

***Supporting information for***

**Cobalt-Copper Dual Light-Driven  
Catalytic Reduction of Aldehydes and  
Aromatic Ketones in Aqueous Media**

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***SI.3. DFT studies***

## **Table of Contents**

1. Computational details.....	3
1.1. Protonation and redox reactions .....	3
1.2. Co <sup>II</sup> and Co <sup>I</sup> speciation under catalytic conditions.....	4
2. Relevant optimized geometries.....	6
3. Free energy profiles.....	10
4. Cartesian coordinates .....	15
5. References.....	41

## 1. Computational details

The DFT quantum mechanical exploration of ketone and water reduction mechanisms was carried out using the Gaussian09 program.<sup>[1]</sup> Geometry optimizations were performed in the unrestricted spin formalism, with the B3LYP hybrid exchange-correlation functional<sup>[2]</sup> and the standard 6-31G\* 6d basis set for all atoms. An extra quadratic convergent SCF step was added when the first-order SCF did not converge (“scf=xqc” keyword). The solvation effect of water was introduced in geometry optimizations and energy through the IEFPCM-SMD polarizable continuum model.<sup>[3]</sup> Dispersion effects were also included using the Grimme D<sub>2</sub> correction.<sup>[4]</sup> The geometries have been edited with the Chemcraft program.<sup>[5]</sup>

The located stationary points were characterized by analytical frequency calculations at the same level of theory than geometry optimizations. Gibbs energy values (G) were obtained by including thermal, solvation and Grimme corrections to the potential energy computed with the 6-311+G\*\* 6d basis set on equilibrium geometries:

$$G = E_{6-311+G^{**}} + G_{\text{corr.}} + G_{\text{solv.}} + E_{\text{disp.}} \quad (1)$$

where the thermal correction ( $G_{\text{corr.}}$ ) was obtained from gas phase analytical Hessians calculations at 298.15 K, the solvation energy ( $G_{\text{solv.}}$ ) was calculated as the difference of the total free energy in gas phase and in water at the same level of theory and geometry and  $E_{\text{disp.}}$  is the dispersion correction.

A cluster of three water molecules ( $\text{H}_2\text{O}$ )<sub>3</sub> is employed to model the H-H bond formation event and the microsolvation sphere around the organic substrates. Hirshfeld charges<sup>[6,7]</sup> were computed to rationalize the reactivity trends of Co-H species.

### 1.1. Protonation and redox reactions

The standard dissociation free energy change between an acid (AH) and its conjugate base (A<sup>-</sup>) in aqueous ( $\Delta G^*$ ) may be expressed as:<sup>[8]</sup>

$$\Delta G^* = G(A_{\text{aq}}^-) + G(H_{\text{aq}}^+) - G(AH_{\text{aq}}) + \Delta G^{\text{o/*}} \quad (2)$$

$$G(H_{\text{aq}}^+) = G(H_{\text{gas}}^+) + \Delta G_{\text{solv}}^{H^+} \quad (3)$$

where  $G(AH_{\text{aq}})$  and  $G(A_{\text{aq}}^-)$  are standard free energies of the acid and its conjugate base in aqueous media, respectively. The  $G(H_{\text{aq}}^+)$  is the free energy of the proton in water, obtained from the experimental solvation free energy ( $\Delta G_{\text{solv}}^{H^+} = -265.9 \text{ kcal} \cdot \text{mol}^{-1}$ )<sup>[8]</sup> and its gas-phase free energy ( $G(H_{\text{gas}}^+) = -6.3 \text{ kcal} \cdot \text{mol}^{-1}$ ).  $\Delta G^{\text{o/*}}$  is the free energy change associated with the conversion from a standard state of 1 M in the aqueous phase and 1 atm in gas phase, to the desired concentration in both phases.  $\Delta G^*$  values are derived with the following expression:

$$\Delta G^{\text{o/*}} = RT \ln(24.4 * c) \quad (4)$$

where  $R$  is the universal gas constant ( $1.987 \text{ cal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ ),  $T$  is the temperature in Kelvin and  $c$  the concentration in  $\text{mol} \cdot \text{L}^{-1}$ .

In the free energy balances the following concentrations were used to adjust the final free energies: 16.5 mM for acetophenone,  $10^{-12}$  M for protons (due to the pH ≈ 12), 33.4 M for water and 7.6 M for acetonitrile (the concentrations of water and acetonitrile were derived from the 6:4

$\text{H}_2\text{O}:\text{CH}_3\text{CN}$  solvent mixture used in catalysis). The previous concentrations translate into  $\Delta G^{o/*}$  values (at 298.15 K) of -0.54 kcal·mol<sup>-1</sup> for acetophenone substrate, -14.5 kcal·mol<sup>-1</sup> for protons, 4.0 kcal·mol<sup>-1</sup> for water and 3.1 kcal·mol<sup>-1</sup> for acetonitrile. The concentration correction for a  $(\text{H}_2\text{O})_n$  water cluster can be derived with the formula  $4.0/n$  kcal·mol<sup>-1</sup>, [9] with a  $\Delta G^{o/*}$  value of 1.33 kcal·mol<sup>-1</sup> when n = 3.

The standard one electron redox potentials relative to the SHE electrode were calculated by:

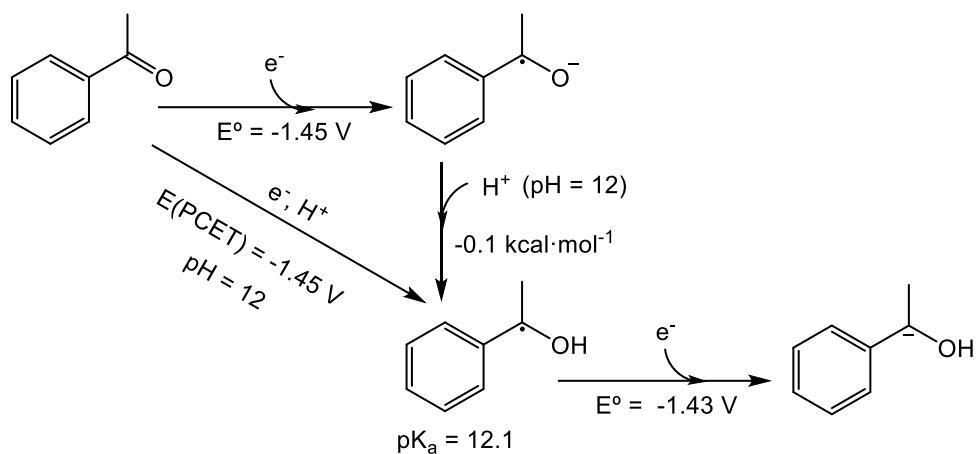
$$E^o = -\frac{\Delta G^o - \Delta G_{\text{SHE}}}{F} \quad (5)$$

where  $\Delta G^o$  is the standard free energy change associated with the reduction reaction, F is the Faraday constant (23.061 kcal·mol<sup>-1</sup>V<sup>-1</sup>) and  $\Delta G_{\text{SHE}}$  is the free energy change associated with the proton reduction to H<sub>2</sub> (-4.24 eV). The  $\Delta G_{\text{SHE}}$  value was derived using the Fermi-Dirac statistics for the treatment of electron thermodynamics. [10]

Energetics for the reduction steps were calculated considering the experimental redox potential of the copper photosensitizer relative to the SHE electrode ( $E(\text{PS}_{\text{Cu}}) = -1.29$  V vs. SHE). The reduction of an acetophenone molecule to the corresponding protonated ketyl radical supposes an energetic cost of 3.8 kcal·mol<sup>-1</sup>. Taking into account the previous value, the relationship  $\Delta G^o = -RT\ln(K)$  and a 16.5 mM for acetophenone, we derived a ketyl radical concentration of 27.5 μM, with a  $\Delta G^{o/*}$  value of -4.3 kcal·mol<sup>-1</sup>. The same values are obtained for the O-protonated ketyl radical at pH = 12.

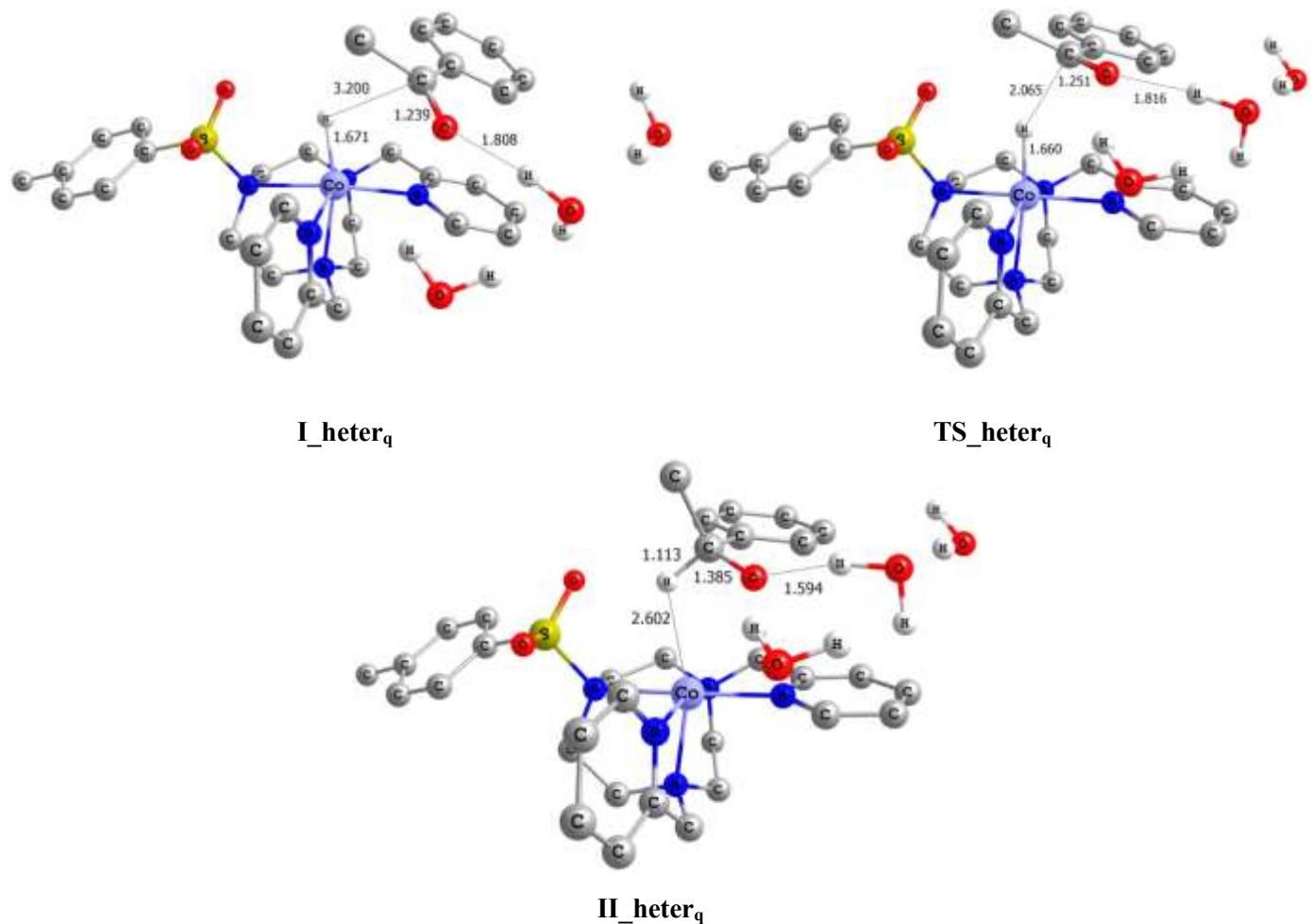
## 1.2. Co<sup>II</sup> and Co<sup>I</sup> speciation under catalytic conditions

DFT calculations were first performed to determine the most stable coordination environment for [1<sup>II</sup>] and [1<sup>I</sup>] species in a  $\text{H}_2\text{O}:\text{CH}_3\text{CN}$  (6:4) solvent mixture, according to the catalytic conditions when using our dual **PS<sub>Cu</sub>/1** catalytic system. The preference for acetonitrile coordination in complexes 1<sup>II</sup> and 1<sup>I</sup> is corroborated by the ligand exchange free energy balances between [1<sup>n</sup>-OH<sub>2</sub>] and [1<sup>n</sup>-NCCH<sub>3</sub>] species ( $\Delta G = -5.3$  kcal·mol<sup>-1</sup> for n = 2 and  $\Delta G = -3.0$  kcal·mol<sup>-1</sup> for n = 1). Therefore, [1<sup>II</sup>-NCCH<sub>3</sub>] and [1<sup>I</sup>-NCCH<sub>3</sub>] are the most stable intermediates under photochemical conditions.

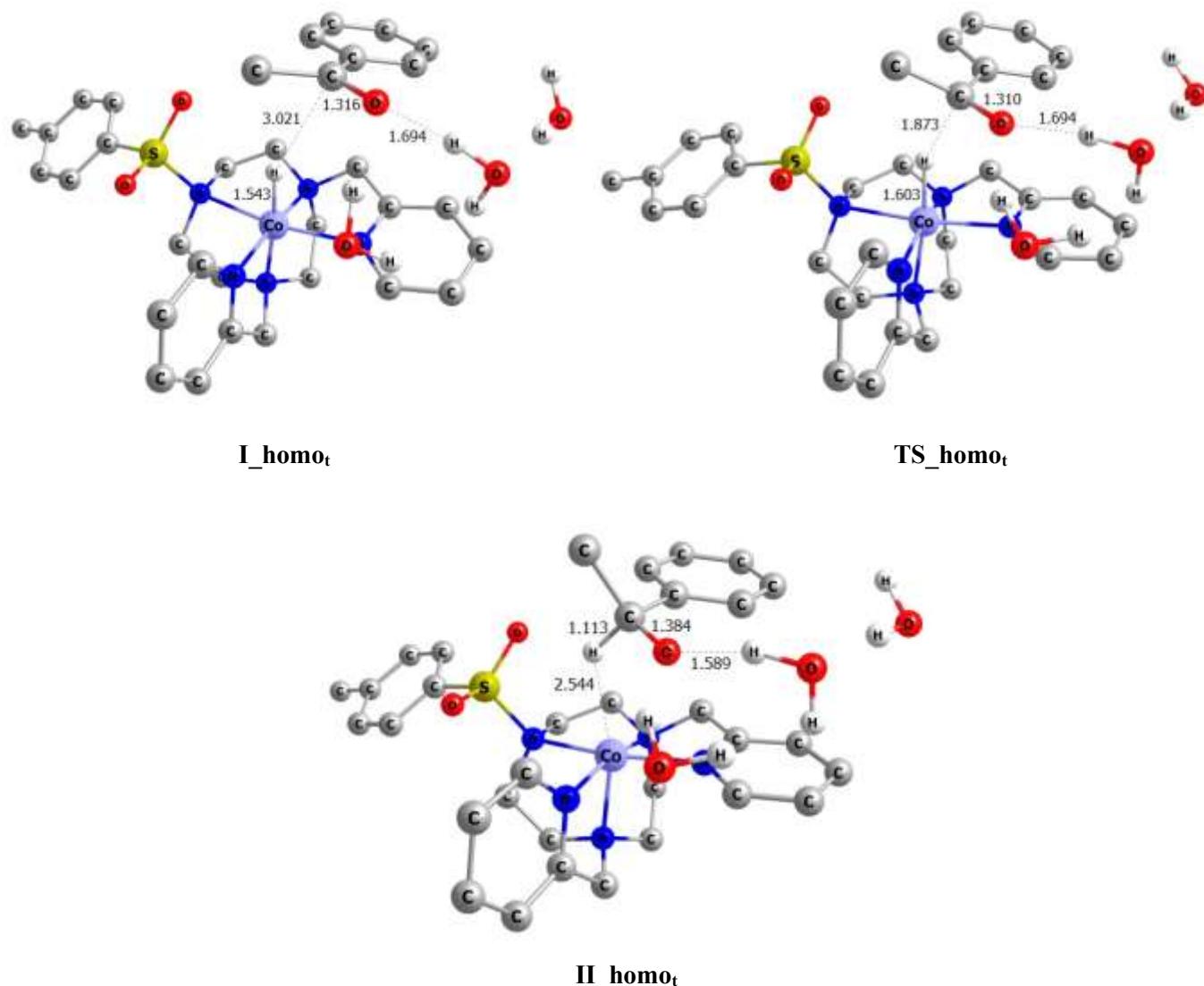


**Figure SI.3.1.** DFT calculated redox potentials and  $\text{pK}_a$  for the above showed redox processes, from top to bottom: one electron reduction of acetophenone, protonation of the ketyl radical ( $\text{pH} = 12$ ), Proton-Coupled Electron Transfer (PCET) from the acetophenone to the protonated ketyl radical at  $\text{pH} = 12$  and one electron reduction of the latter. All the potentials are referred to SHE.

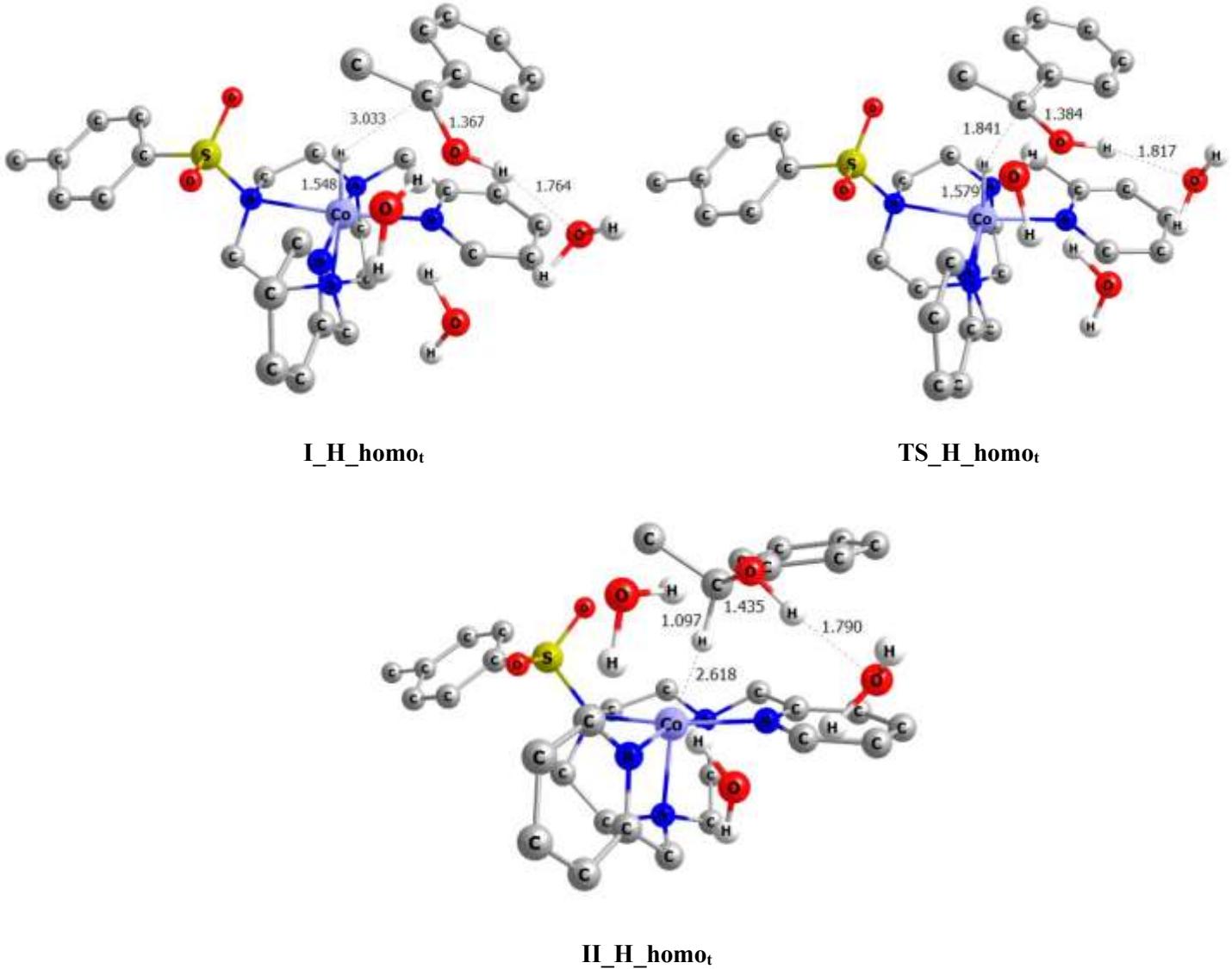
## 2. Relevant optimized geometries



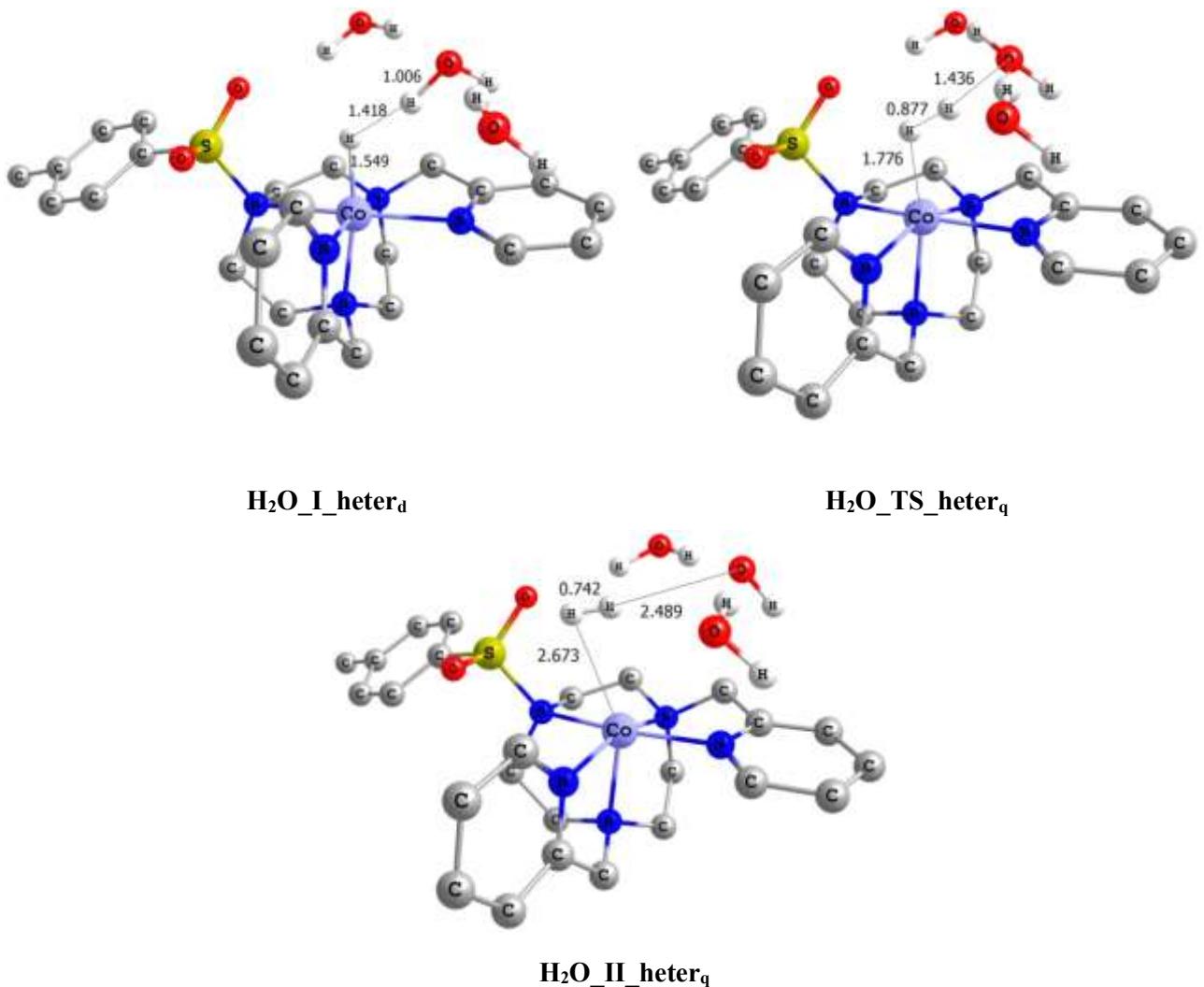
**Figure SI.3.2.** Optimized geometries of the lowest in energy intermediates and transition state involved in the hydride transfer mechanism to acetophenone (**9a**) catalyzed by  $[\text{Co}^{\text{II}}(\text{H})(\text{Py}_2^{\text{Metacn}})]^+$ . Irrelevant hydrogen atoms are omitted for clarity. The most relevant bond distances are in Å.



**Figure SI.3.3.** Optimized geometries of the lowest in energy intermediates and transition state involved in the HAT mechanism for ketyl radical (**9a<sup>ketyl</sup>**) reduction, catalyzed by  $[\text{Co}^{II}(\text{H})(\text{Py}_2\text{Metacn})]^+$ . Irrelevant hydrogen atoms are omitted for clarity. The most relevant bond distances are in Å.

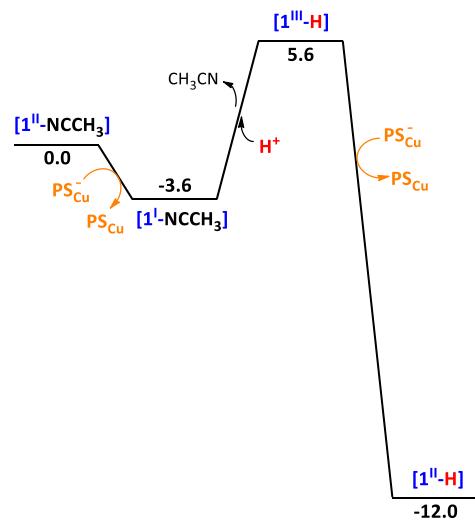


**Figure SI.3.4.** Optimized geometries of the lowest in energy intermediates and transition state involved in the HAT mechanism for the O-protonated ketyl radical reduction, catalyzed by  $[\text{Co}^{\text{II}}(\text{H})(\text{Py}_2^{\text{Metacn}})]^+$ . Irrelevant hydrogen atoms are omitted for clarity. The most relevant bond distances are in Å.

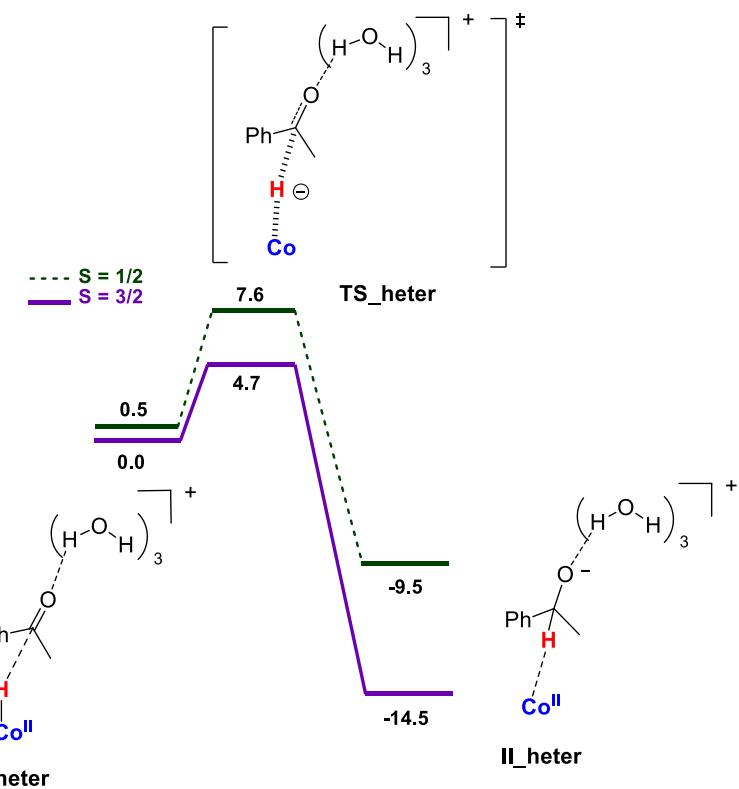


**Figure SI.3.5.** Optimized geometries of the lowest in energy intermediates and transition state involved in the water reduction reaction catalyzed by  $[\text{Co}^{\text{II}}(\text{H})(\text{Py}_2^{\text{Me}}\text{acn})]^+$ . Irrelevant hydrogen atoms are omitted for clarity. The most relevant bond distances are in Å.

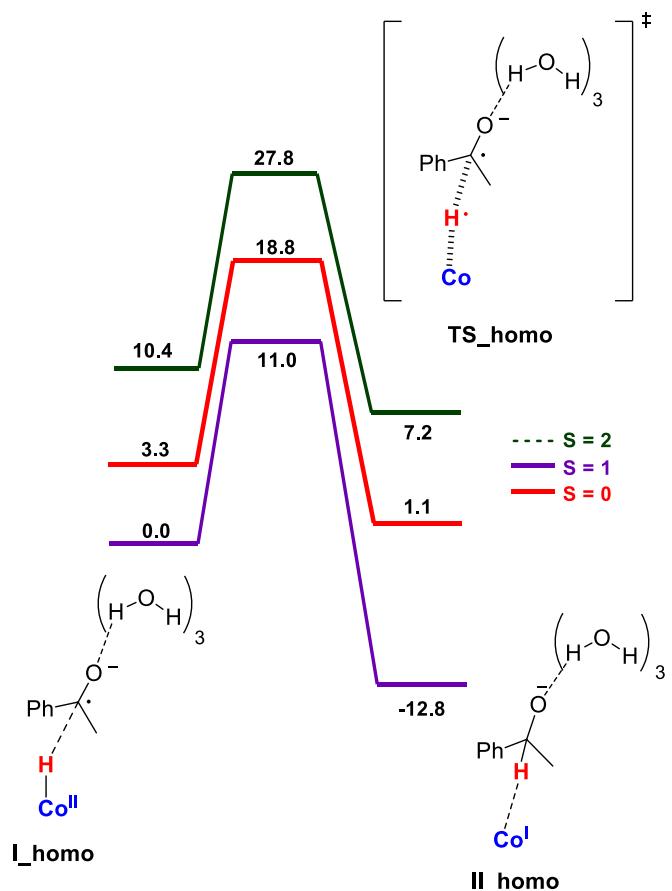
### 3. Free energy profiles



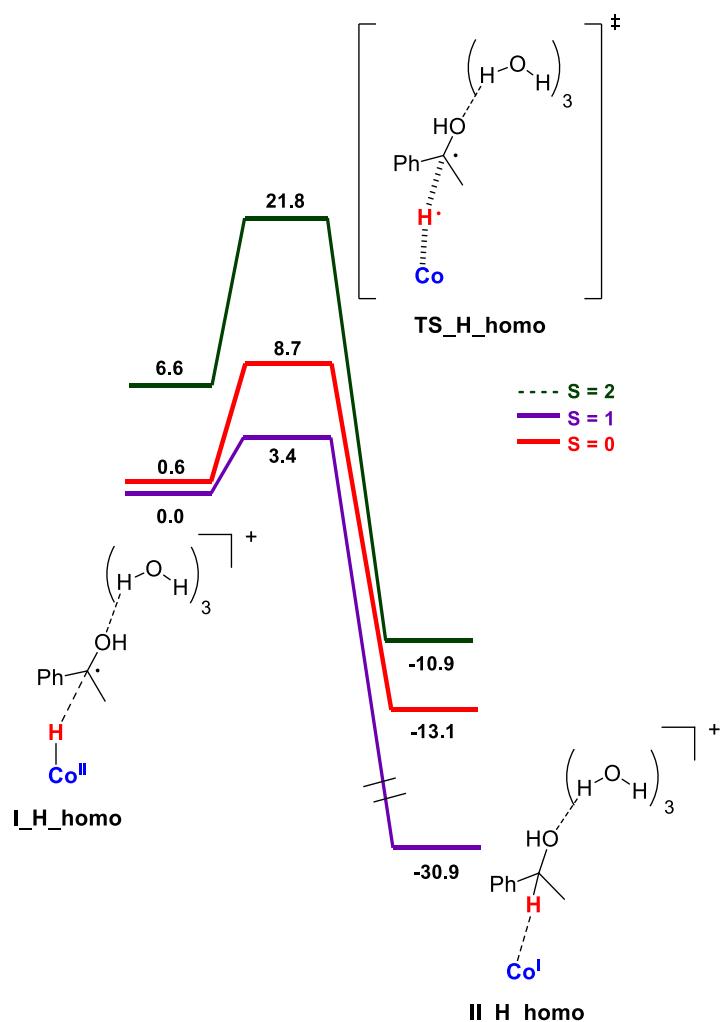
**Figure SI.3.6.** Energy profile for the generation of  $[1^{II}-H]$  species by complex **1** under catalytic conditions ( $PS_{Cu}$  photosensitizer and  $pH = 12$ ). Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .



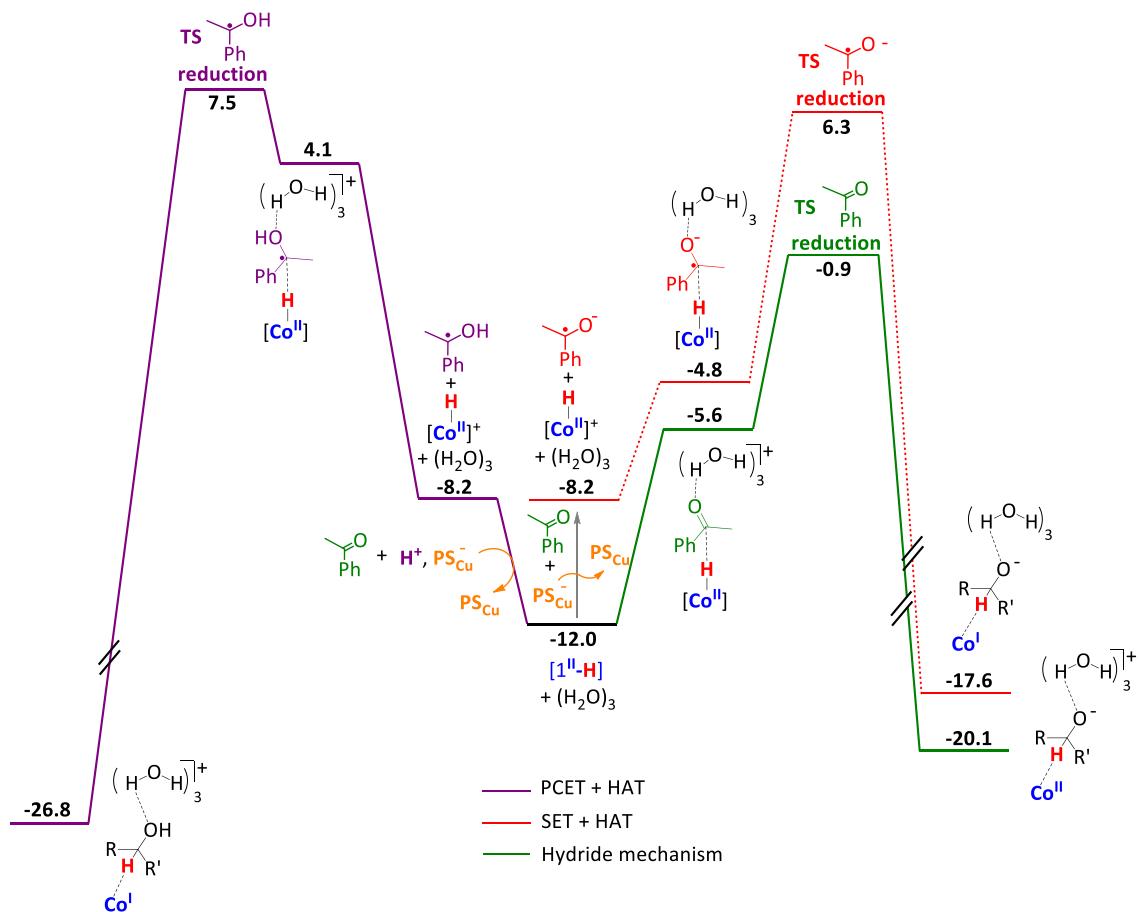
**Figure SI.3.7.** Free energy profiles for the hydride transfer mechanism to acetophenone performed by the  $[\text{Co}^{II}(\text{H})(\text{Py}_2\text{Metacn})]^+$  intermediate in the  $S = 1/2$  and  $S = 3/2$  spin states. Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .



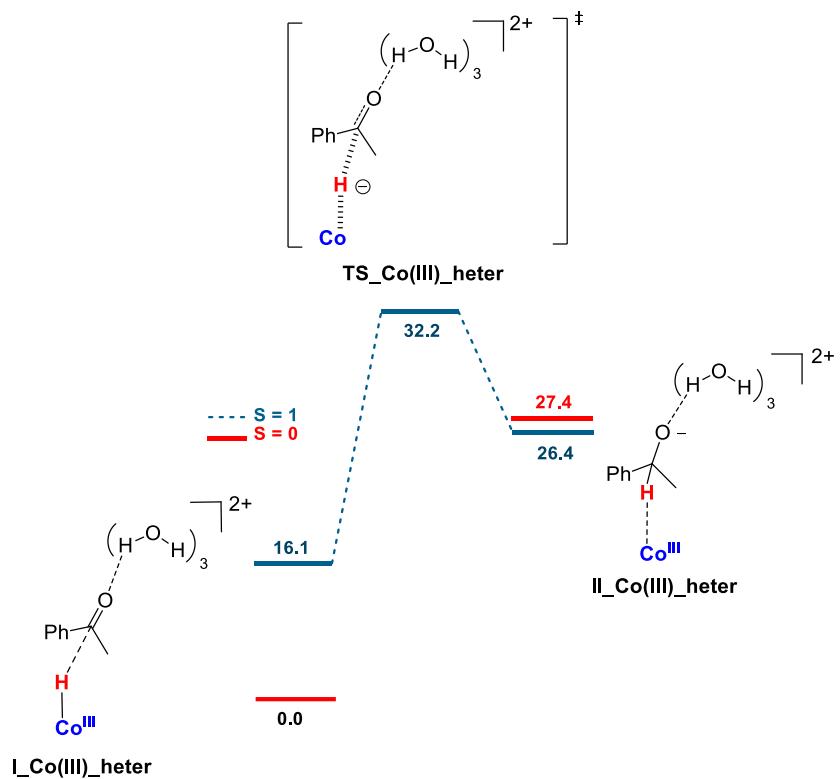
**Figure SI.3.8.** Free energy profiles for the HAT mechanism to the ketyl radical (**9a<sup>ketyl</sup>**) performed by the  $[\text{Co}^{II}(\text{H})(\text{Py}_2^{\text{Me}}\text{acn})]^+$  intermediate in the  $S = 0$ ,  $S = 1$  and  $S = 2$  spin states. Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .



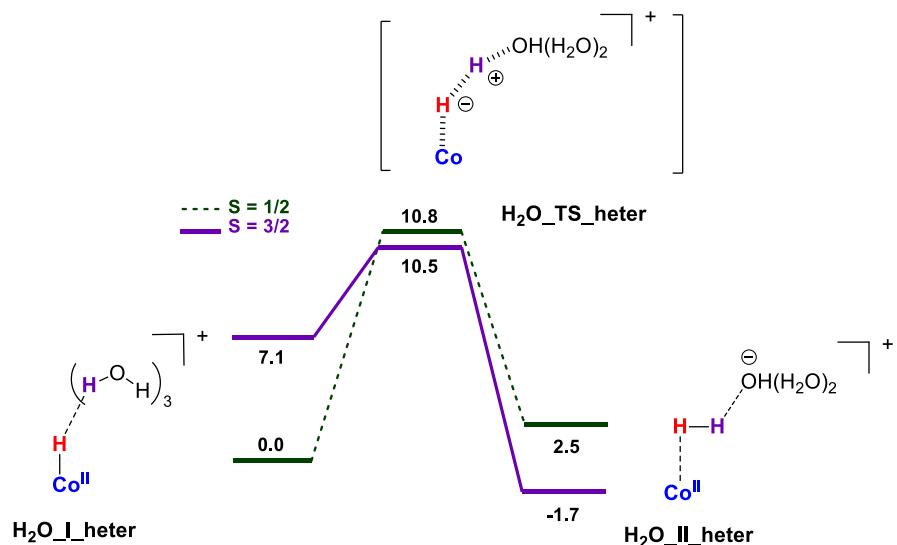
**Figure SI.3.9.** Free energy profiles for the HAT mechanism to the O-protonated ketyl radical performed by the  $[\text{Co}^{\text{II}}(\text{H})(\text{Py}_2^{\text{Me}}\text{tacn})]^+$  intermediate in the  $S = 0$ ,  $S = 1$  and  $S = 2$  spin states. Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .



**Figure SI.3.10.** Comparison of free energy profiles for hydride transfer and HAT mechanisms for acetophenone reduction under catalytic conditions (PS<sub>Cu</sub> photosensitizer and pH = 12). Gibbs energies are in kcal·mol<sup>-1</sup>.



**Figure SI.3.11.** Free energy profiles for the acetophenone reduction reaction performed by the  $[\text{Co}^{\text{III}}(\text{H})(\text{Py}_2^{\text{Metacn}})]^{2+}$  intermediate in the  $S = 0$  and  $S = 1$  spin states. Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .



**Figure SI.3.12.** Free energy profiles for the water reduction reaction performed by the  $[\text{Co}^{\text{II}}(\text{H})(\text{Py}_2^{\text{Metacn}})]^+$  intermediate in the  $S = 1/2$  and  $S = 3/2$  spin states. Gibbs energies are in  $\text{kcal}\cdot\text{mol}^{-1}$ .

#### 4. Cartesian coordinates

In parenthesis are the Gibbs energies (G) in hartrees and the spin state of each cobalt intermediate.

<b>I_heter<sub>d</sub></b>							
(G = -3791.292338) (doublet)							
27	-0.242997000	0.653873000	-0.548285000	6	-3.663233000	-3.472832000	-0.134305000
16	2.654586000	-0.547864000	0.844631000	1	-4.155613000	-1.726102000	1.001089000
7	2.076085000	0.027704000	-0.655041000	6	-2.691825000	-4.441453000	-0.407415000
8	2.422967000	0.511291000	1.837900000	1	-0.709561000	-5.160895000	0.056301000
7	-0.111639000	2.148128000	0.656210000	1	-4.611923000	-3.469844000	-0.663256000
7	-2.327481000	0.769215000	-1.043607000	6	-2.882295000	-5.209658000	-1.151535000
7	0.337079000	1.963649000	-1.967637000	1	-0.665184000	-1.400959000	3.304448000
7	-0.308391000	-0.698338000	-2.060927000	1	0.205369000	-1.352340000	2.642580000
8	2.047710000	-1.875556000	1.040129000	1	-0.655455000	-0.553891000	3.995136000
6	2.599828000	1.374316000	-1.010239000	1	-0.600149000	-2.340495000	3.868639000
1	3.660003000	1.327722000	-1.289662000	1	-0.513046000	-0.366354000	0.572123000
1	2.493314000	2.007109000	-0.128376000	1	-0.444258000	-0.009348000	2.071233000
6	-1.629138000	-1.360200000	-1.933363000	8	-5.233484000	0.484338000	1.751592000
1	-1.579360000	-2.010131000	-1.057782000	1	-4.971645000	0.740101000	0.848158000
1	-1.850021000	-1.979180000	-2.812238000	1	-6.203985000	-0.906406000	0.910474000
6	0.021639000	3.344340000	0.023503000	1	-4.015352000	2.025981000	2.285451000
6	-3.237504000	1.722021000	-0.792488000	1	-3.141625000	2.372283000	2.549679000
1	-2.880684000	2.593438000	-0.252524000	8	-6.587844000	-1.571694000	0.298434000
6	-0.080169000	2.132225000	2.003993000	1	-2.665146000	1.549274000	2.761959000
1	-0.198422000	1.161724000	2.466648000	1	-6.293888000	-2.415535000	0.677212000
6	-0.147414000	3.278266000	-1.470924000				
1	-1.218227000	3.340352000	-1.692684000				
1	0.350207000	4.115402000	-1.973736000				
6	-4.027533000	-0.532818000	-2.130886000				
1	-4.293569000	-1.443527000	-2.657411000				
6	1.820599000	1.971802000	-2.176607000				
1	2.172356000	2.998081000	-2.325630000				
1	2.045582000	1.425858000	-3.093551000				
6	-4.974263000	0.454848000	-1.860159000				
1	-6.006500000	0.327479000	-2.170413000				
6	2.137895000	-1.017362000	-1.719079000				
1	2.883887000	-1.784516000	-1.489609000				
1	2.475927000	-0.539340000	-2.638402000				
6	4.410371000	-0.753959000	0.635862000				
6	-0.363726000	1.531036000	-3.209182000				
1	0.027685000	2.058870000	-4.088198000				
1	-1.417837000	1.781363000	-3.098984000				
6	-0.191857000	0.021047000	-3.381903000				
1	-0.942950000	-0.359123000	-4.082268000				
1	0.785066000	-0.199344000	-3.813368000				
6	4.921089000	-2.003360000	0.271100000				
1	4.263671000	-2.861791000	0.186065000				
6	-2.713566000	-0.336008000	-1.712147000				
6	0.779974000	-1.693469000	-1.898592000				
1	0.824722000	-2.365498000	-2.766547000				
1	0.552230000	-2.281035000	-1.007900000				
6	5.241392000	0.364924000	0.767488000				
1	4.831478000	1.325242000	1.061052000				
6	-4.569350000	1.614037000	-1.190695000				
1	-5.268818000	2.413922000	-0.970271000				
6	0.253335000	4.506677000	2.111391000				
1	0.401670000	5.422483000	2.675407000				
6	0.092622000	3.283607000	2.763639000				
1	0.103913000	3.213133000	3.846068000				
6	0.216825000	4.533381000	0.715972000				
1	0.331489000	5.459407000	0.161981000				
6	6.290278000	-2.126844000	0.039625000				
1	6.701679000	-3.094598000	-0.233397000				
6	7.147517000	-1.022737000	0.157774000				
6	6.605639000	0.217985000	0.530399000				
1	7.262784000	1.076437000	0.638392000				
6	8.619831000	-1.156820000	-0.130273000				
1	8.961050000	-2.186488000	0.023023000				
1	9.209461000	-0.486543000	0.505503000				
1	8.831078000	-0.888419000	-1.174981000				
6	-1.939738000	-1.377856000	2.502339000				
8	-2.779564000	-0.490540000	2.708912000				
6	-2.189862000	-2.452294000	1.506239000				
6	-1.217759000	-3.429685000	1.227685000				
6	-3.409729000	-2.483919000	0.812243000				
6	-1.468711000	-4.415234000	0.273019000				
1	-0.262890000	-3.411462000	1.740917000				

6	0.260043000	4.696343000	0.140122000		6	0.423258000	1.096896000	3.311649000
1	0.380084000	5.772920000	0.215586000		1	0.037979000	1.562028000	4.227293000
6	0.187983000	3.907745000	1.289975000		1	1.485177000	1.326886000	3.228363000
1	0.244809000	4.343565000	2.281597000		6	0.207351000	-0.408559000	3.340807000
6	0.178538000	4.082478000	-1.109712000		1	0.922989000	-0.872741000	4.026014000
1	0.228496000	4.657143000	-2.028723000		1	-0.787159000	-0.646097000	3.717006000
6	6.849559000	-1.531433000	0.802411000		6	-4.978070000	-1.948695000	-0.384318000
1	7.410927000	-2.460450000	0.846314000		1	-4.354720000	-2.835299000	-0.360855000
6	7.524905000	-0.332635000	0.534083000		6	2.763519000	-0.591390000	1.662833000
6	6.788915000	0.862918000	0.484711000		6	-0.723425000	-1.963276000	1.670057000
1	7.302705000	1.798430000	0.280766000		1	-0.775980000	-2.729618000	2.455237000
6	9.015334000	-0.315931000	0.318865000		1	-0.484708000	-2.444339000	0.719654000
1	9.413028000	-1.332090000	0.225844000		6	-5.217374000	0.454426000	-0.744104000
1	9.521811000	0.174191000	1.161475000		1	-4.775404000	1.413567000	-0.991456000
1	9.274691000	0.248735000	-0.585193000		6	4.609962000	1.382381000	1.200454000
6	-2.726956000	0.423346000	2.584343000		1	5.305858000	2.192436000	1.004466000
8	-3.171547000	1.451256000	0.055161000		6	-0.420913000	4.666924000	-1.573876000
6	-3.223083000	-0.922271000	2.201618000		1	-0.637962000	5.638968000	-2.006017000
6	-2.564843000	-2.087841000	2.631940000		6	-0.291466000	3.538219000	-2.381180000
6	-4.343382000	-1.040293000	1.363009000		1	-0.396625000	3.595760000	-3.459113000
6	-3.011603000	-3.341732000	2.214023000		6	-0.267385000	4.522805000	-0.194175000
1	-1.697650000	-2.017393000	3.278667000		1	-0.358819000	5.367139000	0.480854000
6	-4.801692000	-2.291370000	0.963523000		6	-6.348548000	-2.034756000	-0.140972000
1	-4.857070000	-0.154549000	1.022535000		1	-6.792545000	-3.000831000	0.082139000
6	-4.130371000	-3.446358000	1.380744000		6	-7.165855000	-0.895692000	-0.186808000
1	-2.489256000	-4.236404000	2.540013000		6	-6.583000000	0.343851000	-0.496719000
1	-5.672849000	-2.358398000	0.319366000		1	-7.209125000	1.230190000	-0.548978000
1	-4.477514000	-4.424122000	1.058324000		6	-8.639538000	-0.993403000	0.107904000
6	-1.652436000	0.531880000	3.634362000		1	-9.009334000	-2.010734000	-0.059954000
1	-0.736760000	0.053401000	3.265012000		1	-9.213189000	-0.296922000	-0.514332000
1	-1.456951000	1.584639000	3.851724000		1	-8.837788000	-0.734528000	1.157469000
1	-1.957326000	0.004970000	4.546622000		6	1.636468000	-0.799483000	-2.098259000
1	-0.120377000	-0.813951000	1.199999000		8	2.484668000	0.130662000	-2.268628000
1	-4.660101000	1.884410000	1.125130000		6	2.085130000	-2.082779000	-1.448231000
8	-5.361081000	2.323206000	0.586926000		6	1.228448000	-3.191959000	-1.344643000
1	-5.279221000	1.882409000	-0.275258000		6	3.385407000	-2.182283000	-0.941196000
1	-6.745860000	0.986811000	0.831251000		6	1.665197000	-4.366539000	-0.731057000
1	-3.869150000	3.440621000	0.068211000		1	0.211372000	-3.129338000	-1.715424000
8	-2.956892000	3.765030000	-0.077146000		6	3.823300000	-3.356319000	-0.326336000
8	-7.299170000	0.186321000	0.714803000		1	4.051088000	-1.334258000	-1.004827000
1	-2.454379000	3.255475000	0.579672000		6	2.964417000	-4.452561000	-0.215584000
1	-7.013018000	-0.382733000	1.447349000		1	0.988664000	-5.212566000	-0.646791000
					1	4.831487000	-3.400967000	0.076462000
					1	3.299860000	-5.365075000	0.269505000
					6	0.537079000	-0.945603000	-3.146007000
					1	-0.404956000	-1.310871000	-2.739530000
					1	0.377624000	0.004958000	-3.660480000
					1	0.898211000	-1.670005000	-3.890114000
					1	0.658790000	-0.357503000	-0.805636000
					1	4.226776000	0.424152000	-2.047832000
					8	5.135964000	0.806613000	-1.961911000
					1	5.121733000	1.172644000	-1.060596000
					1	6.093750000	-0.629760000	-1.294826000
					1	3.909875000	2.597123000	-2.249264000
					8	2.975169000	2.853203000	-2.342385000
					8	6.548619000	-1.355235000	-0.809249000
					1	2.548397000	1.972251000	-2.410348000
					1	6.179995000	-2.153283000	-1.220306000

### TS\_heter<sub>q</sub>

(G = -3791.285555) (quartet)

27	0.317599000	0.505641000	0.548334000		27	0.256618000	0.443618000	0.434710000
16	-2.670640000	-0.554970000	-0.929722000		16	-2.608687000	-0.617562000	-0.884587000
7	-2.010750000	-0.127401000	0.593814000		7	-1.996572000	-0.121359000	0.654335000
8	-2.411539000	0.569541000	-1.840149000		8	-2.342916000	0.487876000	-1.816298000
7	0.117635000	2.157672000	-0.457701000		7	0.076523000	2.339851000	-0.517157000
7	2.373103000	0.533514000	1.031057000		7	2.304033000	0.515631000	0.962752000
7	-0.255358000	1.650529000	2.109017000		7	-0.346295000	1.770406000	2.133055000
7	0.362362000	-0.993010000	1.957327000		7	0.330817000	-0.958602000	2.126394000
8	-2.132612000	-1.890303000	-1.240713000		8	-2.032650000	-1.948066000	-1.137811000
6	-2.526714000	1.179635000	1.089319000		6	-2.567818000	1.188594000	1.092818000
1	-3.582590000	1.103818000	1.376826000		1	-3.627515000	1.082197000	1.353209000
1	-2.432743000	1.895824000	0.272534000		1	-2.475744000	1.879330000	0.253806000
6	1.691944000	-1.638811000	1.840263000		6	1.663348000	-1.577258000	1.979422000
1	1.670834000	-2.281014000	0.961733000		1	1.628490000	-2.231111000	1.103591000
1	1.903004000	-2.270290000	2.711668000		1	1.927810000	-2.187533000	2.852931000
6	0.008663000	3.264531000	0.324236000		6	-0.126153000	3.392344000	0.302177000
6	3.280445000	1.495267000	0.801372000		6	3.171565000	1.499541000	0.679273000
1	2.921844000	2.375779000	0.277641000		1	2.797829000	2.300411000	0.049323000
6	-0.027675000	2.309669000	-1.786144000					
1	0.067408000	1.413352000	-2.373017000					
6	0.259209000	3.004523000	1.778295000					
1	1.341344000	2.997096000	1.945687000					
1	-0.181953000	3.775825000	2.418822000					
6	4.076084000	-0.787463000	2.087432000					
1	4.344809000	-1.710862000	2.589868000					
6	-1.743524000	1.666781000	2.304007000					
1	-2.077046000	2.685085000	2.527829000					
1	-1.986098000	1.057310000	3.174877000					
6	5.017780000	0.210984000	1.845144000					
1	6.048462000	0.083996000	2.161148000					
6	-2.078517000	-1.269787000	1.556755000					
1	-2.821163000	-2.011370000	1.249945000					
1	-2.426487000	-0.883561000	2.514298000					
6	-4.427082000	-0.699553000	-0.685492000					

6	-0.046153000	2.510702000	-1.842828000		7	-1.925591000	0.238075000	0.654664000
1	0.139529000	1.632292000	-2.451064000		8	-2.383795000	0.872579000	-1.829953000
6	0.125880000	3.122211000	1.764560000		7	0.147231000	2.116602000	-0.534420000
1	1.209622000	3.154740000	1.927960000		7	2.096206000	0.629203000	0.943328000
1	-0.332972000	3.898132000	2.390387000		7	-0.379123000	2.055550000	2.138255000
6	4.004285000	-0.598910000	2.233397000		7	0.197314000	-0.686592000	2.184282000
1	4.288767000	-1.449390000	2.843901000		8	-1.756278000	-1.516779000	-1.210702000
6	-1.822372000	1.739272000	2.309548000		6	-2.557881000	1.545689000	1.047828000
1	-2.207285000	2.749018000	2.495013000		1	-3.620894000	1.402559000	1.266128000
1	-2.063581000	1.147653000	3.193963000		1	-2.448675000	2.225041000	0.203360000
6	4.909441000	0.417740000	1.931656000		6	1.514174000	-1.378316000	2.120726000
1	5.927522000	0.376814000	2.305938000		1	1.457241000	-2.138001000	1.338034000
6	-2.098376000	-1.225763000	1.666878000		1	1.750539000	-1.874386000	3.067324000
1	-2.841859000	-1.970384000	1.369355000		6	0.054078000	3.321591000	0.085570000
1	-2.465550000	-0.792474000	2.596677000		6	2.974972000	1.539830000	0.479104000
6	-4.366675000	-0.788523000	-0.679863000		1	2.578488000	2.317948000	-0.159195000
6	0.371305000	1.242876000	3.316258000		6	0.185677000	2.078476000	-1.878547000
1	0.031484000	1.731056000	4.240211000		1	0.286568000	1.102062000	-2.330425000
1	1.430553000	1.468457000	3.182926000		6	0.184524000	3.302178000	1.589120000
6	0.176812000	-0.270777000	3.439210000		1	1.254188000	3.324479000	1.828554000
1	0.902199000	-0.665484000	4.160489000		1	-0.276039000	4.193432000	2.031797000
1	-0.813458000	-0.491072000	3.840402000		6	3.895855000	-0.486762000	2.081735000
6	-4.902348000	-2.040998000	-0.367435000		1	4.212203000	-1.312247000	2.709588000
1	-4.261458000	-2.913526000	-0.302184000		6	-1.854201000	2.114712000	2.280882000
6	2.706869000	-0.514676000	1.733949000		1	-2.189392000	3.149196000	2.416706000
6	-0.755250000	-1.926245000	1.860569000		1	-2.148280000	1.564111000	3.175378000
1	-0.850720000	-2.655739000	2.677435000		6	4.801047000	0.457371000	1.601375000
1	-0.498084000	-2.460578000	0.942775000		1	5.854447000	0.387493000	1.851575000
6	-5.176086000	0.349311000	-0.787630000		6	-2.196067000	-0.858163000	1.671972000
1	-4.744323000	1.311881000	-1.039527000		1	-2.975118000	-1.543056000	1.330455000
6	4.481203000	1.497290000	1.154479000		1	-2.588826000	-0.378746000	2.567098000
1	5.147063000	2.319532000	0.910982000		6	-4.230934000	-0.667702000	-0.738419000
6	-0.625583000	4.818006000	-1.562381000		6	0.308504000	1.547982000	3.347138000
1	-0.910523000	5.784291000	-1.967874000		1	-0.018901000	2.069410000	4.256104000
6	-0.394096000	3.733036000	-2.409318000		1	1.377288000	1.723154000	3.213641000
1	-0.484433000	3.825255000	-3.486305000		6	0.038951000	0.050321000	3.498481000
6	-0.486899000	4.645814000	-0.183990000		1	0.724495000	-0.373188000	4.237704000
1	-0.655088000	5.462644000	0.510347000		1	-0.972540000	-0.119147000	3.867763000
6	-6.277450000	-2.148590000	-0.162297000		6	-4.624169000	-1.999448000	-0.576308000
1	-6.709610000	-3.117128000	0.072506000		1	-3.887884000	-2.795891000	-0.582391000
6	-7.113916000	-1.027877000	-0.260372000		6	2.556284000	-0.374684000	1.730305000
6	-6.545374000	0.217063000	-0.578974000		6	-0.924092000	-1.637040000	1.952882000
1	-7.185953000	1.090171000	-0.667311000		1	-1.066840000	-2.291353000	2.821444000
6	-8.586289000	-1.145856000	-0.023661000		1	-0.661751000	-2.245038000	1.085003000
1	-9.160433000	-0.666398000	-0.833082000		6	-5.160313000	0.380335000	-0.749470000
1	-8.879169000	-0.640996000	0.910011000		1	-4.839951000	1.406240000	-0.894526000
1	-8.903644000	-2.194411000	0.047629000		6	4.327826000	1.491439000	0.791691000
6	1.855884000	-1.064400000	-2.414672000		1	4.993152000	2.250562000	0.393327000
8	2.657394000	-0.119467000	-2.586524000		6	-0.049955000	4.458881000	-2.027109000
6	2.238668000	-2.217993000	-1.542508000		1	-0.140396000	5.371976000	-2.607382000
6	1.412899000	-3.346305000	-1.393255000		6	0.093530000	3.225197000	-2.658745000
6	3.466147000	-2.183559000	-0.864497000		1	0.133051000	3.139208000	-3.738708000
6	1.809657000	-4.407480000	-0.579388000		6	-0.065061000	4.505079000	-0.632363000
1	0.454541000	-3.393774000	-1.898029000		1	-0.158549000	5.443083000	-0.095487000
6	3.864658000	-3.245706000	-0.054299000		6	-5.979819000	-2.279734000	-0.421032000
1	4.105273000	-1.317572000	-0.956746000		1	-6.303020000	-3.310069000	-0.304132000
6	3.037379000	-4.362423000	0.092697000		6	-6.935753000	-1.253124000	-0.417395000
1	1.159000000	-5.269995000	-0.466330000		6	-6.507898000	0.074404000	-0.586906000
1	4.813883000	-3.185452000	0.470501000		1	-7.242392000	0.874712000	-0.598944000
1	3.340829000	-5.188743000	0.729459000		6	-8.395030000	-1.563961000	-0.219862000
6	0.688790000	-1.203310000	-3.366774000		1	-8.609204000	-2.614046000	-0.445343000
1	-0.184677000	-1.671588000	-2.912326000		1	-9.022484000	-0.926163000	-0.853222000
1	0.417933000	-0.215804000	-3.750169000		1	-8.687513000	-1.376972000	0.822794000
1	1.021019000	-1.826498000	-4.211576000		6	1.609954000	-1.149180000	-2.054538000
1	0.544623000	-0.407308000	-0.961361000		8	2.643247000	-0.248597000	-2.252648000
1	4.358443000	0.341170000	-2.148954000		6	1.987261000	-2.354619000	-1.186194000
8	5.210969000	0.800914000	-1.961375000		6	1.046181000	-3.359539000	-0.898848000
1	5.066145000	1.157019000	-1.067412000		6	3.249473000	-2.446434000	-0.593368000
1	6.167074000	-0.574018000	-1.137531000		6	1.363530000	-4.419997000	-0.046689000
1	3.892111000	2.441950000	-2.410813000		1	0.050430000	-3.299785000	-1.327116000
8	2.962999000	2.678945000	-2.582925000		6	3.573447000	-3.504087000	0.262877000
8	6.593430000	-1.245188000	-0.558996000		1	3.974830000	-1.667608000	-0.776328000
1	2.560511000	1.794248000	-2.691502000		6	2.632583000	-4.497462000	0.541367000
1	6.257083000	-2.082500000	-0.916111000		1	0.617391000	-5.181252000	0.167591000
					1	4.558856000	-3.532856000	0.722108000
					1	2.877440000	-5.317355000	1.211504000
27	0.161890000	0.602183000	0.691549000		6	1.012410000	-1.606908000	-3.401661000
16	-2.509467000	-0.284988000	-0.936899000		1	0.162155000	-2.288955000	-3.281503000
					1	0.671348000	-0.724349000	-3.958818000
					1	1.787347000	-2.111731000	-3.994572000
					1	0.776179000	-0.670413000	-1.495200000

1	4.234818000	-0.207783000	-2.192496000
8	5.205022000	0.094476000	-2.127304000
1	5.153874000	0.7711774000	-1.432239000
1	6.026594000	-1.076183000	-1.046558000
1	4.116241000	2.017573000	-2.910635000
8	3.172374000	2.247407000	-2.888482000
8	6.446759000	-1.681876000	-0.386823000
1	2.768124000	1.347923000	-2.707383000
1	6.096803000	-2.550011000	-0.642881000

6	1.969837000	-2.001694000	-1.524649000
6	1.069173000	-3.071984000	-1.390569000
6	3.240692000	-2.136395000	-0.959106000
6	1.436013000	-4.242762000	-0.722241000
1	0.071623000	-2.983126000	-1.810120000
6	3.615954000	-3.304961000	-0.288548000
1	3.936994000	-1.313692000	-1.024785000
6	2.716780000	-4.366905000	-0.168485000
1	0.720466000	-5.055743000	-0.626101000
1	4.607495000	-3.369046000	0.153334000
1	3.001869000	-5.274500000	0.357083000
6	1.288411000	-1.088221000	-3.762386000
1	0.531602000	-1.876561000	-3.865731000
1	0.935752000	-0.192781000	-4.291331000
1	2.217737000	-1.429223000	-4.239226000
1	0.577799000	-0.436773000	-1.858315000
1	4.067054000	0.371856000	-2.210478000
8	5.042065000	0.664630000	-2.122186000
1	5.023263000	1.176617000	-1.296289000
1	5.948623000	-0.670094000	-1.314161000
1	3.930575000	2.666073000	-2.494760000
8	2.982938000	2.873883000	-2.435014000
8	6.415821000	-1.364087000	-0.787399000
1	2.593429000	1.952507000	-2.426700000
1	6.031486000	-2.185914000	-1.131690000

**II\_heter<sub>q</sub>**  
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27	0.367142000	0.452438000	0.577829000
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8	-2.393422000	0.752144000	-1.842133000
7	0.184809000	2.271257000	-0.431287000
7	2.369221000	0.363763000	1.144835000
7	-0.295339000	1.683933000	2.215129000
7	0.292779000	-1.061199000	2.136137000
8	-1.999499000	-1.716877000	-1.372113000
6	-2.501715000	1.250392000	1.073633000
1	-3.567490000	1.148580000	1.308458000
1	-2.379838000	1.988051000	0.280992000
6	1.603356000	-1.740340000	2.053397000
1	1.586135000	-2.396224000	1.178850000
1	1.794591000	-2.356646000	2.940606000
6	0.011746000	3.317294000	0.409711000
6	3.306568000	1.280564000	0.849128000
1	2.976208000	2.135155000	0.267759000
6	0.049923000	2.462385000	-1.753229000
1	0.216021000	1.595585000	-2.379670000
6	0.250746000	3.019469000	1.871161000
1	1.333283000	2.990494000	2.041433000
1	-0.176799000	3.803536000	2.506622000
6	4.012873000	-0.946504000	2.286017000
1	4.249549000	-1.843042000	2.848976000
6	-1.779062000	1.714201000	2.337787000
1	-2.119559000	2.733539000	2.551938000
1	-2.073031000	1.100167000	3.189340000
6	4.991282000	-0.006371000	1.966638000
1	6.018958000	-0.156535000	2.282078000
6	-2.122513000	-1.199364000	1.521777000
1	-2.867699000	-1.910139000	1.155696000
1	-2.526818000	-0.800222000	2.451113000
6	-4.354127000	-0.668219000	-0.753968000
6	0.347193000	1.095173000	3.415752000
1	-0.025887000	1.566161000	4.334203000
1	1.418372000	1.288461000	3.341462000
6	0.088532000	-0.414714000	3.468565000
1	0.759878000	-0.862605000	4.209095000
1	-0.929847000	-0.614131000	3.806050000
6	-4.846496000	-1.959762000	-0.540896000
1	-4.181872000	-2.816102000	-0.577665000
6	2.707882000	-0.733122000	1.849121000
6	-0.819783000	-1.960781000	1.752858000
1	-0.994367000	-2.725917000	2.521745000
1	-0.526373000	-2.458330000	0.824862000
6	-5.194722000	0.451234000	-0.734463000
1	-4.798440000	1.443485000	-0.920206000
6	4.631261000	1.134853000	1.243601000
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6	1.563007000	-0.732155000	-2.284920000
8	2.475097000	0.304837000	-2.174746000

27	0.071771000	0.454995000	0.711381000
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7	-1.934791000	0.078215000	0.659771000
7	-2.266555000	0.676913000	-1.868306000
7	0.082107000	1.999381000	-0.458370000
7	1.993553000	0.538732000	0.965185000
7	-0.385670000	1.811076000	2.163382000
7	0.141406000	-0.890275000	2.130316000
8	-1.923107000	-1.755194000	-1.184918000
6	-2.579080000	1.376621000	1.067492000
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6	2.844241000	1.511887000	0.586414000
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6	0.174237000	1.994391000	-1.800733000
1	0.214770000	1.026322000	-2.271261000
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6	2.474902000	-0.495569000	1.701183000
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6	4.179212000	1.515439000	0.973344000
1	4.814323000	2.337977000	0.660164000
6	0.132489000	4.390174000	-1.876940000

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8	2.728270000	-0.141340000	-2.401842000		6	0.129535000	4.645571000	-1.687161000
6	2.226109000	-2.269879000	-1.481166000		1	1.064280000	5.621784000	-2.161252000
6	1.295860000	-3.317421000	-1.353319000		6	0.166777000	3.483167000	-2.459669000
6	3.407933000	-2.304529000	-0.725432000		1	0.181149000	3.522264000	-3.542976000
6	1.552949000	-4.378564000	-0.485221000		6	0.122902000	4.540866000	-0.296582000
1	0.370857000	-3.298134000	-1.918987000		1	0.099656000	5.418372000	0.340434000
6	3.670141000	-3.370617000	0.130494000		6	-6.278760000	-1.982554000	-0.343730000
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6	2.742111000	-4.410510000	0.252772000		6	-7.100017000	-0.847634000	-0.421542000
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16	-2.587030000	-0.466241000	-0.923620000		1	-0.219176000	-0.959040000	-2.777991000
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7	0.170631000	2.149438000	-0.473576000		1	0.357637000	-0.359416000	-0.544547000
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1	4.063146000	-1.210177000	-1.018027000		1	-6.281668000	-3.321354000	-0.384832000
6	2.968248000	-4.380953000	-0.471180000		6	-6.932376000	-1.267409000	-0.452423000
1	0.986202000	-5.100485000	-0.938944000		6	-6.517761000	0.068270000	-0.593633000
1	4.841732000	-3.363037000	-0.102104000		1	-7.259732000	0.861408000	-0.588393000
1	3.304804000	-5.329961000	-0.063595000		6	-8.388004000	-1.595207000	-0.261477000
6	0.556049000	-0.670749000	-3.149752000		1	-8.589285000	-2.647113000	-0.489445000
1	-0.382668000	-1.081102000	-2.783189000		1	-9.019193000	-0.962199000	-0.895895000
1	0.392448000	0.318731000	-3.579918000		1	-8.685100000	-1.411817000	0.780444000
1	0.940424000	-1.327311000	-3.941010000		6	1.675220000	-1.086524000	-1.892115000
1	0.948827000	-0.173623000	-0.983310000		8	2.679420000	-0.158311000	-1.926388000
1	4.324909000	0.637873000	-2.044363000		6	2.027517000	-2.368595000	-1.133798000
8	5.240037000	1.000772000	-2.057046000		6	1.055534000	-3.357822000	-0.905979000
1	5.303231000	1.464805000	-1.205881000		6	3.293354000	-2.536113000	-0.567764000
1	6.198832000	-1.983316000	-1.271973000		6	1.344257000	-4.475545000	-0.119854000
8	6.536256000	-1.195123000	-0.817301000		1	0.059266000	-3.234839000	-1.320570000
1	6.117591000	-0.457929000	-1.317248000		6	3.588629000	-3.652559000	0.221175000
1	3.918705000	2.840956000	-2.212720000		1	4.039719000	-1.769487000	-0.714193000
8	2.977383000	3.088147000	-2.205389000		6	2.613932000	-4.625508000	0.453497000
1	2.553725000	2.210107000	-2.291033000		1	0.575934000	-5.224137000	0.056848000
					1	4.578001000	-3.745221000	0.663796000
					1	2.834897000	-5.489132000	1.075201000
27	0.102954000	0.630691000	0.748508000		6	1.131185000	-1.406162000	-3.302176000
16	-2.531944000	-0.256678000	-1.000022000		1	0.291503000	-2.110413000	-3.276698000
7	-1.916472000	0.245010000	0.642934000		1	0.796491000	-0.477837000	-3.782954000
					1	1.937027000	-1.839145000	-3.909871000
					1	0.785832000	-0.693368000	-1.325576000
					1	4.280936000	-0.199490000	-2.105373000

8	5.264163000	0.044564000	-2.135575000
1	5.302460000	0.790777000	-1.514502000
1	6.062325000	-1.103880000	-1.019393000
1	4.141368000	2.041540000	-2.932384000
8	3.214611000	2.284180000	-2.771643000
8	6.475904000	-1.709032000	-0.354629000
1	2.827509000	1.399182000	-2.511675000
1	6.137322000	-2.579448000	-0.618965000

6	1.251570000	-3.062427000	-1.423801000
6	3.406052000	-2.106399000	-0.902212000
6	1.589571000	-4.209620000	-0.697175000
1	0.277507000	-3.000588000	-1.895090000
6	3.743294000	-3.247456000	-0.175349000
1	4.109140000	-1.285378000	-0.956462000
6	2.837184000	-4.308991000	-0.075678000
1	0.872840000	-5.022022000	-0.615731000
1	4.707031000	-3.295142000	0.323851000
1	3.095749000	-5.198075000	0.492655000
6	0.639670000	-0.856958000	-3.305776000
1	-0.280462000	-1.058816000	-2.756111000
1	0.534100000	0.085400000	-3.851029000

## II\_Co(III)\_heter<sub>t</sub>

(G = -3791.117875) (triplet)

27	0.207299000	0.425113000	0.592978000
16	-2.598405000	-0.551077000	-0.961314000
7	-1.983712000	-0.133477000	0.620150000
8	-2.279059000	0.592904000	-1.825911000
7	0.115257000	2.284652000	-0.384825000
7	2.246641000	0.341774000	0.969190000
7	-0.379560000	1.652177000	2.242199000
7	0.252770000	-1.088197000	2.160238000
8	-2.021792000	-1.872288000	-1.253529000
6	-2.573518000	1.159021000	1.110650000
1	-3.637743000	1.030600000	1.335640000
1	-2.460557000	1.890124000	0.309377000
6	1.584782000	-1.717633000	2.037761000
1	1.560518000	-2.383484000	1.171882000
1	1.834628000	-2.313984000	2.923368000
6	-0.034705000	3.325242000	0.465301000
6	3.126631000	1.305991000	0.648490000

1	2.767543000	2.082827000	-0.017154000
6	0.064446000	2.510508000	-1.709067000
1	0.181111000	1.646619000	-2.349438000
6	0.137857000	3.006732000	1.929811000
1	1.212645000	3.012280000	2.145714000
1	-0.335790000	3.770793000	2.556590000
6	3.925931000	-0.742549000	2.289418000
1	4.197997000	-1.572189000	2.932824000
6	-1.865241000	1.649442000	2.374695000
1	-2.229894000	2.661269000	2.581230000
1	-2.142659000	1.033715000	3.230683000
6	4.842656000	0.252441000	1.953632000
1	5.857903000	0.215675000	2.335583000
6	-2.157024000	-1.282319000	1.585586000
1	-2.901061000	-1.994571000	1.220588000
1	-2.559422000	-0.876929000	2.512643000
6	-4.356301000	-0.701180000	-0.788814000
6	0.298746000	1.064862000	3.427399000
1	-0.048044000	1.539182000	4.354068000
1	1.366716000	1.263689000	3.317452000
6	0.058741000	-0.444578000	3.494374000
1	0.747593000	-0.880677000	4.225999000
1	-0.951607000	-0.656831000	3.846949000
6	-4.913004000	-1.958419000	-0.535295000
1	-4.286264000	-2.842716000	-0.496138000
6	2.633208000	-0.665823000	1.780116000
6	-0.842253000	-2.023922000	1.811606000
1	-0.988333000	-2.777192000	2.597344000
1	-0.554097000	-2.530495000	0.887165000
6	-5.145135000	0.454202000	-0.862332000
1	-4.695250000	1.418924000	-1.070341000
6	4.432487000	1.304491000	1.130310000
1	5.109233000	2.108231000	0.857741000
6	-0.314808000	4.850645000	-1.366186000
1	-0.489757000	5.852152000	-1.747325000
6	-0.142820000	3.777712000	-2.241621000
1	-0.173899000	3.911783000	-3.317257000
6	-0.261100000	4.619917000	0.008809000
1	-0.389266000	5.424081000	0.725695000
6	-6.291606000	-2.051221000	-0.351529000
1	-6.741709000	-3.021022000	-0.160288000
6	-7.108800000	-0.913546000	-0.412974000
6	-6.518022000	0.334595000	-0.675096000
1	-7.143740000	1.220653000	-0.734584000
6	-8.594958000	-1.016920000	-0.197702000
1	-8.912059000	-2.061797000	-0.117903000
1	-9.142142000	-0.543957000	-1.022668000
1	-8.887503000	-0.495603000	0.723622000
6	1.834995000	-0.751692000	-2.340604000
8	2.911413000	-0.161875000	-2.957185000
6	2.166200000	-2.006592000	-1.545732000

1	0.818245000	-1.668235000	-4.020030000
1	1.564246000	0.046708000	-1.602589000
1	4.635453000	0.258970000	-2.344047000
8	5.358946000	0.803785000	-1.964791000
1	5.052598000	0.950024000	-1.052479000
1	6.212294000	-2.170892000	-0.958636000
8	6.608229000	-1.378800000	-0.561511000
1	6.291218000	-0.660314000	-1.148466000
1	4.019357000	2.292243000	-2.342713000
8	3.141926000	2.682811000	-2.521605000
1	2.657575000	1.918028000	-2.880051000

## I\_homo<sub>s</sub>

(G = -3791.400991) (singlet)

27	0.205434000	0.822805000	0.446905000
16	-2.689984000	-0.535584000	-0.891275000
7	-2.097106000	0.089629000	0.582747000
8	-2.586662000	0.538146000	-1.891332000
7	-0.034907000	2.278686000	-0.785976000
7	2.288872000	1.057901000	0.927739000
7	-0.430560000	2.125907000	1.846342000
7	0.350136000	-0.493436000	1.976109000
8	-1.983905000	-1.808387000	-1.113378000
6	-2.677287000	1.414480000	0.932936000
1	-3.728555000	1.321014000	1.233904000
1	-2.618596000	2.040273000	0.042083000
6	3.155423000	2.042315000	0.645249000
1	2.750799000	2.895260000	0.107974000
6	-0.105902000	2.228725000	-2.131913000
1	0.036839000	1.251160000	-2.574047000
6	-0.014184000	3.451487000	1.317654000
1	1.056153000	3.565648000	1.520626000
1	-0.541866000	4.274855000	1.812688000
6	4.060796000	-0.159070000	1.998860000
1	4.377133000	-1.053935000	2.523898000
6	-1.909057000	2.066094000	2.076654000
1	-2.307477000	3.076884000	2.214979000
1	-2.093204000	1.525752000	3.006134000
6	4.958569000	0.868446000	1.707326000
1	6.000098000	0.787492000	2.002251000
6	-2.083243000	-0.940657000	1.663750000
1	-2.788506000	-1.751683000	1.457049000
1	-2.437513000	-0.467658000	2.580077000
6	-4.412347000	-0.885064000	-0.606951000
6	0.301504000	1.752733000	3.088698000
1	-0.110637000	2.276239000	3.960901000
1	1.339925000	2.056369000	2.965659000
6	0.211405000	0.238530000	3.287633000
1	0.991821000	-0.088782000	3.982688000
1	-0.746491000	-0.028124000	3.735910000
6	-4.802142000	-2.172814000	-0.226585000
1	-4.073343000	-2.974455000	-0.175946000
6	2.732410000	-0.022791000	1.601339000
6	-0.689795000	-1.542516000	1.836197000
1	-0.693313000	-2.204955000	2.712871000
1	-0.439135000	-2.130458000	0.952231000
6	-5.337699000	0.161880000	-0.694420000
1	-5.023074000	1.152709000	-1.004125000
6	4.496910000	1.996635000	1.021582000
1	5.158969000	2.820583000	0.777018000
6	-0.541928000	4.585019000	-2.279635000
1	-0.743478000	5.480701000	-2.859334000

6	-0.347494000	3.355151000	-2.910155000		1	1.454941000	1.449573000	3.202767000
1	-0.388296000	3.260642000	-3.990104000		6	0.220841000	-0.315626000	3.359314000
6	-0.475390000	4.644197000	-0.886383000		1	0.948673000	-0.737597000	4.061724000
1	-0.619913000	5.575925000	-0.349133000		1	-0.767087000	-0.561388000	3.750294000
6	-6.144416000	-2.408753000	0.066702000		6	-4.942832000	-1.997393000	-0.324062000
1	-6.461354000	-3.407613000	0.353467000		1	-4.309085000	-2.875670000	-0.269145000
6	-7.093644000	-1.378356000	-0.004237000		6	2.769777000	-0.507481000	1.683365000
6	-6.672966000	-0.097035000	-0.395232000		6	-0.691724000	-1.923319000	1.740240000
1	-7.402491000	0.704833000	-0.468697000		1	-0.758958000	-2.672057000	2.544064000
6	-8.534326000	-1.632931000	0.354272000		1	-0.445617000	-2.433247000	0.806370000
1	-8.798816000	-2.685997000	0.208224000		6	-5.203649000	0.389071000	-0.760855000
1	-9.206067000	-1.009143000	-0.246339000		1	-4.771455000	1.345973000	-1.032936000
1	-8.714318000	-1.388231000	1.410579000		6	4.585469000	1.482422000	1.169392000
6	2.396224000	-1.686824000	-2.528087000		1	5.267567000	2.298478000	0.950454000
8	3.460282000	-0.984657000	-2.855900000		6	-0.602182000	4.670666000	-1.639056000
6	2.380897000	-2.590824000	-1.427752000		1	-0.890429000	5.623471000	-2.072666000
6	1.215371000	-3.351369000	-0.176518000		6	-0.378767000	3.552938000	-2.443279000
6	3.531602000	-2.772688000	-0.594135000		1	-0.477278000	3.602915000	-3.522815000
6	1.220909000	-4.219363000	0.007932000		6	-0.443219000	4.535179000	-0.257720000
1	0.308068000	-3.237362000	-1.661237000		1	-0.599436000	5.371100000	0.416849000
6	3.520745000	-3.641325000	0.485621000		6	-6.309808000	-2.090202000	-0.077983000
1	4.421269000	-2.197915000	-0.803751000		1	-6.741711000	-3.053084000	0.181379000
6	2.368966000	-4.385701000	0.806243000		6	-7.141012000	-0.9611192000	-0.164910000
1	0.314697000	-4.773319000	0.245526000		6	-6.570366000	0.272257000	-0.510483000
1	4.417761000	-3.727553000	1.096543000		1	-7.205228000	1.150496000	-0.585999000
1	2.360214000	-5.061897000	1.656511000		6	-8.618341000	-1.085124000	0.102217000
6	1.149229000	-1.488845000	-3.365774000		1	-9.119629000	-0.115103000	0.018415000
1	0.329985000	-1.046390000	-2.778446000		1	-8.799234000	-1.486356000	1.107756000
1	1.375749000	-0.820503000	-4.203698000		1	-9.084279000	-1.779059000	-0.609571000
1	0.767165000	-2.437562000	-3.772209000		6	1.669089000	-0.856962000	-2.098872000
1	0.549949000	-0.205123000	-0.651045000		8	2.591229000	0.069354000	-2.356781000
1	4.795779000	-0.518630000	-1.924336000		6	2.100451000	-2.116442000	-1.467005000
8	5.552026000	-0.076081000	-1.440172000		6	1.226148000	-3.225926000	-1.325926000
1	5.095717000	0.395870000	-0.723920000		6	3.391806000	-2.239902000	-0.904080000
1	6.251746000	-1.273090000	-0.254529000		6	1.625228000	-4.378470000	-0.652471000
1	3.791917000	1.815333000	-1.898844000		1	0.219970000	-3.171090000	-1.728519000
8	3.135131000	1.681395000	-2.600313000		6	3.787772000	-3.394568000	-0.233650000
8	6.564866000	-1.880224000	0.458170000		1	4.076725000	-1.407976000	-0.970056000
1	3.200296000	0.701748000	-2.769689000		6	2.910573000	-4.479155000	-0.096114000
1	6.342759000	-2.758359000	0.109761000		1	0.927108000	-5.207395000	-0.555815000
					1	4.786190000	-3.438510000	0.1969570000
					1	3.216342000	-5.378315000	0.431949000
					6	0.587681000	-1.000864000	-3.172307000
					1	-0.368606000	-1.349065000	-2.776095000
					1	0.427975000	-0.040473000	-3.672789000
					1	0.916940000	-1.717230000	-3.942648000
					1	0.780245000	-0.282557000	-0.854560000
					1	4.208641000	0.299748000	-2.072654000
					8	5.137890000	0.664597000	-1.934093000
					1	5.074535000	1.055992000	-1.045665000
					1	6.091168000	-0.715361000	-1.224625000
					1	3.920088000	2.515028000	-2.280885000
					8	2.979955000	2.717486000	-2.428373000
					8	6.557651000	-1.429218000	-0.728024000
					1	2.604586000	1.797514000	-2.450572000
					1	6.154830000	-2.235005000	-1.089318000

**TS\_homo<sub>s</sub>**  
(G = -3791.376265) (singlet)

27	0.368092000	0.560683000	0.502166000		1	0.916940000	-1.717230000	-3.942648000
16	-2.643401000	-0.597202000	-0.905224000		1	0.780245000	-0.282557000	-0.854560000
7	-1.989547000	-0.126646000	0.601999000		1	4.208641000	0.299748000	-2.072654000
8	-2.396452000	0.503837000	-1.848816000		8	5.137890000	0.664597000	-1.934093000
7	0.116442000	2.198363000	-0.511508000		1	5.074535000	1.055992000	-1.045665000
7	2.353897000	0.600436000	1.032007000		1	6.091168000	-0.715361000	-1.224625000
7	-0.298596000	1.733055000	2.107656000		1	3.920088000	2.515028000	-2.280885000
7	0.382155000	-0.945143000	2.007193000		8	2.979955000	2.717486000	-2.428373000
8	-2.098756000	-1.937439000	-1.185941000		8	6.557651000	-1.429218000	-0.728024000
6	-2.524260000	1.187451000	1.059292000		1	2.604586000	1.797514000	-2.450572000
1	-3.587730000	1.108661000	1.319153000		1	6.154830000	-2.235005000	-1.089318000
1	-2.415056000	1.885858000	0.229150000		1	4.786190000	-3.438510000	0.1969570000
6	1.715872000	-1.567875000	1.886295000		6	3.216342000	-5.378315000	0.431949000
1	1.700836000	-2.216102000	1.009213000		6	0.587681000	-1.000864000	-3.172307000
1	1.954786000	-2.187505000	2.761862000		1	-0.368606000	-1.349065000	-2.776095000
6	-0.075844000	3.302190000	0.264799000		1	0.427975000	-0.040473000	-3.672789000
6	3.250642000	1.571197000	0.783178000		1	0.916940000	-1.717230000	-3.942648000
1	2.873280000	2.439569000	0.252798000		6	2.127834000	0.776735000	
6	-0.024782000	2.348872000	-1.844628000		7	-2.143288000	0.766002000	-0.591816000
1	0.156952000	1.463940000	-2.433197000		7	0.312553000	2.170767000	-1.930650000
6	0.190226000	3.075160000	1.726257000		7	-0.388125000	-0.558416000	-2.061060000
1	1.274904000	3.084398000	1.881586000		8	1.849493000	-1.624807000	1.154565000
1	-0.251004000	3.868831000	2.342984000		6	2.520142000	1.522222000	-1.011624000
6	4.089681000	-0.678194000	2.095248000		1	3.566057000	1.359975000	-1.291681000
1	4.374823000	-1.590125000	2.610176000		1	2.475277000	2.174733000	-0.139921000
6	-1.776308000	1.713594000	2.281911000		6	6.155711000	-1.886947000	-1.076248000
1	-2.150146000	2.725032000	2.482091000		1	-2.024879000	-1.730343000	-2.818048000
1	-2.022235000	1.111528000	3.158159000		6	0.032742000	3.354965000	0.213083000
6	5.018673000	0.325842000	1.825490000		6	-2.924135000	1.870955000	-0.275767000
1	6.055178000	0.215592000	2.128717000		1	-2.516751000	2.536484000	0.474593000
6	-2.049922000	-1.241075000	1.595876000		6	-0.090738000	2.019493000	2.116612000
1	-2.788290000	-1.995996000	1.311094000		1	-0.202573000	1.016844000	2.511044000
1	-2.400310000	-0.829027000	2.541904000					
6	-4.401675000	-0.752395000	-0.667314000					
6	0.397682000	1.200596000	3.299077000					
1	0.021353000	1.657382000	4.225127000					

27	-0.242319000	0.680924000	-0.511550000
16	2.554291000	-0.362787000	0.887506000
7	1.871460000	0.219850000	-0.625570000
8	2.465452000	0.744282000	1.848097000
6	-0.086505000		

6	-0.148749000	3.413703000	-1.287605000		7	-0.034907000	2.278686000	-0.785976000
1	-1.225083000	3.511524000	-1.473560000		7	2.288872000	1.057901000	0.927739000
1	0.346124000	4.300830000	-1.702198000		7	-0.430560000	2.125907000	1.846342000
6	-3.890993000	0.139445000	-2.189125000		7	0.350136000	-0.493436000	1.976109000
1	-4.225712000	-0.571653000	-2.939778000		8	-1.983905000	-1.808387000	-1.113378000
6	1.769854000	2.161627000	-2.177931000		6	-2.677287000	1.414480000	0.932936000
1	2.152940000	3.180946000	-2.309677000		1	-3.728555000	1.321014000	1.233904000
1	1.974567000	1.622107000	-3.104235000		1	-2.618596000	2.040273000	0.042083000
6	-4.682468000	1.262695000	-1.842086000		6	1.700330000	-1.093340000	1.844326000
1	-5.644981000	1.447680000	-2.305969000		1	1.678970000	-1.753631000	0.975523000
6	2.026358000	-0.844749000	-1.697314000		1	1.955325000	-1.690116000	2.728912000
1	2.788086000	-1.579353000	-1.427457000		6	-0.210900000	3.480317000	-0.174553000
1	2.388519000	-0.350114000	-2.597932000		6	3.155423000	2.042315000	0.645249000
6	4.269314000	-0.703604000	0.571767000		1	2.750799000	2.895260000	0.107974000
6	-0.490257000	1.736900000	-3.095394000		6	-0.105902000	2.228725000	-2.131913000
1	-0.224051000	2.289560000	-4.007087000		1	0.036839000	1.251160000	-2.574047000
1	-1.537034000	1.935520000	-2.861049000		6	-0.014184000	3.451487000	1.317654000
6	-0.295552000	0.235741000	-3.338831000		1	1.056153000	3.565648000	1.520626000
1	-1.053136000	-0.117069000	-4.045831000		1	-0.541866000	4.274855000	1.812688000
1	0.678812000	0.050747000	-3.793592000		6	4.060796000	-0.159070000	1.998860000
6	4.669749000	-2.007716000	0.263486000		1	4.377133000	-1.053935000	2.523898000
1	3.947441000	-2.816784000	0.250378000		6	-1.909057000	2.066094000	2.076654000
6	-2.682135000	-0.079056000	-1.575182000		1	-2.307477000	3.076884000	2.214979000
6	0.703055000	-1.553048000	-1.939109000		1	-2.093204000	1.525752000	3.006134000
1	0.777471000	-2.176366000	-2.840119000		6	4.958569000	0.868446000	1.707326000
1	0.465317000	-2.191172000	-1.085912000		1	6.000098000	0.787492000	2.002251000
6	5.186051000	0.354478000	0.616006000		6	-2.083243000	-0.940657000	1.663750000
1	4.862869000	1.357174000	0.873566000		1	-2.788506000	-1.751683000	1.457049000
6	-4.142483000	2.137834000	-0.866246000		1	-2.437513000	-0.467658000	2.580077000
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6	0.208211000	4.383339000	2.376379000		6	0.301504000	1.752733000	3.088698000
1	0.332293000	5.264042000	2.999270000		1	-0.110637000	2.276239000	3.960901000
6	0.048383000	3.122864000	2.951801000		1	1.339925000	2.056369000	2.965659000
1	0.035321000	2.987350000	4.027769000		6	0.211405000	0.238530000	3.287633000
6	0.198843000	4.499447000	0.985320000		1	0.991821000	-0.088782000	3.982688000
1	0.306057000	5.461754000	0.495337000		1	-0.746491000	-0.028124000	3.735910000
6	6.014826000	-2.247270000	-0.010217000		6	-4.802142000	-2.172814000	-0.226585000
1	6.340876000	-3.256859000	-0.243332000		1	-4.073343000	-2.974455000	-0.175946000
6	6.955492000	-1.206906000	0.013887000		6	2.732410000	-0.022791000	1.601339000
6	6.523630000	0.090043000	0.337448000		6	-0.689795000	-1.542516000	1.836197000
1	7.246996000	0.899772000	0.374661000		1	-0.693313000	-2.204955000	2.712871000
6	8.400150000	-1.467307000	-0.320565000		1	-0.439135000	-2.130458000	0.952231000
1	8.658919000	-2.520497000	-0.167079000		6	-5.337699000	0.161880000	-0.694420000
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6	-1.967035000	-1.364369000	2.221643000		1	5.158969000	2.820583000	0.777018000
8	-3.216202000	-0.953690000	2.697563000		6	-0.541928000	4.585019000	-2.279635000
6	-2.052345000	-2.603718000	1.317531000		1	-0.743478000	5.480701000	-2.859334000
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6	-3.352356000	-3.984070000	-0.220890000		6	-6.144416000	-2.408753000	0.066702000
1	-4.163141000	-2.409556000	0.990648000		1	-6.461354000	-3.407613000	0.353467000
6	-2.209090000	-4.701629000	-0.580721000		6	-7.093644000	-1.378356000	-0.004237000
1	-0.090388000	4.936434000	-0.235174000		6	-6.672966000	-0.097035000	-0.395232000
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1	-0.953102000	-0.639208000	3.983289000		1	-8.714318000	-1.388231000	1.410579000
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1	-1.500922000	-0.587760000	1.573498000		8	3.460282000	-0.984657000	-2.855900000
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1	-4.794843000	0.512063000	0.586688000		6	3.531602000	-2.772688000	-0.594135000
1	-5.731226000	-1.298028000	0.033668000		6	1.220909000	-4.219363000	0.007932000
1	-3.705808000	1.824630000	2.178805000		1	0.308068000	-3.237362000	-1.661237000
8	-3.228011000	1.634561000	3.002497000		6	3.520745000	-3.641325000	0.485621000
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1	-3.170326000	0.616847000	2.964658000		6	2.368966000	-4.385701000	0.806243000
1	-6.065138000	-2.781454000	-0.207933000		1	0.314697000	-4.773319000	0.245526000
1					1	4.417761000	-3.727553000	1.096543000
I_homo_t					1	2.360214000	-5.061897000	1.656511000
(G = -3791.406244) (triplet)					6	1.149229000	-1.488845000	-3.365774000
27	0.205434000	0.822805000	0.446905000		1	0.329985000	-1.046390000	-2.778446000
16	-2.689984000	-0.535584000	-0.891275000		1	1.375749000	-0.820503000	-4.203698000
7	-2.097106000	0.089629000	0.582747000		1	0.767165000	-2.437562000	-3.772009000
8	-2.586662000	0.538146000	-1.891332000		8	5.552026000	-0.076081000	-1.440172000

1	5.095717000	0.395870000	-0.723920000	6	3.356947000	-2.237176000	-0.866872000
1	6.251746000	-1.273090000	-0.254529000	6	1.613843000	-4.398001000	-0.640077000
1	3.791917000	1.815533000	-1.898844000	1	0.245003000	-3.250642000	-1.821642000
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1	3.200296000	0.701748000	-2.769689000	6	2.873731000	-4.460854000	-0.021997000
1	6.342759000	-2.758359000	0.109761000	1	0.926264000	-5.236534000	-0.553561000
				1	4.716016000	-3.380974000	0.331007000
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				6	0.592228000	-1.059505000	-3.254435000
				1	-0.341965000	-1.444345000	-2.840633000
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27	0.323311000	0.554275000	0.492823000	1	0.909956000	-1.738389000	-4.063807000
16	-2.584954000	-0.603187000	-0.877351000	1	0.619342000	-0.301586000	-0.829432000
7	-1.964073000	-0.104029000	0.641168000	1	4.232324000	0.263029000	-2.109789000
8	-2.331059000	0.4844482000	-1.833592000	8	5.146617000	0.641600000	-1.954790000
7	0.105481000	2.220380000	-0.520977000	1	5.060533000	1.028151000	-1.065841000
7	2.303929000	0.581190000	1.012198000	1	6.079002000	-0.743451000	-1.201383000
7	-0.294670000	1.759749000	2.118140000	1	3.923909000	2.460895000	-2.337015000
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6	-2.515902000	1.213879000	1.070618000	1	2.599411000	1.772147000	-2.540612000
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1	1.949396000	-2.171833000	2.818328000				
6	-0.067567000	3.324610000	0.261003000				
6	3.195911000	1.547806000	0.726527000	27	0.322504000	0.550226000	0.539744000
1	2.813741000	2.391450000	0.160899000	16	-2.572385000	-0.424497000	-0.916594000
6	-0.028745000	2.384208000	-1.855544000	7	-1.954921000	0.027470000	0.627938000
1	0.136371000	1.498046000	-2.450424000	8	-2.374561000	0.720209000	-1.817300000
6	0.206912000	3.092440000	1.721681000	7	0.198716000	2.198473000	-0.498700000
1	1.293319000	3.088243000	1.866790000	7	2.299919000	0.431003000	1.059670000
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6	4.048362000	-0.644305000	2.123406000	7	0.254258000	-0.962164000	2.172622000
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6	-1.772162000	1.758014000	2.289276000	6	-2.487300000	1.354980000	1.069150000
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1	-2.825720000	-1.941619000	1.366410000	6	0.034235000	3.317980000	0.285254000
1	-2.422213000	-0.765993000	2.584648000	6	3.243597000	1.340195000	0.746397000
6	-4.346607000	-0.765417000	-0.669347000	1	2.915869000	2.167179000	0.124707000
6	0.399122000	1.233722000	3.313666000	6	0.082906000	2.382489000	-1.845488000
1	0.037993000	1.713942000	4.234275000	1	0.247554000	1.501326000	-2.453805000
1	1.459596000	1.463758000	3.205238000	6	0.294172000	3.090077000	1.751652000
6	0.202806000	-0.281210000	3.412776000	1	1.378646000	3.011095000	1.900009000
1	0.926802000	-0.690635000	4.128150000	1	-0.074342000	3.935026000	2.350610000
1	-0.788108000	-0.501120000	3.813189000	6	3.953862000	-0.806057000	2.287964000
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1	-0.828519000	-2.643638000	2.650306000	6	4.931278000	0.129995000	1.950247000
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1	5.205067000	2.298923000	0.875782000	6	-4.321064000	-0.687867000	-0.714273000
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1	-0.840960000	5.674764000	-2.063945000	1	0.032626000	1.727726000	4.303588000
6	-0.359269000	3.597719000	-2.447057000	1	1.439017000	1.408148000	3.270659000
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1	-0.558652000	5.400779000	0.425189000	1	-0.919990000	-0.437814000	3.850968000
6	-6.263273000	-2.102716000	-0.107430000	6	-4.805286000	-1.980975000	-0.495211000
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6	1.701395000	-0.938447000	-2.219504000	1	5.285532000	1.993765000	0.892692000
8	2.587558000	0.003917000	-2.424209000	6	-0.436247000	4.724485000	-1.617130000
6	2.091041000	-2.153061000	-1.493502000	1	-0.691110000	5.689790000	-2.043341000
6	1.229180000	-3.273859000	-1.365805000	6	-0.226850000	3.601046000	-2.428810000

1	-0.302848000	3.666100000	-3.510408000		6	0.253293000	0.194647000	3.255539000
6	-0.295194000	4.560046000	-0.230890000		1	1.056349000	-0.061191000	3.956739000
1	-0.431283000	5.392863000	0.453571000		1	-0.679413000	-0.133136000	3.717427000
6	-6.172577000	-2.159762000	-0.290545000		6	-4.726151000	-2.378056000	-0.156431000
1	-6.563209000	-3.160688000	-0.129906000		1	-3.990226000	-3.170153000	-0.070697000
6	-7.054165000	-1.069019000	-0.294018000		6	2.726901000	0.187245000	1.498879000
6	-6.538695000	0.217308000	-0.523091000		6	-0.514771000	-1.658750000	1.821734000
1	-7.214670000	1.067754000	-0.542559000		1	-0.486905000	-2.333584000	2.689678000
6	-8.525447000	-1.265439000	-0.039532000		1	-0.225272000	-2.223050000	0.932357000
1	-8.822393000	-2.305311000	-0.213049000		6	-5.283350000	-0.069766000	-0.725452000
1	-9.127431000	-0.611206000	-0.681001000		1	-4.976170000	0.910538000	-1.073261000
1	-8.770244000	-1.015243000	1.002186000		6	4.207481000	2.403316000	0.825798000
6	1.578248000	-0.858953000	-2.260316000		1	4.755088000	3.295102000	0.540958000
8	2.558926000	0.117331000	-2.291733000		6	-1.232076000	4.896617000	-1.978271000
6	1.970316000	-2.111540000	-1.463825000		1	-1.587208000	5.820512000	-2.425047000
6	1.060626000	-3.170586000	-1.296814000		6	-0.962165000	3.781411000	-2.773996000
6	3.229867000	-2.229071000	-0.868814000		1	-1.096861000	3.807551000	-3.849904000
6	1.407162000	-4.311297000	-0.568801000		6	-1.046558000	4.808872000	-0.598226000
1	0.069208000	-3.095948000	-1.732352000		1	-1.249595000	5.650087000	0.056510000
6	3.584829000	-3.368673000	-0.139766000		6	-6.067435000	-2.615337000	0.138093000
1	3.932102000	-1.413411000	-0.954734000		1	-6.376146000	-3.604851000	0.463344000
6	2.676680000	-4.418089000	0.013303000		6	-7.026783000	-1.598455000	0.018161000
1	0.684374000	-5.114901000	-0.449386000		6	-6.617576000	-0.330399000	-0.423974000
1	4.567389000	-3.419029000	0.323391000		1	-7.354928000	0.459632000	-0.535835000
1	2.946356000	-5.302774000	0.584329000		6	-8.466576000	-1.853887000	0.378434000
6	1.146690000	-1.259422000	-3.688115000		1	-8.731034000	-2.906725000	0.230237000
1	0.331710000	-1.994365000	-3.688508000		1	-9.139206000	-1.228197000	-0.218857000
1	0.808158000	-0.364213000	-4.226227000		1	-8.643318000	-1.613459000	1.436273000
1	2.003430000	-1.685043000	-4.228688000		6	2.645023000	-2.014665000	-2.494536000
1	0.658969000	-0.473354000	-1.764563000		8	3.532500000	-1.132948000	-2.903613000
1	4.143775000	0.186672000	-2.205667000		6	2.772915000	-2.724482000	-1.266171000
8	5.104648000	0.503189000	-2.067996000		6	1.762221000	-3.625421000	-0.787652000
1	5.026852000	1.005012000	-1.238880000		6	3.923840000	-2.562850000	-0.428149000
1	5.977461000	-0.820594000	-1.209538000		6	9.197763000	-4.313364000	0.409555000
1	4.026157000	2.445624000	-2.562323000		1	0.851903000	-3.761471000	-1.363917000
8	3.083428000	2.682746000	-2.587453000		6	4.066556000	-3.259896000	0.760699000
8	6.419571000	-1.508906000	-0.654731000		1	4.694256000	-1.870171000	-0.730898000
1	2.670111000	1.772016000	-2.546816000		6	3.071148000	-4.153729000	1.201081000
1	6.027158000	-2.331906000	-0.986704000		1	1.125795000	-4.982422000	0.740827000
1					1	4.960145000	-3.092041000	1.359644000

### I\_homo<sub>quint</sub>

(G = -3791.389625) (quintuplet)

27	0.146271000	0.763096000	0.221086000	
16	-2.632583000	-0.756333000	-0.901822000	
7	-2.013491000	-0.093404000	0.575001000	
8	-2.542625000	0.313269000	-1.906646000	
7	-0.337565000	2.531094000	-0.826714000	
7	2.163014000	1.155544000	0.746299000	
7	-0.575993000	2.084628000	1.877302000	
7	0.441817000	-0.543625000	1.972400000	
8	-1.923278000	-2.027842000	-1.112366000	
6	-2.732778000	1.158416000	0.963632000	
1	-3.760358000	0.935302000	1.272842000	
1	-2.756702000	1.801963000	0.083360000	
6	1.837764000	-0.993128000	1.802960000	
1	1.864853000	-1.674006000	0.948573000	
1	2.201565000	-1.533401000	2.685664000	
6	-0.591797000	3.609909000	-0.056030000	
6	2.886326000	2.237894000	0.417089000	
1	2.378312000	2.988959000	-0.179687000	
6	-0.520727000	2.616715000	-2.154910000	
1	-0.307760000	1.716181000	-2.719219000	
6	-0.287328000	3.454446000	1.415046000	
1	0.784869000	3.638897000	1.550134000	
1	-0.828892000	4.209507000	1.999998000	
6	4.046233000	0.272795000	1.935698000	
1	4.465842000	-0.531299000	2.529866000	
6	-2.026762000	1.875351000	2.113712000	
1	-2.536744000	2.835895000	2.256027000	
1	-2.162484000	1.314244000	3.039864000	
6	4.798869000	1.397581000	1.596186000	
1	5.830197000	1.485908000	1.922490000	
6	-1.940705000	-1.139859000	1.649360000	
1	-2.598720000	-1.984962000	1.428554000	
1	-2.323985000	-0.697453000	2.568237000	
6	-4.348515000	-1.102024000	-0.586133000	
6	0.234372000	1.714513000	3.058351000	
1	-0.149728000	2.192532000	3.970603000	
1	1.248785000	2.077568000	2.889634000	

### TS\_homo<sub>quint</sub>

(G = -3791.362011) (quintuplet)

27	0.284834000	0.545380000	0.411417000	
16	-2.589458000	-0.664730000	-0.878528000	
7	-1.989667000	-0.139565000	0.651723000	
8	-2.344310000	0.427395000	-1.832137000	
7	0.181905000	2.342466000	-0.545055000	
7	2.296570000	0.584512000	1.011905000	
7	-0.374532000	1.790029000	2.123362000	
7	0.342716000	-0.937775000	2.102653000	
8	-2.002884000	-1.993823000	-1.116695000	
6	-2.572011000	1.172042000	1.068806000	
1	-3.637066000	1.067266000	1.308581000	
1	-2.458301000	1.855239000	0.226329000	
6	1.679478000	-1.544572000	1.967618000	
1	1.660715000	-2.201098000	1.093146000	
1	1.943204000	-2.151121000	2.845027000	
6	-0.235962000	3.386521000	0.283897000	
6	3.163525000	1.568665000	0.720185000	
1	2.766672000	2.383282000	0.124587000	
6	0.025273000	2.549538000	-1.901667000	
1	0.379236000	1.741306000	-2.535247000	
6	0.082351000	3.147541000	1.729151000	

1	1.171921000	3.160032000	1.868440000		7	2.345550000	0.453283000	1.049705000
1	-0.357652000	3.921593000	2.373554000		7	-0.221133000	1.744146000	2.129481000
6	4.028812000	-0.579365000	2.187967000		7	0.323426000	-1.009649000	2.160724000
1	4.326265000	-1.449996000	2.762800000		8	-2.065879000	-1.825702000	-1.234527000
6	-1.846539000	1.739743000	2.289422000		6	-2.453559000	1.279822000	1.052658000
1	-2.248118000	2.746961000	2.458053000		1	-3.516909000	1.209106000	1.309781000
1	-2.090920000	1.154110000	3.177880000		1	-2.332192000	1.973110000	0.220615000
6	4.931282000	0.439850000	1.887945000		6	1.652029000	-1.660741000	2.032399000
1	5.960426000	0.381401000	2.228046000		1	1.603260000	-2.271353000	1.124969000
6	-2.078525000	-1.235296000	1.669679000		1	1.859107000	-2.319746000	2.887791000
1	-2.820868000	-1.987027000	1.386177000		6	0.075658000	3.284927000	0.239957000
1	-2.439894000	-0.797342000	2.599539000		6	3.320753000	1.406618000	0.787360000
6	-4.347104000	-0.849619000	-0.671054000		1	3.018386000	2.213376000	0.125529000
6	0.342450000	1.271148000	3.303791000		6	0.046786000	2.353669000	-1.884249000
1	-0.014019000	1.738978000	4.233339000		1	0.177606000	1.463496000	-2.486642000
1	1.397082000	1.524527000	3.183402000		6	0.341320000	3.046828000	1.708618000
6	0.182331000	-0.248626000	3.415805000		1	1.426555000	2.998413000	1.854748000
1	0.915935000	-0.632951000	4.135139000		1	-0.054856000	3.871245000	2.313614000
1	-0.802525000	-0.486766000	3.820359000		6	3.971967000	-0.719361000	2.432420000
6	-4.874170000	-2.101741000	-0.343313000		1	4.187513000	-1.574525000	3.070135000
1	-4.226810000	-2.968683000	-0.267808000		6	-1.700639000	1.795340000	2.278729000
6	2.716358000	-0.474048000	1.731910000		1	-2.028239000	2.826609000	2.453994000
6	-0.727977000	-1.921387000	1.854584000		1	-1.984056000	1.221277000	3.161448000
1	-0.808925000	-2.645502000	2.679126000		6	4.971759000	0.262514000	2.163826000
1	-0.473829000	-2.460597000	0.939208000		1	5.967819000	0.192231000	2.587166000
6	-5.165709000	0.280403000	-0.792412000		6	-2.097136000	-1.153417000	1.614467000
1	-4.741069000	1.242911000	-1.056215000		1	-2.863589000	-1.866901000	1.300549000
6	4.487349000	1.542253000	1.151390000		1	-2.469982000	-0.702730000	2.533699000
1	5.152594000	2.364337000	0.905549000		6	-4.377328000	-0.662324000	-0.649497000
6	-1.035637000	4.707585000	-1.583322000		6	0.437052000	1.197204000	3.343016000
1	-1.520238000	5.594573000	-1.977939000		1	0.081895000	1.710565000	4.246305000
6	-0.548556000	3.677316000	-2.438998000		1	1.507409000	1.371702000	3.236150000
1	-0.628974000	3.766004000	-3.519779000		6	0.168356000	-0.309985000	3.464439000
6	-0.849767000	4.523418000	-0.190285000		1	0.862538000	-0.730015000	4.202225000
1	-1.164857000	5.281591000	0.523604000		1	-0.840065000	-0.482518000	3.845890000
6	-6.248597000	-2.217155000	-0.136488000		6	-4.915351000	-1.920102000	-0.359596000
1	-6.673567000	-3.186015000	0.110016000		1	-4.281472000	-2.800061000	-0.343021000
6	-7.093496000	-1.103967000	-0.247744000		6	2.722232000	-0.614589000	1.879223000
6	-6.534037000	0.140915000	-0.581846000		6	-0.794543000	-1.916353000	1.851203000
1	-7.181062000	1.008160000	-0.680974000		1	-0.965526000	-2.646949000	2.656343000
6	-8.575002000	-1.229269000	-0.008252000		1	-0.528703000	-2.460655000	0.940933000
1	-9.143166000	-0.750127000	-0.815013000		6	-5.178884000	0.484136000	-0.703533000
1	-8.858265000	-0.728504000	0.927594000		1	-4.747635000	1.448628000	-0.948239000
1	-8.877591000	-2.279374000	0.061137000		6	4.591071000	1.344711000	1.310101000
6	1.873849000	-1.017566000	-2.348627000		1	5.296784000	2.135991000	1.065266000
8	2.682081000	-0.051406000	-2.511965000		6	-0.427732000	4.690584000	-1.639293000
6	2.262497000	-2.180479000	-1.516935000		1	-0.686200000	5.659140000	-2.056875000
6	1.441940000	-3.323294000	-1.385327000		6	-0.270998000	3.578208000	-2.465279000
6	3.491397000	-2.165018000	-0.828450000		1	-0.394157000	3.648828000	-3.540630000
6	1.838856000	-4.396203000	-0.590167000		6	-0.249716000	4.540497000	-0.262661000
1	0.484263000	-3.367059000	-1.892209000		1	-0.362752000	5.376680000	0.419616000
6	3.888599000	-3.241522000	-0.038588000		6	-6.283724000	-2.021752000	-0.116503000
1	4.128342000	-1.295516000	-0.896244000		1	-6.717810000	-2.993945000	0.098950000
6	3.065764000	-4.366192000	0.089019000		6	-7.112244000	-0.890250000	-0.153315000
1	1.187963000	-5.261668000	-0.496476000		6	-6.542694000	0.357460000	-0.455288000
1	4.836958000	-3.187696000	0.489714000		1	-7.177984000	1.237451000	-0.501975000
1	3.369405000	-5.203799000	0.710764000		6	-8.584377000	-1.004622000	0.141993000
6	0.734037000	-1.155779000	-3.337525000		1	-8.946230000	-2.022190000	-0.040830000
1	-0.140838000	-1.657474000	-2.920911000		1	-9.164405000	-0.302913000	-0.468214000
1	0.441493000	-0.163006000	-3.691801000		1	-8.781891000	-0.763758000	1.195967000
1	1.090515000	-1.737894000	-4.202658000		6	1.529995000	-0.847744000	-2.340572000
1	0.538866000	-0.396841000	-0.927924000		8	2.483625000	0.153571000	-2.318312000
1	4.366962000	0.328577000	-2.117289000		6	1.928333000	-2.112596000	-1.565837000
8	5.238968000	0.763298000	-1.933276000		6	1.017479000	-3.172398000	-1.413762000
1	5.100100000	1.138155000	-1.045820000		6	3.192094000	-2.243709000	-0.983548000
1	6.191422000	-0.601598000	-1.121531000		6	1.365663000	-4.325250000	-0.706394000
1	4.034323000	2.448927000	-2.423112000		1	0.024526000	-3.087523000	-1.845179000
8	3.106536000	2.720101000	-2.546586000		6	3.549946000	-3.395875000	-0.276417000
8	6.628061000	-1.281772000	-0.560063000		1	3.894935000	-1.427855000	-1.058544000
1	2.663717000	1.847796000	-2.600041000		6	2.638649000	-4.444404000	-0.133862000
1	6.256055000	-2.110717000	-0.901266000		1	0.642442000	-5.129967000	-0.596910000
					1	4.536704000	-3.456066000	0.176599000
					1	2.909099000	-5.339458000	0.420488000
					6	1.148036000	-1.223377000	-3.789720000
					1	0.355081000	-1.981163000	-3.829863000
					1	0.798704000	-0.324555000	-4.315051000
					1	2.031621000	-1.610278000	-4.315842000
					1	0.583639000	-0.505171000	-1.860956000
					1	4.083345000	0.275464000	-2.143942000
					8	5.009870000	0.628645000	-1.919101000
					1	4.856770000	0.989289000	-1.023228000

1	5.915893000	-0.759127000	-1.184901000
1	3.930964000	2.475485000	-2.411302000
8	3.009585000	2.718697000	-2.611233000
8	6.360190000	-1.485370000	-0.683659000
1	2.592377000	1.809924000	-2.604920000
1	5.988210000	-2.283215000	-1.091802000

## I\_H\_homo<sub>s</sub>

(G = -3791.848114) (singlet)

6	2.478685000	-3.199679000	-2.927290000
1	1.317375000	-1.560383000	-3.667412000
6	4.398437000	-2.633354000	-1.571336000
4	4.756372000	-0.563122000	-1.209781000
6	3.588777000	-3.610192000	-2.170726000
1	1.840242000	-3.941944000	-3.400401000
1	5.258324000	-2.933360000	-0.978930000
1	3.816937000	-4.665473000	-2.052057000
6	1.476805000	0.980713000	-3.458055000
1	1.398280000	2.070711000	-3.414201000
1	1.602986000	0.679975000	-4.507891000
1	0.525872000	0.547903000	-3.114706000
1	0.367450000	-0.448677000	-0.827967000
1	4.070778000	1.306364000	-1.445343000
1	2.885062000	2.793877000	-0.185068000
8	3.387326000	3.364045000	0.407433000
5	5.904480000	2.246531000	-0.960182000
8	5.418980000	1.652908000	-0.362196000
1	4.832489000	2.264142000	0.144165000
1	2.948499000	3.310401000	-2.467037000
8	2.659700000	4.242926000	-2.541565000
1	2.493728000	4.476583000	-1.613826000
1	2.888733000	3.336515000	1.242002000

### TS\_H\_homo\_s

(G = -3791.835250) (singlet)

27	0.417652000	0.216007000	0.704550000
16	-2.586958000	-0.329148000	-0.961130000
7	-1.937096000	-0.277096000	0.622793000
8	-2.262684000	0.952173000	-1.605901000
7	0.317936000	2.048882000	0.082760000
7	2.447985000	0.028395000	1.190968000
7	-0.145550000	1.038868000	2.510552000
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6	-2.401000000	0.917108000	1.385186000
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1	1.626299000	-2.607222000	0.475479000
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6	0.268097000	2.968128000	1.084613000
6	3.404059000	0.970190000	1.195424000
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6	0.450761000	2.394514000	2.461036000
1	1.525512000	2.289259000	2.645281000
1	0.036720000	3.055572000	3.232230000
6	4.036187000	-1.541598000	2.073605000
1	4.239108000	-2.552856000	2.410893000
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1	-1.920335000	0.317279000	3.402121000
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1	-2.406818000	-1.402826000	2.335364000
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6	0.494365000	0.189397000	3.545332000
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1	5.443159000	1.517754000	1.601869000
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1	5.038996000	-3.364054000	-0.425931000		6	-6.308523000	-0.765545000	0.575653000
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6	0.620361000	-0.588978000	-3.244117000		6	-8.432903000	0.559273000	0.253101000
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27	0.363194000	-0.361420000	-0.809325000		1	-0.345905000	1.949919000	3.089571000
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7	-1.788270000	-0.112379000	-0.752261000		1	3.372937000	0.439315000	2.121894000
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8	-3.384959000	3.367065000	-0.403151000		6	1.358936000	-3.071393000	-2.098588000
1	-5.901609000	2.248699000	0.967689000		6	3.452817000	-2.118407000	-1.332834000
8	-5.416242000	1.656009000	0.368671000		6	1.782822000	-4.329496000	-1.685236000
1	-4.830064000	2.268046000	-0.137086000		1	0.374261000	-2.962900000	-2.540199000
1	-2.943101000	3.307911000	2.470151000		6	3.868955000	-3.384351000	-0.927463000
8	-2.655126000	4.240605000	2.546438000		1	4.115615000	-1.279074000	-1.157025000
1	-2.491078000	4.476785000	1.618995000		6	3.042967000	-4.501586000	-1.093010000
1	-2.889700000	3.338859000	-1.239674000		1	1.124937000	-5.184187000	-1.822405000
					1	4.845757000	-3.494332000	-0.463430000
					1	3.370836000	-5.484811000	-0.767659000
					6	0.581731000	-0.492255000	-3.324316000
					1	0.351258000	0.559877000	-3.510199000
					1	0.912011000	-0.931934000	-4.279323000
					1	-0.336683000	-0.993467000	-3.016420000
					1	0.660109000	-0.292755000	-0.782693000

	3.414922000	0.343573000	-1.946508000	8	3.299439000	1.150505000	-2.575665000
1	2.743229000	2.399046000	-1.406372000	6	2.645608000	-1.178238000	-2.160407000
8	3.379695000	3.129658000	-1.300108000	6	1.681347000	-2.197144000	-2.152941000
1	5.339125000	1.073842000	-2.477369000	6	3.996399000	-1.532235000	-2.055946000
8	5.091290000	0.920941000	-1.549402000	6	2.060323000	-3.538341000	-2.065604000
1	4.716831000	1.785545000	-1.268285000	1	0.626920000	-1.943388000	-2.208576000
1	2.124728000	1.837671000	-3.549215000	6	4.376982000	-2.873501000	-1.949491000
8	1.904143000	2.678338000	-4.000415000	1	4.755364000	-0.757324000	-2.053134000
1	2.129207000	3.332961000	-3.318917000	6	3.411083000	-3.883114000	-1.958052000
1	3.045214000	3.603723000	-0.519529000	1	1.297391000	-4.312532000	-2.067623000
				1	5.430233000	-3.1217173000	-1.861554000
				1	3.706675000	-4.926015000	-1.882394000
				6	1.141487000	0.497459000	-3.319364000
				1	0.966842000	1.570711000	-3.446198000
				1	1.473066000	0.082309000	-4.278790000
27	0.246879000	-0.082871000	0.738571000	1	0.198687000	0.021275000	-3.034083000
16	-2.556071000	-0.022242000	-1.024055000	1	1.800113000	0.558665000	-1.268528000
7	-2.036598000	-0.316698000	0.597566000	1	3.924868000	1.233733000	-1.814168000
8	-2.192772000	1.362116000	-1.355714000	1	2.688455000	3.049401000	-0.360458000
7	0.365597000	1.862277000	0.530606000	8	3.348661000	3.453979000	0.229824000
7	2.161293000	-0.757348000	1.014992000	1	5.671870000	2.365896000	-1.421865000
7	-0.250605000	0.412045000	2.761544000	8	5.271007000	1.772595000	-0.763954000
7	-0.098957000	-2.160036000	1.590023000	1	4.668453000	2.369565000	-0.255326000
8	-1.987187000	-1.127983000	-1.815147000	1	2.723851000	2.826443000	-2.787826000
6	-2.429156000	0.772429000	1.548406000	8	2.426585000	3.741653000	-3.008611000
1	-3.511662000	0.756803000	1.723652000	1	2.247180000	4.140969000	-2.143849000
1	-2.152989000	1.718625000	0.085646000	1	2.962568000	3.317268000	1.112536000
6	1.101928000	-2.926015000	1.224608000				
1	0.996098000	-3.245828000	0.183848000				
1	1.219044000	-3.828621000	1.841080000				
6	0.365968000	2.539955000	1.732699000				
6	3.234113000	0.054298000	1.043657000				
1	3.043869000	1.090920000	0.793142000	27	-0.085259000	-0.425131000	-0.331525000
6	0.304073000	2.645629000	-0.589947000	16	2.866362000	0.045844000	1.211929000
1	0.301903000	2.116940000	-1.530427000	7	2.270955000	-0.601462000	-0.279639000
6	0.528768000	1.654360000	2.936764000	8	2.349668000	1.419932000	1.303664000
1	1.582824000	1.357163000	3.009005000	7	-0.275614000	1.644692000	-0.690056000
1	0.256134000	2.187476000	3.858337000	7	-2.049797000	-1.080894000	-0.848088000
6	3.580349000	-2.586484000	1.655742000	7	0.436155000	-0.289359000	-2.519958000
1	3.666618000	-3.642003000	1.893804000	7	0.240553300	-2.544795000	-0.842234000
6	-1.711316000	0.625981000	2.899066000	8	2.534139000	-0.938361000	2.252896000
1	-1.915938000	1.539631000	3.471444000	6	2.640505000	0.265350000	-1.439774000
1	-2.142658000	-0.201934000	3.464509000	1	3.718118000	0.217892000	-1.634020000
6	4.688845000	-1.740133000	1.682196000	1	2.372502000	1.288712000	-1.174391000
1	5.670305000	-2.125466000	1.942054000	6	-0.989452000	-3.179052000	-0.321466000
6	-2.459264000	-1.689331000	1.040639000	1	-0.972754000	-3.095354000	0.772043000
1	-3.301449000	-2.061773000	0.450300000	1	-1.046927000	-4.240895000	-0.594383000
1	-2.832612000	-1.599888000	2.060367000	6	-0.221094000	2.020339000	-1.986824000
6	-4.330094000	-0.152340000	-1.024618000	6	-3.059030000	-0.324894000	-1.305598000
6	0.258177000	-0.696319000	3.589663000	1	-2.909639000	0.748344000	-1.273528000
1	-0.029939000	-0.586143000	4.645742000	6	-3.017810000	2.589410000	0.264237000
1	1.348696000	-0.668024000	3.529732000	1	-0.345190000	2.228910000	1.284197000
6	-0.243124000	-2.044461000	3.066798000	6	-0.284696000	0.902705000	-3.000398000
1	0.313793000	-2.845299000	3.569107000	1	-1.339362000	0.634387000	-3.129482000
1	-1.291962000	-2.183998000	3.336358000	1	0.091105000	1.246092000	-3.973219000
6	-4.942256000	-1.345145000	-1.417023000	6	-3.323157000	-3.049244000	-1.347533000
1	-4.345740000	-2.179312000	-1.770732000	1	-3.381048000	-4.132625000	1.348517000
6	2.334962000	-2.062935000	1.318995000	6	1.902479000	-0.155697000	-2.707453000
6	-1.311248000	-2.686272000	0.945954000	1	2.125664000	0.592873000	-3.477252000
1	-1.638476000	-3.637700000	1.393469000	1	2.302391000	-1.103743000	-3.070753000
1	-1.078549000	-2.859237000	-0.107417000	6	-4.360961000	-2.261795000	-1.849067000
6	-5.078119000	0.940390000	-0.566873000	1	-5.256200000	-2.725712000	-2.251852000
1	-4.588064000	1.862260000	-0.272904000	6	2.633082000	-0.205200500	-0.423344000
6	4.510051000	-0.390755000	1.372473000	1	3.467152000	-2.319831000	0.231011000
1	5.338288000	0.307939000	1.370893000	1	2.992651000	-2.207160000	-1.439972000
6	0.172012000	4.699980000	0.669031000	6	4.635895000	0.111742000	1.037748000
1	0.091821000	5.780736000	0.724038000	6	-0.074533000	-1.537558000	-3.127807000
6	0.200825000	4.028630000	-0.560830000	1	0.276468000	-1.648692000	-4.163512000
1	0.154388000	4.568710000	-1.501984000	1	-1.163079000	-1.478621000	-3.146531000
6	0.258985000	3.916253000	1.831108000	6	0.375036000	-2.757990000	-2.314757000
1	0.247340000	4.368146000	2.819076000	1	-0.215506000	-3.628237000	-2.623789000
6	-6.332556000	-1.436731000	-1.352983000	1	1.415898000	-2.991712000	-2.543975000
1	-6.832206000	-2.356298000	-1.659137000	6	5.410268000	-0.959586000	1.492781000
6	-7.108712000	-0.362000000	-0.897413000	1	4.945656000	-1.800527000	1.995657000
6	-6.463147000	0.823812000	-0.507790000	6	-2.183877000	-2.424616000	-0.852431000
1	-7.055603000	1.664120000	-0.156279000	6	1.446593000	-2.960733000	-0.100746000
6	-8.609837000	-0.462471000	-0.836795000	1	1.724843000	-3.988783000	-0.333018000
1	-8.983970000	-0.140655000	0.143055000	1	1.217349000	-2.887374000	0.964523000
1	-8.945845000	-1.487888000	-1.022795000	6	5.215009000	1.213543000	0.396950000
1	-9.071195000	0.191692000	-1.588897000	1	4.600282000	2.038733000	0.054253000
6	2.209311000	0.277774000	-2.247085000	6	-4.229427000	-0.874104000	-1.822814000

1	-5.014107000	-0.219665000	-2.184040000		1	-2.417480000	-1.357938000	2.413140000
6	-0.196974000	4.340782000	-1.364724000		6	-4.287649000	-0.482442000	-0.751984000
1	-0.160702000	5.392569000	-1.631939000		6	0.517671000	0.260584000	3.566776000
6	-0.268387000	3.949634000	-0.027528000		1	0.179246000	0.534117000	4.575845000
1	-0.311069000	4.675789000	0.775790000		1	1.590999000	0.443809000	3.508537000
6	-0.171371000	3.361286000	-2.359677000		6	0.229315000	-1.224711000	3.325176000
1	-0.115001000	3.622735000	-3.411274000		1	0.922554000	-1.821733000	3.928895000
6	6.790518000	-0.917406000	1.301497000		1	-0.775533000	-1.467706000	3.675004000
1	7.404422000	-1.741841000	1.652915000		6	-4.910521000	-1.735572000	-0.724129000
6	7.400114000	0.172265000	0.663207000		1	-4.330607000	-2.641303000	-0.862832000
6	6.594892000	1.232578000	0.215622000		6	2.752668000	-1.251373000	1.670939000
1	7.057034000	2.081587000	-0.280311000		6	-0.793118000	-2.418111000	1.426227000
6	8.893896000	0.221651000	0.480015000		1	-0.946372000	-3.295174000	2.071485000
1	9.155804000	0.646070000	-0.496216000		1	-0.564296000	-2.760330000	0.413861000
1	9.336382000	-0.776520000	0.566526000		6	-5.015709000	0.701164000	-0.593844000
1	9.353249000	0.860840000	1.246929000		1	-4.518734000	1.664626000	-0.627460000
6	-3.130227000	1.039472000	2.343138000		6	4.691589000	0.693573000	1.565926000
8	-3.789066000	1.974482000	1.589857000		1	5.425705000	1.489801000	1.505857000
6	-3.467888000	-0.335772000	2.346497000		6	-0.118715000	4.966005000	-0.319020000
6	-2.694297000	-1.251406000	3.128570000		1	-0.297472000	6.025690000	-0.475801000
6	-4.543622000	-0.885900000	1.583645000		6	0.007986000	4.098589000	-1.404693000
6	-2.962241000	-2.613373000	3.117132000		1	-0.048293000	4.450040000	-2.429153000
1	-1.877863000	-0.875256000	3.735133000		6	-0.012890000	4.454912000	0.976553000
6	-4.798113000	-2.250726000	1.587136000		1	-0.102135000	5.095441000	1.847952000
1	-5.172697000	-0.242139000	0.981021000		6	-6.288876000	-1.792758000	-0.537402000
6	-4.012363000	-3.134189000	2.343468000		1	-6.787461000	-2.758029000	-0.523603000
1	-2.348787000	-3.279803000	3.718853000		6	-7.047440000	-0.622401000	-0.372461000
1	-5.615884000	-2.635816000	0.983931000		6	-6.394416000	0.618518000	-0.407301000
1	-4.215474000	-4.201165000	2.333668000		1	-6.974395000	1.529674000	-0.291870000
6	-2.072371000	1.643583000	3.214113000		6	-8.534600000	-0.707640000	-0.152587000
1	-1.913149000	2.689194000	2.935659000		1	-9.008064000	0.274387000	-0.256436000
1	-2.350810000	1.606371000	4.278465000		1	-8.752584000	-1.086891000	0.855150000
1	-1.119865000	1.108428000	3.109789000		1	-8.996138000	-1.401308000	-0.865787000
1	-0.233049000	-0.451297000	1.347972000		6	1.693897000	-0.707976000	-2.322297000
1	-4.480326000	1.630233000	0.963810000		8	2.535093000	0.404266000	-2.440163000
1	-2.996516000	2.765329000	-0.309074000		6	2.260922000	-1.985873000	-1.966445000
8	-3.371084000	3.196412000	-1.098391000		6	1.426115000	-3.146414000	-1.952650000
1	-6.161042000	2.399471000	-0.116284000		6	3.565336000	-2.133932000	-1.408771000
8	-5.573065000	1.690426000	-0.428044000		6	1.878367000	-4.359996000	-1.446923000
1	-4.872443000	2.174598000	-0.927339000		1	0.413099000	-3.084386000	-2.336405000
1	-3.349045000	3.821783000	1.712362000		6	4.004320000	-3.352719000	-0.908595000
8	-2.978781000	4.721459000	1.612059000		1	4.242503000	-1.288229000	-1.352279000
1	-2.726349000	4.735832000	0.674091000		6	3.172783000	-4.486619000	-0.915890000
1	-2.737561000	2.979179000	-1.803011000		1	1.210214000	-5.218771000	-1.457541000
1	5.007821000				1	5.007821000	-3.420172000	-0.494030000

### TS\_H\_homo<sub>quint</sub>

(G = -3791.814436) (quintuplet)

27	0.444185000	0.194894000	0.590461000		1	3.521789000	-5.435972000	-0.519736000
16	-2.520536000	-0.389705000	-0.930559000		6	0.622546000	-0.607198000	-3.380886000
7	-1.885092000	-0.297763000	0.674785000		1	0.213378000	0.408290000	-3.398698000
8	-2.178812000	0.880390000	-1.588242000		1	1.046005000	-0.824999000	-4.372947000
7	0.323040000	2.254441000	0.091895000		1	-0.202769000	-1.293997000	-3.188909000
7	2.427031000	-0.017094000	1.211795000		1	0.788762000	-0.333644000	-1.071073000
7	-0.136058000	1.100383000	2.537367000		1	3.413225000	0.316628000	-2.003054000
7	0.349457000	-1.604143000	1.884875000		1	2.696621000	2.345160000	-1.493170000
8	-2.036509000	-1.664416000	-1.483023000		8	3.294977000	3.114320000	-1.457006000
6	-2.377600000	0.912244000	1.401093000		1	5.325281000	1.092890000	-2.537484000
1	-3.444179000	0.815021000	1.635831000		8	5.106820000	0.985899000	1.595888000
1	-2.235584000	1.765635000	0.737223000		1	4.681172000	1.841298000	-1.363859000
6	1.643394000	-2.263655000	1.606738000		1	1.999347000	1.777571000	-3.617530000
1	1.597248000	-2.654827000	0.582504000		8	1.728398000	2.626667000	-4.023482000
1	1.830114000	-3.099340000	2.294109000		1	2.054490000	3.266794000	-3.368214000
6	0.218110000	3.093016000	1.144407000		1	2.987043000	3.608210000	-0.677951000

### II\_H\_homo<sub>quint</sub>

(G = -3791.866418) (quintuplet)

27	0.402717000	-0.005907000	0.745611000		27	0.402717000	-0.005907000	0.745611000
16	-2.546499000	-0.067753000	-0.986963000		16	-2.546499000	-0.067753000	-0.986963000
7	-1.936407000	-0.262339000	0.622365000		7	-1.936407000	-0.262339000	0.622365000
6	-2.148085000	1.277943000	-1.422830000		8	-2.148085000	1.277943000	-1.422830000
1	0.431020000	2.060903000	0.415923000		7	0.431020000	2.060903000	0.415923000
1	2.316209000	-0.459759000	1.095939000		7	2.316209000	-0.459759000	1.095939000
6	-0.123692000	0.661986000	2.713752000		7	-0.123692000	0.661986000	2.713752000
1	0.125413000	-1.954115000	1.696484000		7	0.125413000	-1.954115000	1.696484000
6	-2.061095000	-1.246661000	-1.722672000		8	-2.061095000	-1.246661000	-1.722672000
1	-2.342310000	0.867915000	1.521513000		6	-2.342310000	0.867915000	1.521513000
1	-3.417963000	0.825355000	1.727696000		1	-3.417963000	0.825355000	1.727696000
6	-2.114691000	1.794385000	0.994534000		1	-2.114691000	1.794385000	0.994534000
1	1.380292000	-2.666735000	1.331312000		6	1.380292000	-2.666735000	1.331312000
6	1.301937000	-2.890520000	0.260888000		1	1.301937000	-2.890520000	0.260888000
1	1.475821000	-3.611280000	1.884478000		1	1.475821000	-3.611280000	1.884478000

				H <sub>2</sub> O_I_heter_d	
6	0.483502000	2.762194000	1.570060000	(G = -3406.377530) (doublet)	
1	3.381118000	0.426607000	1.204975000		
1	3.191600000	1.430329000	0.843282000		
6	0.398356000	2.729640000	-0.749608000		
1	0.348849000	2.127099000	-1.644874000	27	-1.012577000
6	0.601192000	1.946751000	2.836553000	16	2.193073000
1	1.663416000	1.715330000	2.980550000	7	1.359977000
1	0.254572000	2.524050000	3.702421000	8	1.862992000
6	3.737439000	-2.154875000	2.118527000	7	-1.103615000
1	3.829924000	-3.181819000	2.466938000	7	-3.113324000
6	-1.594749000	0.827929000	2.859476000	7	-0.886442000
1	-1.822446000	1.763897000	3.382655000	7	-0.931169000
1	-1.979448000	0.018789000	3.481581000	8	1.879451000
6	4.835057000	-1.245946000	2.209942000	6	1.542881000
1	5.786229000	-1.541797000	2.639663000	1	2.551195000
6	-2.271432000	-1.627576000	1.162775000	1	1.400823000
1	-3.105844000	-2.076070000	0.616818000	6	-2.057640000
1	-2.621547000	-1.495393000	2.186168000	1	-1.784992000
6	-4.316565000	-0.141833000	-0.865228000	1	-2.223783000
6	0.431800000	-0.376826000	3.616206000	6	-1.305939000
1	0.121176000	-0.202412000	4.655007000	6	-4.179696000
1	1.518275000	-0.303202000	3.556886000	1	-3.970052000
6	-0.001907000	-1.777049000	3.170699000	6	-0.936207000
1	0.619776000	-2.514924000	3.691390000	1	-0.773500000
1	-1.035059000	-1.967641000	3.467498000	6	-1.599024000
6	-4.970642000	-1.358157000	-0.107956000	1	-2.673597000
1	-4.412265000	-2.240151000	-1.373660000	1	-1.349944000
6	2.547983000	-1.757522000	1.565542000	6	-4.587417000
6	-1.071600000	-2.567886000	1.094307000	1	-4.701337000
1	-1.338002000	-3.511874000	1.591826000	6	0.530804000
1	-0.839564000	-2.779434000	0.047129000	1	0.628048000
6	-5.016303000	1.014933000	-0.497580000	1	0.769659000
1	-4.493275000	1.952762000	-0.344899000	6	-5.693412000
6	4.603814000	0.076754000	1.725932000	1	-6.698757000
1	5.388615000	0.829329000	1.763538000	6	1.547948000
6	0.482815000	4.844160000	0.370316000	1	2.462030000
1	0.504062000	5.929693000	0.356502000	1	1.687758900
6	0.431256000	4.117599000	-0.819819000	6	3.925566000
1	0.431845000	4.602837000	-1.789356000	6	-1.595814000
6	0.501488000	4.154629000	1.583187000	1	-1.418468000
1	0.534520000	4.678691000	2.532754000	1	-2.662770000
6	-6.355244000	-1.408741000	-0.923220000	6	-1.112380000
1	-6.878939000	-2.344930000	-0.1093701000	1	-1.826662800
6	-7.083992000	-0.270319000	-0.551676000	1	-0.158160000
6	-6.396921000	0.938350000	-0.345660000	6	4.629360000
1	-6.953520000	1.828586000	-0.065964000	1	4.144060000
6	-8.577267000	-0.332616000	-0.370717000	6	-3.312627000
1	-8.846981000	-0.144516000	0.676986000	6	0.361898000
1	-8.970333000	-1.313618000	-0.657141000	1	0.469708000
1	-9.075356000	0.436379000	-0.974453000	1	0.355846000
6	1.915944000	-0.072914000	-2.446278000	6	4.534845000
8	3.082298000	0.510451000	-3.069659000	1	3.977591000
6	2.126460000	-1.558804000	-2.174894000	6	-5.487351000
6	1.170953000	-2.527535000	-2.516033000	1	-6.318733000
6	3.307782000	-1.978960000	-1.546931000	6	-1.139310000
6	1.395067000	-3.881708000	-2.242381000	1	-1.144895000
1	0.244303000	-2.233051000	-2.995816000	6	-0.955108000
6	3.535803000	-3.327651000	-1.274144000	1	-0.817794000
1	4.050159000	-1.243239000	-1.255426000	6	-1.315722000
6	2.579681000	-4.287720000	-1.623972000	1	-1.464772200
1	0.641744000	-4.616059000	-2.515691000	6	5.970482000
1	4.454804000	-3.627235000	-0.777886000	1	6.532766000
1	2.754329000	-5.338765000	-1.409681000	6	6.607464000
6	0.738547000	0.226148000	-3.364351000	6	5.873405000
1	0.705459000	1.297940000	-3.577053000	1	6.360848000
1	0.847536000	-0.314942000	-4.312149000	6	8.050425000
1	-0.204629000	-0.069001000	-2.899221000	1	8.530142000
1	1.759852000	0.423997000	-1.479146000	1	8.608254000
1	3.802838000	0.606120000	-2.400347000	1	8.129910000
1	2.896550000	2.400019000	-1.063923000	1	-0.868535000
8	3.535712000	3.113083000	-0.893506000	8	-2.691550000
1	5.758955000	1.424292000	-2.199174000	1	-3.378554000
8	5.290197000	1.024773000	-1.446410000	1	-2.041696000
1	4.849295000	1.791666000	-1.018901000	1	-3.475182000
1	2.643757000	2.262022000	-3.426016000	8	-3.879032000
8	2.366633000	3.199019000	-3.557465000	1	-4.619327000
1	2.641914000	3.613175000	-2.721334000	8	-0.411897000
1	3.220807000	3.499661000	-0.057995000	1	-2.128023400
				1	0.150775000
				1	-2.307392000
				1	3.005061000
				1	2.538298000

**H<sub>2</sub>O\_II\_heter<sub>q</sub>**

(G = -3406.366295) (quartet)

27	0.991602000	-0.029533000	-0.040473000
16	-2.171054000	-0.185033000	-1.094011000
7	-1.283373000	-0.284986000	0.392910000
8	-1.825010000	1.111425000	-1.695060000
7	1.159132000	2.040616000	-0.405481000
7	3.046421000	-0.455634000	0.245474000
7	0.866271000	0.786738000	2.036738000
7	0.945326000	-1.897568000	1.139896000
8	-1.896845000	-1.435313000	-1.821649000
6	-1.528834000	0.906284000	1.266935000
1	-2.551355000	0.892402000	1.660649000
1	-1.395501000	1.793845000	0.647151000
6	2.095586000	-2.650983000	0.602097000
1	1.834908000	-2.973785000	-0.413072000
1	2.317762000	-3.541735000	1.204606000
6	1.292946000	2.813900000	0.693056000
6	4.065322000	0.410655000	0.133332000
1	3.792841000	1.440779000	-0.072651000
6	0.995763000	2.625165000	-1.604747000
1	0.882805000	1.950854000	-2.446816000
6	1.569343000	2.083562000	1.985572000
1	2.647239000	1.887521000	2.023121000
1	1.320779000	2.718403000	2.845667000
6	4.608051000	-2.218257000	0.680137000
1	4.776274000	-3.265891000	0.907569000
6	-0.553909000	0.943731000	2.443486000
1	-0.705034000	1.901340000	2.955926000
1	-0.805860000	0.164566000	3.164410000
6	5.668818000	-1.321234000	0.547090000
1	6.692836000	-1.662117000	0.665331000
6	-1.510970000	-1.608981000	1.067768000
1	-2.430437000	-2.083476000	0.714526000
1	-1.665697000	-1.413752000	2.128239000
6	-3.887048000	-0.171383000	-0.630348000
6	1.575001000	-0.194568000	2.889829000
1	1.423186000	0.023366000	3.956290000
1	2.640593000	-0.108213000	2.676542000
6	1.101262000	-1.623309000	2.600179000
1	1.818530000	-2.327084000	3.038342000
1	0.145438000	-1.806473000	3.094178000
6	-4.601493000	-1.372372000	-0.611652000
1	-4.133458000	-2.297418000	-0.930131000
6	3.306044000	-1.750424000	0.522179000
6	-0.339650000	-2.560204000	0.838092000
1	-0.484103000	-3.453056000	1.463171000
1	-0.315503000	-2.866462000	-0.207509000
6	-4.474014000	1.038203000	-0.236220000
1	-3.907945000	1.962906000	-0.264117000
6	5.393939000	0.020896000	0.275225000
1	6.187164000	0.754308000	0.178107000
6	1.090388000	4.808653000	-0.626602000
1	1.056787000	5.890902000	-0.709524000
6	0.962941000	4.006217000	-1.762497000
1	0.830932000	4.437507000	-2.748930000
6	1.254784000	4.203890000	0.619779000
1	1.353424000	4.791159000	1.526870000
6	-5.929792000	-1.354206000	-0.187580000
1	-6.498773000	-2.279296000	-0.171964000
6	-6.544087000	-0.161530000	0.218464000
6	-5.800316000	1.030447000	0.183784000
1	-6.269577000	1.961657000	0.489031000
6	-7.976730000	-0.147428000	0.681829000
1	-8.408053000	-1.153716000	0.664149000
1	-8.586072000	0.503946000	0.041830000
1	-8.050132000	0.245887000	1.703986000
1	0.869547000	-0.489922000	-1.651969000
8	2.658200000	-1.733249000	-2.703868000
1	3.288134000	-2.069661000	-2.043527000
1	1.978711000	-1.214762000	-2.155282000
1	3.507068000	-0.133332000	-3.008166000
8	3.878784000	0.778713000	-3.018990000
1	4.577584000	0.728024000	-2.347199000
8	0.326162000	-3.396571000	-2.560935000
1	1.203967000	-2.971804000	-2.662997000
1	-0.242278000	-2.644047000	-2.316767000

**H<sub>2</sub>O\_TS\_heter<sub>d</sub>**

(G = -3406.360360) (doublet)

27	-0.995267000	-0.066350000	-0.210618000
16	2.128227000	-0.069621000	1.071841000
7	1.249837000	-0.242593000	-0.423961000
8	1.788383000	1.258225000	1.599565000
7	-1.084243000	1.772046000	0.348841000
7	-3.008100000	-0.337711000	-0.253829000
7	-0.832534000	0.732419000	-2.119661000
7	-0.979392000	-1.827339000	-1.094913000
8	1.817879000	-1.274608000	1.857628000
6	1.549382000	0.887270000	-1.361026000
1	2.575690000	0.818048000	-1.736988000
1	1.431830000	1.814282000	-0.799024000
6	-2.143881000	-2.564060000	-0.525574000
1	-1.873630000	-2.855180000	0.495419000
1	-2.362791000	-3.466546000	-1.105681000
6	-1.263681000	2.656591000	-0.664532000
6	-3.993549000	0.566138000	-0.135997000
1	-3.688800000	1.594790000	0.020686000
6	-0.981088000	2.232167000	1.610276000
1	-0.836548000	1.483721000	2.377223000
6	-1.508904000	2.047873000	-2.019916000
1	-2.587628000	1.883833000	-2.121174000
1	-1.200699000	2.727447000	-2.822294000
6	-4.646145000	-2.066879000	-0.548508000
1	-4.856950000	-3.117048000	-0.720759000
6	0.587526000	0.867651000	-2.546494000
1	0.728746000	1.794853000	-3.111701000
1	0.831181000	0.046457000	-3.220883000
6	-5.669479000	-1.127270000	-0.414846000
1	-6.708349000	-1.435780000	-0.478637000
6	1.485508000	-1.607143000	-1.023063000
1	2.391268000	-2.070827000	-0.624480000
1	1.660630000	-1.474029000	-2.090031000
6	3.847553000	-0.099323000	0.628150000
6	-1.572196000	-0.246797000	-2.958996000
1	-1.404930000	-0.064175000	-4.027820000
1	-2.635172000	-0.125310000	-2.749537000
6	-1.124673000	-1.661020000	-2.594661000
1	-1.847960000	-2.388563000	-2.973452000
1	-0.164434000	-1.891892000	-3.057100000
6	4.554525000	-1.303905000	0.690506000
1	4.076022000	-2.206893000	1.053811000
6	-3.327054000	-1.635692000	-0.460502000
6	0.296772000	-2.518949000	-0.753811000
1	0.395795000	-3.441335000	-1.338714000
1	0.254025000	-2.770485000	0.305517000
6	4.449014000	1.084423000	0.181845000
1	3.889510000	2.013013000	0.152591000
6	-5.338016000	0.213267000	-0.208388000
1	-6.101364000	0.977053000	-0.107262000
6	-1.197730000	4.502041000	0.868403000
1	-1.233774000	5.568363000	1.069118000
6	-1.039354000	3.587334000	1.910095000
1	-0.953230000	3.911994000	2.941071000
6	-1.310575000	4.027224000	-0.438131000
1	-1.441679000	4.700255000	-1.278736000
6	5.889990000	-1.315368000	0.290957000
1	6.455137000	-2.241581000	0.340773000
6	6.518078000	-0.149903000	-0.171714000
6	5.782672000	1.046463000	-0.212543000
1	6.264208000	1.958063000	-0.555035000
6	7.951100000	-0.176412000	-0.633195000
1	8.464259000	-1.076591000	-0.278793000
1	8.493507000	0.707988000	-0.278691000
1	7.999198000	-0.168813000	-1.731007000
1	-0.684662000	-0.573247000	1.505839000
8	-2.512483000	-1.669698000	2.757067000
1	-3.102873000	-2.022655000	2.073030000
1	-1.341324000	-0.899518000	1.824702000
1	-3.217430000	-0.218527000	2.953324000
8	-3.657185000	0.694870000	3.007368000
1	-4.405606000	0.601962000	2.396696000
8	-0.394696000	-3.263426000	2.637448000
1	-1.236693000	-2.711351000	2.714797000
1	0.267162000	-2.591377000	2.402469000

**H<sub>2</sub>O\_TS\_heter<sub>q</sub>**  
(G = -3406.360789) (quartet)

27	-1.002041000	-0.024487000	-0.035973000
16	2.142329000	-0.165299000	1.055591000
7	1.239094000	-0.281764000	-0.431376000
8	1.793113000	1.137873000	1.638015000
7	-1.133344000	2.002821000	0.383871000
7	-3.053405000	-0.449409000	-0.193202000
7	-0.905860000	0.770367000	-2.071563000
7	-0.986457000	-1.906931000	-1.157888000
8	1.854325000	-1.403932000	1.795893000
6	1.497739000	0.893530000	-1.328098000
1	2.516553000	0.853077000	-1.728384000
1	1.385143000	1.793492000	-0.722391000
6	-2.133966000	-2.651341000	-0.597511000
1	-1.851873000	-2.987208000	0.407296000
1	-2.380225000	-3.532944000	-1.203061000
6	-1.305500000	2.786393000	-0.704180000
6	-4.059448000	0.423656000	-0.027096000
1	-3.772408000	1.450817000	0.172918000
6	-0.948812000	2.574542000	1.587182000
1	-0.804426000	1.893622000	2.417578000
6	-1.604948000	2.070061000	-2.0000125000
1	-2.683821000	1.876634000	-2.023754000
1	-1.364626000	2.710124000	-2.857907000
6	-4.642435000	-2.196714000	-0.580855000
1	-4.827312000	-3.240431000	-0.812797000
6	0.511520000	0.923340000	-2.497084000
1	0.654833000	1.876384000	-3.019020000
1	0.752917000	0.136696000	-3.213044000
6	-5.689526000	-1.294824000	-0.388919000
1	-6.720022000	-1.627781000	-0.465976000
6	1.470257000	-1.615698000	-1.093470000
1	2.391625000	-2.081690000	-0.734257000
1	1.622546000	-1.431260000	-2.156121000
6	3.855907000	-0.165257000	0.593363000
6	-1.632043000	-0.214697000	-2.909159000
1	-1.499977000	-0.000382000	-3.978226000
1	-2.693032000	-0.126316000	-2.673011000
6	-1.153207000	-1.642191000	-2.619479000
1	-1.873633000	-2.348953000	-3.046550000
1	-0.199998000	-1.827331000	-3.117757000
6	4.570042000	-1.366457000	0.617521000
1	4.095811000	-2.284147000	0.947757000
6	-3.331909000	-1.740027000	-0.471205000
6	0.301961000	-2.566077000	-0.851194000
1	0.444426000	-3.465240000	-1.466564000
1	0.279486000	-2.859233000	0.198615000
6	4.448806000	1.036512000	0.184199000
1	3.882138000	1.961274000	0.180720000
6	-5.394529000	0.041789000	-0.111279000
1	-6.178039000	0.778074000	0.030772000
6	-1.097808000	4.766751000	0.634888000
1	-1.077228000	5.848270000	0.729683000
6	-0.932192000	3.953692000	1.758303000
1	-0.782891000	4.375998000	2.745955000
6	-1.283823000	4.174904000	-0.614526000
1	-1.412315000	4.770961000	-1.511968000
6	5.907024000	-1.355967000	0.222406000
1	6.477313000	-2.280134000	0.240808000
6	6.529189000	-0.171386000	-0.1955546000
6	5.783565000	1.020019000	-0.206811000
1	6.259005000	1.944358000	-0.522945000
6	7.973448000	-0.164343000	-0.620522000
1	8.401425000	-1.171510000	-0.584272000
1	8.566612000	0.489294000	0.032415000
1	8.075672000	0.223327000	-1.642237000
1	-0.764833000	-0.524891000	1.651279000
8	-2.440489000	-1.659334000	2.755443000
1	-3.051839000	-1.972605000	2.068577000
1	-1.451953000	-0.950263000	1.993200000
1	-3.128671000	-0.153726000	3.025046000
8	-3.496628000	0.778021000	3.106899000
1	-4.276514000	0.752312000	2.530037000
8	-0.371336000	-3.367717000	2.555244000
1	-1.193055000	-2.808678000	2.671800000
1	0.293080000	-2.700206000	2.311922000

**H<sub>2</sub>O\_II\_heter<sub>d</sub>**  
(G = -3406.373572) (doublet)

27	0.902668000	0.084914000	0.257954000
16	-2.064707000	-0.211055000	-1.021924000
7	-1.192642000	-0.065762000	0.511225000
8	-1.794282000	1.024027000	-1.766134000
7	0.952785000	1.806857000	-0.643470000
7	2.848935000	-0.134100000	0.185672000
7	0.775252000	1.261999000	2.021013000
7	0.979317000	-1.480748000	1.459889000
8	-1.643195000	-1.509609000	-1.567444000
6	-1.578388000	1.202591000	1.223701000
1	-2.613090000	1.141357000	1.574444000
1	-1.483771000	2.018692000	0.507282000
6	2.152222000	-2.278259000	1.006563000
1	1.860385000	-2.809135000	0.095613000
1	2.453280000	-3.011630000	1.761517000
6	1.129777000	2.863978000	0.188313000
6	3.776114000	0.773235000	-0.177173000
1	3.410232000	1.716521000	-0.561773000
6	0.884336000	2.025283000	-1.970248000
1	0.763298000	1.149066000	-2.592117000
6	1.402735000	2.539678000	1.637950000
1	2.488250000	2.432731000	1.747573000
1	1.086053000	3.364689000	2.286989000
6	4.611379000	-1.652769000	0.790341000
1	4.892662000	-2.623125000	1.184905000
6	-0.645169000	1.429797000	2.413876000
1	-0.824569000	2.439290000	2.800425000
1	-0.876443000	0.734012000	3.221213000
6	5.567671000	-0.709336000	0.415597000
1	6.625921000	-0.931974000	0.509444000
6	-1.464258000	-1.296744000	1.359936000
1	-2.375555000	-1.809860000	1.045393000
1	-1.644703000	-0.954219000	2.377436000
6	-3.789649000	-0.275337000	-0.613747000
1	1.892560000	-1.640881000	3.390159000
1	0.199730000	-1.172055000	3.410928000
6	-4.426640000	-1.516510000	-0.510842000
1	-3.878449000	-2.434911000	-0.690889000
6	3.264751000	-1.332840000	0.665090000
6	-0.285519000	-2.247979000	1.283806000
1	-0.378556000	-3.024222000	2.053137000
1	-0.246969000	-2.723232000	0.303862000
6	-4.478423000	0.926533000	-0.409472000
1	-3.972807000	1.880584000	-0.510220000
6	5.140581000	0.527291000	-0.071779000
1	5.846078000	1.293510000	-0.372874000
6	1.094559000	4.393463000	-1.663478000
1	1.140111000	5.403883000	-2.057937000
6	0.958513000	3.299236000	-2.518894000
1	0.901431000	3.423708000	-3.594530000
6	1.182202000	4.168875000	-0.290496000
1	1.307512000	4.985934000	0.412287000
6	-5.782549000	-1.544992000	-0.193728000
1	-6.294412000	-2.500131000	-0.119851000
6	-6.500496000	-0.359187000	0.024400000
6	-5.832333000	0.870620000	-0.092509000
1	-6.383219000	1.794226000	0.060155000
6	-7.958069000	-0.403034000	0.397269000
1	-8.437128000	-1.311029000	0.015186000
1	-8.490040000	0.473932000	0.011977000
1	-8.070487000	-0.402720000	1.490638000
1	0.720500000	-0.923337000	-2.166272000
8	3.091479000	-3.231838000	-2.092599000
1	3.498519000	-3.286638000	-1.215015000
1	1.420961000	-1.163732000	-2.140305000
1	3.552222000	-1.827662000	-2.579844000
8	3.866714000	-0.898031000	-2.902735000
1	4.522141000	-0.649849000	-2.232536000
8	0.591889000	-3.827908000	-1.726903000
1	1.584790000	-3.588299000	-1.867197000
1	0.153923000	-2.964230000	-1.777737000

**H<sub>2</sub>O\_II\_heter<sub>q</sub>**  
(G = -3406.380229) (quartet)

27	-1.012796000	-0.015083000	-0.071491000
16	2.174784000	-0.181169000	1.064718000
7	1.254651000	-0.276399000	-0.410510000
8	1.857432000	1.128708000	1.650899000
7	-1.069853000	2.023804000	0.411798000
7	-3.054914000	-0.407935000	-0.154410000
7	-0.862096000	0.807127000	-2.063294000
7	-1.019067000	-1.862154000	-1.212360000
8	1.843211000	-1.411112000	1.802236000
6	1.533350000	0.898645000	-1.301309000
1	2.554562000	0.845846000	-1.694189000
1	1.427571000	1.798115000	-0.694339000
6	-2.187761000	-2.600084000	-0.681237000
1	-1.922488000	-2.969370000	0.316051000
1	-2.447559000	-3.456727000	-1.315149000
6	-1.203808000	2.819639000	-0.674406000
6	-4.038443000	0.486261000	0.035663000
1	-3.726639000	1.488772000	0.309922000
6	-0.889308000	2.593387000	1.617099000
1	-0.790047000	1.916349000	2.455771000
6	-1.531928000	2.125960000	-1.974025000
1	-2.614702000	1.955108000	-1.990722000
1	-1.279963000	2.762101000	-2.830385000
6	-4.683020000	-2.073463000	-0.706142000
1	-4.892484000	-3.093631000	-1.010150000
6	0.561760000	0.943338000	-2.478910000
1	0.717791000	1.895786000	-2.997151000
1	0.797174000	0.155343000	-3.194487000
6	-5.707237000	-1.150288000	-0.489706000
1	-6.744400000	-1.443072000	-0.621614000
6	1.454349000	-1.610809000	-1.086803000
1	2.351559000	-2.111608000	-0.713456000
1	1.635708000	-1.419966000	-2.144102000
6	3.887219000	-0.226251000	0.606806000
6	-1.606939000	-0.139329000	-2.933371000
1	-1.466931000	0.108349000	-3.993382000
1	-2.666340000	-0.037107000	-2.693080000
6	-1.153767000	-1.578921000	-2.673094000
1	-1.879226000	-2.266281000	-3.121699000
1	-0.195058000	-1.773052000	-3.157394000
6	4.572048000	-1.444798000	0.641164000
1	4.073127000	-2.349399000	0.971121000
6	-3.363935000	-1.667156000	-0.528697000
6	0.258381000	-2.537010000	-0.881112000
1	0.400579000	-3.433635000	-1.499514000
1	0.204644000	-2.838693000	0.165711000
6	4.512701000	0.960429000	0.203787000
1	3.969539000	1.899199000	0.197634000
6	-5.380981000	0.155974000	-0.119600000
1	-6.145774000	0.907718000	0.041794000
6	-0.938528000	4.792888000	0.664832000
1	-0.878532000	5.872810000	0.760358000
6	-0.824170000	3.971914000	1.787773000
1	-0.677852000	4.385565000	2.779539000
6	-1.129945000	4.206276000	-0.585440000
1	-1.227331000	4.803778000	-1.485805000
6	5.913373000	-1.466156000	0.263972000
1	6.463416000	-2.402128000	0.297135000
6	6.567869000	-0.297114000	-0.150873000
6	5.851769000	0.911457000	-0.171057000
1	6.354035000	1.824507000	-0.477921000
6	8.009979000	-0.333788000	-0.581399000
1	8.508709000	-1.237530000	-0.215406000
1	8.550954000	0.546910000	-0.216077000
1	8.081819000	-0.328932000	-1.677926000
1	-0.360533000	-0.130906000	2.517845000
8	-2.960500000	-2.001441000	2.764329000
1	-3.475886000	-2.203887000	1.968822000
1	-1.031876000	-0.437409000	2.592149000
1	-3.305103000	-0.493223000	2.991011000
8	-3.533164000	0.504742000	3.122381000
1	-4.328720000	0.613652000	2.578313000
8	-0.647930000	-3.145236000	2.421497000
1	-1.557526000	-2.680471000	2.534937000
1	-0.038866000	-2.409329000	2.247810000

[Co<sup>II</sup>(CH<sub>3</sub>CN)(Py<sub>2</sub><sup>Ts</sup>tacn)]<sup>2+</sup>  
(G = -3309.075646) (doublet)

27	-1.224635000	-0.048518000	0.011022000
16	2.137479000	-0.103040000	1.045925000
7	1.126396000	-0.381885000	-0.323010000
8	1.845138000	1.263234000	1.504240000
7	-1.185596000	1.865279000	0.373197000
7	-3.363409000	-0.383738000	0.063978000
7	-1.179145000	0.499874000	-1.892292000
7	-1.271756000	-1.931460000	-0.689077000
8	1.920518000	-1.242844000	1.951222000
6	1.298458000	0.672182000	-1.364528000
1	2.273904000	0.583689000	-1.857233000
1	1.238545000	1.637643000	-0.860852000
6	-2.417087000	-2.602802000	-0.010230000
1	-2.130304000	-2.781652000	1.030863000
1	-2.630191000	-3.568946000	-0.479968000
6	-1.427716000	2.621507000	-0.727427000
6	-4.383636000	0.486553000	0.069170000
1	-4.117478000	1.537429000	0.142004000
6	-0.880089000	2.483548000	1.530173000
1	-0.691342000	1.844096000	2.381675000
6	-1.844679000	1.834545000	-1.934828000
1	-2.926063000	1.670334000	-1.880612000
1	-1.626364000	2.362595000	-2.868204000
6	-4.927526000	-2.190633000	-0.143701000
1	-5.096246000	-3.258224000	-0.240217000
6	0.222600000	0.573800000	-2.438785000
1	0.314358000	1.447928000	-3.089555000
1	0.392196000	-0.304113000	-3.061484000
6	-5.987664000	-1.282411000	-0.129904000
1	-7.011416000	-1.634903000	-0.211704000
6	1.220685000	-1.796045000	-0.807544000
1	2.124029000	-2.288656000	-0.437764000
1	1.313834000	-1.776560000	-1.893054000
6	3.805326000	-0.169236000	0.435371000
6	-1.963670000	-0.531927000	-2.637886000
1	-1.826725000	-0.410802000	-3.718375000
1	-3.016546000	-0.383261000	-2.403449000
6	-1.500945000	-1.912502000	-2.186529000
1	-2.247695000	-2.664554000	-2.455877000
1	-0.572110000	-2.188727000	-2.685789000
6	4.948885000	-1.382829000	0.470866000
1	4.052866000	-2.260955000	0.924794000
6	-3.628270000	-1.702085000	-0.040169000
6	0.011237000	-2.609930000	-0.351435000
1	0.045380000	-3.604061000	-0.813035000
1	0.042114000	-2.722922000	0.733289000
6	4.371321000	0.982379000	-0.125024000
1	3.824256000	1.918744000	-0.132446000
6	-5.713236000	0.081730000	-0.020519000
1	-6.507679000	0.820348000	-0.013518000
6	-1.038637000	4.644353000	0.499060000
1	-0.974625000	5.726973000	0.546794000
6	-0.806938000	3.867406000	1.634492000
1	-0.561023000	4.318267000	2.589598000
6	-1.353927000	4.008580000	-0.702070000
1	-1.542272000	4.569329000	-1.611240000
6	5.783372000	-1.435211000	-0.068142000
1	6.338083000	-2.368715000	-0.039000000
6	6.375077000	-0.301052000	-0.643009000
6	5.655246000	0.905128000	-0.656963000
1	6.109585000	1.793476000	-1.086758000
6	7.750742000	-0.374262000	-1.251222000
1	8.287112000	-1.265625000	-0.908916000
1	8.340291000	0.515394000	-1.000061000
1	7.682350000	-0.420356000	-2.346990000
6	-0.876023000	-0.879522000	2.922772000
7	-1.086967000	-0.565664000	1.830756000
6	-0.570821000	-1.268535000	4.285499000
1	0.311541000	-0.714854000	4.625551000
1	-1.421035000	-1.042670000	4.938251000
1	-0.360258000	-2.343400000	4.317400000

[Co<sup>II</sup>(CH<sub>3</sub>CN)(Py<sub>2</sub><sup>Ts</sup>tacn)]<sup>2+</sup>  
(G = -3309.078216) (quartet)

27	-1.179906000	-0.098565000	0.118849000
16	2.082525000	-0.221804000	1.047634000
7	1.053671000	-0.460313000	-0.342698000
8	1.735244000	1.107113000	1.571006000
7	-1.236402000	1.982178000	0.367667000
7	-3.266911000	-0.474511000	0.194822000
7	-1.167115000	0.517533000	-1.961279000
7	-1.286532000	-2.049501000	-0.806873000
8	1.902771000	-1.415922000	1.887071000
6	1.278687000	0.618450000	-1.362109000
1	2.269163000	0.512818000	-1.817833000
1	1.224091000	1.573511000	-0.837732000
6	-2.434484000	-2.711353000	-0.144476000
1	-2.132028000	-2.959830000	0.879528000
1	-2.713997000	-3.639306000	-0.657192000
6	-1.417214000	2.671203000	-0.780409000
6	-4.234271000	0.452711000	0.278165000
1	-3.906882000	1.466061000	0.490572000
6	-0.991836000	2.654009000	1.506774000
1	-0.859114000	2.049990000	2.397699000
6	-1.810167000	1.852765000	-1.987486000
1	-2.895862000	1.705253000	-1.945632000
1	-1.582749000	2.392273000	-2.914203000
6	-4.919700000	-2.141949000	-0.283101000
1	-5.144623000	-3.177411000	-0.516133000
6	0.231121000	0.571512000	-2.473118000
1	0.375333000	1.463293000	-3.092530000
1	0.403763000	-0.289592000	-3.119520000
6	-5.925670000	-1.177788000	-0.192507000
1	-6.963794000	-1.453474000	-0.351241000
6	1.190407000	-1.856509000	-0.889915000
1	2.104422000	-2.335315000	-0.530694000
1	1.294779000	-1.781518000	-1.971494000
6	3.743867000	-0.198805000	0.424468000
6	-1.974837000	-0.509382000	-2.668059000
1	-1.903269000	-0.387257000	-3.756612000
1	-3.015685000	-0.364480000	-2.375706000
6	-1.512639000	-1.917630000	-2.282020000
1	-2.265720000	-2.641690000	-2.610776000
1	-0.587436000	-2.167811000	-2.803092000
6	4.465735000	-1.394784000	0.366386000
1	4.043750000	-2.315631000	0.753595000
6	-3.599189000	-1.753224000	-0.084074000
6	-0.002517000	-2.723137000	-0.494092000
1	0.072112000	-3.690643000	-1.007791000
1	0.021517000	-2.895724000	0.585030000
6	4.277523000	1.006619000	-0.048949000
1	3.705406000	1.925829000	0.011518000
6	-5.579143000	0.143263000	0.094707000
1	-6.329185000	0.923331000	0.167515000
6	-1.068994000	4.754915000	0.358485000
1	-0.994540000	5.838120000	0.350838000
6	-0.905295000	4.040773000	1.547418000
1	-0.705552000	4.543369000	2.487480000
6	-1.329858000	4.059751000	-0.822286000
1	-1.467800000	4.576319000	-1.766379000
6	5.748334000	-1.373854000	-0.179236000
1	6.324756000	-2.293269000	-0.224491000
6	6.309220000	-0.184966000	-0.666630000
6	5.559885000	1.001412000	-0.587927000
1	5.989822000	1.929938000	-0.953090000
6	7.687417000	-0.170942000	-1.272486000
1	8.185586000	-1.138169000	-1.148461000
1	8.308202000	0.607805000	-0.812303000
1	7.632642000	0.052666000	-2.346385000
6	-0.735833000	-0.848473000	3.178537000
7	-1.040529000	-0.552936000	2.102471000
6	-0.339458000	-1.220946000	4.521896000
1	0.560619000	-0.661855000	4.800842000
1	-1.149421000	-0.990832000	5.222565000
1	-0.125185000	-2.295173000	4.549914000

[Co<sup>II</sup>(H<sub>2</sub>O)(Py<sub>2</sub><sup>Ts</sup>tacn)]<sup>2+</sup>  
(G = -3252.754191) (doublet)

27	1.213341000	-0.103063000	-0.177110000
16	-2.092548000	0.213122000	-1.057404000
7	-1.094069000	-0.312433000	0.239822000
8	-1.847479000	1.651144000	-1.226632000
7	1.293671000	1.829040000	-0.302584000
7	3.279180000	-0.518413000	-0.484525000
7	1.292228000	0.200327000	1.788829000
7	1.190001000	-2.059039000	0.274134000
8	-1.775185000	-0.709254000	-2.170801000
6	-1.181477000	0.586954000	1.428885000
1	-2.144789000	0.469037000	1.938780000
1	-1.086748000	1.611681000	1.070369000
6	2.258487000	-2.697960000	-0.547214000
1	1.899537000	-2.751026000	-1.580421000
1	2.452832000	-3.719869000	-0.205627000
6	1.617713000	2.432077000	0.869418000
6	4.326755000	0.319139000	-0.454705000
1	4.091196000	1.379746000	-0.435376000
6	1.003837000	2.597638000	-1.369409000
1	0.751948000	2.069286000	-2.279120000
6	2.035529000	1.481340000	1.953492000
1	3.101476000	1.266619000	1.820422000
1	1.895020000	1.904308000	2.953218000
6	4.790039000	-2.383615000	-0.473611000
1	4.927001000	-3.459956000	-0.468897000
6	-0.068281000	0.276686000	2.423389000
1	-0.073388000	1.057323000	3.189616000
1	-0.269710000	-0.665392000	2.932111000
6	5.878074000	-1.508396000	-0.449254000
1	6.892172000	-1.895819000	-0.428450000
6	-1.274651000	-1.775442000	0.529675000
1	-2.228219000	-2.147770000	0.144285000
1	-1.324102000	-1.892113000	1.611818000
6	-3.773607000	-0.044607000	-0.557611000
6	2.060978000	-0.957889000	2.334091000
1	2.011322000	-0.975719000	3.429033000
1	3.101305000	-0.832572000	2.034614000
6	1.493541000	-2.244520000	1.745170000
1	2.209511000	-3.060656000	1.876228000
1	0.578600000	-2.539878000	2.259044000
6	-4.445479000	-1.206092000	-0.948548000
1	-3.963981000	-1.930740000	-1.595954000
6	3.505769000	-1.849805000	-0.493724000
6	-0.148823000	-2.607446000	-0.078661000
1	-0.240750000	-3.645318000	0.263927000
1	-0.229384000	-2.585787000	-1.166654000
6	-4.375429000	0.913472000	0.269219000
1	-3.843645000	1.815176000	0.553462000
6	5.644420000	-0.132277000	-0.441184000
1	6.462188000	0.579971000	-0.415820000
6	1.331685000	4.606562000	-0.098520000
1	1.339125000	5.689053000	-0.016701000
6	1.020801000	3.986554000	-1.309085000
1	0.782777000	4.563071000	-2.196244000
6	1.633917000	3.813773000	1.009173000
1	1.885091000	4.249723000	1.970152000
6	-5.751841000	-1.401802000	-0.502491000
1	-6.292023000	-2.293987000	-0.805873000
6	-6.382253000	-0.464605000	0.328184000
6	-5.678317000	0.692658000	0.703112000
1	-6.161511000	1.430330000	1.337586000
6	-7.786322000	-0.689857000	0.822700000
1	-8.260405000	-1.529041000	0.303234000
1	-8.399046000	0.208420000	0.678996000
1	-7.782864000	-0.910239000	1.898842000
8	0.974104000	-0.311790000	-2.188502000
1	0.082722000	-0.647485000	-2.428474000
1	1.608320000	-0.910057000	-2.618912000

**[Co<sup>II</sup>(H<sub>2</sub>O)(Py<sub>2</sub><sup>Ts</sup>tacn)]<sup>2+</sup>**

(G = -3252.755099) (quartet)

27	1.213150000	-0.123291000	-0.314434000	8	1.858070000	1.047725000	1.594337000
16	-2.076794000	0.059416000	-1.171304000	7	-1.232906000	2.001359000	0.463194000
7	-1.030891000	-0.390221000	0.150676000	7	-3.378541000	-0.385896000	0.203380000
8	-1.791651000	1.470549000	-1.459027000	7	-1.243642000	0.540346000	-1.876379000
7	1.291398000	1.976790000	-0.338933000	7	-1.377868000	-2.013068000	-0.721846000
7	3.252373000	-0.532417000	-0.474508000	8	1.981519000	-1.482450000	1.860804000
7	1.255716000	0.254912000	1.810072000	6	1.210047000	0.627429000	-1.295581000
7	1.237854000	-2.182936000	0.395322000	1	2.190427000	0.579232000	-1.787051000
8	-1.818162000	-0.960060000	-2.210102000	1	1.137230000	1.567069000	-0.746689000
6	-1.196016000	0.557524000	1.303669000	6	-2.525758000	-2.629768000	-0.030562000
1	-2.180149000	0.427279000	1.767251000	1	-2.228859000	-2.796194000	1.011975000
1	-1.116650000	1.568349000	0.903396000	1	-2.801384000	-3.598257000	-0.472855000
6	2.357432000	-2.790950000	-0.351381000	6	-1.343015000	2.686619000	-0.705054000
1	2.026381000	-2.953440000	-1.383610000	6	-4.371977000	0.526755000	0.164536000
1	2.647694000	-3.762519000	0.067426000	1	-4.078228000	1.551555000	0.373116000
6	1.547830000	2.516624000	0.873022000	6	-0.814954000	2.681652000	1.551317000
6	4.250125000	0.367856000	-0.503683000	1	-0.741260000	2.103002000	2.467056000
1	3.949577000	1.408524000	-0.575911000	1	-5.185488000	-3.127027000	-0.597035000
6	0.993305000	2.792332000	-1.364146000	6	0.142920000	0.586202000	-2.388965000
1	0.791391000	2.308851000	-2.313624000	1	0.294580000	1.478695000	-3.010277000
6	1.972411000	1.543932000	1.948233000	1	0.312065000	-0.273105000	-3.040499000
1	3.042651000	1.346667000	1.816015000	6	-6.014812000	-1.128673000	-0.404515000
1	1.831444000	1.977530000	2.945132000	1	-7.033459000	-1.417574000	-0.645074000
6	4.858638000	-2.298415000	-0.297069000	6	1.102380000	-1.863317000	-0.853782000
1	5.057445000	-3.360699000	-0.201632000	1	2.007468000	-2.392140000	-0.540939000
6	-0.125760000	0.329097000	2.368005000	1	1.162860000	-1.792556000	-1.939434000
1	-0.197912000	1.153060000	3.086146000	6	3.775246000	-0.279028000	0.342329000
1	-0.334065000	-0.587335000	2.920334000	6	-2.057254000	-0.469168000	-2.579594000
6	5.894690000	-1.363450000	-0.334968000	1	-1.980684000	-0.364027000	-3.672386000
1	6.927940000	-1.691435000	-0.274441000	1	-3.099105000	-0.306389000	-2.300570000
6	-1.221545000	-1.843309000	0.516334000	6	-1.624659000	-1.889507000	-2.182567000
1	-2.161098000	-2.232255000	0.116167000	1	-2.401413000	-2.596145000	-2.501439000
1	-1.313971000	-1.899562000	1.600187000	1	-0.717061000	-2.163813000	-2.723891000
6	-3.739668000	-0.110248000	-0.585321000	6	4.472698000	-1.485782000	0.237007000
6	2.018100000	-0.881270000	2.391382000	1	4.044143000	-2.404766000	0.621529000
1	1.964370000	-0.865604000	3.487403000	6	-3.698005000	-1.679784000	-0.066587000
1	3.062218000	-0.758878000	2.099469000	6	-10.081440000	-2.682548000	-0.406371000
6	1.477632000	-2.218166000	1.868027000	1	-0.041020000	-3.678522000	-0.872529000
1	2.195319000	-3.008606000	2.114769000	1	-0.065455000	-2.805823000	0.678873000
1	0.545744000	-2.471096000	2.375878000	6	4.319676000	0.921378000	-0.130457000
6	-4.432568000	-1.303722000	-0.809967000	1	3.769111000	1.850772000	-0.033881000
1	-3.980918000	-2.106857000	-1.381760000	6	-5.692550000	0.202800000	-0.131732000
6	3.543841000	-1.849529000	-0.368455000	1	-6.447284000	0.982643000	-0.152415000
6	-0.080785000	-2.717937000	0.000463000	6	-0.584680000	4.727122000	0.316530000
1	-0.235788000	-3.740181000	0.373380000	1	-0.325735000	5.779919000	0.255597000
1	-0.107884000	-2.732930000	-1.091823000	6	-0.487037000	4.033144000	1.525012000
6	-4.307611000	0.950398000	0.133469000	1	-0.154708000	4.525007000	2.433744000
1	-3.760023000	1.874113000	0.285286000	6	-1.021592000	4.034509000	-0.815986000
6	5.587960000	-0.005448000	-0.438835000	1	-1.112832000	4.525876000	-1.779932000
1	6.364457000	0.751243000	-0.461813000	6	5.738844000	-1.481257000	-0.347721000
6	1.187124000	4.733327000	0.027650000	1	6.295363000	-2.410918000	-0.426080000
1	1.139718000	5.808050000	0.175291000	6	6.309592000	-0.295407000	-0.830487000
6	0.939188000	4.176017000	-1.227862000	6	5.584999000	0.902184000	-0.710041000
1	0.697528000	4.795554000	-2.084710000	1	6.021591000	1.828960000	-1.072408000
6	1.494170000	3.889358000	1.095328000	6	7.671429000	-0.296611000	-1.474130000
1	1.692157000	4.278913000	2.088541000	1	8.160487000	-1.270521000	-1.365627000
6	-5.722303000	-1.430230000	-0.297230000	1	8.315206000	0.471995000	-1.028553000
1	-6.278375000	-2.347124000	-0.469043000	1	7.592201000	-0.069918000	-2.545934000
6	-6.316612000	-0.391730000	0.433741000	6	-0.640527000	-0.839624000	3.155874000
6	-5.595130000	0.797091000	0.636257000	7	-1.010485000	-0.560325000	2.085802000
1	-6.052331000	1.611238000	1.191560000	6	-0.123153000	-1.199824000	4.466265000
6	-7.701617000	-0.541803000	1.002853000	1	0.817733000	-0.668123000	4.652103000
1	-8.186871000	-1.449565000	0.629745000	1	-0.842368000	-0.934038000	5.249814000
1	-8.324585000	0.324475000	0.748395000	1	0.067031000	-2.278998000	4.511070000
1	-7.661044000	-0.598867000	2.099020000				
8	0.942959000	-0.499550000	-2.461329000				
1	0.055312000	-0.899032000	-2.583674000				
1	1.566657000	-1.204144000	-2.709981000				

**[Co<sup>I</sup>(H<sub>2</sub>O)(Py<sub>2</sub><sup>Ts</sup>tacn)]<sup>+</sup>**

(G = -3252.873019) (triplet)

27	1.258045000	-0.022030000	-0.340344000
16	-2.057147000	0.067015000	-1.123060000
7	-1.031411000	-0.368778000	0.185152000
8	-1.820762000	1.488216000	-1.410314000
7	1.286882000	1.924726000	-0.371731000
7	3.256865000	-0.536354000	-0.506877000
7	1.282110000	0.264862000	1.831211000
7	1.232841000	-2.146619000	0.365402000

8	-1.782864000	-0.934423000	-2.177851000		6	4.426745000	0.363102000	-0.374860000
6	-1.153535000	0.590341000	1.327886000		1	4.192605000	1.419585000	-0.273030000
1	-2.139429000	0.501959000	1.800444000		6	0.976503000	2.643417000	-1.437988000
1	-1.038016000	1.593065000	0.917443000		1	0.754894000	2.133869000	-2.366397000
6	2.326308000	-2.764248000	-0.405618000		6	1.983932000	1.480489000	1.881329000
1	1.982318000	-2.885704000	-1.439599000		1	3.057620000	1.298945000	1.764597000
1	2.590032000	-3.760083000	-0.022201000		1	1.818210000	1.893807000	2.882612000
6	1.509133000	2.507374000	0.861600000		6	4.891132000	-2.324654000	-0.606102000
6	4.282292000	0.336277000	-0.494739000		1	5.027402000	-3.398466000	-0.687519000
1	4.009415000	1.384373000	-0.577045000		6	-0.083707000	0.204991000	2.302563000
6	0.967491000	2.783696000	-1.391174000		1	-0.133255000	0.974123000	3.080211000
1	0.815873000	2.318889000	-2.359895000		1	-0.262263000	-0.750803000	2.795348000
6	2.004764000	1.549870000	1.913186000		6	5.980843000	-1.454559000	-0.538690000
1	3.060867000	1.331819000	1.709111000		1	6.995203000	-1.841117000	-0.569062000
1	1.937973000	1.997786000	2.915248000		6	-1.201763000	-1.878008000	0.384872000
6	4.835412000	-2.333517000	-0.263096000		1	-2.138645000	-2.285016000	-0.007814000
1	5.005475000	-3.400455000	-0.157666000		1	-1.248914000	-2.013019000	1.465134000
6	-0.081821000	0.348787000	2.391985000		6	-3.743992000	-0.098549000	-0.627837000
1	-0.155657000	1.176085000	3.110212000		6	2.071862000	-0.962214000	2.238258000
1	-0.301525000	-0.565089000	2.947165000		1	1.988117000	-1.011118000	3.331220000
6	5.894727000	-1.422956000	-0.258926000		1	3.117233000	-0.799152000	1.979847000
1	6.918566000	-1.770103000	-0.156916000		6	1.565193000	-2.258867000	1.606779000
6	-1.214233000	-1.813798000	0.551438000		1	2.310991000	-3.049551000	1.737282000
1	-2.167181000	-2.206152000	0.184898000		1	0.657495000	-2.597236000	2.108067000
1	-1.270363000	-1.872102000	1.637783000		6	-4.443650000	-1.273403000	-0.915483000
6	-3.733241000	-0.136792000	-0.569631000		1	-3.994340000	-2.043234000	-1.533272000
6	2.048866000	-0.872430000	2.367994000		6	3.605227000	-1.792582000	-0.561962000
1	2.031293000	-0.896802000	3.468142000		6	-0.038393000	-2.656076000	-0.229935000
1	3.086031000	-0.747783000	2.051330000		1	-0.098004000	-3.703499000	0.095686000
6	1.502698000	-2.202029000	1.828724000		1	-0.117517000	-2.616064000	-1.317348000
1	2.225813000	-2.996428000	2.052352000		6	-4.309351000	0.915231000	0.156592000
1	0.582714000	-2.465278000	2.354487000		1	-3.758227000	1.826336000	0.363498000
6	-4.408853000	-1.334202000	-0.820383000		6	5.745716000	-0.083060000	-0.423704000
1	-3.940049000	-2.119555000	-1.403005000		1	6.563231000	0.627833000	-0.362890000
6	3.534717000	-1.856731000	-0.391522000		6	1.217156000	4.630236000	-0.112284000
6	-0.087057000	-2.681722000	-0.000390000		1	1.189232000	5.709975000	-0.002142000
1	-0.234528000	-3.710273000	0.364333000		6	0.948069000	4.030375000	-1.343195000
1	-0.146040000	-2.686687000	-1.091818000		1	0.707684000	4.621565000	-2.220422000
6	-4.323828000	0.898776000	0.166793000		6	1.523556000	3.815365000	0.978400000
1	-3.790922000	1.827230000	0.340891000		1	1.741907000	4.232729000	1.955923000
6	5.610867000	-0.060805000	-0.375987000		6	-5.733780000	-1.427806000	-0.408118000
1	6.399823000	0.684170000	-0.367575000		1	-6.292006000	-2.332666000	-0.631202000
6	1.003632000	4.723758000	0.043690000		6	-6.324745000	-0.432896000	0.382629000
1	0.883798000	5.790136000	0.206597000		6	-5.597258000	0.738474000	0.653096000
6	0.823090000	4.150399000	-1.226932000		1	-6.049364000	1.520648000	1.256949000
1	0.564299000	4.762484000	-2.086708000		6	-7.712097000	-0.609372000	0.941189000
6	1.357480000	3.861495000	1.096683000		1	-8.180603000	-1.521544000	0.557080000
1	1.529342000	4.239623000	2.101160000		1	-8.348385000	0.247416000	0.685994000
6	-5.701544000	-1.489989000	-0.321254000		1	-7.681906000	-0.672522000	2.037173000
1	-6.242386000	-2.411786000	-0.515304000		1	1.107366000	-0.275913000	-1.853210000
6	-6.317163000	-0.475441000	0.424919000					
6	-5.613484000	0.718658000	0.656350000					
1	-6.085943000	1.515821000	1.223692000					
6	-7.705157000	-0.655804000	0.979507000					
1	-8.167560000	-1.573058000	0.600343000					
1	-8.344641000	0.196624000	0.718623000					
1	-7.676552000	-0.713006000	0.207600200					
8	0.977484000	-0.449712000	-2.555546000					
1	0.085898000	-0.848718000	-2.613971000					
1	1.587141000	-1.179742000	-2.749353000					
<b>[Co<sup>II</sup>(H)(Py<sub>2</sub>T<sup>t</sup>acn)]<sup>+</sup></b>								
(G = -3176.983890) (quartet)								
27	1.259371000	-0.081944000	-0.304627000		27	1.234578000	-0.104244000	-0.521051000
16	-2.064949000	0.083222000	-1.192351000		16	-2.038127000	-0.140709000	-1.272117000
7	-1.078847000	-0.413949000	0.112971000		7	-0.997272000	-0.537591000	0.057745000
8	-1.796673000	1.512473000	-1.413775000		8	-1.726083000	1.249535000	-1.635759000
7	1.273948000	1.847866000	-0.390026000		7	1.248468000	2.010730000	-0.4230364000
7	3.376671000	-0.468646000	-0.442785000		7	3.322291000	-0.476447000	-0.520373000
7	1.286390000	0.181021000	1.694318000		7	1.280170000	0.242403000	1.692516000
7	1.270914000	-2.064418000	0.138860000		7	1.340543000	-2.171242000	0.235021000
8	-1.828471000	-0.880973000	-2.279095000		8	-1.869981000	-1.217106000	-2.259436000
6	-1.189216000	0.487261000	1.293260000		6	-1.180468000	0.418382000	1.193960000
1	-2.156944100	0.364280000	1.795621000		1	-2.156790000	0.271747000	1.669816000
1	-1.106200000	1.511390000	0.928853000		1	-1.136139000	1.424873000	0.776350000
6	2.364420000	-2.643930000	-0.680365000		6	2.469437000	-2.735929000	-0.533315000
1	2.029652000	-2.635858000	-1.723292000		1	2.145582000	-2.831395000	-1.576757000
1	2.571945000	-3.680988000	-0.388419000		1	2.756302000	-3.729612000	-0.165140000
6	1.555854000	2.437213000	0.802735000		6	1.473673000	2.528775000	0.804248000
					6	4.303068000	0.439974000	-0.485479000
					1	3.985096000	1.478045000	-0.504434000
					6	0.908993000	2.836280000	-1.427692000
					1	0.738753000	2.365379000	-2.389904000
					6	1.939971000	1.550513000	1.855332000
					1	3.017537000	1.405505000	1.716325000
					1	1.788294000	1.964776000	2.860484000
					6	4.965070000	-2.217184000	-0.401200000
					1	5.180838000	-3.279603000	-0.354445000
					6	-0.094805000	0.245310000	2.253448000

1	-0.214596000	1.061386000	2.976183000		1	3.099246000	-1.022652000	1.990648000
1	-0.257379000	-0.682172000	2.804682000		6	1.497656000	-2.432384000	1.615393000
6	5.984290000	-1.263556000	-0.377021000		1	2.219755000	-3.249932000	1.682753000
1	7.023038000	-1.573665000	-0.315599000		1	0.587245000	-2.764212000	2.114586000
6	-1.122480000	-1.988908000	0.429129000		6	-4.312393000	-1.067034000	-1.052555000
1	-2.054627000	-2.417782000	0.051110000		1	-3.866467000	-1.803949000	-1.711662000
1	-1.184255000	-2.049240000	1.515157000		6	3.384644000	-1.744673000	-0.685847000
6	-3.694347000	-0.207220000	-0.628878000		6	-0.168199000	-2.721023000	-0.214289000
6	2.091636000	-0.862365000	2.248889000		1	-0.269912000	-3.756012000	0.129995000
1	2.040495000	-0.879534000	3.346678000		1	-0.245998000	-2.687635000	-1.300986000
1	3.129939000	-0.689595000	1.964373000		6	-4.139300000	1.025949000	0.201962000
6	1.613821000	-2.212436000	1.703990000		1	-3.565772000	1.895845000	0.502718000
1	2.372160000	-2.972599000	1.924183000		6	5.316673000	0.195649000	-0.699369000
1	0.706499000	-2.519887000	2.226484000		1	6.044402000	0.999316000	-0.701496000
6	-4.428538000	-1.391038000	-0.744431000		6	1.589795000	4.425854000	-0.086559000
1	-4.016194000	-2.248145000	-1.265411000		1	1.718669000	5.501779000	-0.022617000
6	3.643658000	-1.787572000	-0.478116000		6	1.255226000	3.822031000	-1.299469000
6	0.051181000	-2.802579000	-0.114085000		1	1.123960000	4.403134000	-2.205288000
1	-0.015197000	-3.827540000	0.277782000		6	1.773957000	3.627566000	1.042006000
1	-0.011938000	-2.837393000	-1.203961000		1	2.061052000	4.050774000	1.998479000
6	-4.215655000	0.917919000	0.022193000		6	-5.628979000	-1.202752000	-0.616768000
1	-3.636793000	1.832301000	0.093455000		1	-6.212537000	-2.060169000	-0.938905000
6	5.648682000	0.090839000	-0.419020000		6	-6.213826000	-0.249321000	0.228851000
1	6.408335000	0.864624000	-0.390999000		6	-5.454011000	0.864863000	0.625050000
6	0.994418000	4.745126000	0.016321000		1	-5.902539000	1.616735000	1.268144000
1	0.887698000	5.811369000	0.192621000		6	-7.628864000	-0.410911000	0.714852000
6	0.777202000	4.210026000	-1.254697000		1	-8.132435000	-1.237669000	0.203447000
1	0.502992000	4.839028000	-0.2094713000		1	-8.203877000	0.509223000	0.553954000
6	1.346539000	3.890864000	1.061813000		1	-7.641251000	-0.614711000	1.794074000
1	1.522780000	4.264407000	2.065225000		1	0.917304000	-0.419432000	-1.617632000
6	-5.709354000	-1.440567000	-0.195207000					
1	-6.295043000	-2.351012000	-0.284350000					
6	-6.257393000	-0.332304000	0.466010000					
6	-5.496040000	0.844521000	0.561765000					
1	-5.915359000	1.712961000	1.062194000					
6	-7.632820000	-0.397688000	1.075264000					
1	-8.173641000	-1.287540000	0.736440000		27	1.148457000	-0.140567000	-0.243456000
1	-8.218316000	0.493272000	0.817801000		16	-1.967192000	0.095702000	-1.203329000
1	-7.565787000	-0.435124000	2.171186000		7	-0.981481000	-0.418396000	0.166459000
1	1.052824000	-0.321421000	-2.211231000		8	-1.643612000	1.510802000	-1.416399000
					7	1.291348000	1.858444000	-0.319527000
					7	3.149668000	-0.540740000	-0.632813000
					7	1.308976000	0.137448000	1.770664000
					7	1.209397000	-2.192575000	0.258255000
					8	-1.699890000	-0.893380000	-2.255196000
					6	-1.150886000	0.492769000	1.350811000
					1	-2.133579000	0.342869000	1.809959000
					1	-1.074353000	1.518151000	0.988364000
					6	2.283138000	-2.784877000	-0.576938000
					1	1.895452000	-2.885772000	-1.596878000
					1	2.568674000	-3.776951000	-0.211110000
					6	1.624622000	2.405403000	0.877583000
					6	4.127788000	0.378186000	-0.712106000
					1	3.814041000	1.416370000	-0.726319000
					6	1.046551000	2.663740000	-1.372123000
					1	0.795504000	2.169449000	-2.301048000
					6	2.038442000	1.425271000	1.943549000
					1	3.108311000	1.225875000	1.813774000
					1	1.891196000	1.832998000	2.948274000
					6	4.785766000	-2.286089000	-0.656339000
					1	5.000622000	-3.348878000	-0.624328000
					6	-0.064023000	0.206718000	2.383235000
					1	-0.092283000	0.997830000	3.137760000
					1	-0.263548000	-0.732330000	2.897963000
					6	5.803909000	-1.334684000	-0.731728000
					1	6.843004000	-1.647421000	-0.760737000
					6	-1.230344000	-1.871227000	0.488199000
					1	-2.193465000	-2.204354000	0.094032000
					1	-1.298139000	-1.960679000	1.571474000
					6	-3.646555000	-0.053948000	-0.655251000
					6	2.091870000	-1.023904000	2.288326000
					1	2.073428000	-1.042167000	3.383965000
					1	3.123325000	-0.890280000	1.960114000
					6	1.523485000	-2.325521000	1.725438000
					1	2.246672000	-3.132433000	1.878016000
					1	0.613748000	-2.609718000	2.255158000
					6	-4.370204000	-1.206961000	-0.973844000
					1	-3.924796000	-1.988348000	-1.579788000
					6	3.465652000	-1.852386000	-0.610646000
					6	-0.124182000	-2.749190000	-0.083440000
					1	-0.233022000	-3.769227000	0.304809000
					1	-0.202009000	-2.768721000	-1.171562000

6	-4.202157000	0.979476000	0.110442000		1	-2.303374000	1.666646000	0.882410000
1	-3.631411000	1.873901000	0.335507000		1	-2.303307000	1.666558000	-0.882638000
6	5.470491000	0.020341000	-0.764865000		1	-3.592809000	0.789468000	-0.000114000
1	6.230913000	0.791297000	-0.822099000					
6	1.409750000	4.614487000	-0.027850000					
1	1.445161000	5.693059000	0.089939000					
6	1.102105000	4.046803000	-1.266149000					
1	0.899747000	4.661134000	-2.136269000					
6	1.677461000	3.782015000	1.059002000					
1	1.931762000	4.183409000	2.033904000					
6	-5.678900000	-1.321224000	-0.508912000					
1	-6.258011000	-2.206498000	-0.754811000					
6	-6.262390000	-0.309566000	0.267183000					
6	-5.509422000	0.839277000	0.564428000					
1	-5.957688000	1.634071000	1.153910000					
6	-7.667628000	-0.449281000	0.787372000					
1	-8.192499000	-1.274760000	0.295376000					
1	-8.235446000	0.476265000	0.634274000					
1	-7.656486000	-0.647532000	1.867917000					
1	0.968536000	-0.228937000	-1.703741000					
<b>H<sub>2</sub>O</b>								
(G = -76.468827) (singlet)								
8	0.000000000	0.000000000	0.121359000					
1	0.000000000	0.757766000	-0.485437000					
1	0.000000000	-0.757766000	-0.485437000					
<b>(H<sub>2</sub>O)<sub>3</sub></b>								
(G = -229.388173) (singlet)								
8	1.432539000	-1.037400000	0.002469000					
1	1.335635000	-0.065848000	-0.085725000					
8	-1.460496000	-0.566402000	-0.002749000					
1	0.495613000	-1.302201000	0.011285000					
1	-1.934604000	-0.426529000	0.834122000					
8	0.303114000	1.560259000	-0.102813000					
1	0.479151000	1.696894000	0.842870000					
1	-0.432739000	0.899253000	-0.093608000					
1	-2.144316000	-0.453224000	-0.684198000					
<b>CH<sub>3</sub>CN</b>								
(G = -132.782109) (singlet)								
6	0.000000000	0.000000000	0.276959000					
7	0.000000000	0.000000000	1.440477000					
6	0.000000000	0.000000000	-1.180973000					
1	0.000000000	1.030628000	-1.553086000					
1	0.892550000	-0.515314000	-1.553086000					
1	-0.892550000	-0.515314000	-1.553086000					
<b>Acetophenone (9a)</b>								
(G = -384.922192) (singlet)								
6	2.587772000	0.119064000	-0.000005000					
6	1.810554000	1.281268000	0.000047000					
6	0.418155000	1.190364000	0.000004800					
6	-0.209275000	-0.067389000	0.000005000					
6	0.581583000	-1.230001000	-0.0000043000					
6	1.971002000	-1.138089000	-0.0000052000					
1	3.671907000	0.191684000	-0.000010000					
1	2.288279000	2.256711000	0.000086000					
1	-0.177549000	2.097150000	0.0000087000					
1	0.091961000	-2.198529000	-0.0000080000					
1	2.574852000	-2.041124000	-0.0000095000					
8	-2.230089000	-1.311664000	0.0000107000					
6	-1.695042000	-0.200805000	0.000007000					
6	-2.532958000	1.056379000	-0.0000093000					
<b>Ketyl radical (9a<sup>ketyl</sup>)</b>								
(G = -385.024638) (doublet)								
6	2.617047000	0.110918000	0.000095000					
6	1.818579000	1.273773000	0.000098000					
6	0.432934000	1.197905000	-0.000031000					
6	-0.249046000	-0.068670000	-0.000183000					
6	0.588159000	-1.238444000	-0.000141000					
6	1.969987000	-1.144323000	-0.000011000					
1	3.701616000	0.178944000	0.0000199000					
1	2.295321000	2.253127000	0.000195000					
1	-0.149411000	2.115614000	-0.000027000					
1	0.105861000	-2.212436000	-0.000241000					
1	2.566214000	-2.056106000	0.000004000					
8	-2.280405000	-1.333790000	0.000318000					
6	-1.672478000	-0.188465000	-0.000339000					
6	-2.515211000	1.082612000	0.000014000					
1	-2.319830000	1.714707000	0.880529000					
1	-2.319773000	1.715202000	-0.880127000					
1	-3.576582000	0.809432000	-0.000082000					
<b>O-protonated ketyl radical</b>								
(G = -385.481597) (doublet)								
6	-2.662136000	-0.053950000	0.002060000					
6	-1.920127000	-1.246471000	0.012302000					
6	-0.532085000	-1.224957000	0.008893000					
6	0.185983000	0.010945000	-0.008320000					
6	-0.589258000	1.213813000	-0.013932000					
6	-1.976793000	1.171556000	-0.010231000					
1	-3.748069000	-0.079505000	0.005530000					
1	-2.435412000	-2.203887000	0.026473000					
1	0.010639000	-2.164119000	0.026897000					
1	-0.080902000	2.171919000	-0.025235000					
1	-2.536436000	2.104004000	-0.016675000					
8	2.182497000	1.299613000	0.037176000					
6	1.599989000	0.050581000	-0.016872000					
6	2.530146000	-1.117056000	-0.015998000					
1	2.959979000	-1.288133000	0.984211000					
1	2.036933000	-2.037996000	-0.335967000					
1	3.370584000	-0.924736000	-0.699091000					
1	3.148389000	1.198787000	-0.010968000					
<b>C-deprotonated alcohol</b>								
(G = -385.584845) (singlet)								
6	2.685824000	0.044656000	-0.031943000					
6	1.930230000	1.239916000	-0.023837000					
6	0.547047000	1.244364000	0.016081000					
6	-0.232806000	0.012569000	0.060441000					
6	0.577149000	-1.201430000	0.043145000					
6	1.962677000	-1.164987000	0.000989000					
1	3.771814000	0.058862000	-0.066410000					
1	2.448908000	2.199353000	-0.056160000					
1	0.023146000	2.197910000	0.006033000					
1	0.069764000	-2.162476000	0.083600000					
1	2.504694000	-2.112180000	-0.005717000					
8	-2.272949000	-1.298701000	0.023447000					
6	-1.613040000	-0.027144000	0.103565000					
6	-2.559701000	1.123622000	-0.033182000					
1	-3.437062000	1.010796000	0.626807000					
1	-2.078041000	2.071509000	0.236752000					
1	-2.970931000	1.252554000	-1.057265000					
1	-1.932982000	-1.756105000	-0.766768000					

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