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SUPPLEMENTARY INFORMATION FOR THE ARTICLE:

Photoexcitation and Relaxation kinetics of molecular systems in solution: towards a complete in silico model

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Massimiliano Aschi, Vincenzo Barone, Benedetta Carlotti, Isabella Daidone, Fausto Elisei, Andrea Amadei

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1. SCHEMATIC SUMMARY OF THE MAIN STEPS ADOPTED IN THE PRESENT STUDY.

Step 1.

Parametrization of DASPMI in the S0 electronic state.

> Parametrization of DASPMI in the ground electronic state (S0) is carried out through the scan of the S0 potential energy surface along the semiclassical coordinates ξ_2 and ξ_3 representing, by previous studies, the DASPMI conformational space accessible at room temperature. This step has produced the atomic charges and the ξ_2, ξ_3 dihedral energy functions to be used within the force-field termed as FF-S0 used in the Step 5.

Step 2.

Parametrization of DASPMI in the S1 electronic state.

> Parametrization of DASPMI in the first electronic excited state (S1) is carried out through the scan of the S1 potential energy surface along the semiclassical coordinates ξ_2 and ξ_3 which, similarly to the S0 state, represent the DASPMI conformational space. This procedure, carried out using TD-DFT calculations with CAM-B3LYP functional and 6-31G* has produced the atomic charges and the ξ_2, ξ_3 dihedral energy functions to be used within the force-fields termed termed as FF1 and FF2 (see text) utilized in the Step 8.

Step 3.

Evaluation of the unperturbed basis set for MD-PMM calculations in the S0 surface.

> Using the S0 surface of Step 1 we evaluate (using the TD-DFT CAM-B3LYP/6-31G* level of theory) the electronic energies of six electronic states and the corresponding electric dipole matrix.
> All the terms are evaluated on a grid of 45 points and subsequently interpolated with a cubic spline providing the unperturbed matrix elements $\epsilon^0_{S0-i}(\xi_2, \xi_3)$ $\mu^0_{S0-i,j}(\xi_2, \xi_3)$ for the energies and electric dipoles, respectively (with i=1,6 and j=1,6).

Step 4.

Evaluation of the unperturbed basis set for MD-PMM calculations in the S1 surface.

> Using the S1 surface of Step 2 we evaluate (using the TD-DFT CAM-B3LYP/6-31G* level of theory) the electronic energies of six vertical excited states and the corresponding electric dipole matrix.
> All the terms are evaluated on a grid of 45 points and subsequently interpolated with a cubic spline providing the unperturbed matrix elements $\epsilon^0_{S1-i}(\xi_2, \xi_3)$ $\mu^0_{S1-i,j}(\xi_2, \xi_3)$ for the energies and electric dipoles, respectively (with i=1,6 and j=1,6).

Step 5.

Molecular Dynamics simulation of DASPMI in the ground state, in water.

Molecular dynamics simulation of DASPMI in water at 300 K, using the FF-S0 force field, hereafter termed as *EqMD* is performed. The *EqMD* simulation produces a trajectory of DASPMI and solvent molecules. An *a posteriori* analysis of *EqMD* reveals that, according to FF-S0, DASPMI internal motion is dominated by two relevant internal coordinates basically coincident with ξ_2 and ξ_3 (at each *EqMD* frame DASPMI can be located at a specific point of the ξ_2, ξ_3 space)

Step 6.

MD-PMM calculations of aqueous DASPMI absorption spectrum.

Using the *EqMD* we evaluate the absorption spectrum according to the following procedure:

- Step 6.1

At each *EqMD* frame DASPMI we assigned the DASPMI ξ_2, ξ_3 values and the corresponding values of the unperturbed elements (Step 3) and we evaluated the electric field $\boldsymbol{E}$ and potential $\mathcal{V}$ produced by the solvent onto DASPMI center of mass.

- Step 6.2.

The perturbed Hamiltonian matrix of generic elements

$$H_{i,j} = \quad \epsilon^0_{S0-i}\delta_{i,j} - \boldsymbol{E}\cdot\boldsymbol{\mu}^0_{S0-i,j} \quad + q\;\mathcal{V}\delta_{i,j}$$

is constructed and diagonalized (note that q is the charge of DASPMI equal to +1). This operation provides, at each step of *EqMD*, a set of eigenvalues, $\epsilon_{S0-i}(\xi_2,\xi_3)$ and associated eigenvectors hereafter termed as *perturbed* eigenvalues and eigenvectors. The perturbed eigenvalues are utilized for calculating the (vertical) excitation energy of DASPMI perturbed by water ($\Delta\epsilon_{0-i}=\epsilon_{S0-i}-\epsilon_{S0-0}$) and the perturbed eigenvectors are utilized for calculating the perturbed transition dipole $\boldsymbol{\mu}_{S0-i,j}$.

- Step 6.3.

Using all the frames of *EqMD*, and equation (3) reported in the text, we evaluate the DASPMI absorption spectrum for the 0-i transition.
Note that the variance in the equation (3) has been also calculated by considering three different DASPMI configurations (along the *EqMD*) showing the same ξ_2, ξ_3 instantanoeus values but (obviously) sightly different values of the remaining semiclassical internal coordintes. Using this structures, after a local minimization, the excitation energies have been calculated in vacuo and used for evaluating σ.

Step 7.

Extraction of excited state DASPMI initial conditions at 400 nm of pump.

For reproducing the experimental setup, using the perturbed excitation energies previously calculated ($\Delta\epsilon_{0-1}=\epsilon_{S0-1}-\epsilon_{S0-0}$) at each frame of *EqMD*, we extract all the instantaneous DASPMI-solvent configuration showing an excitation wavelength of 400 nm. A total of 134 points has been extracted.

Step 8.

Non-equilibrium MD simulations of aqueous DASPMI in the first excited states.

Starting from each of the 134 DASPMI-solvent configurations (Step 7), and exchanging the

DASPMI force field from FF-S0 to FF2 (see text) we performed 134 MD simulations (termed in the text as *NeqMD*).

Step 9.
MD-PMM applied to each of the NeqMD simulations.

For each of the 134 *NeqMD* we carried out the PMM procedure similarly to Step 6 but now using the unperturbed basis set evaluated on the S1 potential energy surface (Step 4) according to the steps below reported.

- Step 9.1

At each *NeqMD* frame DASPMI we assigned the DASPMI ξ_2, ξ_3 values and the corresponding values of the unperturbed elements (Step 5) and we evaluated the electric field $\boldsymbol{E}$ and potential $\mathcal{V}$ produced by the solvent onto DASPMI center of mass.

- Step 9.2 (DASPMI CR kinetics).
The perturbed Hamiltonian matrix of generic elements

$$H_{i,j} = \epsilon^0_{S1-i}\delta_{i,j} - \boldsymbol{E}\cdot\boldsymbol{\mu}^0_{S1-i,j} + q\,\mathcal{V}\delta_{i,j}$$

is constructed and utilized for calculating the Diabatic Perturbed Energy difference (ΔDPE, see text) in each *NeqMD*.
When ΔDPE becomes equal to zero (the energy crossing is reached, see red lines in the Figure) the remaining portion of the same trajectory is disregarded.
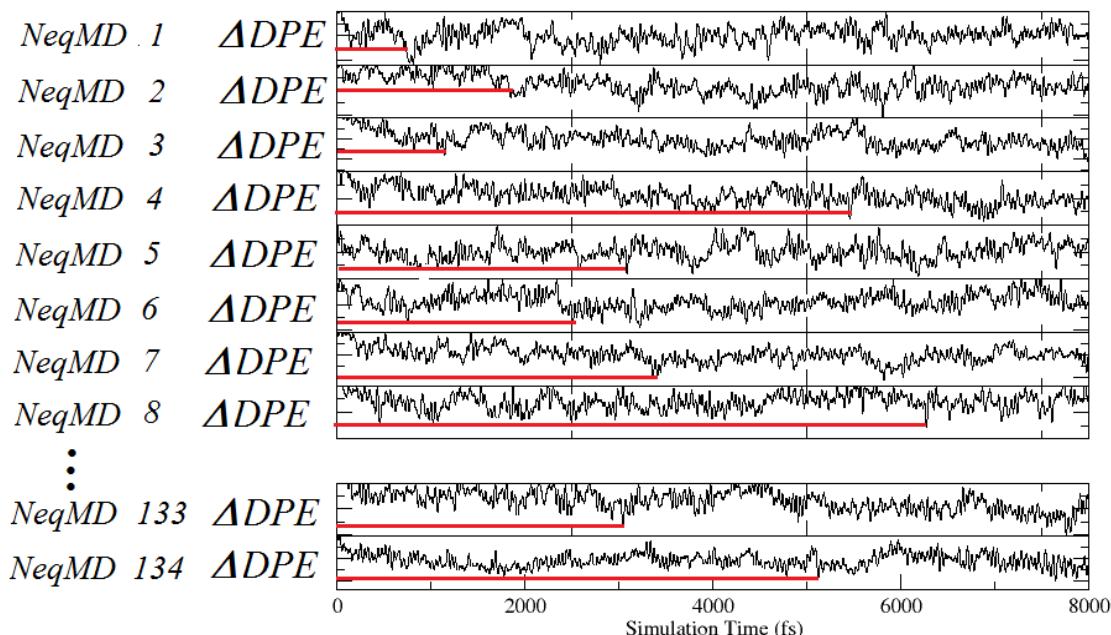
The selected crossing times are used to calculate the CR kinetics (see text).

- Step 9.3 (DASPMI Time Dependent Fluorescence spectra).
For each *NeqMD*, the perturbed Hamiltonian matrix of generic elements, described in the in Step 9.2, is now diagonalized at each step of *NeqMD*.
This operation provides, at each step of *NeqMD*, a set of eigenvalues and associated eigenvectors hereafter termed as *perturbed* eigenvalues and eigenvectors.
The perturbed eigenvalues are utilized for calculating the 0-1 (vertical) energy

difference of DASPMI perturbed by water ($\Delta\varepsilon_{0\text{-}1} = \epsilon_{S1\text{-}1} - \epsilon_{S1\text{-}0}$) and the perturbed eigenvectors are utilized for calculating the perturbed transition dipole $\mu_{S1-i,j}$.

These values of $\Delta\varepsilon_{0\text{-}1}$ provide the instantaneous fluorescence frequency.

The time sequence of $\Delta\varepsilon_{0\text{-}1}$ are reported in the Figure below.
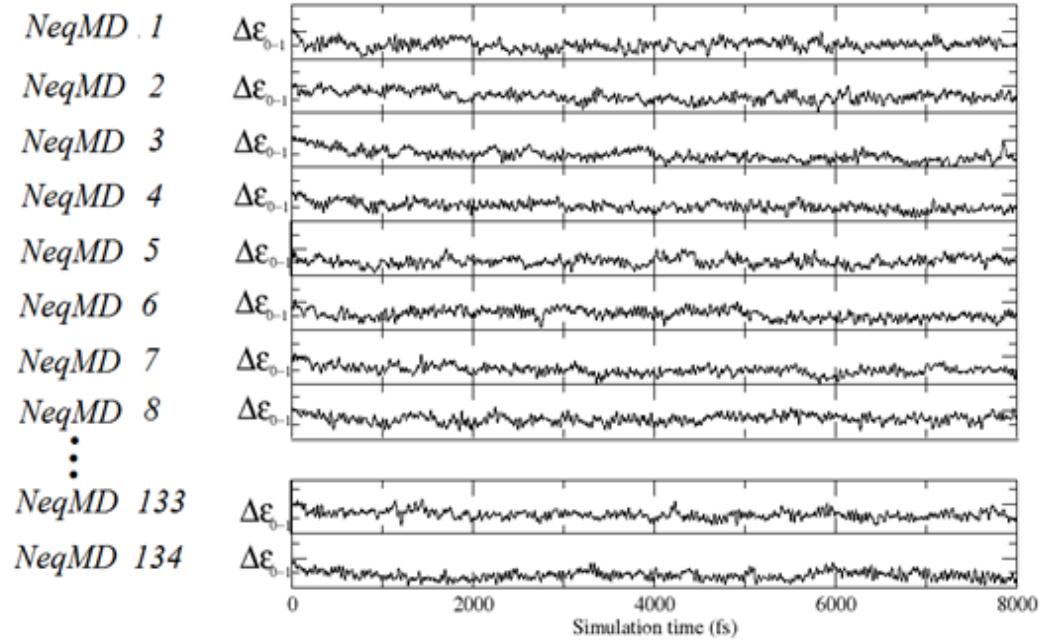
Finally we utilize the $\Delta\varepsilon_{0\text{-}1}$ values in the above Figure (disregarding the portion of the time frames of the *NeqMD* trajectories beyond the DPE crossing, see Step 9.2) for evaluating the Time Dependent fluorescence spectra using equation (4) reported in the text, and schematically reported in the Figure below. More precisely: all the values of $\Delta\varepsilon_{0\text{-}1}$ falling within a given time interval $t_i+\Delta t$ (e.g. 0-300 fs in the red square in the figure) are concatenated and utilized for calculating the emission spectrum (equation 4). Such a spectrum is then assigned as the emission signal at the time $t_i+\Delta t/2$ (e.g. in the case of the red square in the figure the corresponding time is equal to 150 fs).
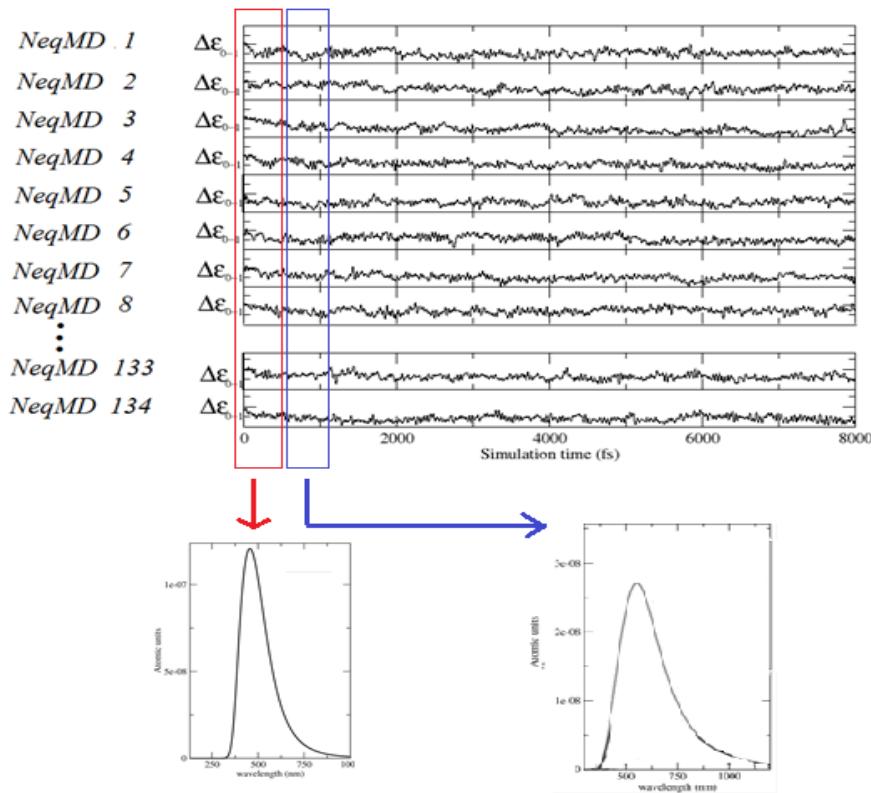
2. GROMACS-FORMAT TOPOLOGIES

2.1 DASPMI Ground state (FF-S0)

```
[ moleculetype ]
; Name   nrexcl
XLMC    3
[ atoms ]
; nr type resnr resid atom cgnr charge    mass    total_charge
   1   HC   1   XLMC   H12   1 0.045000  1.0080
   2   C    1   XLMC   C11   1 0.063119  12.0110
   3   HC   1   XLMC   H10   1 0.045000  1.0080
   4   HC   1   XLMC   H11   1 0.045000  1.0080
   5   NT   1   XLMC    N1   2 -0.282468  14.0067
   6   C    1   XLMC    C7   2 0.361566  12.0110
   7   C    1   XLMC   C10   2 0.071197  12.0110
   8   HC   1   XLMC    H7   2 0.055000  1.0080
   9   HC   1   XLMC    H8   2 0.055000  1.0080
  10   HC   1   XLMC    H9   2 0.055000  1.0080
  11   C    1   XLMC    C8   3 -0.232864  12.0110
  12   HC   1   XLMC    H5   3 0.141586  1.0080
  13   C    1   XLMC    C9   3 -0.114481  12.0110
  14   HC   1   XLMC    H6   3 0.115604  1.0080
  15   C    1   XLMC    C4   4 0.155660  12.0110
  16   C    1   XLMC    C1   4 -0.125579  12.0110
```

```
17   HC   1   XLMC    H1    4  0.150428  1.0080
18   C    1   XLMC    C2    4 -0.295712  12.0110
19   HC   1   XLMC    H2    4  0.146281  1.0080
20   C    1   XLMC    C3    5  0.311103  12.0110
21   NT   1   XLMC    N2    5  0.017762  14.0067
22   C    1   XLMC    C     5 -0.040315  12.011
23   C    1   XLMC    C12   5 -0.053162  12.0110
24   HC   1   XLMC    H14   5  0.154506  1.0080
25   C    1   XLMC    C15   6 -0.249371  12.0110
26   HC   1   XLMC    H17   6  0.153899  1.0080
27   C    1   XLMC    C14   7  0.059080  12.0110
28   HC   1   XLMC    H16   7  0.116388  1.0080
29   C    1   XLMC    C13   7 -0.113642  12.0110
30   HC   1   XLMC    H15   7  0.133453  1.0080
31   C    1   XLMC    C6    8 -0.210490  12.0110
32   HC   1   XLMC    H4    8  0.145778  1.0080
33   C    1   XLMC    C5    8 -0.163654  12.0110
34   HC   1   XLMC    H3    8  0.113328  1.0080
35   HC   1   XLMC    H3    8  0.057000  1.0080
36   HC   1   XLMC    H3    8  0.057000  1.0080
37   HC   1   XLMC    H3    8  0.057000  1.0080

[ bonds ]
; ai  aj  funct  c0       c1
  1    2   2  0.1090  1.2300e+07
  2    3   2  0.1090  1.2300e+07
  2    4   2  0.1090  1.2300e+07
  2    5   2  0.1480  5.7300e+06
  5    6   2  0.1450  5.2319e+06
  5    7   2  0.1480  5.7300e+06
  6   11   2  0.1390  8.6600e+06
  6   31   2  0.1390  8.6600e+06
  7    8   2  0.1090  1.2300e+07
  7    9   2  0.1090  1.2300e+07
  7   10   2  0.1090  1.2300e+07
 11   12   2  0.1080  1.5003e+07
 11   13   2  0.1390  8.6600e+06
 13   14   2  0.1090  1.2300e+07
 13   15   2  0.1390  8.6600e+06
 15   16   2  0.1480  5.7300e+06
 15   33   2  0.1390  8.6600e+06
 16   17   2  0.1090  1.2300e+07
 16   18   2  0.1330  1.1800e+07
 18   19   2  0.1080  1.5003e+07
 18   20   2  0.1480  5.7300e+06
 20   21   2  0.1360  1.0200e+07
 20   25   2  0.1400  8.5400e+06
 22   21   2  0.1480  5.7300e+06
 21   23   2  0.1380  1.1000e+07
 23   24   2  0.1090  1.2300e+07
 23   29   2  0.1360  1.0200e+07
 25   26   2  0.1090  1.2300e+07
```

```
25  27   2  0.1380  1.1000e+07
27  28   2  0.1090  1.2300e+07
27  29   2  0.1410  6.5389e+06
29  30   2  0.1090  1.2300e+07
31  32   2  0.1080  1.5003e+07
31  33   2  0.1390  8.6600e+06
33  34   2  0.1090  1.2300e+07
35  22   2  0.1090  1.2300e+07
36  22   2  0.1090  1.2300e+07
37  22   2  0.1090  1.2300e+07
```

[pairs]
; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp
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 1   7   1
 2   8   1
 2   9   1
 2  10   1
 2  11   1
 2  31   1
 3   6   1
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 4   6   1
 4   7   1
 5  12   1
 5  13   1
 5  32   1
 5  33   1
 6   8   1
 6   9   1
 6  10   1
 6  14   1
 6  34   1
 7  11   1
 7  31   1
11  16   1
11  32   1
12  14   1
12  15   1
12  31   1
13  17   1
13  18   1
13  34   1
14  16   1
14  33   1
15  19   1
15  32   1
16  21   1
16  25   1
16  31   1
16  34   1
17  19   1
```

```
17  20   1
17  33   1
18  22   1
18  26   1
18  27   1
18  33   1
19  21   1
19  25   1
20  24   1
20  28   1
21  26   1
21  30   1
22  24   1
22  25   1
22  29   1
23  28   1
24  27   1
24  30   1
25  30   1
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26  29   1
28  30   1
32  34   1
35  23   1
35  20   1
36  23   1
36  20   1
37  23   1
37  20   1
```

[angles]
```
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   1   2   4   2   108.53  443.00
   1   2   5   2   108.53  443.00
   3   2   4   2   108.53  443.00
   3   2   5   2   108.53  443.00
   4   2   5   2   108.53  443.00
   2   5   6   2   116.00  620.00
   2   5   7   2   111.00  530.00
   6   5   7   2   116.00  620.00
   5   6  11   2   120.00  560.00
   5   6  31   2   120.00  560.00
  11   6  31   2   120.00  560.00
   5   7   8   2   108.53  443.00
   5   7   9   2   108.53  443.00
   5   7  10   2   108.53  443.00
   8   7   9   2   108.53  443.00
   8   7  10   2   108.53  443.00
   9   7  10   2   108.53  443.00
   6  11  12   2   120.00  505.00
```

```
  6  11  13   2  120.00  560.00
 12  11  13   2  120.00  505.00
 11  13  14   2  120.00  505.00
 11  13  15   2  120.00  560.00
 14  13  15   2  120.00  505.00
 13  15  16   2  120.00  560.00
 13  15  33   2  120.00  560.00
 16  15  33   2  120.00  560.00
 15  16  17   2  114.00 1559.41
 15  16  18   2  126.00  640.00
 17  16  18   2  120.00  505.00
 16  18  19   2  120.00  505.00
 16  18  20   2  126.00  640.00
 19  18  20   2  113.00 1559.41
 18  20  21   2  120.00  560.00
 18  20  25   2  120.00  560.00
 21  20  25   2  115.00  610.00
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 20  21  23   2  124.00  730.00
 22  21  23   2  116.00  465.00
 21  23  24   2  120.00  505.00
 21  23  29   2  120.00  560.00
 24  23  29   2  126.00  575.00
 20  25  26   2  120.00  505.00
 20  25  27   2  120.00  560.00
 26  25  27   2  120.00  505.00
 25  27  28   2  120.00  505.00
 25  27  29   2  120.00  560.00
 28  27  29   2  120.00  505.00
 23  29  27   2  120.00  560.00
 23  29  30   2  120.00  505.00
 27  29  30   2  120.00  505.00
  6  31  32   2  120.00  505.00
  6  31  33   2  120.00  560.00
 32  31  33   2  120.00  505.00
 15  33  31   2  120.00  560.00
 15  33  34   2  120.00  505.00
 31  33  34   2  120.00  505.00
 35  22  21   2  108.53  443.00
 36  22  21   2  108.53  443.00
 37  22  21   2  108.53  443.00
 35  22  36   2  108.53  443.00
 35  22  37   2  108.53  443.00
 36  22  37   2  108.53  443.00
```

[dihedrals]
; GROMOS improper dihedrals
; ai aj ak al funct angle   fc
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 18  16  20  19   2    0.00  167.36
 20  18  21  25   2    0.00  900.36
 15  16  33  13   2    0.00  900.36
```

```
33  15  31  34   2    0.00  167.36
31  33   6  32   2    0.00  167.36
 6  31  11   5   2    0.00  900.36
11   6  13  12   2    0.00  167.36
13  15  11  14   2    0.00  167.36
21  20  23  22   2    0.00  167.36
23  21  29  24   2    0.00  167.36
29  23  27  30   2    0.00  167.36
27  29  25  28   2    0.00  167.36
25  20  27  26   2    0.00  167.36
 7   5   6  11   2    0.0   900.0
```

[dihedrals]
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; ai  aj  ak  al funct  ph0     cp    mult
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  7   5   6  31   1  180.00   33.50   2
  6   5   7   8   1  180.00    1.00   6
 31   6  11  13   1  180.00   41.80   2
 11   6  31  33   1  180.00   41.80   2
  6  11  13  15   1  180.00   41.80   2
 11  13  15  33   1  180.00   41.80   2
 33  15  16  18   1  180.00   30.00   2
 13  15  33  31   1  180.00   41.80   2
 15  16  18  20   1  180.00   41.80   2
 16  18  20  21   1  180.00   30.00   2
 25  20  21  23   1  180.00   41.80   2
 21  20  25  27   1  180.00   41.80   2
 20  21  23  29   1  180.00   41.80   2
 21  23  29  27   1  180.00   41.80   2
 20  25  27  29   1  180.00   41.80   2
 25  27  29  23   1  180.00   41.80   2
  6  31  33  15   1  180.00   41.80   2
 35  22  21  23   1  180.00    1.00   6
```

[exclusions]
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; ai  aj  funct ;  GROMOS 1-4 exclusions
  6  15
 11  33
 13  31
 15  20
 20  29
 21  27
 23  25
```

2.2 DASPMI L.E. CONDITION (FF1)

[moleculetype]
```
; Name   nrexcl
XLMC    3
```
[atoms]
```
; nr type  resnr resid atom cgnr charge   mass   total_charge
  1  HC   1   XLMC   H12   1 0.084733 1.0080
```

```
 2   C   1   XLMC   C11  1 0.028575  12.0110
 3   HC  1   XLMC   H10  1 0.037931   1.0080
 4   HC  1   XLMC   H11  1 0.037867   1.0080
 5   NT  1   XLMC   N1   2 -0.215134  14.0067
 6   C   1   XLMC   C7   2 0.317788  12.0110
 7   C   1   XLMC   C10  2 0.049606  12.0110
 8   HC  1   XLMC   H7   2 0.078219   1.0080
 9   HC  1   XLMC   H8   2 0.033372   1.0080
10   HC  1   XLMC   H9   2 0.033395   1.0080
11   C   1   XLMC   C8   3 -0.207289  12.0110
12   HC  1   XLMC   H5   3 0.153980   1.0080
13   C   1   XLMC   C9   3 -0.191872  12.0110
14   HC  1   XLMC   H6   3 0.121595   1.0080
15   C   1   XLMC   C4   4 0.324886  12.0110
16   C   1   XLMC   C1   4 -0.244732  12.0110
17   HC  1   XLMC   H1   4 0.139763   1.0080
18   C   1   XLMC   C2   4 -0.227940  12.0110
19   HC  1   XLMC   H2   4 0.165308   1.0080
20   C   1   XLMC   C3   5 0.265962  12.0110
21   NT  1   XLMC   N2   5 -0.028406  14.0067
22   C   1   XLMC   H13  5 -0.078949  12.0080
23   C   1   XLMC   C12  5 -0.020526  12.0110
24   HC  1   XLMC   H14  5 0.142782   1.0080
25   C   1   XLMC   C15  6 -0.206560  12.0110
26   HC  1   XLMC   H17  6 0.147201   1.0080
27   C   1   XLMC   C14  7 0.018385  12.0110
28   HC  1   XLMC   H16  7 0.108745   1.0080
29   C   1   XLMC   C13  7 -0.136992  12.0110
30   HC  1   XLMC   H15  7 0.133105   1.0080
31   C   1   XLMC   C6   8 -0.156072  12.0110
32   HC  1   XLMC   H4   8 0.151127   1.0080
33   C   1   XLMC   C5   8 -0.245247  12.0110
34   HC  1   XLMC   H3   8 0.146669   1.0080
35   HC  1   XLMC   H3   8 0.109994   1.0080
36   HC  1   XLMC   H3   8 0.064385   1.0080
37   HC  1   XLMC   H3   8 0.064350   1.0080

[ bonds ]
; ai  aj  funct  c0       c1
  1   2   2  0.1090  1.2300e+07
  2   3   2  0.1090  1.2300e+07
  2   4   2  0.1090  1.2300e+07
  2   5   2  0.1480  5.7300e+06
  5   6   2  0.1450  5.2319e+06
  5   7   2  0.1480  5.7300e+06
  6  11   2  0.1390  8.6600e+06
  6  31   2  0.1390  8.6600e+06
  7   8   2  0.1090  1.2300e+07
  7   9   2  0.1090  1.2300e+07
  7  10   2  0.1090  1.2300e+07
 11  12   2  0.1080  1.5003e+07
 11  13   2  0.1390  8.6600e+06
```

```
13   14   2   0.1090   1.2300e+07
13   15   2   0.1390   8.6600e+06
15   16   2   0.1480   5.7300e+06
15   33   2   0.1390   8.6600e+06
16   17   2   0.1090   1.2300e+07
16   18   2   0.1330   1.1800e+07
18   19   2   0.1080   1.5003e+07
18   20   2   0.1480   5.7300e+06
20   21   2   0.1360   1.0200e+07
20   25   2   0.1400   8.5400e+06
22   21   2   0.1480   5.7300e+06
21   23   2   0.1380   1.1000e+07
23   24   2   0.1090   1.2300e+07
23   29   2   0.1360   1.0200e+07
25   26   2   0.1090   1.2300e+07
25   27   2   0.1380   1.1000e+07
27   28   2   0.1090   1.2300e+07
27   29   2   0.1410   6.5389e+06
29   30   2   0.1090   1.2300e+07
31   32   2   0.1080   1.5003e+07
31   33   2   0.1390   8.6600e+06
33   34   2   0.1090   1.2300e+07
35   22   2   0.1090   1.2300e+07
36   22   2   0.1090   1.2300e+07
37   22   2   0.1090   1.2300e+07
```

[pairs]
; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp
```
 1    6   1
 1    7   1
 2    8   1
 2    9   1
 2   10   1
 2   11   1
 2   31   1
 3    6   1
 3    7   1
 4    6   1
 4    7   1
 5   12   1
 5   13   1
 5   32   1
 5   33   1
 6    8   1
 6    9   1
 6   10   1
 6   14   1
 6   34   1
 7   11   1
 7   31   1
11   16   1
```

```
   11   32   1
   12   14   1
   12   15   1
   12   31   1
   13   17   1
   13   18   1
   13   34   1
   14   16   1
   14   33   1
   15   19   1
   15   32   1
   16   21   1
   16   25   1
   16   31   1
   16   34   1
   17   19   1
   17   20   1
   17   33   1
   18   22   1
   18   23   1
   18   26   1
   18   27   1
   18   33   1
   19   21   1
   19   25   1
   20   24   1
   20   28   1
   21   26   1
   21   30   1
   22   24   1
   22   25   1
   22   29   1
   23   28   1
   24   27   1
   24   30   1
   25   30   1
   26   28   1
   26   29   1
   28   30   1
   32   34   1
   35   23   1
   35   20   1
   36   23   1
   36   20   1
   37   23   1
   37   20   1


[ angles ]
; ai  aj  ak  funct  angle    fc
   1   2   3   2   108.53   443.00
   1   2   4   2   108.53   443.00
```

1	2	5	2	108.53	443.00
3	2	4	2	108.53	443.00
3	2	5	2	108.53	443.00
4	2	5	2	108.53	443.00
2	5	6	2	116.00	620.00
2	5	7	2	111.00	530.00
6	5	7	2	116.00	620.00
5	6	11	2	120.00	560.00
5	6	31	2	120.00	560.00
11	6	31	2	120.00	560.00
5	7	8	2	108.53	443.00
5	7	9	2	108.53	443.00
5	7	10	2	108.53	443.00
8	7	9	2	108.53	443.00
8	7	10	2	108.53	443.00
9	7	10	2	108.53	443.00
6	11	12	2	120.00	505.00
6	11	13	2	120.00	560.00
12	11	13	2	120.00	505.00
11	13	14	2	120.00	505.00
11	13	15	2	120.00	560.00
14	13	15	2	120.00	505.00
13	15	16	2	120.00	560.00
13	15	33	2	120.00	560.00
16	15	33	2	120.00	560.00
15	16	17	2	114.00	1559.41
15	16	18	2	126.00	640.00
17	16	18	2	120.00	505.00
16	18	19	2	117.00	505.00
16	18	20	2	134.00	640.00
19	18	20	2	109.00	1559.41
18	20	21	2	123.00	560.00
18	20	25	2	117.00	560.00
21	20	25	2	120.00	610.00
20	21	22	2	124.00	390.00
20	21	23	2	120.00	730.00
22	21	23	2	116.00	465.00
21	23	24	2	120.00	505.00
21	23	29	2	120.00	560.00
24	23	29	2	126.00	575.00
20	25	26	2	120.00	505.00
20	25	27	2	120.00	560.00
26	25	27	2	120.00	505.00
25	27	28	2	120.00	505.00
25	27	29	2	120.00	560.00
28	27	29	2	120.00	505.00
23	29	27	2	120.00	560.00
23	29	30	2	120.00	505.00
27	29	30	2	120.00	505.00
6	31	32	2	120.00	505.00
6	31	33	2	120.00	560.00
32	31	33	2	120.00	505.00

```
 15  33  31   2   120.00  560.00
 15  33  34   2   120.00  505.00
 31  33  34   2   120.00  505.00
 35  22  21   2   108.53  443.00
 36  22  21   2   108.53  443.00
 37  22  21   2   108.53  443.00
35  22  36   2   108.53  443.00
 35  22  37   2   108.53  443.00
 36  22  37   2   108.53  443.00


[ dihedrals ]
; GROMOS improper dihedrals
; ai  aj  ak  al funct  angle    fc
 16  18  17  15   2    0.00  167.36
 18  16  20  19   2    0.00  167.36
 20  18  21  25   2    0.00  900.36
 15  16  33  13   2    0.00  900.36
 33  15  31  34   2    0.00  167.36
 31  33   6  32   2    0.00  167.36
  6  31  11   5   2    0.00  900.36
 11   6  13  12   2    0.00  167.36
 13  15  11  14   2    0.00  167.36
 21  20  23  22   2    0.00  167.36
 23  21  29  24   2    0.00  167.36
 29  23  27  30   2    0.00  167.36
 27  29  25  28   2    0.00  167.36
 25  20  27  26   2    0.00  167.36
  7   5   6  11   2    0.0   900.0


[ dihedrals ]
; ai  aj  ak  al funct  ph0     cp     mult
  3   2   5   6   1   180.00   1.00   6
  7   5   6  31   1   180.00  33.50   2
  6   5   7   8   1   180.00   1.00   6
 31   6  11  13   1   180.00  41.80   2
 11   6  31  33   1   180.00  41.80   2
  6  11  13  15   1   180.00  41.80   2
 11  13  15  33   1   180.00  41.80   2
 ; 33  15  16  18   1 180.00  32.20   2
 33  15  16  18   1   180.0    7.0    2
 13  15  33  31   1   180.00  41.80   2
 15  16  18  20   1   180.00  41.80   2
  ; 16  18  20  21   1 180.00  32.00   2
 16  18  20  21   1   180.0    6.5    2
 25  20  21  23   1   180.00  41.80   2
 21  20  25  27   1   180.00  41.80   2
 20  21  23  29   1   180.00  41.80   2
 21  23  29  27   1   180.00  41.80   2
 20  25  27  29   1   180.00  41.80   2
 25  27  29  23   1   180.00  41.80   2
  6  31  33  15   1   180.00  41.80   2
 35  22  21  23   1   180.00   1.00   6
```

[exclusions]
; ai   aj funct ; GROMOS 1-4 exclusions
   6   15
  11   33
  13   31
  15   20
  20   29
  21   27
  23   25

2.3 DASPMI CT1 CONDITION (FF2)

; Name   nrexcl
XLMC   3
[atoms]
; nr type resnr resid atom cgnr charge   mass   total_charge
   1   HC   1   XLMC   H12   1 0.097076 1.0080
   2   C   1   XLMC   C11   1 0.000889 12.0110
   3   HC   1   XLMC   H10   1 0.065322 1.0080
   4   HC   1   XLMC   H11   1 0.062973 1.0080
   5   NT   1   XLMC   N1   2 -0.173243 14.0067
   6   C   1   XLMC   C7   2 0.352118 12.0110
   7   C   1   XLMC   C10   2 -0.022222 12.0110
   8   HC   1   XLMC   H7   2 0.105586 1.0080
   9   HC   1   XLMC   H8   2 0.068768 1.0080
  10   HC   1   XLMC   H9   2 0.068551 1.0080
  11   C   1   XLMC   C8   3 -0.167298 12.0110
  12   HC   1   XLMC   H5   3 0.149092 1.0080
  13   C   1   XLMC   C9   3 -0.189466 12.0110
  14   HC   1   XLMC   H6   3 0.161711 1.0080
  15   C   1   XLMC   C4   4 0.297952 12.0110
  16   C   1   XLMC   C1   4 -0.216187 12.0110
  17   HC   1   XLMC   H1   4 0.103074 1.0080
  18   C   1   XLMC   C2   4 0.121018 12.0110
  19   HC   1   XLMC   H2   4 0.044773 1.0080
  20   C   1   XLMC   C3   5 0.085354 12.0110
  21   NT   1   XLMC   N2   5 -0.005816 14.0067
  22   C   1   XLMC   H13   5 -0.046668 12.080
  23   C   1   XLMC   C12   5 -0.166124 12.0110
  24   HC   1   XLMC   H14   5 0.140180 1.0080
  25   C   1   XLMC   C15   6 -0.182534 12.0110
  26   HC   1   XLMC   H17   6 0.103128 1.0080
  27   C   1   XLMC   C14   7 -0.112779 12.0110
  28   HC   1   XLMC   H16   7 0.099369 1.0080
  29   C   1   XLMC   C13   7 -0.084591 12.0110
  30   HC   1   XLMC   H15   7 0.112745 1.0080
  31   C   1   XLMC   C6   8 -0.189075 12.0110
  32   HC   1   XLMC   H4   8 0.153190 1.0080
  33   C   1   XLMC   C5   8 -0.148915 12.0110
  34   HC   1   XLMC   H3   8 0.156558 1.0080
  35   HC   1   XLMC   H3   8 0.084936   1.0080

```
36  HC  1  XLMC   H3  8 0.018079   1.0080
37  HC  1  XLMC   H3  8 0.052474   1.0080
```

[bonds]
```
; ai  aj  funct  c0       c1
   1   2   2  0.1090  1.2300e+07
   2   3   2  0.1090  1.2300e+07
   2   4   2  0.1090  1.2300e+07
   2   5   2  0.1480  5.7300e+06
   5   6   2  0.1450  5.2319e+06
   5   7   2  0.1480  5.7300e+06
   6  11   2  0.1390  8.6600e+06
   6  31   2  0.1390  8.6600e+06
   7   8   2  0.1090  1.2300e+07
   7   9   2  0.1090  1.2300e+07
   7  10   2  0.1090  1.2300e+07
  11  12   2  0.1080  1.5003e+07
  11  13   2  0.1390  8.6600e+06
  13  14   2  0.1090  1.2300e+07
  13  15   2  0.1390  8.6600e+06
  15  16   2  0.1480  5.7300e+06
  15  33   2  0.1390  8.6600e+06
  16  17   2  0.1090  1.2300e+07
  16  18   2  0.1330  1.1800e+07
  18  19   2  0.1080  1.5003e+07
  18  20   2  0.1480  5.7300e+06
  20  21   2  0.1360  1.0200e+07
  20  25   2  0.1400  8.5400e+06
  22  21   2  0.1480  5.7300e+06
  21  23   2  0.1380  1.1000e+07
  23  24   2  0.1090  1.2300e+07
  23  29   2  0.1360  1.0200e+07
  25  26   2  0.1090  1.2300e+07
  25  27   2  0.1380  1.1000e+07
  27  28   2  0.1090  1.2300e+07
  27  29   2  0.1410  6.5389e+06
  29  30   2  0.1090  1.2300e+07
  31  32   2  0.1080  1.5003e+07
  31  33   2  0.1390  8.6600e+06
  33  34   2  0.1090  1.2300e+07
  35  22   2  0.1090  1.2300e+07
  36  22   2  0.1090  1.2300e+07
  37  22   2  0.1090  1.2300e+07
```

[pairs]
```
; ai  aj  funct ;  all 1-4 pairs but the ones excluded in GROMOS itp
   1   6   1
   1   7   1
   2   8   1
   2   9   1
   2  10   1
   2  11   1
   2  31   1
```

```
3    6    1
3    7    1
4    6    1
4    7    1
5    12   1
5    13   1
5    32   1
5    33   1
6    8    1
6    9    1
6    10   1
6    14   1
6    34   1
7    11   1
7    31   1
11   16   1
11   32   1
12   14   1
12   15   1
12   31   1
13   17   1
13   18   1
13   34   1
14   16   1
14   33   1
15   19   1
15   32   1
16   21   1
16   25   1
16   31   1
16   34   1
17   19   1
17   20   1
17   33   1
18   22   1
18   23   1
18   26   1
18   27   1
18   33   1
19   21   1
19   25   1
20   24   1
20   28   1
21   26   1
21   30   1
22   24   1
22   25   1
22   29   1
23   28   1
24   27   1
24   30   1
25   30   1
```

```
26  28  1
26  29  1
28  30  1
32  34  1
35  23  1
35  20  1
36  23  1
36  20  1
37  23  1
37  20  1


[ angles ]
; ai  aj  ak funct  angle    fc
  1   2   3   2   108.53   443.00
  1   2   4   2   108.53   443.00
  1   2   5   2   108.53   443.00
  3   2   4   2   108.53   443.00
  3   2   5   2   108.53   443.00
  4   2   5   2   108.53   443.00
  2   5   6   2   116.00   620.00
  2   5   7   2   111.00   530.00
  6   5   7   2   116.00   620.00
  5   6  11   2   120.00   560.00
  5   6  31   2   120.00   560.00
 11   6  31   2   120.00   560.00
  5   7   8   2   108.53   443.00
  5   7   9   2   108.53   443.00
  5   7  10   2   108.53   443.00
  8   7   9   2   108.53   443.00
  8   7  10   2   108.53   443.00
  9   7  10   2   108.53   443.00
  6  11  12   2   120.00   505.00
  6  11  13   2   120.00   560.00
 12  11  13   2   120.00   505.00
 11  13  14   2   120.00   505.00
 11  13  15   2   120.00   560.00
 14  13  15   2   120.00   505.00
 13  15  16   2   120.00   560.00
 13  15  33   2   120.00   560.00
 16  15  33   2   120.00   560.00
 15  16  17   2   114.00  1559.41
 15  16  18   2   126.00   640.00
 17  16  18   2   120.00   505.00
 16  18  19   2   117.00   505.00
 16  18  20   2   134.00   640.00
 19  18  20   2   109.00  1559.41
 18  20  21   2   123.00   560.00
 18  20  25   2   117.00   560.00
 21  20  25   2   120.00   610.00
 20  21  22   2   124.00   390.00
 20  21  23   2   120.00   730.00
```

```
22  21  23   2   116.00  465.00
21  23  24   2   120.00  505.00
21  23  29   2   120.00  560.00
24  23  29   2   126.00  575.00
20  25  26   2   120.00  505.00
20  25  27   2   120.00  560.00
26  25  27   2   120.00  505.00
25  27  28   2   120.00  505.00
25  27  29   2   120.00  560.00
28  27  29   2   120.00  505.00
23  29  27   2   120.00  560.00
23  29  30   2   120.00  505.00
27  29  30   2   120.00  505.00
 6  31  32   2   120.00  505.00
 6  31  33   2   120.00  560.00
32  31  33   2   120.00  505.00
15  33  31   2   120.00  560.00
15  33  34   2   120.00  505.00
31  33  34   2   120.00  505.00
35  22  21   2   108.53  443.00
36  22  21   2   108.53  443.00
37  22  21   2   108.53  443.00
35  22  36   2   108.53  443.00
35  22  37   2   108.53  443.00
36  22  37   2   108.53  443.00
```

[dihedrals]
; GROMOS improper dihedrals
; ai aj ak al funct angle   fc
```
 16  18  17  15   2    0.00  167.36
 18  16  20  19   2    0.00  167.36
 20  18  21  25   2    0.00  900.36
 15  16  33  13   2    0.00  900.36
 33  15  31  34   2    0.00  167.36
 31  33   6  32   2    0.00  167.36
  6  31  11   5   2    0.00  900.36
 11   6  13  12   2    0.00  167.36
 13  15  11  14   2    0.00  167.36
 21  20  23  22   2    0.00  167.36
 23  21  29  24   2    0.00  167.36
 29  23  27  30   2    0.00  167.36
 27  29  25  28   2    0.00  167.36
 25  20  27  26   2    0.00  167.36
  7   5   6  11   2    0.0   900.0
```

[dihedrals]
; ai aj ak al funct ph0   cp   mult
```
  3   2   5   6   1  180.00   1.00   6
  7   5   6  31   1  180.00  33.50   2
  6   5   7   8   1  180.00   1.00   6
 31   6  11  13   1  180.00  41.80   2
 11   6  31  33   1  180.00  41.80   2
```

```
 6  11  13  15   1   180.00   41.80   2
11  13  15  33   1   180.00   41.80   2
  33  15  16  18   1  180.00   24.00   2
13  15  33  31   1   180.00   41.80   2
15  16  18  20   1   180.00   41.80   2
  16  18  20  21   1  180.00   -7.00   2
25  20  21  23   1   180.00   41.80   2
21  20  25  27   1   180.00   41.80   2
20  21  23  29   1   180.00   41.80   2
21  23  29  27   1   180.00   41.80   2
20  25  27  29   1   180.00   41.80   2
25  27  29  23   1   180.00   41.80   2
 6  31  33  15   1   180.00   41.80   2
35  22  21  23   1   180.00    1.00   6
[ exclusions ]
; ai  aj  funct ;  GROMOS 1-4 exclusions
  6   15
 11   33
 13   31
 15   20
 20   29
 21   27
 23   25
```

3. SIMULATION BOX DASPMI IN WATER (.gro format)

```
DASPMI in water
 2170
  1XLMC  H12   1   1.504   0.448   2.215  -0.5801   0.8433  -1.5442
  1XLMC  C11   2   1.518   0.362   2.149   0.0440   0.0042  -0.3481
  1XLMC  H10   3   1.472   0.388   2.054  -1.2067   3.0023   0.9710
  1XLMC  H11   4   1.464   0.278   2.193  -0.8137   0.2080  -0.9900
  1XLMC   N1   5   1.660   0.323   2.136   0.0185  -0.1773  -0.1043
  1XLMC   C7   6   1.757   0.372   2.231  -0.6797   0.5777   0.2248
  1XLMC  C10   7   1.698   0.273   2.001   0.5943  -0.7031   0.2463
  1XLMC   H7   8   1.627   0.310   1.927  -0.0953   0.3571   1.3857
  1XLMC   H8   9   1.799   0.308   1.980   0.7602  -0.1899   1.7122
  1XLMC   H9  10   1.688   0.165   1.992  -0.2133  -0.6255   0.1416
  1XLMC   C8  11   1.893   0.370   2.203  -0.6666  -0.8890   0.3166
  1XLMC   H5  12   1.926   0.344   2.103  -0.0920  -0.2807   0.3399
  1XLMC   C9  13   1.993   0.399   2.295  -0.2604  -0.4579  -0.2467
  1XLMC   H6  14   2.096   0.396   2.261  -0.8299   2.5517  -2.7703
  1XLMC   C4  15   1.959   0.429   2.427   0.2164  -0.4500  -0.1246
  1XLMC   C1  16   2.057   0.435   2.538   0.2163   0.4536  -0.1654
  1XLMC   H1  17   2.019   0.474   2.632  -1.5131  -4.3996   1.4823
  1XLMC   C2  18   2.184   0.402   2.520   0.0655  -0.3458   0.2135
  1XLMC   H2  19   2.209   0.339   2.436   1.5471   0.1096   0.2836
  1XLMC   C3  20   2.293   0.396   2.621   0.0956  -0.2775   0.1839
  1XLMC   N2  21   2.426   0.392   2.594   0.0677  -0.0437   0.0132
```

```
1XLMC    C   22   2.480   0.427   2.461  0.4503 -0.2349  0.1168
1XLMC   C12  23   2.529   0.358   2.679 -0.1435 -0.6298  0.0357
1XLMC   H14  24   2.622   0.318   2.638 -0.1728 -0.8073  0.1389
1XLMC   C15  25   2.266   0.388   2.758  0.1618  0.5299  0.2464
1XLMC   H17  26   2.166   0.418   2.790 -0.5075  0.0221 -1.2618
1XLMC   C14  27   2.368   0.369   2.849  0.4569  0.1609 -0.1596
1XLMC   H16  28   2.347   0.368   2.956  0.0298 -1.6586 -0.2355
1XLMC   C13  29   2.504   0.352   2.812  0.5399  0.0460  0.2029
1XLMC   H15  30   2.576   0.328   2.890  1.1521  2.0490  0.2930
1XLMC    C6  31   1.729   0.425   2.357 -0.1703  0.5912  0.3370
1XLMC    H4  32   1.628   0.421   2.397  0.5869  0.9935  2.4062
1XLMC    C5  33   1.825   0.453   2.453  0.3118 -0.1389  0.0805
1XLMC    H3  34   1.787   0.460   2.555  1.2156 -2.0223  0.5832
1XLMC    H3  35   2.580   0.469   2.452 -0.0172  1.3012  1.6308
1XLMC    H3  36   2.467   0.341   2.394  3.1644 -0.4945 -0.1915
1XLMC    H3  37   2.415   0.508   2.427 -0.5615  0.3646  3.2101
2SOL    OW   38   1.826   1.757   0.439  0.1429  0.0016  0.2258
2SOL    HW1  39   1.778   1.823   0.497  0.3459 -0.1060  0.5184
2SOL    HW2  40   1.899   1.714   0.491 -0.4208 -0.9618  0.2535
3SOL    OW   41   1.625   2.293   1.095 -0.0513  0.0378  0.0422
3SOL    HW1  42   1.579   2.371   1.139  0.3951  0.8403 -0.8720
3SOL    HW2  43   1.558   2.222   1.075 -0.3658 -0.0681  1.4224
4SOL    OW   44   2.814   2.468   1.284 -0.4225 -0.0802 -0.1454
4SOL    HW1  45   2.846   2.549   1.334  1.8058 -0.8877 -0.1464
4SOL    HW2  46   2.714   2.465   1.286 -0.5030  1.5765  1.5738
5SOL    OW   47   1.322   2.486   1.041 -0.1365 -0.7969  0.3563
5SOL    HW1  48   1.301   2.440   1.127  2.1560 -0.7840  1.0066
5SOL    HW2  49   1.403   2.544   1.054 -1.0884  1.0106 -1.2363
6SOL    OW   50   1.868   2.042   0.046  0.4227 -0.3068 -0.5422
6SOL    HW1  51   1.769   2.029   0.050  0.4755 -0.7674 -0.6766
6SOL    HW2  52   1.891   2.109  -0.024  0.0294  1.8223  1.2362
7SOL    OW   53   2.614   2.406   0.191  0.0501  0.5145  0.2123
7SOL    HW1  54   2.535   2.410   0.252  0.0525  1.8627  0.1563
7SOL    HW2  55   2.625   2.313   0.158 -1.8234  0.3892 -0.1818
8SOL    OW   56   1.338   2.023   1.820 -0.1490  0.8239 -0.1709
8SOL    HW1  57   1.337   2.085   1.899 -0.9999 -0.0476  0.5328
8SOL    HW2  58   1.249   2.026   1.774 -0.1222  0.2933 -0.2627
9SOL    OW   59   0.130   1.605   0.645 -0.7229  0.3288 -0.3250
9SOL    HW1  60   0.052   1.636   0.699 -0.6957  1.1311 -0.7255
9SOL    HW2  61   0.127   1.505   0.636  0.1792 -0.0448  2.5512
10SOL   OW   62   0.629   2.711   0.716 -0.5153  0.4722  0.5417
10SOL   HW1  63   0.664   2.678   0.804  0.7723 -0.2686 -0.2175
10SOL   HW2  64   0.535   2.679   0.703 -0.0716 -1.0277  0.8335
11SOL   OW   65   0.548   0.166   0.065  0.2432  0.5891 -0.2805
11SOL   HW1  66   0.574   0.183  -0.030 -2.2926  0.9422 -0.9647
11SOL   HW2  67   0.609   0.217   0.125  0.9580  1.5613 -1.7609
12SOL   OW   68   2.738   1.779   0.493  0.0775 -0.1508 -0.6415
12SOL   HW1  69   2.745   1.680   0.511 -2.0777 -0.4563 -1.2105
12SOL   HW2  70   2.764   1.829   0.576 -1.5608 -1.2993  0.6384
13SOL   OW   71   1.290   0.557   0.500  0.9540 -0.3140  0.3624
13SOL   HW1  72   1.276   0.520   0.591  1.1224  0.0935  0.5573
13SOL   HW2  73   1.224   0.518   0.437 -0.7401  1.1624  1.1470
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14SOL    OW   74   2.678  1.182   0.576  0.4895  0.1934 -0.1517
14SOL   HW1   75   2.647  1.249   0.509  1.2620  1.7565  0.9947
14SOL   HW2   76   2.711  1.229   0.658  1.5043 -1.5787  0.5138
15SOL    OW   77   2.022  1.106   1.046  0.0477 -0.0021  0.2861
15SOL   HW1   78   2.066  1.023   1.080  1.0761  0.0420 -0.8701
15SOL   HW2   79   2.073  1.186   1.077  1.6011  0.0048 -2.0730
16SOL    OW   80   1.806  3.114   2.120  0.3070 -0.2134 -0.1079
16SOL   HW1   81   1.736  3.065   2.068 -1.6644 -0.3077  2.4130
16SOL   HW2   82   1.889  3.122   2.065 -1.2987 -1.0209 -2.8629
17SOL    OW   83   1.354  1.726   1.289 -0.0898 -0.2622  0.1905
17SOL   HW1   84   1.280  1.723   1.221 -2.6176 -0.6272  2.7626
17SOL   HW2   85   1.383  1.632   1.310 -2.2048 -0.5094  2.4112
18SOL    OW   86   1.210  2.094   0.955  0.4635  0.5917  0.7022
18SOL   HW1   87   1.251  2.158   0.890 -0.6958 -0.9157 -1.6367
18SOL   HW2   88   1.119  2.126   0.981 -0.6163 -0.5388 -1.3872
19SOL    OW   89   1.210  3.096   0.215 -0.3228 -0.7937  0.2609
19SOL   HW1   90   1.116  3.062   0.216 -1.0613  1.0898  1.7415
19SOL   HW2   91   1.212  3.188   0.175  1.0711 -1.1643 -0.6148
20SOL    OW   92   1.318  2.400   1.299  0.0702 -0.4977  0.1412
20SOL   HW1   93   1.384  2.466   1.335 -0.1253  0.3467 -0.9933
20SOL   HW2   94   1.311  2.323   1.362  0.2927  0.5539  1.5074
21SOL    OW   95   2.481  3.015   1.450  0.1472  0.7923  0.0411
21SOL   HW1   96   2.525  3.028   1.539 -0.9838  0.1660  0.7190
21SOL   HW2   97   2.507  3.090   1.388 -0.1671  2.0147  1.3486
22SOL    OW   98   1.233  2.622   0.371 -0.0574 -0.0341 -0.0994
22SOL   HW1   99   1.257  2.719   0.374 -0.4157  0.1423 -1.9375
22SOL   HW2  100   1.134  2.611   0.382  0.1749 -0.3732  2.0803
23SOL    OW  101   2.501  1.319   0.861 -0.3579  0.2487  0.2241
23SOL   HW1  102   2.443  1.299   0.782 -2.1789  2.7686  0.7803
23SOL   HW2  103   2.533  1.414   0.856  1.7174 -0.3318  1.2215
24SOL    OW  104   0.031  0.708   0.894  0.2529 -0.3563  0.5118
24SOL   HW1  105   0.092  0.786   0.883 -1.0674  0.6324 -0.0713
24SOL   HW2  106  -0.055  0.738   0.936 -0.5041 -1.3819 -0.2434
25SOL    OW  107   0.264  1.893   1.739  0.4366 -0.4749  0.1874
25SOL   HW1  108   0.254  1.956   1.662 -1.0114  0.1665  0.8752
25SOL   HW2  109   0.358  1.896   1.773  0.8636 -0.1128 -0.9809
26SOL    OW  110   2.369  2.499   1.984  0.2397  0.0421 -0.5512
26SOL   HW1  111   2.305  2.551   1.927  0.2439 -1.1037 -1.6474
26SOL   HW2  112   2.447  2.469   1.929 -0.1840 -1.8468 -0.2082
27SOL    OW  113   0.603  0.609   1.101  0.6454  0.1564  0.4349
27SOL   HW1  114   0.651  0.654   1.176  0.6517  1.6345 -0.4263
27SOL   HW2  115   0.590  0.673   1.025 -0.6964 -0.8547 -0.2479
28SOL    OW  116   0.980  2.698   1.916  0.2965  0.3509 -0.0608
28SOL   HW1  117   1.034  2.673   1.996  1.6765  0.7363 -0.8348
28SOL   HW2  118   0.894  2.648   1.916  0.1117  0.6139  1.8424
29SOL    OW  119   0.068  0.417   1.075  0.3293  0.6099 -0.3223
29SOL   HW1  120   0.094  0.382   0.985 -1.4628 -1.7758 -0.0292
29SOL   HW2  121   0.130  0.380   1.145 -0.7471 -1.0269 -0.1720
30SOL    OW  122   0.543  2.830   1.794 -0.2415  0.1790 -0.1609
30SOL   HW1  123   0.629  2.869   1.826 -1.2494  0.8430  1.8983
30SOL   HW2  124   0.471  2.847   1.861 -2.3975  1.0764 -2.5165
31SOL    OW  125   2.086  0.690   1.909 -0.4729  0.0393  0.8900
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31SOL    HW1 126  1.997   0.716   1.946 -0.4994  0.0179  0.8412
31SOL    HW2 127  2.149   0.768   1.915 -0.9068  0.5179 -0.3949
32SOL     OW 128  2.144   2.444   1.466  0.3370 -0.1036 -0.5367
32SOL    HW1 129  2.087   2.525   1.455  0.5388 -0.0026 -0.8357
32SOL    HW2 130  2.240   2.467   1.448  0.7332  0.1285  1.5555
33SOL     OW 131  2.665   2.276   1.528  0.2933 -0.1467 -0.4594
33SOL    HW1 132  2.620   2.324   1.604  1.8568  5.0582 -2.3835
33SOL    HW2 133  2.762   2.266   1.549  0.6285  0.8284 -1.4630
34SOL     OW 134  1.510   0.692   1.290  0.1773  0.1102 -0.9151
34SOL    HW1 135  1.431   0.706   1.230  2.1039  1.7056 -3.2629
34SOL    HW2 136  1.586   0.655   1.238  1.1910 -0.9274  1.1726
35SOL     OW 137  1.327   0.990   0.251  0.3113 -0.6238 -0.1309
35SOL    HW1 138  1.227   0.990   0.254  0.3075 -0.2359 -0.2827
35SOL    HW2 139  1.358   0.988   0.156  0.4463 -0.1792 -0.0993
36SOL     OW 140  2.547   1.155   1.976 -0.1219  0.1299 -0.0220
36SOL    HW1 141  2.508   1.233   2.024  1.3142  1.6434 -1.1742
36SOL    HW2 142  2.516   1.070   2.018 -1.7778  1.3058  1.2434
37SOL     OW 143  1.794   2.139   1.231 -0.0137 -0.6677  0.1844
37SOL    HW1 144  1.779   2.045   1.202  0.7449 -0.8121  0.2315
37SOL    HW2 145  1.726   2.199   1.189 -0.2179 -1.1748 -0.2076
38SOL     OW 146  2.006   2.877   1.170  0.1507 -0.4765  0.7176
38SOL    HW1 147  2.086   2.875   1.230  2.0269  0.7698 -1.6100
38SOL    HW2 148  1.933   2.929   1.215  0.7714 -1.1719  2.6647
39SOL     OW 149  1.566   2.626   0.996  0.2330 -0.2547  0.4631
39SOL    HW1 150  1.541   2.626   0.899  1.1246 -2.0798  0.2025
39SOL    HW2 151  1.650   2.679   1.009  0.3099 -0.3027  0.1747
40SOL     OW 152  2.970   0.855   1.040  0.0218  0.0910 -0.6090
40SOL    HW1 153  2.993   0.949   1.012 -0.9044  1.2319  2.1534
40SOL    HW2 154  2.871   0.847   1.050 -0.0868 -1.7709 -2.4589
41SOL     OW 155  2.552   1.974   0.415  0.2659  0.0426 -0.2347
41SOL    HW1 156  2.618   1.905   0.442 -0.4763 -0.4849  0.2740
41SOL    HW2 157  2.581   2.063   0.449  0.2952 -0.3208  0.7230
42SOL     OW 158  0.482   1.455   1.127 -0.0166  0.0963  0.0355
42SOL    HW1 159  0.426   1.496   1.056 -1.6768 -0.4000  1.0004
42SOL    HW2 160  0.533   1.378   1.089  0.5449  0.9548 -1.0025
43SOL     OW 161  1.527   1.749   0.976  0.1598  0.2751 -0.0045
43SOL    HW1 162  1.506   1.671   1.035 -1.9586  0.6895 -0.1284
43SOL    HW2 163  1.527   1.833   1.030 -1.1747  0.5806 -0.4275
44SOL     OW 164  0.464   1.728   0.850 -0.6278  0.4666 -0.1458
44SOL    HW1 165  0.417   1.640   0.861  0.4572 -0.3555 -1.7344
44SOL    HW2 166  0.470   1.773   0.939 -0.8524 -1.2496  0.7930
45SOL     OW 167  2.517   2.120   2.097 -0.2401 -0.3225 -0.6246
45SOL    HW1 168  2.599   2.168   2.065  0.2391 -0.0805  0.8949
45SOL    HW2 169  2.440   2.184   2.099  0.2443  0.2644  0.7595
46SOL     OW 170  2.714   2.678   2.007 -0.0328  0.4651  0.3979
46SOL    HW1 171  2.698   2.612   2.081  0.0660 -0.2701 -0.2322
46SOL    HW2 172  2.768   2.754   2.042  1.4600 -0.6924  0.6859
47SOL     OW 173  0.789   3.032   1.154 -0.4860  0.1094 -0.2790
47SOL    HW1 174  0.832   2.954   1.199  0.8380  1.1501  0.3300
47SOL    HW2 175  0.742   3.088   1.221  1.6642  1.7787 -0.0410
48SOL     OW 176  1.058   0.956   1.003  0.2728  0.1470 -0.1637
48SOL    HW1 177  1.154   0.957   0.973 -0.3535 -1.4266 -2.4823
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48SOL   HW2 178   1.032   0.863   1.027 -0.4733  0.7084  1.2945
49SOL   OW  179   2.904   1.910   1.427 -0.3122 -0.1513  0.7375
49SOL   HW1 180   2.920   1.815   1.453 -2.5003 -0.7630  0.1307
49SOL   HW2 181   2.911   1.919   1.328  0.6114  0.5078  0.8505
50SOL   OW  182   2.211   1.790   2.033 -0.1261  0.0973  0.2785
50SOL   HW1 183   2.309   1.808   2.034 -0.1399  0.2027  1.6715
50SOL   HW2 184   2.170   1.834   1.953  0.9210  0.2590 -0.1793
51SOL   OW  185   1.546   2.440   1.691 -0.1208  0.2915 -0.2293
51SOL   HW1 186   1.587   2.468   1.778  1.4742  0.1304 -0.9080
51SOL   HW2 187   1.532   2.341   1.692  0.5003  0.2016 -0.4043
52SOL   OW  188   0.009   2.823   1.725 -0.3992 -0.8272  0.0302
52SOL   HW1 189  -0.040   2.795   1.808  0.7077 -1.5897  0.4359
52SOL   HW2 190   0.096   2.864   1.749 -0.0274 -1.1260 -0.7617
53SOL   OW  191   0.773   0.647   0.204 -0.5747 -0.0073  0.1559
53SOL   HW1 192   0.745   0.672   0.112 -0.3351 -2.6789 -0.7385
53SOL   HW2 193   0.693   0.622   0.258 -0.6703  1.0751  0.5261
54SOL   OW  194   2.421   0.993   1.644  0.5333  0.4423  0.5237
54SOL   HW1 195   2.496   0.963   1.704 -0.6298 -2.5789  0.6725
54SOL   HW2 196   2.412   0.929   1.568 -1.4235  1.1308  0.1188
55SOL   OW  197   2.125   0.891   1.114  0.3372  0.0661 -0.5925
55SOL   HW1 198   2.031   0.864   1.089 -0.0793  1.0362 -0.1289
55SOL   HW2 199   2.183   0.810   1.116 -0.6067 -0.6292 -0.3981
56SOL   OW  200   2.361   1.099   0.433 -0.0059 -0.2416  0.1274
56SOL   HW1 201   2.373   1.136   0.525  2.7845  0.2109 -0.3255
56SOL   HW2 202   2.324   1.171   0.374  0.2567  0.1366  0.4168
57SOL   OW  203   2.016   0.983   2.107  0.1546  0.7697 -0.0170
57SOL   HW1 204   2.107   0.940   2.108 -0.4971 -0.7091 -1.2917
57SOL   HW2 205   2.004   1.033   2.021 -0.6599 -0.0174 -0.3715
58SOL   OW  206   1.022   2.840   1.215 -0.3103 -0.1533 -0.0919
58SOL   HW1 207   1.058   2.899   1.142  1.6115  1.4920  2.0415
58SOL   HW2 208   0.999   2.751   1.177  1.3856  0.3449 -2.5639
59SOL   OW  209   2.963   2.997   0.956 -0.2837 -0.2822  0.0616
59SOL   HW1 210   2.952   2.923   1.022  2.3683 -1.1076 -0.2888
59SOL   HW2 211   3.060   3.020   0.948 -0.5737  0.3034 -2.9688
60SOL   OW  212   1.621   2.627   0.729  0.4182 -0.0047  0.3175
60SOL   HW1 213   1.634   2.530   0.748  1.9215  0.1497  0.2069
60SOL   HW2 214   1.708   2.675   0.741  0.4202  0.8704 -2.4676
61SOL   OW  215   2.754   2.448   0.554  0.0418  0.1971  0.6375
61SOL   HW1 216   2.683   2.479   0.618 -0.1643 -0.5224  0.7633
61SOL   HW2 217   2.787   2.526   0.500 -0.9579  0.5004  0.4591
62SOL   OW  218   1.209   2.916   1.440 -0.4840  0.2788 -0.6704
62SOL   HW1 219   1.149   2.871   1.374  0.3716 -0.9411 -0.6359
62SOL   HW2 220   1.249   2.848   1.501  0.9779  1.0516 -0.7240
63SOL   OW  221   1.804   1.516   1.213 -0.1193  0.3814  0.4593
63SOL   HW1 222   1.853   1.440   1.255  0.3948  0.5317  0.1371
63SOL   HW2 223   1.771   1.488   1.123  1.2627  0.9617 -0.2566
64SOL   OW  224   2.021   2.487   0.683 -0.1945 -0.4708 -0.4804
64SOL   HW1 225   2.095   2.555   0.681 -0.4873 -0.1567 -0.8328
64SOL   HW2 226   2.041   2.419   0.754 -0.1603  0.2834  0.2600
65SOL   OW  227   1.310   2.209   1.478 -0.5461 -0.2833  1.0939
65SOL   HW1 228   1.284   2.119   1.444 -0.7105 -0.0769  0.6677
65SOL   HW2 229   1.387   2.199   1.542 -0.1926 -0.6701  0.6222
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66SOL    OW  230   0.495   3.126   2.000  0.0150  0.0503 -0.2330
66SOL   HW1  231   0.533   3.146   1.909 -0.5208 -0.2394 -0.5226
66SOL   HW2  232   0.408   3.079   1.990  1.5609 -3.2127  0.4083
67SOL    OW  233   3.105   1.457   1.932  0.7531 -0.0464 -0.3379
67SOL   HW1  234   3.051   1.540   1.941  0.5049 -0.2130 -0.2834
67SOL   HW2  235   3.060   1.382   1.981  0.9053 -0.2446 -0.4998
68SOL    OW  236   0.822   2.348   0.988 -0.2874 -0.8003  0.0030
68SOL   HW1  237   0.885   2.424   1.002  0.6989 -1.3164 -1.3644
68SOL   HW2  238   0.761   2.340   1.066  0.2972  0.7172  0.6477
69SOL    OW  239   2.266   0.464   1.887 -0.1740  0.1357 -0.1800
69SOL   HW1  240   2.189   0.527   1.901  0.3760  0.6171  0.8035
69SOL   HW2  241   2.320   0.495   1.808 -1.2449 -0.4972 -1.2048
70SOL    OW  242   0.600   1.550   1.374 -0.2141  0.4514 -0.5861
70SOL   HW1  243   0.568   1.547   1.279 -1.6336 -0.5643 -0.1076
70SOL   HW2  244   0.582   1.462   1.417 -0.5063  1.2190  0.9065
71SOL    OW  245   2.031   1.566   0.071 -0.0634  0.0690  0.6012
71SOL   HW1  246   2.051   1.472   0.096  1.2139  0.1084 -0.1832
71SOL   HW2  247   2.045   1.579  -0.027 -1.5414  0.7634  0.4485
72SOL    OW  248   1.583   1.843   0.282  0.1193 -0.1598  0.3961
72SOL   HW1  249   1.643   1.795   0.345  0.5048  1.7294  1.5540
72SOL   HW2  250   1.488   1.831   0.309  0.1360 -1.0559  0.0793
73SOL    OW  251   1.834   1.697   0.861  0.2430  0.1663  0.3684
73SOL   HW1  252   1.740   1.712   0.830  0.3174  0.3668  0.2362
73SOL   HW2  253   1.890   1.669   0.783  0.3082  0.1109  0.4352
74SOL    OW  254   0.804   1.843   2.077  0.1811  0.2308  0.1068
74SOL   HW1  255   0.708   1.813   2.082 -0.3759  1.7582 -0.7396
74SOL   HW2  256   0.826   1.895   2.160 -0.1583  1.0157 -0.2804
75SOL    OW  257   0.332   1.778   0.612  0.2879 -0.1634  0.2097
75SOL   HW1  258   0.390   1.771   0.693  0.2958  1.7028  0.4129
75SOL   HW2  259   0.252   1.718   0.623  1.1880 -1.2991  0.7669
76SOL    OW  260   0.413   1.325   2.083  0.2500 -0.5194  0.0058
76SOL   HW1  261   0.429   1.282   2.172 -3.2282 -1.7729  0.1612
76SOL   HW2  262   0.350   1.268   2.030  0.1127  1.5565 -2.1869
77SOL    OW  263   0.884   0.319   2.185 -0.3170  0.0810 -0.7959
77SOL   HW1  264   0.830   0.299   2.103  0.4103  1.2115 -1.5743
77SOL   HW2  265   0.834   0.382   2.244 -0.1685  0.5281 -1.1474
78SOL    OW  266   1.528   0.971   1.363 -0.2575  0.4312  0.0689
78SOL   HW1  267   1.620   1.006   1.380 -0.1280  0.6461 -0.9997
78SOL   HW2  268   1.531   0.871   1.365 -0.1796  0.4389  0.8675
79SOL    OW  269   0.325   0.956   2.108  0.3013 -0.0356 -0.5274
79SOL   HW1  270   0.232   0.920   2.102 -0.0660  0.5453  1.2785
79SOL   HW2  271   0.336   1.028   2.039 -0.6771  0.1061 -0.5571
80SOL    OW  272   3.059   0.470   0.745 -0.3903 -0.1427  0.0585
80SOL   HW1  273   3.108   0.550   0.778  0.0866  0.0131 -0.9962
80SOL   HW2  274   2.961   0.490   0.742 -0.2517  0.4815 -0.4307
81SOL    OW  275   0.252   0.407   0.574 -0.7413 -0.9980 -0.6221
81SOL   HW1  276   0.326   0.432   0.636 -2.8413 -0.2615  1.7957
81SOL   HW2  277   0.241   0.307   0.575 -0.0616 -1.0764 -0.6518
82SOL    OW  278   2.515   0.081   2.040  0.0167 -0.3333  0.1291
82SOL   HW1  279   2.454   0.099   1.963 -0.3046 -0.3765  0.3726
82SOL   HW2  280   2.574   0.160   2.055  2.0348 -1.3552 -1.9296
83SOL    OW  281   0.474   3.060   0.209 -0.1551 -0.0032 -0.3193
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83SOL    HW1 282  0.507  3.146  0.169  1.7486 -0.2068  0.7197
83SOL    HW2 283  0.394  3.028  0.158 -0.7610  2.2479 -0.8785
84SOL     OW 284  1.263  2.733  1.627 -0.0730 -0.1664 -0.1815
84SOL    HW1 285  1.287  2.797  1.700 -1.2732 -0.5906  0.6150
84SOL    HW2 286  1.261  2.640  1.665  0.5932 -0.5585 -1.0773
85SOL     OW 287  1.834  2.497  1.409  0.6072  0.3278 -0.4952
85SOL    HW1 288  1.847  2.410  1.458 -1.3951  0.3602  0.1958
85SOL    HW2 289  1.875  2.571  1.462  0.7429  0.0180 -0.1612
86SOL     OW 290  0.739  2.625  0.940  0.1314 -0.4335  0.0948
86SOL    HW1 291  0.714  2.536  0.978 -1.8121  0.2031  0.4270
86SOL    HW2 292  0.734  2.694  1.012  0.0235  0.1999 -0.5113
87SOL     OW 293  1.540  0.175  0.032 -0.0215 -0.2792 -0.0033
87SOL    HW1 294  1.566  0.128  0.116 -0.0866  1.4925  1.0701
87SOL    HW2 295  1.442  0.163  0.016  0.0035 -0.6798  0.1438
88SOL     OW 296  1.335  1.098  0.636  0.0908  0.3846  0.5000
88SOL    HW1 297  1.431  1.109  0.659  0.1447  3.3800 -0.6715
88SOL    HW2 298  1.326  1.034  0.559  1.3576  1.4313 -0.5516
89SOL     OW 299  0.572  2.182  1.809  0.0196 -0.5783 -0.1811
89SOL    HW1 300  0.580  2.084  1.829 -0.0688 -0.4246  0.6183
89SOL    HW2 301  0.653  2.229  1.844 -0.5750 -0.1703  0.6620
90SOL     OW 302  2.015  2.772  0.101 -0.4118 -0.1029  0.0908
90SOL    HW1 303  1.970  2.684  0.115 -1.6966  0.6537  0.9406
90SOL    HW2 304  2.001  2.829  0.182 -0.3144  1.1935 -0.7856
91SOL     OW 305  2.049  1.922  0.984 -0.5248  0.4413  0.2610
91SOL    HW1 306  1.952  1.919  1.008 -0.3090  0.0595  1.1364
91SOL    HW2 307  2.059  1.933  0.886 -1.4593 -0.8526 -0.0032
92SOL     OW 308  2.993  2.294  0.606  0.7138  0.0365 -0.3594
92SOL    HW1 309  2.900  2.329  0.600  0.4796  0.5089  3.4353
92SOL    HW2 310  2.992  2.195  0.593 -0.3179  0.0283 -0.3144
93SOL     OW 311  1.921  1.999  0.310  0.2570  0.1832 -0.0714
93SOL    HW1 312  1.921  2.028  0.214 -0.2113 -0.6034 -0.3237
93SOL    HW2 313  1.873  1.911  0.317  1.4509 -0.4217  0.6857
94SOL     OW 314  2.336  2.880  0.304  0.7228  0.0424 -0.6763
94SOL    HW1 315  2.365  2.851  0.213  1.1508 -2.2468  0.1202
94SOL    HW2 316  2.398  2.841  0.373 -0.9662 -0.3143  0.7327
95SOL     OW 317  2.791  0.456  1.931 -1.0276 -0.2020 -0.2198
95SOL    HW1 318  2.758  0.410  2.013 -1.0648  1.9795  1.0589
95SOL    HW2 319  2.753  0.549  1.927  0.9433  0.6167 -1.3764
96SOL     OW 320  2.706  0.343  1.712  0.3628  0.6089  0.7699
96SOL    HW1 321  2.650  0.413  1.667 -1.3551 -0.6608  0.8388
96SOL    HW2 322  2.741  0.379  1.798 -0.0414  1.5602  0.5545
97SOL     OW 323  0.899  2.352  0.119  0.2349  0.3366 -0.2006
97SOL    HW1 324  0.805  2.354  0.085  0.2432 -3.0545 -0.6944
97SOL    HW2 325  0.899  2.335  0.217  0.3800  1.3164 -0.0123
98SOL     OW 326  0.379  2.856  0.852 -0.1135 -0.6686  0.1992
98SOL    HW1 327  0.449  2.915  0.812 -1.1867  0.0101 -0.7314
98SOL    HW2 328  0.351  2.787  0.784 -1.0094 -0.3409  0.2282
99SOL     OW 329  0.422  0.286  2.058  0.0537  0.4214  0.5728
99SOL    HW1 330  0.376  0.203  2.091 -0.2776  0.2669 -0.2513
99SOL    HW2 331  0.388  0.365  2.108 -0.6840  0.2383  0.3694
100SOL    OW 332  1.570  1.973  2.124  0.7524 -0.7931  0.4487
100SOL   HW1 333  1.500  2.035  2.088 -0.9326 -2.1342  1.3126
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100SOL   HW2 334   1.601   1.912   2.051 -0.8059 -1.8233  0.6149
101SOL    OW 335   3.042   2.309   1.329  0.2272 -0.1961 -0.0558
101SOL   HW1 336   2.951   2.328   1.293 -1.0003 -2.8870  1.3554
101SOL   HW2 337   3.106   2.296   1.253 -1.0794 -0.5895 -1.1198
102SOL    OW 338   2.528   0.886   2.069 -0.6458 -0.2486  0.1848
102SOL   HW1 339   2.544   0.874   2.167  0.4601 -0.9051 -0.0674
102SOL   HW2 340   2.579   0.818   2.018  0.9009  1.6970 -1.0001
103SOL    OW 341   1.611   2.832   0.136  0.2805  0.4630  0.2275
103SOL   HW1 342   1.669   2.761   0.095  0.5030  0.3426  0.7513
103SOL   HW2 343   1.584   2.804   0.228  1.1665  1.5056  0.8163
104SOL    OW 344   2.051   3.140   0.023  0.0048  0.3020  0.5329
104SOL   HW1 345   2.000   3.165   0.106 -0.2778  1.8070 -0.0612
104SOL   HW2 346   2.021   3.050  -0.008 -1.7066  0.7722  0.6884
105SOL    OW 347   2.670   1.074   0.879 -0.0104 -0.3882 -0.3267
105SOL   HW1 348   2.652   1.173   0.880  0.8065 -0.2330  0.5131
105SOL   HW2 349   2.723   1.051   0.798 -0.8166 -0.2620 -0.9008
106SOL    OW 350   1.973   0.460   1.221 -0.0864  0.1120 -0.1954
106SOL   HW1 351   2.042   0.507   1.276  0.2721  1.2817 -1.5764
106SOL   HW2 352   2.005   0.453   1.126 -1.0630 -1.0509 -0.4654
107SOL    OW 353   2.898   1.613   1.951  0.1354 -0.2211 -0.0200
107SOL   HW1 354   2.866   1.694   1.902 -0.1457 -1.9971 -2.9526
107SOL   HW2 355   2.872   1.621   2.048 -0.0560  3.0331 -0.2355
108SOL    OW 356   2.269   2.779   0.024  0.2647 -0.3631 -0.0795
108SOL   HW1 357   2.262   2.727  -0.061 -1.6326 -0.0471 -0.1542
108SOL   HW2 358   2.189   2.762   0.081 -0.1114  1.9542  0.1914
109SOL    OW 359   0.009   0.962   0.567  0.5902  0.3974  0.8546
109SOL   HW1 360   0.058   0.875   0.571 -0.9895 -0.4744  2.4984
109SOL   HW2 361   0.059   1.030   0.621  0.9356  0.0479  0.9811
110SOL    OW 362   1.450   2.964   0.700  0.6310 -0.0604  0.2827
110SOL   HW1 363   1.433   2.892   0.632 -1.9794  0.5159  0.2012
110SOL   HW2 364   1.459   2.922   0.790  0.6436 -0.6108  0.0345
111SOL    OW 365   1.695   2.920   1.813  0.3829 -0.4508  0.0817
111SOL   HW1 366   1.794   2.914   1.824  0.2119 -0.4099  1.9561
111SOL   HW2 367   1.658   2.829   1.794  0.6770 -0.6484  0.4384
112SOL    OW 368   1.628   0.369   0.210 -0.6129 -0.4214  0.1331
112SOL   HW1 369   1.585   0.335   0.127 -0.4974 -0.1816 -0.0284
112SOL   HW2 370   1.721   0.335   0.216 -0.9554 -1.2660  0.6890
113SOL    OW 371   1.628   3.082   1.009  0.5485  0.5865  0.4367
113SOL   HW1 372   1.596   3.162   1.059  0.4196  1.2786 -0.7045
113SOL   HW2 373   1.634   3.104   0.911 -1.8854 -1.5003 -0.3077
114SOL    OW 374   0.227   1.539   1.981 -0.0152  0.1647  0.5427
114SOL   HW1 375   0.264   1.490   2.060 -0.1764 -1.2376 -0.2332
114SOL   HW2 376   0.137   1.503   1.959  1.6696 -2.5086 -2.8573
115SOL    OW 377   2.293   2.279   1.695  0.0172 -0.3272  0.1305
115SOL   HW1 378   2.249   2.246   1.611  0.3946  1.7041 -0.9174
115SOL   HW2 379   2.250   2.364   1.724  1.5063  0.2983  0.5916
116SOL    OW 380   2.918   0.354   1.088 -0.0010  0.3189  0.5807
116SOL   HW1 381   2.896   0.292   1.012  0.1223  0.8160  0.1297
116SOL   HW2 382   3.000   0.407   1.065 -0.0452  0.5744  1.0042
117SOL    OW 383   0.100   1.955   0.896 -0.0149  0.1717 -0.2680
117SOL   HW1 384   0.145   2.000   0.973 -2.6277  1.3452  0.7013
117SOL   HW2 385   0.152   1.972   0.812  2.1048  0.1105  0.9738
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118SOL    OW  386  2.741  1.105  1.431 -0.0258 -0.0468 -0.0069
118SOL    HW1 387  2.696  1.146  1.510  1.1277 -0.7341  1.0304
118SOL    HW2 388  2.672  1.067  1.369 -0.9368  0.5363  0.6309
119SOL    OW  389  2.596  1.626  1.578 -0.1338  0.7552  0.2607
119SOL    HW1 390  2.546  1.684  1.514 -1.9545 -0.1741  0.7448
119SOL    HW2 391  2.693  1.626  1.556 -0.3755  2.4077 -0.9359
120SOL    OW  392  2.423  0.282  1.017 -0.2992  0.2214 -0.3448
120SOL    HW1 393  2.482  0.237  0.950 -0.0852  0.2160 -0.1539
120SOL    HW2 394  2.358  0.341  0.969  1.5552  2.3116 -0.4832
121SOL    OW  395  1.729  0.586  1.174 -0.3051 -0.2996 -0.4291
121SOL    HW1 396  1.790  0.530  1.229 -1.5178 -0.2904  0.9949
121SOL    HW2 397  1.749  0.683  1.190 -1.4842 -0.2621  1.0705
122SOL    OW  398  1.948  0.971  1.577  0.0474  0.7582  0.0883
122SOL    HW1 399  1.965  0.881  1.536  0.3708  1.3204 -1.0514
122SOL    HW2 400  2.034  1.021  1.581 -0.1442  1.0453  0.6732
123SOL    OW  401  0.259  2.316  0.500  0.3095  0.0164  0.2493
123SOL    HW1 402  0.180  2.290  0.555  0.3283  2.0238  1.3142
123SOL    HW2 403  0.228  2.342  0.408 -0.2837  0.7459  0.6431
124SOL    OW  404  3.035  1.243  1.198 -0.1162 -0.0903  0.2266
124SOL    HW1 405  3.134  1.255  1.191 -0.0382 -0.7785  0.1003
124SOL    HW2 406  3.009  1.231  1.294 -0.2926  1.7900  0.4537
125SOL    OW  407  3.041  1.761  0.712  0.3593 -0.3574 -0.5929
125SOL    HW1 408  3.018  1.758  0.615 -0.3526  0.1708 -0.4501
125SOL    HW2 409  3.038  1.856  0.744  2.6339 -0.2554 -0.5168
126SOL    OW  410  0.233  3.001  0.118 -0.0442 -0.1784 -0.6008
126SOL    HW1 411  0.205  2.933  0.050 -2.3986  0.3895 -0.2907
126SOL    HW2 412  0.184  2.985  0.204  1.0312  0.6049  0.1937
127SOL    OW  413  0.315  1.152  1.060  0.4553 -0.0910  0.4023
127SOL    HW1 414  0.275  1.064  1.088  0.4198  0.2450  1.4629
127SOL    HW2 415  0.355  1.143  0.969  0.7013 -1.2943  0.6055
128SOL    OW  416  0.815  2.731  1.441  0.1745  0.1312  0.6963
128SOL    HW1 417  0.861  2.818  1.425  0.9793 -0.4331 -0.1648
128SOL    HW2 418  0.870  2.675  1.503 -0.5119  0.3444  1.5367
129SOL    OW  419  0.695  0.999  1.170 -0.7356  0.0484 -0.1264
129SOL    HW1 420  0.787  1.026  1.198 -1.0317  0.4998  0.4298
129SOL    HW2 421  0.683  0.901  1.185 -1.0795  0.3735  1.9347
130SOL    OW  422  1.620  2.287  2.139  0.6381 -0.3946  0.1885
130SOL    HW1 423  1.630  2.360  2.206 -0.4846  0.4040 -0.4792
130SOL    HW2 424  1.691  2.218  2.153  2.0370  1.0640  0.5107
131SOL    OW  425  2.941  1.686  0.972 -0.0068  0.6269 -0.3112
131SOL    HW1 426  3.007  1.695  0.898  0.4650  2.3162  0.2646
131SOL    HW2 427  2.857  1.734  0.947 -0.4552 -0.1882 -0.3997
132SOL    OW  428  2.602  0.072  1.270  0.3061  0.8115  0.1112
132SOL    HW1 429  2.697  0.102  1.275 -0.2187  2.7196 -0.3333
132SOL    HW2 430  2.588  0.020  1.186  1.0960 -0.1533  0.5512
133SOL    OW  431  0.864  1.597  0.873  0.1318  0.2437 -0.1198
133SOL    HW1 432  0.949  1.615  0.825 -0.8801  0.4699 -1.9327
133SOL    HW2 433  0.830  1.681  0.916  0.9769  0.0693  0.9284
134SOL    OW  434  3.017  3.058  0.209 -0.9196  0.2335  0.4375
134SOL    HW1 435  2.977  3.121  0.142 -2.0252  0.7661  1.5660
134SOL    HW2 436  2.964  2.973  0.212  0.2371 -0.5614 -0.6756
135SOL    OW  437  3.095  2.013  0.531 -0.1631 -0.0495  0.4511
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135SOL    HW1  438   3.053   1.927   0.500 -2.6877  0.8124  1.2368
135SOL    HW2  439   3.191   1.996   0.555 -1.0220 -3.1141  2.2905
136SOL     OW  440   0.730   2.586   1.888 -0.2087  0.1725 -0.2447
136SOL    HW1  441   0.721   2.525   1.966  1.5055  0.4488  0.2150
136SOL    HW2  442   0.640   2.626   1.866 -0.8631 -0.5087  1.0694
137SOL     OW  443   2.336   1.294   0.641  0.4745  0.1690 -0.0845
137SOL    HW1  444   2.264   1.305   0.709  0.0367  2.7972 -0.8462
137SOL    HW2  445   2.357   1.383   0.600  0.2241 -1.3197 -3.8915
138SOL     OW  446   1.004   1.184   0.211  0.1241 -0.3551 -0.1997
138SOL    HW1  447   1.058   1.238   0.276 -1.1544 -0.2204  0.7986
138SOL    HW2  448   0.907   1.204   0.225 -0.1704 -0.0641 -2.4267
139SOL     OW  449   1.144   1.829   1.117  0.3228 -0.3363  0.1287
139SOL    HW1  450   1.145   1.897   1.191  0.6448 -0.2515  0.0499
139SOL    HW2  451   1.144   1.875   1.029  2.1983 -0.3984  0.0448
140SOL     OW  452   1.552   0.219   0.633 -0.3774 -0.5527  0.3509
140SOL    HW1  453   1.572   0.307   0.589 -1.3416 -0.3354  0.3311
140SOL    HW2  454   1.494   0.164   0.572 -0.0236 -1.0833  0.4870
141SOL     OW  455   0.808   1.852   1.008  0.0169  0.1040 -0.0959
141SOL    HW1  456   0.724   1.900   0.983 -0.2552 -0.4450 -0.2578
141SOL    HW2  457   0.796   1.806   1.096  0.5884  1.0832  0.5077
142SOL     OW  458   0.459   2.174   0.704  0.0230  0.4199  0.1148
142SOL    HW1  459   0.547   2.206   0.669  0.5233 -0.0004  0.9440
142SOL    HW2  460   0.409   2.250   0.744  0.3838  0.5094  0.4011
143SOL     OW  461   2.252   1.321   0.332 -0.1169 -0.0298  0.0896
143SOL    HW1  462   2.304   1.406   0.336 -1.3553  0.7260  0.6706
143SOL    HW2  463   2.183   1.328   0.260 -0.4839 -0.3984  0.4050
144SOL     OW  464   2.708   2.898   0.842 -0.1298 -0.1212  0.0728
144SOL    HW1  465   2.776   2.947   0.896 -1.4713  0.2228  1.5417
144SOL    HW2  466   2.744   2.881   0.750  2.3880 -1.0820  1.1565
145SOL     OW  467   1.712   1.437   0.943  0.0429 -0.3787 -0.2061
145SOL    HW1  468   1.615   1.439   0.970 -0.5994  0.9536 -2.3378
145SOL    HW2  469   1.736   1.525   0.901  1.9147 -1.0711 -0.6737
146SOL     OW  470   1.892   2.311   1.646  0.2967  0.9378  0.2315
146SOL    HW1  471   1.862   2.265   1.729  0.8948  1.1076  0.5402
146SOL    HW2  472   1.965   2.376   1.667  0.7967  0.6248 -0.4979
147SOL     OW  473   2.573   0.924   0.520  0.2189 -0.0523 -0.0613
147SOL    HW1  474   2.478   0.935   0.489  0.4613  0.1056 -0.7800
147SOL    HW2  475   2.615   1.014   0.530  0.5910 -0.1479 -0.7244
148SOL     OW  476   0.294   2.217   1.749 -0.2952  0.6305  0.3790
148SOL    HW1  477   0.293   2.188   1.653 -2.9065 -0.0679  0.5558
148SOL    HW2  478   0.385   2.200   1.788  0.8495  0.9915 -1.9444
149SOL     OW  479   2.144   0.496   0.180  0.2738 -0.4537  0.1073
149SOL    HW1  480   2.158   0.553   0.260  1.7670 -0.6087 -0.0230
149SOL    HW2  481   2.232   0.463   0.146 -0.5350 -2.8732  0.2026
150SOL     OW  482   2.723   1.809   0.883  0.2692  0.2247 -0.2634
150SOL    HW1  483   2.652   1.835   0.947 -0.5772 -1.4262 -0.4943
150SOL    HW2  484   2.731   1.880   0.812 -1.6166  0.1292 -0.6229
151SOL     OW  485   1.196   2.641   0.808 -0.1827 -0.5643  0.0626
151SOL    HW1  486   1.252   2.657   0.889 -0.2270  0.4800 -0.0886
151SOL    HW2  487   1.254   2.641   0.727 -0.2356 -0.7715  0.0262
152SOL     OW  488   0.534   1.803   1.120  0.1122  1.3430  0.5838
152SOL    HW1  489   0.501   1.884   1.168  1.8623  1.4385  1.7259
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152SOL   HW2 490   0.565   1.734   1.186 -0.9573 -0.1243 -0.3706
153SOL    OW 491   2.787   0.516   0.774  0.2695  0.1581  0.8017
153SOL   HW1 492   2.707   0.505   0.832 -0.2286  1.1083  0.3180
153SOL   HW2 493   2.788   0.608   0.736  0.6070 -0.4211 -0.6645
154SOL    OW 494   2.508   1.632   1.054  0.1420 -0.2411 -0.3527
154SOL   HW1 495   2.538   1.586   0.970 -0.6418 -2.3723  0.4892
154SOL   HW2 496   2.583   1.634   1.119  0.4794  0.6168 -0.7509
155SOL    OW 497   2.407   2.646   1.673  0.3502 -0.4464 -0.6826
155SOL   HW1 498   2.411   2.581   1.596 -0.5730  0.2562 -1.3402
155SOL   HW2 499   2.364   2.731   1.643 -0.1966 -0.2228  0.6713
156SOL    OW 500   2.390   0.970   0.032 -0.6006  0.6508 -0.1921
156SOL   HW1 501   2.343   0.899  -0.020  2.5411 -1.3252 -0.6212
156SOL   HW2 502   2.370   0.959   0.129 -1.4914  0.2736 -0.4100
157SOL    OW 503   0.843   1.338   0.827  0.1149 -0.0778 -0.4484
157SOL   HW1 504   0.825   1.436   0.842  1.2404 -0.0462  0.9020
157SOL   HW2 505   0.855   1.321   0.730 -0.8062  0.9954 -0.7724
158SOL    OW 506   1.122   0.922  -0.017 -0.2736  0.2359 -0.0913
158SOL   HW1 507   1.088   0.910   0.077 -0.0499  0.6670  0.0486
158SOL   HW2 508   1.222   0.929  -0.014 -0.0948 -1.5599 -0.5455
159SOL    OW 509   0.476   1.125   1.286 -0.1535 -0.0635  0.5756
159SOL   HW1 510   0.547   1.076   1.237 -1.2870 -4.8828  3.1508
159SOL   HW2 511   0.406   1.157   1.221  2.1534  1.0785 -1.5169
160SOL    OW 512   1.550   2.851   0.430 -0.1212  0.3277  0.3427
160SOL   HW1 513   1.546   2.752   0.417  0.4654  0.2397  0.7521
160SOL   HW2 514   1.627   2.873   0.491  0.3918  1.1152 -0.5610
161SOL    OW 515   1.044   0.112   1.820 -0.3316  0.0168 -0.2072
161SOL   HW1 516   1.091   0.199   1.833 -0.9744  0.5572 -1.3841
161SOL   HW2 517   0.953   0.128   1.780 -0.0961 -1.2404 -1.3256
162SOL    OW 518   1.759   1.974   0.591 -0.2845 -0.4517  0.1732
162SOL   HW1 519   1.725   2.043   0.527 -1.0345 -0.0844  0.9523
162SOL   HW2 520   1.726   1.995   0.683  1.0730 -0.7713  0.7497
163SOL    OW 521   0.476   0.462   0.730  0.0059 -0.8331  0.4541
163SOL   HW1 522   0.439   0.454   0.823 -0.1011 -0.7294  0.4192
163SOL   HW2 523   0.548   0.393   0.718 -1.5422 -2.4315 -0.1400
164SOL    OW 524   0.738   0.060   1.806  0.0092  0.4053 -0.3043
164SOL   HW1 525   0.778  -0.028   1.832  1.1530  0.9668 -0.0734
164SOL   HW2 526   0.687   0.049   1.720  1.4926 -0.1652 -1.1599
165SOL    OW 527   0.559   3.096   0.927 -0.1949  0.4252 -0.3469
165SOL   HW1 528   0.572   3.073   1.024 -0.1168 -1.2793 -0.7465
165SOL   HW2 529   0.646   3.126   0.888 -0.1329  0.6934 -0.0161
166SOL    OW 530   1.903   1.329   1.885 -0.2162 -0.0640 -0.2650
166SOL   HW1 531   1.936   1.238   1.861 -2.3028 -1.1526  0.7969
166SOL   HW2 532   1.957   1.365   1.961 -0.8661 -1.4809  0.9281
167SOL    OW 533   1.438   2.684   2.188 -0.4141 -0.2633 -0.2162
167SOL   HW1 534   1.438   2.721   2.095 -0.3967  0.0235 -0.1045
167SOL   HW2 535   1.441   2.760   2.253  0.8382 -0.4889  0.0155
168SOL    OW 536   1.816   1.165   0.846  0.7363 -0.2451  0.1817
168SOL   HW1 537   1.868   1.121   0.919 -0.2172 -1.1851  0.3126
168SOL   HW2 538   1.794   1.259   0.873  0.9256 -0.3840  0.8346
169SOL    OW 539   2.465   1.860   2.036  0.0111  0.2238 -0.7682
169SOL   HW1 540   2.519   1.813   1.966 -0.2635  1.1826 -1.6477
169SOL   HW2 541   2.491   1.957   2.038 -2.2998  0.9322 -1.8709
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170SOL    OW  542   2.368   0.970   0.808 -0.3269  0.3186  0.0423
170SOL    HW1 543   2.426   1.038   0.855 -0.6266  1.1327 -0.7296
170SOL    HW2 544   2.275   1.006   0.802 -0.6956 -0.5576  0.3949
171SOL    OW  545   1.137   1.423   0.237  0.0973 -0.6171  0.2693
171SOL    HW1 546   1.231   1.419   0.202  0.1172  0.6381  0.1296
171SOL    HW2 547   1.073   1.404   0.163  0.1689  1.1896 -0.2915
172SOL    OW  548   0.807   1.697   1.266 -0.5358 -0.7610  0.2290
172SOL    HW1 549   0.890   1.642   1.256 -1.2483 -1.6815 -0.9034
172SOL    HW2 550   0.744   1.652   1.329  1.4322  2.0132  4.6519
173SOL    OW  551   1.081   1.088   0.732 -0.3284 -0.4753 -0.2373
173SOL    HW1 552   1.168   1.095   0.683 -0.2477 -0.4219 -0.0878
173SOL    HW2 553   1.098   1.060   0.827 -0.5607 -1.5814 -0.5113
174SOL    OW  554   1.985   0.720   1.509 -0.2333 -0.5012  0.1500
174SOL    HW1 555   1.947   0.662   1.581  0.6382 -1.8655 -0.4619
174SOL    HW2 556   2.068   0.679   1.473  0.3199  1.0527 -0.4357
175SOL    OW  557   2.259   1.557   1.231 -0.4381 -0.4399 -0.1282
175SOL    HW1 558   2.224   1.615   1.157 -3.1581 -2.0322 -0.1914
175SOL    HW2 559   2.356   1.539   1.214 -0.3798  1.1761 -1.9874
176SOL    OW  560   0.697   0.905   0.356 -0.2951 -0.2679 -0.1084
176SOL    HW1 561   0.739   0.841   0.292 -1.0387 -1.6051  0.6792
176SOL    HW2 562   0.753   0.912   0.438 -0.7442 -0.7613  0.2499
177SOL    OW  563   0.686   0.281   1.415  0.2905 -0.6608 -0.0006
177SOL    HW1 564   0.714   0.377   1.423 -0.2709 -0.6352  2.2022
177SOL    HW2 565   0.765   0.226   1.386  1.0845  0.2263  0.3995
178SOL    OW  566   2.059   1.438   2.073  0.3610  0.2851 -0.2433
178SOL    HW1 567   2.052   1.411   2.169 -0.9840 -1.9749 -0.9064
178SOL    HW2 568   2.156   1.443   2.048  0.7844  1.8718  1.4010
179SOL    OW  569   2.516   1.442   1.313 -0.0430 -0.0296 -0.3702
179SOL    HW1 570   2.495   1.365   1.254 -2.9620  1.3476 -1.3444
179SOL    HW2 571   2.486   1.422   1.406 -2.6730  0.5018 -1.0045
180SOL    OW  572   1.261   2.085   0.124 -0.4218  0.5888 -0.3138
180SOL    HW1 573   1.288   2.111   0.217 -3.0564 -0.0479  0.7189
180SOL    HW2 574   1.260   1.986   0.117 -1.1010  0.6175 -0.7065
181SOL    OW  575   0.353   0.055   1.657 -0.8373  0.1109 -0.5094
181SOL    HW1 576   0.314   0.098   1.575 -0.0977  0.9598 -0.4335
181SOL    HW2 577   0.348   0.119   1.734 -0.3343 -0.1836 -0.2235
182SOL    OW  578   1.438   2.803   1.935  0.6779 -0.1342  0.4570
182SOL    HW1 579   1.341   2.821   1.916  0.2641 -1.4758  1.1408
182SOL    HW2 580   1.482   2.769   1.853  0.4790  0.1164  0.2425
183SOL    OW  581   1.410   1.232   0.336  0.6215  0.0440  0.1654
183SOL    HW1 582   1.406   1.288   0.253 -0.4908 -0.0046  0.1651
183SOL    HW2 583   1.393   1.136   0.314  2.4355 -0.3191  0.1806
184SOL    OW  584   1.680   0.685   1.761  0.0644  0.1252  0.4511
184SOL    HW1 585   1.602   0.646   1.712 -0.2526  1.5366 -0.2144
184SOL    HW2 586   1.759   0.625   1.751  0.4072  0.9857 -2.9578
185SOL    OW  587   1.338   1.793   0.408 -0.5974  0.5135 -0.1997
185SOL    HW1 588   1.285   1.729   0.464 -0.3101  0.3530 -0.1091
185SOL    HW2 589   1.323   1.886   0.442  0.6181  0.2984  1.0194
186SOL    OW  590   1.931   0.326   0.286  0.0135  0.1485  0.8700
186SOL    HW1 591   2.013   0.356   0.237 -0.8257  1.9897  0.5322
186SOL    HW2 592   1.914   0.387   0.363 -0.7914 -0.4984  1.2185
187SOL    OW  593   2.028   1.926   0.711 -0.1612  0.4192 -0.2812
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187SOL    HW1 594   2.065   1.852   0.653 -1.1488 -0.9774  0.8027
187SOL    HW2 595   1.941   1.958   0.673  0.6237  1.5939 -1.1631
188SOL     OW 596   0.326   0.966   0.524 -0.2700 -0.2783 -0.2135
188SOL    HW1 597   0.359   1.046   0.473  0.7330  0.1598  1.0628
188SOL    HW2 598   0.241   0.934   0.483  0.9934 -0.5985 -2.7960
189SOL     OW 599   0.583   2.700   2.186 -0.3531 -0.1991 -0.7019
189SOL    HW1 600   0.552   2.621   2.240 -0.2281  0.5839  0.5517
189SOL    HW2 601   0.678   2.686   2.158  0.7766  0.8166  2.2277
190SOL     OW 602   0.382   2.448   1.350 -0.6682 -0.7693  0.8997
190SOL    HW1 603   0.349   2.525   1.404 -0.6999 -1.6785  2.2057
190SOL    HW2 604   0.429   2.382   1.409 -0.5996 -1.7409 -0.1907
191SOL     OW 605   0.506   1.804   2.104 -0.1578 -0.2198  0.2531
191SOL    HW1 606   0.408   1.806   2.085 -0.1121 -3.4842 -0.9462
191SOL    HW2 607   0.528   1.724   2.159  1.8724  0.4932  0.5863
192SOL     OW 608   0.833   1.055   0.869  0.5047 -0.1707 -0.8692
192SOL    HW1 609   0.913   1.015   0.914 -0.7460  0.4542  2.1809
192SOL    HW2 610   0.851   1.151   0.848  0.3550  0.1630  0.4654
193SOL     OW 611   3.109   0.639   1.184 -0.0656  0.4972  0.1054
193SOL    HW1 612   3.051   0.705   1.136  0.6556  0.8778 -0.2606
193SOL    HW2 613   3.134   0.565   1.123  0.8541  0.9826 -0.1267
194SOL     OW 614   3.000   1.394   0.458  0.2821 -1.0208  0.1790
194SOL    HW1 615   3.042   1.427   0.542 -1.5704 -0.0934  0.7788
194SOL    HW2 616   2.992   1.469   0.393  0.3260 -1.3900 -0.2622
195SOL     OW 617   3.005   1.591   0.257 -0.1752  0.4738  0.0325
195SOL    HW1 618   2.922   1.620   0.209 -2.4436 -3.0238  1.4280
195SOL    HW2 619   3.047   1.515   0.207  1.2102  1.0453  0.2873
196SOL     OW 620   1.096   1.992   1.730 -0.2791 -0.1300  0.3166
196SOL    HW1 621   1.089   1.922   1.659 -1.5218  1.0340 -0.7660
196SOL    HW2 622   1.055   2.077   1.697 -3.3632 -0.2419  3.3231
197SOL     OW 623   2.420   0.508   0.538 -0.0226  0.1154 -0.3790
197SOL    HW1 624   2.338   0.451   0.539  0.1941 -0.2130 -0.7916
197SOL    HW2 625   2.417   0.573   0.614 -1.2929  0.9955 -1.1479
198SOL     OW 626   0.815   0.114   0.452  0.3863 -0.5504  0.3568
198SOL    HW1 627   0.738   0.160   0.408  0.7208 -0.1177  0.2240
198SOL    HW2 628   0.901   0.157   0.424  0.6117 -0.3135  1.3642
199SOL     OW 629   0.700   2.767   1.159 -0.2630  0.2228 -0.3905
199SOL    HW1 630   0.647   2.850   1.178  0.0910  0.2504  0.5062
199SOL    HW2 631   0.738   2.731   1.244 -0.9914 -1.2580 -0.6573
200SOL     OW 632   0.901   2.314   0.722 -0.0813  0.0363 -0.0486
200SOL    HW1 633   0.876   2.319   0.819 -2.4324 -1.0536 -0.5318
200SOL    HW2 634   0.843   2.376   0.669 -0.4061 -1.0734 -1.0204
201SOL     OW 635   0.228   2.021   0.667  0.1189 -0.1614  0.0162
201SOL    HW1 636   0.306   2.082   0.683  0.6466 -1.1925  1.5993
201SOL    HW2 637   0.260   1.932   0.636 -0.5166 -0.2150 -0.5075
202SOL     OW 638   0.325   2.354   0.817  0.7342 -0.0069  0.4300
202SOL    HW1 639   0.301   2.366   0.914 -0.6843  1.4323 -0.0486
202SOL    HW2 640   0.241   2.347   0.764  1.5047 -1.0751 -0.6876
203SOL     OW 641   1.189   1.241   1.665  0.2979 -0.1340  0.0415
203SOL    HW1 642   1.163   1.315   1.603  0.8846 -0.4988 -0.6527
203SOL    HW2 643   1.288   1.235   1.670  0.2819  0.3516  1.5965
204SOL     OW 644   2.206   0.102   0.485  0.0976  0.1601  1.0157
204SOL    HW1 645   2.274   0.076   0.554  0.2165  1.0571  1.2513
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204SOL   HW2 646  2.232  0.065   0.396  1.2990  1.1055  0.9508
205SOL    OW 647  2.874  1.028   0.672  0.4328  0.0137  0.0260
205SOL   HW1 648  2.806  1.060   0.606 -1.5739 -1.3147  1.3456
205SOL   HW2 649  2.963  1.020   0.627 -0.7642 -0.5276 -2.4224
206SOL    OW 650  2.633  2.217   0.558  0.3929 -0.2545  0.8051
206SOL   HW1 651  2.571  2.254   0.627  0.0797  0.3154  0.2273
206SOL   HW2 652  2.693  2.290   0.525  1.6036 -0.8621  1.5820
207SOL    OW 653  2.563  0.928   1.287 -0.0566  0.2329  0.7757
207SOL   HW1 654  2.469  0.962   1.291 -0.1812  0.0420 -0.2680
207SOL   HW2 655  2.565  0.832   1.316 -0.0485  0.4660  1.5743
208SOL    OW 656  0.146  2.641   0.567  0.3154  0.2927 -0.3191
208SOL   HW1 657  0.079  2.615   0.497 -1.3296  0.9448  0.9427
208SOL   HW2 658  0.174  2.736   0.551  0.9352  0.0215 -0.8455
209SOL    OW 659  1.227  1.810   0.146  0.1124 -0.4938 -0.2298
209SOL   HW1 660  1.272  1.744   0.085  0.6523 -0.3542  0.0147
209SOL   HW2 661  1.255  1.793   0.240  2.6902  1.9382 -0.4195
210SOL    OW 662  3.034  0.390   1.818 -0.6264  0.1108 -0.4944
210SOL   HW1 663  2.942  0.402   1.857 -1.4317 -0.3179 -2.2062
210SOL   HW2 664  3.065  0.296   1.835 -1.0393 -0.1211 -0.9925
211SOL    OW 665  0.305  1.515   1.352 -0.0281  0.0548 -0.0187
211SOL   HW1 666  0.370  1.499   1.277  0.1166  2.3693 -0.4406
211SOL   HW2 667  0.345  1.578   1.418 -1.5707  0.9784  0.0769
212SOL    OW 668  0.412  0.984   1.527  0.3537 -0.2843  0.2181
212SOL   HW1 669  0.468  0.902   1.538  0.6402  0.0316  1.1987
212SOL   HW2 670  0.430  1.024   1.437 -1.4029 -2.4693 -1.1992
213SOL    OW 671  3.066  2.505   0.426  0.1480  0.2693  0.2448
213SOL   HW1 672  3.038  2.503   0.330  1.1365 -1.3651 -0.0672
213SOL   HW2 673  3.049  2.415   0.467  2.6508 -0.1101  0.6485
214SOL    OW 674  2.392  2.414   0.354 -0.6496 -0.7045  0.4895
214SOL   HW1 675  2.385  2.410   0.454  0.0135  2.1759  0.7395
214SOL   HW2 676  2.300  2.419   0.315 -0.9074  0.8170  1.1965
215SOL    OW 677  2.844  1.998   2.141  0.5433  0.2961  0.2193
215SOL   HW1 678  2.889  2.060   2.076 -1.8377  2.5783  0.6014
215SOL   HW2 679  2.804  2.051   2.216 -0.0788 -1.9179  1.5417
216SOL    OW 680  0.126  0.753   1.546 -0.2727  0.1872  0.5281
216SOL   HW1 681  0.162  0.743   1.454 -1.4774  0.9851 -0.0581
216SOL   HW2 682  0.159  0.839   1.586  1.4969 -0.8828  1.4626
217SOL    OW 683  0.371  2.634   0.275  0.1691 -0.1767  0.1827
217SOL   HW1 684  0.375  2.639   0.374  0.2766 -1.5618  0.2683
217SOL   HW2 685  0.296  2.573   0.248 -1.1266  1.6800 -0.6467
218SOL    OW 686  2.832  2.731   1.451  0.1139  0.3543  0.4843
218SOL   HW1 687  2.915  2.682   1.480 -0.2678 -0.4511  0.2520
218SOL   HW2 688  2.857  2.805   1.389  0.5920 -0.4849 -0.3422
219SOL    OW 689  1.359  2.907   0.050 -0.3323 -0.1369 -0.2148
219SOL   HW1 690  1.336  2.986   0.107 -0.5940 -0.0795 -0.3953
219SOL   HW2 691  1.456  2.887   0.058 -0.7360 -1.4873  1.9605
220SOL    OW 692  2.183  1.295   1.206 -0.3045  0.2787 -0.0121
220SOL   HW1 693  2.260  1.232   1.198 -0.8578 -0.2522 -1.3006
220SOL   HW2 694  2.218  1.388   1.218  0.5327  0.0134 -0.3057
221SOL    OW 695  0.301  2.869   0.578 -0.5562  0.0080  0.9067
221SOL   HW1 696  0.394  2.902   0.560 -0.2672 -1.5782 -0.7997
221SOL   HW2 697  0.249  2.940   0.625  1.2244  1.2978  1.0136
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222SOL   OW  698  1.115  2.285  1.634  0.3124 -0.3583  0.3353
222SOL   HW1 699  1.141  2.368  1.683  1.8180 -0.0938 -0.8167
222SOL   HW2 700  1.179  2.269  1.558 -1.3658 -1.2484 -0.9820
223SOL   OW  701  2.148  2.431  0.248  0.1614  0.1943 -0.2213
223SOL   HW1 702  2.157  2.438  0.149 -2.1181 -0.9426 -0.5811
223SOL   HW2 703  2.111  2.517  0.284  0.0981  0.2803 -0.4913
224SOL   OW  704  1.136  2.236  0.597  0.0001 -0.4408  0.0895
224SOL   HW1 705  1.040  2.236  0.625 -0.6019  0.5044 -1.8362
224SOL   HW2 706  1.190  2.285  0.666 -0.8467 -1.0827  1.2541
225SOL   OW  707  2.047  0.014  2.020  0.3653 -0.4127 -0.0673
225SOL   HW1 708  2.064  0.103  1.979 -0.4143 -0.2509 -0.0613
225SOL   HW2 709  2.127 -0.015  2.071  0.3534  0.6652  0.6097
226SOL   OW  710  1.925  0.582  1.709  0.1781  1.0038 -0.5604
226SOL   HW1 711  1.936  0.483  1.704  0.7250  1.0095  0.2935
226SOL   HW2 712  1.997  0.620  1.766 -0.4807  1.8070 -0.2448
227SOL   OW  713  0.605  1.576  0.418  0.2740  0.3427  0.1074
227SOL   HW1 714  0.608  1.562  0.517  0.3934 -3.6176 -0.3083
227SOL   HW2 715  0.518  1.619  0.393 -0.9367 -1.0008  1.7594
228SOL   OW  716  2.416  2.901  0.788 -0.3223 -0.8790 -0.4883
228SOL   HW1 717  2.504  2.873  0.826 -0.3670 -0.4120 -0.0256
228SOL   HW2 718  2.385  2.833  0.722  1.7184  0.2695 -2.7809
229SOL   OW  719  0.828  0.889  1.650 -0.2629  0.1125  0.1288
229SOL   HW1 720  0.903  0.839  1.692 -1.7210  0.1573  2.9783
229SOL   HW2 721  0.845  0.988  1.658 -0.4334  0.1202  0.3890
230SOL   OW  722  1.139  0.561  1.520 -0.0515  0.2470  0.1921
230SOL   HW1 723  1.079  0.536  1.596  0.0420 -0.8969 -0.0788
230SOL   HW2 724  1.125  0.657  1.496 -1.0635  0.2620  0.7652
231SOL   OW  725  2.090  1.553  0.405 -0.0682  0.8615 -0.2699
231SOL   HW1 726  2.179  1.548  0.360  1.2690  0.4845  2.2069
231SOL   HW2 727  2.030  1.482  0.369  1.0609  0.3226 -1.1473
232SOL   OW  728  1.826  1.736  1.332  0.0137 -0.5426  0.4553
232SOL   HW1 729  1.900  1.721  1.397  0.1147  0.1742  0.5135
232SOL   HW2 730  1.809  1.652  1.281  1.3407 -0.5226 -0.0516
233SOL   OW  731  1.919  0.473  0.537  0.2216  0.5276  0.0946
233SOL   HW1 732  1.845  0.456  0.601  0.2489  1.1010  0.2773
233SOL   HW2 733  1.959  0.563  0.554 -0.1818  0.9659 -1.1202
234SOL   OW  734  0.155  1.342  1.173  0.3937  0.3749  0.3503
234SOL   HW1 735  0.189  1.370  1.262  0.0664  0.0641  0.5716
234SOL   HW2 736  0.227  1.294  1.123 -0.1332 -1.5522  1.3754
235SOL   OW  737  0.401  0.481  1.206  0.3151 -0.3435  0.5345
235SOL   HW1 738  0.481  0.525  1.166 -0.4867 -0.3729 -1.1914
235SOL   HW2 739  0.381  0.396  1.157 -0.5874 -0.4980  1.1356
236SOL   OW  740  1.632  3.119  0.225  0.4700  0.5102 -0.2557
236SOL   HW1 741  1.654  3.022  0.214  1.6941  0.9983 -2.7164
236SOL   HW2 742  1.569  3.130  0.303 -0.5636 -2.3485 -0.5551
237SOL   OW  743  0.822  1.080  0.024  0.1477  0.5740  0.3641
237SOL   HW1 744  0.908  1.100  0.071  0.2485  0.3086  0.2906
237SOL   HW2 745  0.827  0.990 -0.018 -0.1952  0.5248  0.4262
238SOL   OW  746  1.717  1.424  1.714  0.3361 -0.2533 -0.9345
238SOL   HW1 747  1.700  1.521  1.694 -0.3997  0.7082  3.3896
238SOL   HW2 748  1.808  1.414  1.754 -0.6361 -0.7684  1.2808
239SOL   OW  749  0.937  2.153  1.320  0.6893  0.3101  0.6566
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239SOL   HW1 750   1.022   2.131   1.370  0.5022 -0.7132  0.5495
239SOL   HW2 751   0.955   2.151   1.222  0.2096 -1.4894  0.5740
240SOL    OW 752   2.069   2.877   0.911 -0.3524  0.2067  0.2751
240SOL   HW1 753   2.084   2.973   0.890 -0.7547  0.4658  1.1083
240SOL   HW2 754   2.067   2.865   1.010  0.6542 -0.8182  0.1920
241SOL    OW 755   0.434   2.809   0.051 -0.1970  0.8423 -0.3084
241SOL   HW1 756   0.482   2.738  -0.001 -0.8726 -0.7145  1.0762
241SOL   HW2 757   0.403   2.770   0.138 -1.4892  2.5805  0.0533
242SOL    OW 758   0.124   2.327   1.924 -0.1631  0.1977 -0.6692
242SOL   HW1 759   0.174   2.267   1.861 -1.4370 -2.2821  0.5552
242SOL   HW2 760   0.062   2.386   1.872 -1.7668 -2.3302 -1.7982
243SOL    OW 761   0.532   2.248   1.492  0.0493  0.3564 -0.3229
243SOL   HW1 762   0.615   2.252   1.437  1.2364 -0.6672  1.3379
243SOL   HW2 763   0.553   2.217   1.584 -2.4222 -1.9164 -0.3845
244SOL    OW 764   2.104   2.481   1.736 -0.1978  0.0076 -0.2796
244SOL   HW1 765   2.088   2.514   1.643 -0.2655  0.0391 -0.2570
244SOL   HW2 766   2.063   2.544   1.801 -1.5433 -0.8233 -0.2831
245SOL    OW 767   2.118   0.733   0.390 -0.1058 -0.3881 -0.1483
245SOL   HW1 768   2.160   0.752   0.479  0.6131 -1.3612 -0.2554
245SOL   HW2 769   2.022   0.760   0.392 -0.0460 -0.1911  0.8475
246SOL    OW 770   0.282   2.452   1.091  0.4531 -0.1828 -0.4185
246SOL   HW1 771   0.324   2.457   1.181  1.4974 -1.0138 -0.8460
246SOL   HW2 772   0.238   2.540   1.070 -1.1391 -0.4357  1.5020
247SOL    OW 773   1.575   0.633   0.186  0.0845  0.3548 -0.4754
247SOL   HW1 774   1.620   0.670   0.267  0.7074  0.0610 -0.6845
247SOL   HW2 775   1.583   0.533   0.186 -2.2478  0.0841  0.4859
248SOL    OW 776   0.940   0.692   1.065  0.2282 -0.3056  0.7143
248SOL   HW1 777   0.963   0.621   0.999 -0.5941 -0.7000  0.8335
248SOL   HW2 778   0.921   0.650   1.154 -2.8642 -0.2847  0.1755
249SOL    OW 779   1.005   0.679   0.334  0.2036  0.2791  0.0040
249SOL   HW1 780   0.923   0.663   0.279 -0.1705 -1.2465  0.9560
249SOL   HW2 781   0.982   0.670   0.431  1.3763  0.4103  0.3035
250SOL    OW 782   2.978   0.601   1.451  0.5600 -0.0220 -0.5073
250SOL   HW1 783   3.032   0.588   1.368  4.8567  0.6366  1.8784
250SOL   HW2 784   2.951   0.697   1.457  1.4937  0.2549 -0.5203
251SOL    OW 785   2.101   1.047   0.776 -0.0454 -0.0706 -0.1724
251SOL   HW1 786   2.087   1.105   0.695 -2.0938 -1.3775 -0.8357
251SOL   HW2 787   2.072   1.097   0.858  1.1012  0.8982 -0.3241
252SOL    OW 788   0.433   0.357   1.524  0.0713 -0.2100  0.2512
252SOL   HW1 789   0.517   0.315   1.491 -0.2626 -1.1484  0.5416
252SOL   HW2 790   0.355   0.317   1.475 -0.1971  0.8276 -0.1927
253SOL    OW 791   2.901   2.977   1.315  0.9144 -0.1159 -0.0260
253SOL   HW1 792   2.926   2.928   1.231  1.9511 -0.4868  0.4813
253SOL   HW2 793   2.885   3.073   1.293 -0.4998 -0.5286 -0.9241
254SOL    OW 794   0.943   0.136   1.378 -0.2092  0.1431 -0.1571
254SOL   HW1 795   0.902   0.051   1.410  0.6756 -0.3203 -0.1992
254SOL   HW2 796   0.993   0.179   1.453  1.2861 -0.5883 -0.6878
255SOL    OW 797   1.681   0.972   1.673 -0.3941  0.0318  0.1230
255SOL   HW1 798   1.650   0.889   1.719 -0.6977 -0.1013 -0.3173
255SOL   HW2 799   1.765   0.952   1.623  0.1509  0.2721  0.9202
256SOL    OW 800   0.513   2.037   0.925 -0.5079 -0.2053 -0.0790
256SOL   HW1 801   0.488   2.111   0.987  2.3411  1.5024 -0.7991
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256SOL   HW2 802  0.492  2.063  0.831 -1.0411 -1.0658 -0.2139
257SOL   OW  803  2.410  0.430  0.111  0.0136  0.3666 -0.9790
257SOL   HW1 804  2.444  0.524  0.111 -0.2527  0.4684 -0.0353
257SOL   HW2 805  2.483  0.368  0.139  0.0309  0.3467 -1.0668
258SOL   OW  806  2.338  0.638  1.135 -0.1702 -0.0902  0.2706
258SOL   HW1 807  2.258  0.615  1.080 -0.1897 -1.3405  0.7691
258SOL   HW2 808  2.420  0.633  1.079 -0.3990  0.9056 -0.1721
259SOL   OW  809  0.073  0.549  0.172 -0.2705 -0.1560 -0.3443
259SOL   HW1 810 -0.026  0.544  0.184 -0.8178  4.8189 -0.7687
259SOL   HW2 811  0.099  0.510  0.084 -1.4252 -3.3206  0.5867
260SOL   OW  812  2.858  0.118  0.912 -0.4167 -0.3511  0.2054
260SOL   HW1 813  2.939  0.159  0.870  0.2240  0.7187  2.3347
260SOL   HW2 814  2.877  0.023  0.935  0.0451 -0.2620  0.2006
261SOL   OW  815  0.211  0.267  0.878  0.1868 -0.0083 -0.2974
261SOL   HW1 816  0.244  0.262  0.972  1.2561 -0.2988 -0.6741
261SOL   HW2 817  0.266  0.206  0.820 -1.7652 -1.4216 -0.7583
262SOL   OW  818  2.298  2.934  1.947 -0.5170 -0.0175 -0.0198
262SOL   HW1 819  2.299  3.016  1.889  2.4187  0.8426  1.0382
262SOL   HW2 820  2.384  2.884  1.934 -1.4222 -1.8684  0.8272
263SOL   OW  821  0.068  1.751  1.096  0.5650 -0.4360 -0.6800
263SOL   HW1 822  0.141  1.770  1.162  1.9953 -1.3794 -1.9101
263SOL   HW2 823  0.057  1.830  1.036  0.7567 -0.3882 -0.6551
264SOL   OW  824  1.052  0.799  1.787  0.1307 -0.2751 -0.4697
264SOL   HW1 825  0.998  0.851  1.853 -2.0488 -0.2700 -2.1383
264SOL   HW2 826  1.135  0.850  1.765  0.0035  0.5728  0.8637
265SOL   OW  827  0.953  3.029  0.257  0.1262 -0.5238 -0.3121
265SOL   HW1 828  0.951  3.020  0.356  1.8526  1.1924 -0.0712
265SOL   HW2 829  0.871  2.986  0.218 -0.8395 -0.7801  1.8629
266SOL   OW  830  1.829  0.789  0.336 -0.3353 -0.6945  0.0902
266SOL   HW1 831  1.794  0.725  0.404 -0.8466  0.7624  1.2600
266SOL   HW2 832  1.814  0.883  0.368 -0.9656  0.0650 -2.2261
267SOL   OW  833  1.463  0.050  1.803 -0.1885  0.1645  0.1936
267SOL   HW1 834  1.508  0.020  1.888 -0.4032 -1.1686 -0.1335
267SOL   HW2 835  1.524  0.032  1.726 -0.2900  0.6998 -0.0146
268SOL   OW  836  2.871  0.754  0.262 -0.2600 -0.3625  0.2053
268SOL   HW1 837  2.798  0.743  0.329 -0.2342 -1.7379  0.0353
268SOL   HW2 838  2.888  0.666  0.217  0.8332  0.1678 -0.4467
269SOL   OW  839  2.392  0.764  1.500 -0.1534 -0.1372 -0.0626
269SOL   HW1 840  2.487  0.754  1.469 -0.0276 -2.6500  0.8791
269SOL   HW2 841  2.332  0.714  1.437 -1.0908  2.5451 -1.4235
270SOL   OW  842  1.523  3.044  2.024 -0.4851  0.6239  0.0593
270SOL   HW1 843  1.476  2.973  1.972  0.3135 -0.0458  0.2296
270SOL   HW2 844  1.519  3.021  2.122 -0.7014  1.1035  0.1646
271SOL   OW  845  2.068  1.345  1.635  0.3352  0.6405  0.3397
271SOL   HW1 846  2.157  1.390  1.642  2.0429 -2.5975  2.2670
271SOL   HW2 847  2.016  1.360  1.719  0.6165 -0.2721  0.6953
272SOL   OW  848  2.691  1.217  1.751 -0.5506 -0.1399  0.2824
272SOL   HW1 849  2.725  1.127  1.723  1.7598  0.9447 -0.6627
272SOL   HW2 850  2.629  1.206  1.829  0.4705 -2.4597  0.8684
273SOL   OW  851  0.218  2.824  1.298  0.6730  0.0192 -0.0257
273SOL   HW1 852  0.249  2.764  1.371 -3.2118 -0.7308  1.2514
273SOL   HW2 853  0.216  2.773  1.211  0.6156 -0.6383  0.3560
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274SOL    OW  854   1.612   1.561   0.048 -0.7269  0.2483 -0.0222
274SOL   HW1  855   1.668   1.599   0.122 -0.8050 -0.2087  0.2739
274SOL   HW2  856   1.671   1.518  -0.020 -0.7576 -1.6243  1.0592
275SOL    OW  857   0.404   0.669   2.099 -0.6242  0.6114 -0.5513
275SOL   HW1  858   0.343   0.706   2.030  1.2739  0.4874 -2.3993
275SOL   HW2  859   0.465   0.741   2.133  0.4952  0.0469 -1.3046
276SOL    OW  860   0.478   1.918   1.417 -0.2371 -0.3290 -0.3200
276SOL   HW1  861   0.487   1.830   1.464  0.6411  0.0907  0.3286
276SOL   HW2  862   0.568   1.958   1.405 -0.5966  0.2891 -1.0005
277SOL    OW  863   1.963   2.878   2.209  0.1277 -0.0658  0.5303
277SOL   HW1  864   1.932   2.970   2.184 -1.9337 -1.2103 -1.5089
277SOL   HW2  865   2.062   2.878   2.218  0.2253  2.2602  0.1802
278SOL    OW  866   1.421   2.898   0.979 -0.5560 -0.0705 -0.3528
278SOL   HW1  867   1.477   2.980   0.991 -2.4614  1.1000  0.9882
278SOL   HW2  868   1.422   2.844   1.063 -0.6546 -0.5754 -0.6674
279SOL    OW  869   1.611   2.354   0.769  0.0395 -0.3320 -0.4705
279SOL   HW1  870   1.535   2.335   0.831 -0.1023  0.9564 -0.2236
279SOL   HW2  871   1.697   2.350   0.820 -0.0519  0.4196 -0.2470
280SOL    OW  872   1.709   0.670   0.552 -0.3021 -0.6136  0.6861
280SOL   HW1  873   1.718   0.724   0.636  1.4539 -1.3272  1.0029
280SOL   HW2  874   1.652   0.589   0.570  1.1957 -1.5087  1.6231
281SOL    OW  875   1.468   0.600   1.564  0.3258 -0.5092  0.3820
281SOL   HW1  876   1.500   0.648   1.483  2.9879 -1.2171  0.9038
281SOL   HW2  877   1.377   0.563   1.548  0.4607  0.0520 -1.9684
282SOL    OW  878   1.716   1.653   2.188 -0.0867 -0.2618 -0.1042
282SOL   HW1  879   1.687   1.632   2.094 -0.0366  1.3480 -0.5046
282SOL   HW2  880   1.755   1.571   2.230 -0.7346 -1.1851 -1.2474
283SOL    OW  881   0.546   1.344   0.280 -0.1729 -0.0512 -0.0571
283SOL   HW1  882   0.533   1.411   0.353  0.3464  1.0549 -0.9556
283SOL   HW2  883   0.545   1.390   0.192  2.2638 -0.9008 -0.6089
284SOL    OW  884   2.505   2.778   0.512  0.2232 -0.4695 -0.1671
284SOL   HW1  885   2.556   2.692   0.515 -0.1877 -0.7211  2.6227
284SOL   HW2  886   2.563   2.852   0.545 -0.2549 -0.2167  0.1296
285SOL    OW  887   1.213   0.003   1.991 -0.7366 -0.0572 -0.1573
285SOL   HW1  888   1.291   0.032   1.935 -0.8978 -1.6884 -1.2899
285SOL   HW2  889   1.129   0.014   1.938 -0.7886 -2.6430 -0.7083
286SOL    OW  890   0.493   0.752   0.609  0.8919  0.1471  1.1969
286SOL   HW1  891   0.444   0.678   0.654  0.9689  0.2420  1.4344
286SOL   HW2  892   0.427   0.814   0.566  0.8609 -0.8252 -0.2329
287SOL    OW  893   1.870   2.136   2.109  0.4017 -0.6270 -0.1468
287SOL   HW1  894   1.968   2.151   2.097  0.6697 -2.0513  0.0673
287SOL   HW2  895   1.854   2.043   2.142 -1.0935 -0.8331 -1.3116
288SOL    OW  896   0.478   3.162   0.469  0.2407  1.0525 -0.2680
288SOL   HW1  897   0.449   3.128   0.380 -0.8861  1.0021  0.1145
288SOL   HW2  898   0.519   3.087   0.522 -0.4327  0.7433 -0.1815
289SOL    OW  899   2.948   2.786   1.129 -0.3762 -0.2528 -0.6817
289SOL   HW1  900   2.918   2.736   1.048  0.2606  0.8241 -1.6049
289SOL   HW2  901   3.014   2.730   1.180 -0.0056 -0.5333 -1.4555
290SOL    OW  902   0.691   0.310   0.742 -0.1560  0.2517  0.5315
290SOL   HW1  903   0.729   0.348   0.826 -0.6882  0.4597  0.6860
290SOL   HW2  904   0.713   0.213   0.736 -1.3158 -0.1008  1.6315
291SOL    OW  905   0.432   1.097   0.745  0.1914 -0.1118  0.7684
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291SOL    HW1 906  0.389  1.036  0.678 -0.4770  0.2182  0.8935
291SOL    HW2 907  0.501  1.046  0.796  1.5458 -0.0865 -0.9443
292SOL     OW 908  2.861  0.157  1.283  0.5525 -0.2678  0.0032
292SOL    HW1 909  2.870  0.236  1.222  0.7623  0.0438  0.4273
292SOL    HW2 910  2.885  0.185  1.376  0.9000 -0.9047  0.1075
293SOL     OW 911  0.462  2.926  1.310 -0.3194 -0.4521 -0.3501
293SOL    HW1 912  0.492  2.851  1.371 -0.8953 -0.0257  0.4826
293SOL    HW2 913  0.363  2.920  1.297 -0.5310  0.7180  0.5252
294SOL     OW 914  2.820  1.321  0.778 -0.0823  0.7086 -0.5380
294SOL    HW1 915  2.823  1.317  0.878  2.4189 -2.5135 -0.5509
294SOL    HW2 916  2.896  1.377  0.744  1.6779 -1.5114 -0.5203
295SOL     OW 917  2.761  0.628  1.619  0.0829  0.1674 -0.4295
295SOL    HW1 918  2.775  0.669  1.710  1.0949  1.6626 -1.2191
295SOL    HW2 919  2.850  0.603  1.580 -0.1345  1.6231 -1.9309
296SOL     OW 920  1.437  1.475  0.986 -0.5315 -0.2510  0.0588
296SOL    HW1 921  1.411  1.524  0.902  1.6374 -0.0640 -0.5588
296SOL    HW2 922  1.379  1.395  0.997 -2.1897  0.8134 -0.5050
297SOL     OW 923  2.684  0.462  1.193 -0.1694  0.6551 -0.2831
297SOL    HW1 924  2.621  0.390  1.222 -0.9469  0.6180 -1.9423
297SOL    HW2 925  2.772  0.421  1.168 -0.4817  0.3048 -0.8447
298SOL     OW 926  0.178  1.806  2.081  0.3105 -0.9237  0.3374
298SOL    HW1 927  0.117  1.800  2.160 -0.5461  1.6880 -0.0137
298SOL    HW2 928  0.147  1.742  2.010 -1.4439 -0.4103  0.5835
299SOL     OW 929  0.814  3.030  1.437 -0.2267  0.1071 -0.3487
299SOL    HW1 930  0.887  3.029  1.506 -0.6557 -1.5208  0.1073
299SOL    HW2 931  0.728  3.054  1.481 -0.1336  1.1995 -0.7366
300SOL     OW 932  0.171  2.711  1.052  0.3116 -0.2563  0.1121
300SOL    HW1 933  0.091  2.697  0.995  0.4686  0.8826 -0.4219
300SOL    HW2 934  0.239  2.763  1.001  0.3285  1.0845  1.4440
301SOL     OW 935  1.497  1.935  1.273 -0.1576  0.2718 -0.0851
301SOL    HW1 936  1.440  1.853  1.282 -1.8199  1.4528  0.7559
301SOL    HW2 937  1.567  1.935  1.345 -0.6847 -0.0211  0.4407
302SOL     OW 938  2.335  0.121  2.234 -0.5249 -0.5743  0.4743
302SOL    HW1 939  2.267  0.188  2.203 -0.5659 -1.4204 -1.4169
302SOL    HW2 940  2.410  0.117  2.168  1.0268 -0.2308  2.1340
303SOL     OW 941  2.441  0.284  1.271 -0.3076  0.1224 -0.5096
303SOL    HW1 942  2.414  0.288  1.175 -1.5947 -0.1426 -0.1648
303SOL    HW2 943  2.497  0.202  1.286  1.0404  0.8526 -1.2878
304SOL     OW 944  1.489  1.091  1.073  0.4605 -0.2742  0.1288
304SOL    HW1 945  1.476  1.050  1.163 -1.2679 -1.4391 -0.6042
304SOL    HW2 946  1.424  1.167  1.061  1.0432  0.2182  0.0484
305SOL     OW 947  1.897  0.643  0.827  0.0152  0.4898 -0.0836
305SOL    HW1 948  1.837  0.566  0.802  0.5726  0.1011 -0.2278
305SOL    HW2 949  1.845  0.728  0.820 -0.8231  0.0733  0.7735
306SOL     OW 950  2.278  2.823  1.260  0.1984  0.0329 -0.0748
306SOL    HW1 951  2.297  2.743  1.204 -0.5957 -0.6060  0.5439
306SOL    HW2 952  2.315  2.904  1.215 -1.2672 -0.3046 -2.0385
307SOL     OW 953  1.674  0.911  1.017 -0.3622  0.2355  0.0155
307SOL    HW1 954  1.750  0.910  1.082 -1.1281  0.4063  0.9560
307SOL    HW2 955  1.620  0.994  1.031 -0.4486  0.3491 -0.9672
308SOL     OW 956  0.225  0.675  1.293  0.0808 -0.1388  0.1870
308SOL    HW1 957  0.280  0.593  1.279 -0.7416 -0.6294 -0.2120
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308SOL    HW2  958  0.134  0.662  1.254 -0.2191  0.7861  0.5437
309SOL    OW   959  3.066  0.683  1.764 -0.3427  0.0541  0.9656
309SOL    HW1  960  3.114  0.688  1.676 -0.8645  0.4293  0.6961
309SOL    HW2  961  3.067  0.588  1.797 -1.9502 -0.5321 -0.4843
310SOL    OW   962  2.386  0.527  1.648 -0.7380 -0.3703 -0.5138
310SOL    HW1  963  2.416  0.604  1.592 -2.8850  0.8519 -0.0879
310SOL    HW2  964  2.361  0.451  1.589  2.6606 -1.3531 -0.9043
311SOL    OW   965  2.574  2.577  0.727 -0.2744  0.1346  0.0923
311SOL    HW1  966  2.634  2.637  0.780  1.3946  1.6002 -3.1654
311SOL    HW2  967  2.484  2.573  0.771  0.9957  0.9722  3.0683
312SOL    OW   968  0.756  0.542  1.510 -0.4811 -0.1246 -0.1712
312SOL    HW1  969  0.668  0.588  1.516  0.1162  1.2218 -1.2506
312SOL    HW2  970  0.807  0.557  1.595 -0.1437  1.5717 -0.6463
313SOL    OW   971  1.951  0.864  0.090 -0.0166  0.1407  0.9759
313SOL    HW1  972  1.904  0.848  0.176  1.0629  0.3329  1.6272
313SOL    HW2  973  1.962  0.777  0.041  0.5525 -0.2004  1.6831
314SOL    OW   974  0.300  2.667  1.501  0.3179  0.0520 -0.0323
314SOL    HW1  975  0.261  2.621  1.581  0.0651 -0.3085 -0.3616
314SOL    HW2  976  0.392  2.699  1.523  0.3694 -0.3226  0.3035
315SOL    OW   977  1.017  1.771  1.552 -0.7285  0.1676  0.0680
315SOL    HW1  978  0.940  1.711  1.571 -1.7381  1.4510  0.2027
315SOL    HW2  979  1.102  1.730  1.585 -1.3622 -1.2283  0.0018
316SOL    OW   980  2.109  2.168  1.977 -0.2879 -0.2807 -0.6359
316SOL    HW1  981  2.092  2.234  1.904  1.7196 -1.3879 -2.1901
316SOL    HW2  982  2.093  2.076  1.943 -0.7975 -0.7693  0.8228
317SOL    OW   983  1.404  2.195  2.028  1.0773 -0.1442 -0.2017
317SOL    HW1  984  1.475  2.254  2.067  0.4326 -0.0786  0.9087
317SOL    HW2  985  1.329  2.251  1.993  0.9026 -0.2642 -0.0219
318SOL    OW   986  3.059  2.744  2.010  0.3654 -0.2037 -0.4043
318SOL    HW1  987  3.141  2.742  2.066 -0.9555 -0.3065  1.6114
318SOL    HW2  988  3.022  2.837  2.008  0.0277 -0.3404 -0.5591
319SOL    OW   989  1.074  1.558  1.181 -0.3990  0.3928  0.6512
319SOL    HW1  990  1.096  1.634  1.120 -0.2662 -0.7907 -0.8235
319SOL    HW2  991  1.051  1.477  1.127 -0.5063 -0.6373  2.1793
320SOL    OW   992  1.129  0.231  0.829  0.0166  0.3270  0.2218
320SOL    HW1  993  1.211  0.175  0.827  0.0769  0.4062 -1.6893
320SOL    HW2  994  1.062  0.191  0.890  0.9415 -0.5062  0.7154
321SOL    OW   995  2.381  2.990  1.040 -0.0168 -0.0569 -0.3710
321SOL    HW1  996  2.316  3.061  1.012  0.4392  0.3383 -0.4395
321SOL    HW2  997  2.406  2.934  0.960 -1.1118 -0.9190 -0.1385
322SOL    OW   998  2.443  1.916  1.146 -0.2222 -0.2656 -0.3596
322SOL    HW1  999  2.420  1.822  1.124 -0.1481 -0.0021 -1.6234
322SOL    HW2 1000  2.360  1.970  1.155 -0.2196  0.0187 -1.8594
323SOL    OW  1001  0.206  0.727  0.340 -0.2264  0.4924  0.4397
323SOL    HW1 1002  0.299  0.754  0.312 -0.5214 -0.2552 -1.4258
323SOL    HW2 1003  0.172  0.657  0.278 -2.8399  2.1831 -0.1956
324SOL    OW  1004  2.712  0.960  1.696 -0.7251  0.3838  0.5337
324SOL    HW1 1005  2.784  0.947  1.628 -2.0123  0.6259 -0.9314
324SOL    HW2 1006  2.732  0.904  1.776  1.6578  1.3024  0.6727
325SOL    OW  1007  2.790  2.596  0.987  0.1845 -0.2172 -0.7812
325SOL    HW1 1008  2.709  2.604  1.046 -1.7494 -0.5520 -3.2107
325SOL    HW2 1009  2.834  2.508  1.003 -0.2635 -0.2865  0.1686
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326SOL    OW 1010   2.296   0.457   0.816   0.2332  0.0727 -0.1973
326SOL    HW1 1011  2.347   0.542   0.808  -0.2160  0.3315 -0.3244
326SOL    HW2 1012  2.263   0.429   0.726  -0.1073  0.0652 -0.0707
327SOL    OW 1013   1.807   0.227   1.289   0.3189 -0.2128  0.2420
327SOL    HW1 1014  1.853   0.315   1.278  -1.4611  0.9802  1.7277
327SOL    HW2 1015  1.742   0.214   1.215  -0.4391  0.4268  0.7787
328SOL    OW 1016   0.053   2.288   1.105   0.3008  0.2942  0.0973
328SOL    HW1 1017  0.114   2.208   1.094   0.0423 -0.0527  1.0846
328SOL    HW2 1018  0.108   2.371   1.105   0.6080  0.1042 -0.6193
329SOL    OW 1019   1.905   0.045   0.261  -0.0272  0.6197 -0.2047
329SOL    HW1 1020  1.914   0.142   0.284  -0.7725  0.4816  0.7384
329SOL    HW2 1021  1.808   0.019   0.264   0.3055 -0.6153  1.5744
330SOL    OW 1022   0.981   0.530   1.753   0.7962  0.0262  0.0167
330SOL    HW1 1023  1.011   0.623   1.777   1.5713 -0.5250  1.2910
330SOL    HW2 1024  0.906   0.503   1.812   0.4333 -0.0941 -0.4904
331SOL    OW 1025   0.485   0.061   1.252  -0.5341 -0.1270  0.4541
331SOL    HW1 1026  0.476  -0.033   1.285   1.5799 -0.1537  1.0634
331SOL    HW2 1027  0.546   0.112   1.312  -0.4732  1.2395 -0.7080
332SOL    OW 1028   0.901   0.908   0.553   0.2294  0.0920  0.1593
332SOL    HW1 1029  0.930   0.952   0.639  -0.3775 -0.2223  0.5368
332SOL    HW2 1030  0.882   0.811   0.570  -0.0211  0.0568 -0.2999
333SOL    OW 1031   3.018   0.190   0.384   0.1928 -0.2685 -0.4759
333SOL    HW1 1032  3.030   0.129   0.306  -0.4761 -0.6354 -0.2892
333SOL    HW2 1033  3.084   0.266   0.377   1.1323 -1.0807 -0.6257
334SOL    OW 1034   2.700   2.309   1.978  -0.0601 -0.5024  0.0104
334SOL    HW1 1035  2.716   2.362   2.062  -0.8633  1.6582 -1.1033
334SOL    HW2 1036  2.784   2.262   1.951   0.7601  0.3560  0.9871
335SOL    OW 1037   0.868   1.385   1.528   0.1212 -0.6005  0.0349
335SOL    HW1 1038  0.965   1.408   1.529  -0.0443  0.1399  1.2670
335SOL    HW2 1039  0.840   1.361   1.435   0.8285  1.9819 -0.9186
336SOL    OW 1040   2.462   2.272   0.748  -0.2365 -0.0258 -1.0597
336SOL    HW1 1041  2.425   2.358   0.781   1.0743  0.0985  0.1971
336SOL    HW2 1042  2.390   2.219   0.702  -1.3823  1.1187 -0.6280
337SOL    OW 1043   1.166   1.619   1.722   0.6685  0.1168 -0.6389
337SOL    HW1 1044  1.097   1.660   1.782   0.4050  0.3154 -1.0713
337SOL    HW2 1045  1.246   1.593   1.776  -0.1475 -1.0734  0.0635
338SOL    OW 1046   1.363   1.581   1.889   0.5476  0.3664 -0.0810
338SOL    HW1 1047  1.329   1.575   1.983  -0.5891  0.3590 -0.4801
338SOL    HW2 1048  1.453   1.538   1.884   0.2372 -0.4170  0.8142
339SOL    OW 1049   1.324   2.409   0.182  -0.0161 -0.2499  0.2402
339SOL    HW1 1050  1.300   2.494   0.230   1.9969  0.6715 -0.3084
339SOL    HW2 1051  1.325   2.333   0.247  -1.9342  0.0715  0.7204
340SOL    OW 1052   0.235   0.529   1.681   0.1615 -0.4110  0.2185
340SOL    HW1 1053  0.186   0.604   1.637  -0.6992  0.0621  1.8816
340SOL    HW2 1054  0.296   0.485   1.615  -1.0549  0.2438 -1.3974
341SOL    OW 1055   1.515   2.164   1.701  -0.2789  0.5147 -0.7783
341SOL    HW1 1056  1.606   2.141   1.735  -0.2557  1.1514 -0.4073
341SOL    HW2 1057  1.446   2.121   1.759  -0.2245  0.5743 -0.6699
342SOL    OW 1058   1.431   0.812   0.740   0.1384 -0.2608  0.5782
342SOL    HW1 1059  1.377   0.797   0.657   1.8772  1.1221 -0.8636
342SOL    HW2 1060  1.519   0.852   0.717   0.5604  0.4970  3.1410
343SOL    OW 1061   1.594   1.732   0.718  -0.0649 -0.2075 -0.0063
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343SOL   HW1 1062   1.550   1.733   0.808  0.5666  0.7841  0.3199
343SOL   HW2 1063   1.635   1.822   0.701  1.0664 -0.8190 -0.6578
344SOL    OW 1064   1.592   2.063   0.068 -0.0157  0.2452 -0.0415
344SOL   HW1 1065   1.603   1.977   0.117  0.7035  1.3043  1.7324
344SOL   HW2 1066   1.496   2.074   0.042 -0.1669 -0.9426 -0.0442
345SOL    OW 1067   3.000   1.217   0.246 -0.5267  0.2768 -0.2999
345SOL   HW1 1068   2.999   1.269   0.332 -0.4463  1.0077 -0.7383
345SOL   HW2 1069   3.030   1.124   0.265 -1.1755  0.2274  0.5826
346SOL    OW 1070   1.920   3.046   1.555 -0.2660  1.0633 -0.0345
346SOL   HW1 1071   1.826   3.012   1.562 -0.1571  0.1660 -2.0519
346SOL   HW2 1072   1.975   3.007   1.629 -1.0610 -0.0141  0.0184
347SOL    OW 1073   1.814   2.221   0.371 -0.3018  0.2672  0.1149
347SOL   HW1 1074   1.874   2.148   0.340  1.0861  1.6611 -0.6219
347SOL   HW2 1075   1.762   2.257   0.293 -0.4453  0.5242  0.3269
348SOL    OW 1076   2.909   2.356   1.067  0.6037 -0.1234  0.4616
348SOL   HW1 1077   2.887   2.404   1.151  1.1114  0.9249  0.0212
348SOL   HW2 1078   3.006   2.328   1.069  0.5784 -0.2268  0.2858
349SOL    OW 1079   0.642   2.285   0.016 -0.3358 -0.8560  0.5489
349SOL   HW1 1080   0.561   2.238  -0.018 -0.4796 -0.2844  0.0742
349SOL   HW2 1081   0.620   2.330   0.102 -1.1700  1.0464 -0.5899
350SOL    OW 1082   2.273   2.891   2.209  0.1864 -0.5978 -0.1630
350SOL   HW1 1083   2.285   2.925   2.115  0.0230 -2.5530 -0.9521
350SOL   HW2 1084   2.300   2.795   2.212  0.2273 -0.5536  1.8378
351SOL    OW 1085   0.600   2.462   0.228  0.0712 -0.1120  0.0453
351SOL   HW1 1086   0.679   2.524   0.237  1.3691 -1.5936 -0.6049
351SOL   HW2 1087   0.516   2.516   0.219  1.0964  1.5303 -0.1443
352SOL    OW 1088   1.837   2.245   0.898  0.8290 -0.2641 -0.1884
352SOL   HW1 1089   1.810   2.280   0.987 -0.3919  0.0042 -0.6478
352SOL   HW2 1090   1.936   2.255   0.887  1.0991 -0.9957  1.4143
353SOL    OW 1091   1.845   2.564   0.219  0.4491  0.1509 -0.5489
353SOL   HW1 1092   1.800   2.484   0.178 -0.0069  0.2137 -0.1868
353SOL   HW2 1093   1.858   2.547   0.317 -0.3638  0.8254 -0.3098
354SOL    OW 1094   1.853   0.809   1.273 -0.4317  0.2567  0.0117
354SOL   HW1 1095   1.900   0.757   1.344 -0.2322  1.2086  0.5866
354SOL   HW2 1096   1.835   0.902   1.305 -3.2245 -0.2222  0.0245
355SOL    OW 1097   3.051   2.617   0.901  0.0096 -0.6097  0.6192
355SOL   HW1 1098   2.954   2.607   0.879  0.4482 -2.7193 -0.5843
355SOL   HW2 1099   3.104   2.551   0.849  1.9453 -0.6675  2.5419
356SOL    OW 1100   0.972   1.220   2.206 -0.4001 -0.4452 -0.2739
356SOL   HW1 1101   0.872   1.228   2.210 -0.3246  0.5754 -0.1561
356SOL   HW2 1102   1.001   1.224   2.110 -0.4559 -0.4127 -0.2902
357SOL    OW 1103   2.865   2.013   0.189 -0.1599  0.3965  0.3276
357SOL   HW1 1104   2.820   1.992   0.103  0.6205  0.0010  0.0012
357SOL   HW2 1105   2.803   1.996   0.265 -0.2672 -1.0178 -0.0532
358SOL    OW 1106   3.002   1.783   0.443  0.1043  0.2253 -0.4259
358SOL   HW1 1107   3.040   1.727   0.370  0.6178  1.8329 -1.4474
358SOL   HW2 1108   2.902   1.787   0.434 -0.2780 -2.5821  1.2337
359SOL    OW 1109   2.488   1.984   0.868 -0.4600 -0.8608  0.0156
359SOL   HW1 1110   2.436   1.993   0.953 -0.7142  1.2595 -0.3023
359SOL   HW2 1111   2.499   2.075   0.827  0.2859 -1.7566 -1.8441
360SOL    OW 1112   0.014   1.424   0.072 -0.4998 -0.2389 -0.0589
360SOL   HW1 1113   0.078   1.499   0.054 -0.1159 -0.6754 -0.5160
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360SOL    HW2 1114   0.065   1.341   0.094 -0.9169  0.0895  2.4880
361SOL     OW 1115   2.979   2.527   0.153 -0.4706  0.8626  0.6253
361SOL    HW1 1116   3.043   2.599   0.128 -0.7805  1.9147  2.6939
361SOL    HW2 1117   2.886   2.557   0.133 -0.5235  0.5332  0.3707
362SOL     OW 1118   0.928   1.272   0.568 -0.0803 -0.3978 -0.1214
362SOL    HW1 1119   0.978   1.196   0.610  0.2885 -0.5973 -0.9065
362SOL    HW2 1120   0.900   1.246   0.476  0.0721  0.4333 -0.4070
363SOL     OW 1121   2.293   2.568   1.122  0.1352 -0.0204  0.4480
363SOL    HW1 1122   2.199   2.558   1.091  0.2268 -1.8715  0.7021
363SOL    HW2 1123   2.308   2.512   1.204  1.4682  0.2282  0.3977
364SOL     OW 1124   0.113   0.920   0.112 -0.0874  0.2703 -0.0126
364SOL    HW1 1125   0.035   0.927   0.173 -1.0490  0.2072 -1.1834
364SOL    HW2 1126   0.192   0.883   0.161 -0.0210  2.6963  1.8384
365SOL     OW 1127   2.138   2.814   0.478 -0.7532 -0.9787 -0.1733
365SOL    HW1 1128   2.048   2.837   0.440 -1.7602 -3.3664  0.5486
365SOL    HW2 1129   2.208   2.830   0.408 -2.0068 -1.0372 -1.5053
366SOL     OW 1130   2.595   1.565   0.777 -0.1887 -0.0376  0.4374
366SOL    HW1 1131   2.642   1.512   0.707  2.5521 -2.0106  3.4332
366SOL    HW2 1132   2.650   1.645   0.801 -0.9022  0.4261  0.5569
367SOL     OW 1133   3.149   0.898   2.097  0.2460 -0.1991 -0.2267
367SOL    HW1 1134   3.055   0.911   2.131  0.1973  0.7137 -0.6728
367SOL    HW2 1135   3.150   0.909   1.998  0.6848 -1.0786 -0.3237
368SOL     OW 1136   1.266   1.361   0.545 -0.0430 -0.0545  0.0637
368SOL    HW1 1137   1.292   1.265   0.557  0.8226  0.3406  1.8326
368SOL    HW2 1138   1.210   1.371   0.464  0.9774 -1.8388 -0.9275
369SOL     OW 1139   2.202   1.689   0.981  0.2296 -0.3315 -0.2679
369SOL    HW1 1140   2.131   1.760   0.983 -0.8716 -1.2323 -3.2160
369SOL    HW2 1141   2.283   1.724   0.934  0.0701 -0.6883 -0.8158
370SOL     OW 1142   1.213   0.568   0.164 -0.2095 -0.3588 -0.5126
370SOL    HW1 1143   1.300   0.616   0.166  0.1736 -1.0453  1.8219
370SOL    HW2 1144   1.145   0.620   0.215 -0.5859 -0.8587 -0.4952
371SOL     OW 1145   2.061   1.208   0.560 -0.0102  0.4351  0.1800
371SOL    HW1 1146   2.124   1.227   0.485  0.9312 -0.9517  0.5909
371SOL    HW2 1147   1.975   1.257   0.544  0.6334  1.1996 -1.1226
372SOL     OW 1148   1.805   1.058   1.366 -0.1739 -0.0419  0.4905
372SOL    HW1 1149   1.844   1.134   1.315 -0.4305  1.3341  2.2293
372SOL    HW2 1150   1.861   1.040   1.447 -0.9165 -0.7236  0.8663
373SOL     OW 1151   0.301   2.517   2.048 -0.3386 -0.3159  0.2703
373SOL    HW1 1152   0.353   2.486   2.127  3.1372 -0.5188 -1.8605
373SOL    HW2 1153   0.275   2.438   1.992 -1.4801 -0.0905  0.4742
374SOL     OW 1154   1.548   0.438   0.477  0.7529 -0.0159  0.0681
374SOL    HW1 1155   1.579   0.417   0.384  1.8595  0.8056  0.2249
374SOL    HW2 1156   1.459   0.483   0.473 -0.4081 -2.2240 -0.4154
375SOL     OW 1157   2.230   1.726   1.438  0.0961  0.1779 -0.6144
375SOL    HW1 1158   2.321   1.766   1.451  0.5124 -0.7359 -0.6780
375SOL    HW2 1159   2.236   1.651   1.373 -0.6714 -0.0415 -0.4388
376SOL     OW 1160   0.178   1.379   0.360  0.5265 -0.5004  0.7602
376SOL    HW1 1161   0.128   1.313   0.304  0.6675 -2.1312  2.4627
376SOL    HW2 1162   0.163   1.359   0.456 -0.7300  2.9948  1.4312
377SOL     OW 1163   2.270   0.887   1.942  0.5062  0.0123 -0.1081
377SOL    HW1 1164   2.299   0.930   1.856 -0.6372  0.8107 -0.1111
377SOL    HW2 1165   2.351   0.867   1.997  1.1064  2.0638 -0.1539
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378SOL    OW 1166   3.084   1.183   1.929 -0.1837  0.0020 -0.1209
378SOL   HW1 1167   2.992   1.191   1.969 -0.8768 -1.6761 -1.2758
378SOL   HW2 1168   3.110   1.087   1.924  1.2809  0.3935 -0.6537
379SOL    OW 1169   1.529   0.775   2.014  0.2572  0.2841  0.9707
379SOL   HW1 1170   1.486   0.751   2.101 -0.1343 -0.5644  0.5586
379SOL   HW2 1171   1.502   0.708   1.945  1.2597  0.4541  0.4041
380SOL    OW 1172   1.047   0.826   1.404  0.3900  0.2914  0.2465
380SOL   HW1 1173   0.980   0.886   1.361 -0.3729 -1.2612 -0.8159
380SOL   HW2 1174   1.125   0.880   1.435 -0.5651  1.8997 -0.0620
381SOL    OW 1175   0.312   0.312   0.020 -0.8428  0.4390 -0.0673
381SOL   HW1 1176   0.389   0.251   0.039 -1.6336 -0.5482  0.0719
381SOL   HW2 1177   0.232   0.257  -0.005 -1.6545  1.4152  0.3364
382SOL    OW 1178  -0.014   2.639   1.242  0.0215 -0.6803 -0.2117
382SOL   HW1 1179  -0.003   2.624   1.340  2.2168  0.9932 -0.1200
382SOL   HW2 1180   0.076   2.652   1.200 -0.9403 -0.2273 -2.2634
383SOL    OW 1181   2.013   3.089   0.633  0.3438 -0.5717 -0.2729
383SOL   HW1 1182   2.041   2.994   0.627 -2.5571 -1.4558 -1.8183
383SOL   HW2 1183   2.079   3.147   0.586  1.8734 -1.8251  0.2267
384SOL    OW 1184   1.990   2.689   1.545 -0.6203  0.7012  0.6533
384SOL   HW1 1185   1.951   2.678   1.636  0.6874 -0.6302  1.0932
384SOL   HW2 1186   2.068   2.752   1.548 -1.1243  1.3547  0.2735
385SOL    OW 1187   2.123   0.584   0.975 -0.4645 -0.1517 -0.1420
385SOL   HW1 1188   2.042   0.628   0.936 -0.8747  2.2092  2.9822
385SOL   HW2 1189   2.175   0.539   0.902 -2.0788  2.2469 -3.0136
386SOL    OW 1190   0.944   2.741   0.771  0.0699  0.0057  0.0757
386SOL   HW1 1191   0.861   2.695   0.803 -0.2621  0.2886 -0.3740
386SOL   HW2 1192   1.021   2.677   0.775 -0.2721 -0.4159  0.0012
387SOL    OW 1193   1.813   1.583   0.238 -0.2461 -0.1435  0.2953
387SOL   HW1 1194   1.808   1.642   0.319 -0.0552  1.1373 -0.5889
387SOL   HW2 1195   1.900   1.599   0.191 -0.5672 -0.4983 -0.4307
388SOL    OW 1196   1.211   2.379   1.998  0.5666  0.0263 -0.2576
388SOL   HW1 1197   1.245   2.398   2.090  0.0946 -0.3183 -0.0091
388SOL   HW2 1198   1.124   2.329   2.004 -0.3436  1.4733 -0.8623
389SOL    OW 1199   2.630   0.673   1.391  0.1459 -0.0967  0.1537
389SOL   HW1 1200   2.651   0.610   1.317  0.5618  1.0405 -0.7267
389SOL   HW2 1201   2.682   0.647   1.472  1.0478 -0.3303 -0.4830
390SOL    OW 1202   1.639   2.821   1.393  0.8298  0.2978  0.2922
390SOL   HW1 1203   1.659   2.791   1.300 -1.7143 -4.2481  0.9454
390SOL   HW2 1204   1.589   2.908   1.389  1.5134  0.6724 -2.4641
391SOL    OW 1205   1.800   2.467   0.523 -0.1844  0.2282 -0.0345
391SOL   HW1 1206   1.872   2.489   0.588 -0.0346  1.4142 -0.5698
391SOL   HW2 1207   1.826   2.387   0.469 -0.4178 -0.9114  1.5028
392SOL    OW 1208   1.188   2.855   1.887 -0.2949  0.3801 -0.2326
392SOL   HW1 1209   1.104   2.802   1.891 -0.2418  0.3678  1.1345
392SOL   HW2 1210   1.177   2.939   1.939  0.5496  0.3636 -0.0111
393SOL    OW 1211   2.266   1.542   1.864 -0.0251 -0.1669 -0.1229
393SOL   HW1 1212   2.355   1.531   1.908  0.5892 -0.3030 -1.3314
393SOL   HW2 1213   2.258   1.635   1.828 -1.3097  0.5587  1.8698
394SOL    OW 1214   0.864   0.364   0.104  0.3125  0.1460  0.2301
394SOL   HW1 1215   0.844   0.456   0.139  0.3346  0.3736 -0.3592
394SOL   HW2 1216   0.865   0.365   0.004 -2.5760 -1.0482  0.0656
395SOL    OW 1217   0.732   2.881   0.183 -0.1456 -0.2757 -0.3558
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395SOL   HW1 1218  0.639   2.900   0.213 -0.0848 -0.5257 -0.0089
395SOL   HW2 1219  0.759   2.789   0.211  1.2498  0.7870  2.2096
396SOL    OW 1220  2.522   1.596   0.034  0.0431  0.3755 -0.2232
396SOL   HW1 1221  2.508   1.689  -0.001 -1.7022  0.6755  1.1159
396SOL   HW2 1222  2.618   1.584   0.061 -0.1028  2.5534  1.5713
397SOL    OW 1223  1.057   1.619   0.420 -0.1282 -0.1213 -0.2454
397SOL   HW1 1224  0.980   1.667   0.378 -0.2869 -0.4637 -0.3456
397SOL   HW2 1225  1.085   1.543   0.362  2.6941  2.1453 -2.1448
398SOL    OW 1226  1.726   0.838   0.763 -0.6186  0.3272 -0.1308
398SOL   HW1 1227  1.746   0.920   0.709 -1.6612  0.1425 -0.8363
398SOL   HW2 1228  1.698   0.864   0.855 -1.7887  0.8324 -0.6087
399SOL    OW 1229  1.798   1.883   1.088 -0.4137 -0.0311 -0.3770
399SOL   HW1 1230  1.804   1.846   1.181 -1.5376  0.9808  0.1273
399SOL   HW2 1231  1.776   1.809   1.024 -0.5398 -0.5940  0.3013
400SOL    OW 1232  2.743   1.274   0.134 -0.9714 -0.4032  0.3629
400SOL   HW1 1233  2.725   1.206   0.064  2.3984  1.3870 -2.5882
400SOL   HW2 1234  2.824   1.247   0.187 -0.4123  0.6201  0.0634
401SOL    OW 1235  2.470   1.384   1.582 -0.2627  0.2015 -0.1846
401SOL   HW1 1236  2.510   1.475   1.580  2.8018 -0.9975 -2.7224
401SOL   HW2 1237  2.523   1.325   1.643 -0.1701 -0.6490 -1.0636
402SOL    OW 1238  2.689   0.301   2.112 -0.2142  0.6559 -0.1626
402SOL   HW1 1239  2.713   0.271   2.204  0.3913  2.0011  0.1564
402SOL   HW2 1240  2.600   0.347   2.114  0.7178  2.5771  0.2294
403SOL    OW 1241  1.790   2.919   0.582  0.1103  0.0915 -0.2600
403SOL   HW1 1242  1.808   3.012   0.614 -0.4124  0.0073  0.2949
403SOL   HW2 1243  1.810   2.853   0.654 -1.4500 -0.0688  0.0628
404SOL    OW 1244  2.361   2.099   0.182  0.7991 -0.1240 -0.5772
404SOL   HW1 1245  2.428   2.076   0.252  0.2718 -0.6661 -0.2533
404SOL   HW2 1246  2.276   2.129   0.225  0.5538 -0.2267 -0.9845
405SOL    OW 1247  0.960   1.091   1.209  0.4167 -0.3946 -0.0272
405SOL   HW1 1248  1.032   1.131   1.265 -0.6059  0.7943  0.4954
405SOL   HW2 1249  0.995   1.071   1.118  1.6891 -0.9027  0.5541
406SOL    OW 1250  0.269   1.162   1.925  0.3611 -0.2294 -0.1133
406SOL   HW1 1251  0.173   1.167   1.895  0.5319 -0.1193 -0.6613
406SOL   HW2 1252  0.329   1.174   1.845  0.8354 -1.8817 -0.0377
407SOL    OW 1253  1.121   1.198   1.956  0.2927  0.2317  0.0370
407SOL   HW1 1254  1.069   1.278   1.926  0.1676 -0.4245 -1.5664
407SOL   HW2 1255  1.216   1.225   1.973 -0.0821  1.0165  1.0436
408SOL    OW 1256  0.902   1.415   1.876 -0.1573  0.1535  0.5313
408SOL   HW1 1257  0.803   1.399   1.878 -0.7015  3.0258  1.6704
408SOL   HW2 1258  0.920   1.511   1.855  2.5256 -0.7194 -1.7139
409SOL    OW 1259  2.187   0.366   0.543  0.2764  0.9117 -0.4347
409SOL   HW1 1260  2.093   0.402   0.544  0.6711  1.9931  0.1080
409SOL   HW2 1261  2.188   0.275   0.503 -1.3274  0.0243  1.3703
410SOL    OW 1262  1.677   2.486   1.934 -0.2845 -0.5705  0.1802
410SOL   HW1 1263  1.634   2.410   1.982 -0.2261  0.2265  1.5589
410SOL   HW2 1264  1.736   2.536   1.998  2.1612 -1.1996 -1.4572
411SOL    OW 1265  1.355   0.091   0.798 -0.2192  0.5413 -0.0612
411SOL   HW1 1266  1.387   0.001   0.767 -0.9761  0.7346 -1.4487
411SOL   HW2 1267  1.402   0.162   0.747 -1.3084  0.8722 -0.6274
412SOL    OW 1268  1.924   2.904   0.320 -0.1619 -0.0691 -0.5929
412SOL   HW1 1269  1.879   2.912   0.409 -2.2408 -1.1103 -1.4967
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412SOL   HW2 1270   1.907   2.987   0.267  0.2556  0.1442 -0.4013
413SOL    OW 1271   0.580   0.578   0.389 -0.0006 -0.0659 -0.2152
413SOL   HW1 1272   0.489   0.551   0.356  0.0464  1.2177 -1.4630
413SOL   HW2 1273   0.570   0.634   0.472 -0.2821 -0.7694  0.2331
414SOL    OW 1274   0.937   0.552   1.301  0.0822 -0.4326  0.3764
414SOL   HW1 1275   0.859   0.533   1.361  0.4398  0.2714  1.0876
414SOL   HW2 1276   1.019   0.566   1.357  0.8289 -1.5845 -0.3707
415SOL    OW 1277   2.131   2.704   1.932  0.4510  0.1188 -0.0140
415SOL   HW1 1278   2.211   2.765   1.933  0.2823  0.3735  1.4952
415SOL   HW2 1279   2.133   2.645   2.013 -0.0846 -0.9806 -0.7739
416SOL    OW 1280   1.779   1.269   0.221 -0.1011 -0.5354  0.3714
416SOL   HW1 1281   1.745   1.246   0.312 -0.4048 -1.5917  0.0114
416SOL   HW2 1282   1.749   1.361   0.196 -0.7587 -0.5724  0.9896
417SOL    OW 1283   2.887   2.695   0.472 -0.1415  0.2320 -0.5232
417SOL   HW1 1284   2.965   2.633   0.476 -1.3434 -1.3271 -0.0184
417SOL   HW2 1285   2.901   2.770   0.537 -0.1344 -1.3915  1.4751
418SOL    OW 1286   2.513   2.801   1.876  0.2118 -0.2055 -0.5274
418SOL   HW1 1287   2.580   2.761   1.938 -0.1409 -1.2069 -0.7683
418SOL   HW2 1288   2.498   2.739   1.798 -1.4963 -0.3704 -0.1245
419SOL    OW 1289   2.983   3.023   1.896  0.1861  0.4829 -0.2485
419SOL   HW1 1290   2.948   2.995   1.807 -1.3042  3.3260 -0.6775
419SOL   HW2 1291   3.043   3.103   1.884 -2.4444  2.8920  1.4076
420SOL    OW 1292   1.257   2.006   0.592  0.4097 -0.0879  0.0353
420SOL   HW1 1293   1.248   1.970   0.685  1.3101  1.0124  0.5693
420SOL   HW2 1294   1.213   2.095   0.587 -0.5529 -0.6006 -0.8932
421SOL    OW 1295   0.925   2.398   0.382 -0.0863  0.6772 -0.4018
421SOL   HW1 1296   0.874   2.458   0.443 -0.4648  1.0643 -1.0866
421SOL   HW2 1297   1.003   2.359   0.431 -0.3993  0.9524  0.3301
422SOL    OW 1298   2.755   0.774   0.682 -0.6930  0.2467  0.2765
422SOL   HW1 1299   2.680   0.780   0.616  0.3561 -0.6035 -1.0498
422SOL   HW2 1300   2.811   0.856   0.676 -0.5240  0.1135  0.0001
423SOL    OW 1301   2.952   2.540   2.201 -0.2296 -0.2601 -0.5473
423SOL   HW1 1302   2.988   2.613   2.142 -0.8600  1.2732  0.9107
423SOL   HW2 1303   2.998   2.454   2.178 -0.3725  0.2835 -3.1757
424SOL    OW 1304   0.235   0.284   1.830 -0.8119 -0.6219 -0.3083
424SOL   HW1 1305   0.311   0.298   1.894  1.0679  0.8053 -2.6647
424SOL   HW2 1306   0.219   0.368   1.778 -3.2720 -1.2638 -0.7372
425SOL    OW 1307   1.947   1.311   1.355 -0.5433 -0.0660  0.2938
425SOL   HW1 1308   1.975   1.312   1.451 -2.1467 -2.9175  0.9118
425SOL   HW2 1309   2.027   1.307   1.296  0.4583 -1.3194  1.6777
426SOL    OW 1310   0.535   0.598   1.740  0.5355 -0.3362 -0.1003
426SOL   HW1 1311   0.443   0.562   1.756  0.8876 -1.4800 -0.5141
426SOL   HW2 1312   0.599   0.554   1.804  0.6671  1.1887  0.8817
427SOL    OW 1313   3.024   0.014   0.614  0.3853  0.3293  0.1011
427SOL   HW1 1314   3.005   0.049   0.522  2.4591 -1.3861 -1.0668
427SOL   HW2 1315   3.049   0.089   0.674  1.1990  1.2687 -1.3531
428SOL    OW 1316   0.810   1.317   1.264 -0.3136 -0.1571 -0.0787
428SOL   HW1 1317   0.856   1.229   1.272  0.0468  0.1322  1.1217
428SOL   HW2 1318   0.732   1.308   1.201  1.3554 -0.6310 -2.1715
429SOL    OW 1319   3.018   1.498   0.724  0.9878  0.0068 -0.5370
429SOL   HW1 1320   3.075   1.480   0.804 -1.2180  2.0952  1.6851
429SOL   HW2 1321   3.008   1.597   0.712 -1.4402 -0.2604 -1.2857
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430SOL    OW 1322   0.598   0.036   1.551  0.1991  0.7362  0.0716
430SOL    HW1 1323  0.597   0.135   1.545 -1.0945  0.6959 -0.9129
430SOL    HW2 1324  0.517   0.004   1.599  2.1442  0.2229  3.3157
431SOL    OW 1325   2.711   2.989   0.082  0.2811 -0.2477  0.4305
431SOL    HW1 1326  2.765   2.953   0.158  1.7703 -0.6500 -0.7719
431SOL    HW2 1327  2.641   2.922   0.056 -1.3702  0.5710  2.4539
432SOL    OW 1328   2.174   1.104   1.561  0.1067  0.7440  0.1125
432SOL    HW1 1329  2.265   1.087   1.598 -0.1419  1.5469  1.1455
432SOL    HW2 1330  2.138   1.189   1.600 -1.6969 -0.3320  0.9353
433SOL    OW 1331   1.827   3.058   1.252  0.3757 -0.5118 -0.0106
433SOL    HW1 1332  1.746   3.084   1.201 -1.2641 -0.8466  2.2725
433SOL    HW2 1333  1.847   3.126   1.322  2.9035  0.2288 -1.3076
434SOL    OW 1334   2.486   1.548   2.027 -0.0503  0.3448  0.3749
434SOL    HW1 1335  2.522   1.595   2.108  0.4201  2.1707 -0.8231
434SOL    HW2 1336  2.514   1.598   1.945  0.6839 -2.2234 -1.0360
435SOL    OW 1337   0.962   2.785   0.503 -0.1019 -0.3561 -0.4114
435SOL    HW1 1338  1.003   2.875   0.521  0.1698 -0.1484 -1.9187
435SOL    HW2 1339  0.926   2.747   0.588 -0.0373  1.0886  0.2924
436SOL    OW 1340   2.554   0.043   0.206 -0.3350  0.0785 -0.0348
436SOL    HW1 1341  2.455   0.027   0.207 -0.4564  0.7261 -0.5842
436SOL    HW2 1342  2.597  -0.022   0.143 -0.8907  2.0684 -2.6620
437SOL    OW 1343   2.038   1.898   1.859  0.0699 -0.1634 -0.0975
437SOL    HW1 1344  1.950   1.930   1.823 -0.5513 -0.1583  1.3521
437SOL    HW2 1345  2.081   1.838   1.792 -0.1617  1.2748 -1.5992
438SOL    OW 1346   1.651   1.146   0.647 -0.8313 -0.1144  0.8606
438SOL    HW1 1347  1.639   1.225   0.587  0.1107 -1.7383 -1.6469
438SOL    HW2 1348  1.709   1.171   0.725 -0.0791  1.5192 -0.1897
439SOL    OW 1349   0.793   1.864   1.730 -0.5304 -0.4478  0.7231
439SOL    HW1 1350  0.769   1.782   1.678  0.5719 -2.1101  2.6558
439SOL    HW2 1351  0.834   1.931   1.669 -2.3055 -0.9293 -1.0848
440SOL    OW 1352   2.785   2.551   1.780 -0.4978 -0.5199 -0.2121
440SOL    HW1 1353  2.776   2.594   1.870 -0.9034 -0.1419 -0.4273
440SOL    HW2 1354  2.694   2.533   1.742 -0.3504  0.4292 -1.0649
441SOL    OW 1355   3.021   1.512   1.263  0.3661  0.2081 -0.2593
441SOL    HW1 1356  3.008   1.587   1.198  0.2706  0.2548 -0.1857
441SOL    HW2 1357  3.016   1.425   1.214 -2.1287  0.1185  0.0276
442SOL    OW 1358   0.354   0.431   0.295 -0.3412 -0.4338  0.0048
442SOL    HW1 1359  0.289   0.414   0.370  0.0212  1.0528  0.6983
442SOL    HW2 1360  0.311   0.409   0.208 -1.0036 -1.5715  0.5958
443SOL    OW 1361   2.062   0.156   1.455 -0.0674  0.1773 -0.2783
443SOL    HW1 1362  2.007   0.184   1.376 -0.4521  0.7308  0.1805
443SOL    HW2 1363  2.041   0.061   1.477 -1.4859  0.6175  0.4067
444SOL    OW 1364   2.650   0.287   0.174  0.2461 -0.3048 -0.3663
444SOL    HW1 1365  2.713   0.313   0.246 -0.6260 -0.2144  0.3808
444SOL    HW2 1366  2.629   0.190   0.181  1.0199 -0.5500 -1.1986
445SOL    OW 1367   0.176   1.018   1.612  0.0608 -0.2881 -0.6528
445SOL    HW1 1368  0.151   1.113   1.630 -1.6600 -0.8595  0.1929
445SOL    HW2 1369  0.268   1.014   1.573  0.5355  1.6571  0.1675
446SOL    OW 1370   0.280   0.840   0.850  0.1965 -0.6197  0.4453
446SOL    HW1 1371  0.246   0.786   0.772 -0.2623  0.7656 -0.3506
446SOL    HW2 1372  0.376   0.861   0.835 -0.1712  0.5949 -0.3343
447SOL    OW 1373   1.766   0.210   1.546  0.7049 -0.4381 -0.1334
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447SOL   HW1 1374   1.733   0.117   1.562 -0.3957 -0.6528 -3.0006
447SOL   HW2 1375   1.782   0.223   1.448  0.7122  2.4254  0.1684
448SOL    OW 1376   3.103   0.052   1.598 -0.0045  0.4465  0.2733
448SOL   HW1 1377   3.020   0.088   1.555  0.0951  0.6373  0.2357
448SOL   HW2 1378   3.142  -0.020   1.541  0.2782  0.8887 -0.1006
449SOL    OW 1379   2.875   1.458   1.703  0.3798  0.2546  1.0509
449SOL   HW1 1380   2.883   1.493   1.796  0.6245  0.6171  0.8947
449SOL   HW2 1381   2.825   1.371   1.704 -1.2773  1.1647  1.3227
450SOL    OW 1382   1.848   2.674   2.049 -0.0985 -0.3802 -0.0817
450SOL   HW1 1383   1.876   2.759   2.095  1.2252 -0.2161 -1.1393
450SOL   HW2 1384   1.917   2.604   2.065  1.2399  0.1384 -3.0586
451SOL    OW 1385   1.286   1.266   1.043 -0.5835 -0.0168  0.6674
451SOL   HW1 1386   1.286   1.263   1.143  0.8331  1.6850  0.7635
451SOL   HW2 1387   1.191   1.269   1.010 -1.0984  2.2513  2.1198
452SOL    OW 1388   2.815   2.904   2.061  0.1951  0.5059 -0.7163
452SOL   HW1 1389   2.721   2.914   2.094 -0.0769  0.7533 -1.5613
452SOL   HW2 1390   2.844   2.989   2.016 -0.6100 -0.8513 -4.0637
453SOL    OW 1391   0.455   2.184   1.200 -0.5349 -0.2409 -0.0281
453SOL   HW1 1392   0.508   2.189   1.285  1.7596 -0.4989 -1.3543
453SOL   HW2 1393   0.373   2.240   1.210  0.8081  1.6102  1.5957
454SOL    OW 1394   0.736   0.029   0.690 -0.3538 -0.0924  0.3129
454SOL   HW1 1395   0.812  -0.029   0.718  0.0071 -0.9324 -2.1535
454SOL   HW2 1396   0.749   0.057   0.595 -2.5499  0.7107  0.1924
455SOL    OW 1397   0.691   0.256   2.007  0.3071 -0.1769  0.2175
455SOL   HW1 1398   0.597   0.256   2.041  0.9540 -2.5018  2.3317
455SOL   HW2 1399   0.704   0.178   1.945  1.2544 -1.0396  1.4539
456SOL    OW 1400   2.254   1.782   1.725  0.2104  0.8463  0.1001
456SOL   HW1 1401   2.351   1.804   1.730  0.4940 -0.1978 -0.4657
456SOL   HW2 1402   2.227   1.770   1.630 -0.1153 -0.3482  0.3241
457SOL    OW 1403   2.535   2.348   1.741  0.0674  0.3323 -0.5831
457SOL   HW1 1404   2.574   2.298   1.818 -1.3513  0.0736 -0.0044
457SOL   HW2 1405   2.442   2.316   1.724 -0.0570  1.2048 -1.6566
458SOL    OW 1406   3.055   0.957   0.308 -0.0980 -0.0890  0.1539
458SOL   HW1 1407   2.974   0.901   0.290 -1.9033  1.9000  1.6125
458SOL   HW2 1408   3.071   0.963   0.406  2.6149 -1.3841 -0.1166
459SOL    OW 1409   1.312   2.228   0.376  0.7488 -0.0387  0.2461
459SOL   HW1 1410   1.392   2.270   0.418  0.7279 -1.3541  1.6814
459SOL   HW2 1411   1.241   2.213   0.446  0.2756 -1.2688 -0.4568
460SOL    OW 1412   0.816   2.928   1.876  0.1986  0.4040  0.6070
460SOL   HW1 1413   0.900   2.874   1.866 -0.5824 -0.7816  0.2136
460SOL   HW2 1414   0.795   2.938   1.973  1.5747  2.0138  0.7906
461SOL    OW 1415   0.138   3.006   0.972 -0.4414  0.0993  0.1149
461SOL   HW1 1416   0.136   3.060   1.055 -1.8873  1.6975 -0.8917
461SOL   HW2 1417   0.231   2.974   0.955  0.1693  1.0265  1.5213
462SOL    OW 1418   2.181   2.700   0.725 -0.0288  0.6424 -0.1473
462SOL   HW1 1419   2.151   2.773   0.787 -2.0299  0.6317 -1.0008
462SOL   HW2 1420   2.179   2.734   0.631 -0.4052 -0.3152 -0.5027
463SOL    OW 1421   1.082   3.040   0.551 -0.4747  0.0148  0.3850
463SOL   HW1 1422   1.117   3.133   0.536  2.0446 -0.5470  2.2175
463SOL   HW2 1423   1.149   2.973   0.520 -1.6937 -1.2339  0.3048
464SOL    OW 1424   1.990   1.543   0.712  0.0656  0.7319  0.7431
464SOL   HW1 1425   2.004   1.474   0.782 -0.1769  0.0814  0.1638
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464SOL   HW2 1426   2.076   1.591   0.694   0.2672   0.4859   1.0416
465SOL    OW 1427   2.945   2.278   0.017   0.0768   0.3774   0.2430
465SOL   HW1 1428   2.951   2.364   0.068   1.3553   0.8904  -0.7062
465SOL   HW2 1429   2.943   2.202   0.082  -1.2229   1.1023   1.1061
466SOL    OW 1430   0.169   0.726   0.635   0.2309   0.0890  -0.5450
466SOL   HW1 1431   0.161   0.700   0.538  -1.4059  -1.1462  -0.1308
466SOL   HW2 1432   0.167   0.643   0.691  -0.0175   0.8576   0.6057
467SOL    OW 1433   2.232   1.439   0.852   0.5655   0.1291  -0.8194
467SOL   HW1 1434   2.311   1.406   0.904   0.3634   0.0049  -0.5863
467SOL   HW2 1435   2.203   1.527   0.890  -0.2148  -0.4415  -0.0414
468SOL    OW 1436   1.253   1.792   0.820  -0.1404   0.4560  -0.2905
468SOL   HW1 1437   1.225   1.699   0.796  -0.3757   0.4761  -0.0962
468SOL   HW2 1438   1.336   1.788   0.876   0.3791   0.4067  -1.0506
469SOL    OW 1439   0.786   0.420   0.504  -0.2268   0.0272   0.0546
469SOL   HW1 1440   0.756   0.362   0.580   0.8559   1.3119   1.5098
469SOL   HW2 1441   0.705   0.461   0.461  -0.9502  -1.7728  -0.4207
470SOL    OW 1442   2.571   2.245   1.022   0.2001  -0.1210   0.2395
470SOL   HW1 1443   2.572   2.304   0.942   3.0934  -1.4335  -0.8336
470SOL   HW2 1444   2.477   2.221   1.045  -0.7768  -2.1377  -4.6918
471SOL    OW 1445   2.840   0.886   2.114   0.2477   0.5487   0.0848
471SOL   HW1 1446   2.829   0.984   2.100  -1.0170   0.4226   0.0491
471SOL   HW2 1447   2.835   0.865   2.212  -1.4452   0.3477  -0.0054
472SOL    OW 1448   0.083   1.510   0.963   0.2867  -0.1390   0.1026
472SOL   HW1 1449   0.103   1.441   1.033  -0.8656  -0.3838   0.2045
472SOL   HW2 1450   0.092   1.601   1.002   1.1662  -0.2324   0.1431
473SOL    OW 1451   1.373   0.119   1.308   0.1335  -0.6539   0.2963
473SOL   HW1 1452   1.322   0.161   1.383   0.9178   0.7597   0.0833
473SOL   HW2 1453   1.311   0.105   1.230  -0.3391  -0.6755   0.6689
474SOL    OW 1454   2.626   3.096   0.458   0.1373   0.3495   0.4512
474SOL   HW1 1455   2.615   3.135   0.366   1.4281  -0.7742  -0.2007
474SOL   HW2 1456   2.576   3.153   0.523  -0.3352   1.5015  -0.8523
475SOL    OW 1457   0.559   2.957   0.639  -0.1484  -0.0857  -0.3240
475SOL   HW1 1458   0.589   2.865   0.663  -0.7560  -0.1935   0.0501
475SOL   HW2 1459   0.627   3.024   0.668   0.3043  -0.4148  -0.6159
476SOL    OW 1460   2.402   0.404   2.118   0.1747   0.0032  -0.4891
476SOL   HW1 1461   2.347   0.398   2.034   1.3521  -1.7991  -1.1929
476SOL   HW2 1462   2.402   0.499   2.151  -0.0390   0.8452  -2.7220
477SOL    OW 1463   1.557   2.548   1.325   0.2891  -0.1031  -0.5286
477SOL   HW1 1464   1.625   2.486   1.365  -0.1892  -0.7534  -0.7091
477SOL   HW2 1465   1.565   2.638   1.368   1.0486  -0.2582  -0.3209
478SOL    OW 1466   0.043   0.415   0.412  -0.2924  -0.7507  -0.2462
478SOL   HW1 1467   0.106   0.437   0.486   0.4789  -0.9880  -0.8194
478SOL   HW2 1468   0.042   0.489   0.345  -1.0245  -0.5131   0.0151
479SOL    OW 1469   0.210   0.225   1.423   0.2969   0.3306   0.0371
479SOL   HW1 1470   0.160   0.170   1.356   0.3147   0.1630   0.1607
479SOL   HW2 1471   0.147   0.285   1.471  -0.0292  -0.9090   1.2143
480SOL    OW 1472   0.743   0.506   1.923  -0.0685   0.0757   0.0997
480SOL   HW1 1473   0.723   0.416   1.963   0.8294  -0.1051   0.1672
480SOL   HW2 1474   0.742   0.576   1.994   0.9113  -0.1498   0.3530
481SOL    OW 1475   2.164   1.742   0.590   0.1429  -0.0100   0.1671
481SOL   HW1 1476   2.128   1.669   0.532  -0.7298  -0.6742   1.4886
481SOL   HW2 1477   2.264   1.740   0.588   0.1531   0.1594  -1.4821
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482SOL    OW 1478   1.144   0.371   2.187  0.1244  0.1564 -0.3148
482SOL   HW1 1479   1.156   0.387   2.089  0.0352  1.2966 -0.1569
482SOL   HW2 1480   1.057   0.324   2.203 -0.5362  1.2218 -0.6883
483SOL    OW 1481   1.889   2.652   1.788  0.2805  0.1269 -0.0020
483SOL   HW1 1482   1.824   2.578   1.774  1.4475 -0.8454 -0.4081
483SOL   HW2 1483   1.886   2.680   1.884 -1.4201  0.7886 -0.2074
484SOL    OW 1484   2.964   0.870   1.467 -0.2014  0.0154 -0.0947
484SOL   HW1 1485   3.056   0.880   1.506 -1.0827  1.7742  1.6522
484SOL   HW2 1486   2.939   0.954   1.419 -1.2831 -0.0489  0.3306
485SOL    OW 1487   1.067   0.906   0.240  0.5336 -0.3377 -0.2959
485SOL   HW1 1488   1.048   0.828   0.300  0.0664  0.2118  0.2893
485SOL   HW2 1489   1.030   0.990   0.281  1.2278  0.2338 -0.8019
486SOL    OW 1490   2.807   1.729   2.196  0.2299 -0.0607  0.1510
486SOL   HW1 1491   2.830   1.817   2.153 -0.6441 -0.2067 -0.6663
486SOL   HW2 1492   2.708   1.717   2.196  0.2593 -0.4317  1.5396
487SOL    OW 1493   1.745   1.681   1.744 -0.3798  0.5692 -0.5495
487SOL   HW1 1494   1.809   1.696   1.668 -0.0731  0.9400 -0.2198
487SOL   HW2 1495   1.797   1.664   1.828 -0.6959 -1.5087 -0.7286
488SOL    OW 1496   0.825   1.663   0.291 -0.4137  0.6898 -0.0848
488SOL   HW1 1497   0.823   1.670   0.191 -1.2353  0.0988 -0.1133
488SOL   HW2 1498   0.740   1.622   0.324  0.7048 -1.1328  0.6891
489SOL    OW 1499   2.588   0.153   0.826  0.2947  0.0222  0.0688
489SOL   HW1 1500   2.672   0.113   0.865 -0.4335 -2.2682 -0.5502
489SOL   HW2 1501   2.601   0.169   0.728  0.0755 -0.1546  0.0107
490SOL    OW 1502   2.184   2.008   1.182  0.3110  0.3285 -0.1236
490SOL   HW1 1503   2.127   1.977   1.106 -0.1008 -0.6586  0.5626
490SOL   HW2 1504   2.134   2.075   1.237 -0.3287 -0.7387  0.6350
491SOL    OW 1505   1.596   0.380   1.685 -0.1248  0.0775  0.0431
491SOL   HW1 1506   1.568   0.461   1.635 -2.0631 -1.4132 -1.4450
491SOL   HW2 1507   1.654   0.323   1.627 -1.4023 -1.0936 -0.1283
492SOL    OW 1508   0.631   1.154   1.769 -0.0300  0.1590 -0.3570
492SOL   HW1 1509   0.723   1.155   1.731 -0.1818 -0.6936 -0.7768
492SOL   HW2 1510   0.565   1.139   1.696 -0.5794  1.5293 -0.1742
493SOL    OW 1511   1.824   1.020   0.496 -0.2526 -0.2256  0.3164
493SOL   HW1 1512   1.766   1.079   0.552 -2.2552  1.5418 -3.2616
493SOL   HW2 1513   1.916   1.058   0.491 -0.7883  1.1136  0.2476
494SOL    OW 1514   2.937   0.460   0.198 -0.0113  0.2445 -0.3640
494SOL   HW1 1515   2.888   0.421   0.276 -1.1720 -1.2059 -1.7434
494SOL   HW2 1516   2.969   0.386   0.139 -0.1278  1.3259 -1.8243
495SOL    OW 1517   1.018   0.369   1.078  0.2453  0.5112  0.3685
495SOL   HW1 1518   1.048   0.277   1.102 -1.2792  0.0790  0.7551
495SOL   HW2 1519   1.011   0.425   1.161  1.5620  1.1188  0.0886
496SOL    OW 1520   0.057   2.423   0.731 -0.0110  0.4922  0.0679
496SOL   HW1 1521  -0.023   2.371   0.704  0.9561 -0.2285 -1.5498
496SOL   HW2 1522   0.083   2.486   0.658  1.1856  0.3541  0.3389
497SOL    OW 1523   2.291   1.032   1.289 -0.1674  0.2450  0.0289
497SOL   HW1 1524   2.245   1.041   1.377  0.1558 -2.5257  0.5845
497SOL   HW2 1525   2.225   1.001   1.220  0.1659 -0.6063  0.0727
498SOL    OW 1526   0.537   1.287   1.500 -0.1556 -0.4032  0.5938
498SOL   HW1 1527   0.452   1.301   1.551  0.2479 -0.3376  1.2577
498SOL   HW2 1528   0.522   1.216   1.431 -0.8383 -0.1653  0.4822
499SOL    OW 1529   2.722   1.579   1.227  0.3463 -0.2794  0.3209
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499SOL    HW1 1530   2.804   1.590   1.283  0.0570  1.0642  0.5163
499SOL    HW2 1531   2.665   1.507   1.266  1.3456 -1.1347  0.2612
500SOL     OW 1532   0.251   2.543   1.735  0.6507 -0.1809 -0.3420
500SOL    HW1 1533   0.255   2.545   1.835 -0.3127 -0.9694 -0.2767
500SOL    HW2 1534   0.249   2.449   1.703  1.8265  0.0474 -1.1680
501SOL     OW 1535   1.147   2.001   2.163 -0.0753 -0.0911 -0.3466
501SOL    HW1 1536   1.108   1.953   2.242 -1.2075 -0.1685 -0.9311
501SOL    HW2 1537   1.198   1.935   2.106  0.2909 -0.1394  0.0325
502SOL     OW 1538   2.131   2.253   0.894 -0.0520  0.1466 -0.6702
502SOL    HW1 1539   2.161   2.256   0.989  0.5325  1.1028 -0.8839
502SOL    HW2 1540   2.165   2.169   0.851  0.0808 -0.0551 -0.1786
503SOL     OW 1541   2.708   1.999   1.593  0.4327  0.3845 -0.0101
503SOL    HW1 1542   2.679   2.094   1.582  0.1320  0.5153  1.6574
503SOL    HW2 1543   2.779   1.978   1.526 -0.5678  1.3053 -1.4035
504SOL     OW 1544   2.150  -0.000   0.876 -0.4224  0.6652  0.4001
504SOL    HW1 1545   2.066   0.053   0.863 -0.1202  0.9147 -0.5968
504SOL    HW2 1546   2.221   0.033   0.814 -0.1174 -0.6789 -0.0080
505SOL     OW 1547   1.548   2.584   0.431 -0.4591 -0.5479  0.0185
505SOL    HW1 1548   1.527   2.505   0.373  1.7732 -1.4597  0.3591
505SOL    HW2 1549   1.617   2.558   0.498 -1.4189  1.0871  1.7036
506SOL     OW 1550   2.463   1.245   1.138 -0.3073 -0.2818 -0.0229
506SOL    HW1 1551   2.467   1.151   1.171  1.2737  0.2981  1.6147
506SOL    HW2 1552   2.507   1.250   1.048  0.9647 -0.8883  0.5407
507SOL     OW 1553   0.255   2.951   1.753 -0.1694 -0.0692 -0.1505
507SOL    HW1 1554   0.256   3.042   1.712 -0.6228  0.6278  1.3290
507SOL    HW2 1555   0.330   2.897   1.715  0.6477  1.2059 -0.4153
508SOL     OW 1556   0.943   0.078   0.961  0.0358 -0.5137 -0.5114
508SOL    HW1 1557   0.947  -0.004   0.904  0.0075 -1.3168  0.6154
508SOL    HW2 1558   0.860   0.076   1.017  0.1061  0.2149 -0.3741
509SOL     OW 1559   1.695   0.436   0.743  0.0032 -0.0184 -0.8685
509SOL    HW1 1560   1.648   0.366   0.689  0.6511 -0.3220 -1.0593
509SOL    HW2 1561   1.663   0.432   0.837 -1.1663  0.5415 -1.2190
510SOL     OW 1562   1.413   0.581   0.924  0.0517 -0.1890 -0.0881
510SOL    HW1 1563   1.452   0.652   0.864  1.1061 -0.2776  0.4596
510SOL    HW2 1564   1.370   0.625   1.003 -1.3095 -0.0737 -0.8726
511SOL     OW 1565   0.765   1.189   0.318  0.2282 -0.2502 -0.2431
511SOL    HW1 1566   0.693   1.253   0.292 -0.3641 -0.6970  0.2466
511SOL    HW2 1567   0.726   1.096   0.323  1.1394 -0.6956 -1.2599
512SOL     OW 1568   0.311   0.237   1.115  0.0927  0.1680 -0.1919
512SOL    HW1 1569   0.230   0.211   1.167  0.0116 -2.2505 -1.3916
512SOL    HW2 1570   0.388   0.181   1.144  0.7111  0.6843 -0.8142
513SOL     OW 1571   2.873   0.897   0.019  0.0336  0.4078  0.0118
513SOL    HW1 1572   2.886   0.874   0.116  0.4896 -1.4263 -0.4270
513SOL    HW2 1573   2.922   0.981  -0.002 -0.0878  0.8440  1.3822
514SOL     OW 1574   0.702   1.038   2.009  0.4108 -0.7448 -0.0881
514SOL    HW1 1575   0.800   1.018   2.002  0.0456 -2.4138 -1.0733
514SOL    HW2 1576   0.672   1.084   1.925  0.1746 -1.1676 -0.2425
515SOL     OW 1577   0.891   2.928   2.147 -0.1855 -0.3121  0.0779
515SOL    HW1 1578   0.896   3.025   2.170 -1.8401  0.0723 -0.9436
515SOL    HW2 1579   0.950   2.875   2.208  3.4329  1.6339 -1.4495
516SOL     OW 1580   2.580   2.965   2.170  0.4128 -0.3047  0.2088
516SOL    HW1 1581   2.492   2.917   2.167  1.1885 -1.7321 -1.6055
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516SOL    HW2 1582   2.565    3.062    2.146 -0.6958 -0.4588  0.1986
517SOL    OW 1583    1.964    0.325    1.659  0.2039  0.1013 -0.6113
517SOL    HW1 1584   1.873    0.286    1.651  0.5841 -0.9001 -0.2421
517SOL    HW2 1585   2.028    0.272    1.602  0.4900  1.0437 -1.1970
518SOL    OW 1586    0.374    1.175    0.391 -0.0085  0.6984 -0.4485
518SOL    HW1 1587   0.293    1.234    0.391 -0.1351  0.6571  2.5245
518SOL    HW2 1588   0.455    1.231    0.377 -0.3220  1.2405 -0.1607
519SOL    OW 1589    2.580    0.603    0.998 -0.3671  0.0251 -0.1597
519SOL    HW1 1590   2.611    0.531    1.060 -1.3405 -0.1244  0.1702
519SOL    HW2 1591   2.637    0.684    1.009 -0.8282  0.1807  1.3027
520SOL    OW 1592    2.674    0.857    1.034 -0.0816 -0.4593 -0.2549
520SOL    HW1 1593   2.637    0.887    1.123  1.3523 -0.6659  0.4434
520SOL    HW2 1594   2.670    0.933    0.970  1.4272  0.5995  0.8309
521SOL    OW 1595    0.214    3.079    2.016  0.2701 -0.0706 -0.1723
521SOL    HW1 1596   0.218    2.987    1.977 -2.6276  0.3292 -1.6852
521SOL    HW2 1597   0.154    3.137    1.960  1.2461  2.5019  1.2554
522SOL    OW 1598    1.402    0.063    0.459 -0.0674 -0.0855 -0.0629
522SOL    HW1 1599   1.370   -0.024    0.498 -1.4640 -0.2368 -1.4491
522SOL    HW2 1600   1.324    0.114    0.423  0.8898  1.1586 -0.4559
523SOL    OW 1601    2.589    0.630    2.170 -0.4337 -0.4877 -0.5193
523SOL    HW1 1602   2.676    0.595    2.204 -1.1576 -1.1065  0.7625
523SOL    HW2 1603   2.547    0.690    2.238 -1.4409 -0.9328 -0.7211
524SOL    OW 1604    2.599    0.273    0.545 -0.8381 -0.1701 -0.0545
524SOL    HW1 1605   2.525    0.340    0.542 -0.0852  0.7587  1.0345
524SOL    HW2 1606   2.674    0.302    0.486 -0.4123  0.0813  0.5982
525SOL    OW 1607    2.347    2.520    0.843 -0.1027 -0.0150 -0.2682
525SOL    HW1 1608   2.287    2.586    0.798 -0.7385 -0.4547 -0.0806
525SOL    HW2 1609   2.319    2.508    0.938  1.1581  0.8190  0.2277
526SOL    OW 1610    1.011    2.224    2.104 -0.6185  0.1390  0.2315
526SOL    HW1 1611   1.060    2.141    2.131 -3.0935 -1.3708  0.3555
526SOL    HW2 1612   0.981    2.274    2.185  1.2961  1.5320  0.1680
527SOL    OW 1613    2.002    1.062    1.854  0.1875  0.8113  0.3818
527SOL    HW1 1614   1.990    0.999    1.777  0.4644 -0.8818  1.6535
527SOL    HW2 1615   2.099    1.087    1.862  0.2643  0.4791  0.5330
528SOL    OW 1616    0.236    0.137    0.555  0.1898 -0.1294 -0.1402
528SOL    HW1 1617   0.316    0.078    0.548 -0.4082 -0.9012 -0.6965
528SOL    HW2 1618   0.157    0.082    0.583 -0.7959  0.0023 -2.4429
529SOL    OW 1619    1.305    0.819    0.501 -1.0946 -0.5029 -0.0977
529SOL    HW1 1620   1.268    0.726    0.504 -0.7982 -0.7629 -2.4021
529SOL    HW2 1621   1.306    0.851    0.406  1.4810  0.7516  0.2672
530SOL    OW 1622    0.533    2.375    0.507  0.1564 -0.5595  0.4442
530SOL    HW1 1623   0.438    2.353    0.525  0.5913 -2.4202  0.6319
530SOL    HW2 1624   0.552    2.367    0.409 -0.3168  1.8288  0.0837
531SOL    OW 1625    1.727    1.239    2.133 -0.0433  0.0102 -0.1520
531SOL    HW1 1626   1.826    1.230    2.123  0.0762 -1.1688  1.5821
531SOL    HW2 1627   1.682    1.159    2.092 -0.0796 -0.6879  1.1899
532SOL    OW 1628    0.151    1.308    0.614 -0.0479  0.2777 -0.2734
532SOL    HW1 1629   0.125    1.238    0.681 -2.0110  1.9496  0.8015
532SOL    HW2 1630   0.251    1.321    0.617  0.0574 -0.5880  1.4132
533SOL    OW 1631    0.973    0.332    0.342  0.1046 -0.2477 -0.2771
533SOL    HW1 1632   0.900    0.372    0.397 -0.1554 -1.9410  0.6648
533SOL    HW2 1633   0.946    0.330    0.246  0.1133  1.7276 -0.3731
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534SOL    OW 1634   2.554   2.635   1.133  0.5773 -0.1025 -0.3390
534SOL   HW1 1635   2.568   2.700   1.207  0.0201  0.4676 -0.7243
534SOL   HW2 1636   2.458   2.608   1.130  0.9002 -1.3808  0.1626
535SOL    OW 1637   1.289   2.341   0.814 -0.0831  0.0096  0.1141
535SOL   HW1 1638   1.317   2.404   0.742 -0.7423  1.8939  1.4108
535SOL   HW2 1639   1.302   2.385   0.903 -0.8199 -1.6139  1.0668
536SOL    OW 1640   0.390   2.838   2.029 -0.0966  0.3264 -0.1784
536SOL   HW1 1641   0.465   2.794   2.077  0.2629  0.1061 -0.9238
536SOL   HW2 1642   0.303   2.814   2.072  0.1966 -0.1268  0.1550
537SOL    OW 1643   0.596   0.231   0.334 -0.2350  0.0857  0.4157
537SOL   HW1 1644   0.553   0.162   0.391 -0.3038 -0.8757 -0.7693
537SOL   HW2 1645   0.546   0.317   0.342 -1.2348 -0.5000  0.5148
538SOL    OW 1646   2.766   1.916   1.846  0.2672 -0.4061  0.2044
538SOL   HW1 1647   2.820   1.972   1.908 -0.8226  0.5962  0.2838
538SOL   HW2 1648   2.752   1.965   1.760 -1.3101 -0.2149  0.5362
539SOL    OW 1649   3.001   1.093   0.934 -0.0663 -0.4023 -0.3713
539SOL   HW1 1650   2.957   1.079   0.845  0.1919 -2.5710 -0.2007
539SOL   HW2 1651   2.943   1.152   0.991 -0.1109  1.2515 -2.0155
540SOL    OW 1652   1.472   2.063   1.050  0.0283  0.0663 -0.5595
540SOL   HW1 1653   1.492   2.021   1.138  1.8159  1.7215 -0.1046
540SOL   HW2 1654   1.375   2.054   1.029 -0.3618 -0.6317  1.4126
541SOL    OW 1655   2.406   1.542   0.521 -0.1571  0.0543 -0.3422
541SOL   HW1 1656   2.406   1.575   0.427  0.7353 -0.0465 -0.3880
541SOL   HW2 1657   2.461   1.603   0.578  1.3464 -1.1831 -0.3833
542SOL    OW 1658   2.622   0.672   0.398 -0.0019  0.0122  0.4126
542SOL   HW1 1659   2.575   0.749   0.439 -0.3374 -0.5004  1.0098
542SOL   HW2 1660   2.603   0.589   0.450 -0.6712 -0.7164 -0.9208
543SOL    OW 1661   0.360   2.613   0.727  0.4075 -0.0077  0.4259
543SOL   HW1 1662   0.362   2.523   0.771 -1.2240  0.0457  0.6693
543SOL   HW2 1663   0.290   2.613   0.656  0.8589  0.8763 -0.0311
544SOL    OW 1664   1.455   3.009   1.400 -0.3064 -0.3017 -0.3237
544SOL   HW1 1665   1.440   3.094   1.350  0.4379 -0.7920 -1.4247
544SOL   HW2 1666   1.367   2.967   1.422 -0.6557 -0.1119 -1.3127
545SOL    OW 1667   2.729   2.630   0.104  0.5463 -0.0886 -0.3368
545SOL   HW1 1668   2.662   2.696   0.068 -1.9063 -0.4712  2.9763
545SOL   HW2 1669   2.681   2.546   0.131  2.4239 -0.5910  1.7195
546SOL    OW 1670   0.418   0.137   0.768 -0.5103 -0.0733  0.1063
546SOL   HW1 1671   0.476   0.093   0.837 -1.6655 -1.0797  0.4722
546SOL   HW2 1672   0.451   0.113   0.677  0.8578  1.0311  0.2858
547SOL    OW 1673   0.612   1.391   1.916  0.6177 -0.3251 -0.1258
547SOL   HW1 1674   0.548   1.365   1.988  1.3847 -2.6435 -0.1957
547SOL   HW2 1675   0.633   1.311   1.859  1.7298  0.9275 -1.5889
548SOL    OW 1676   1.277   2.486   1.744  0.2791 -0.3279  0.0580
548SOL   HW1 1677   1.245   2.461   1.835 -0.3446  2.1082  0.6061
548SOL   HW2 1678   1.374   2.464   1.734  0.4524 -0.2658  1.4649
549SOL    OW 1679   1.662   2.344   0.141  0.0097  0.3667  0.1752
549SOL   HW1 1680   1.619   2.386   0.061 -0.6167  1.6474  1.1455
549SOL   HW2 1681   1.659   2.244   0.132 -2.0609  0.4343 -0.3846
550SOL    OW 1682   0.371   1.675   0.336 -0.5913  0.2758 -0.4255
550SOL   HW1 1683   0.374   1.736   0.415  0.9012  0.8098 -0.8451
550SOL   HW2 1684   0.300   1.607   0.349 -0.9157  0.8455  1.0062
551SOL    OW 1685   2.548   2.344   1.290  0.2731  0.4680 -0.0096
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551SOL    HW1 1686   2.595   2.302   1.368 -0.7010 -0.3650  0.1506
551SOL    HW2 1687   2.583   2.304   1.205 -1.7124 -1.9417  0.1798
552SOL     OW 1688   1.284   2.909   0.416 -0.9002  0.5129  0.3786
552SOL    HW1 1689   1.258   2.966   0.337  0.4630  0.6803  0.0210
552SOL    HW2 1690   1.383   2.899   0.418 -0.9034  0.5936  2.1515
553SOL     OW 1691   3.085   0.209   0.789 -0.1664  0.6095 -0.1191
553SOL    HW1 1692   3.067   0.302   0.758  0.9117  1.8042  2.4718
553SOL    HW2 1693   3.175   0.206   0.832 -0.9779 -1.1243  1.6099
554SOL     OW 1694   1.564   2.721   1.653 -0.4989 -1.0627  0.5683
554SOL    HW1 1695   1.530   2.627   1.658 -0.2920 -1.0892  1.6980
554SOL    HW2 1696   1.571   2.749   1.557 -1.3525 -1.9066  0.2462
555SOL     OW 1697   1.220   0.298   1.527 -0.0374  0.0889  0.7236
555SOL    HW1 1698   1.212   0.397   1.532 -3.8874 -0.0572  0.6669
555SOL    HW2 1699   1.261   0.263   1.611  2.6148  1.7025  0.2001
556SOL     OW 1700   2.986   2.036   0.800  0.1305 -0.3063  0.4426
556SOL    HW1 1701   3.077   2.030   0.839  0.4974  1.2690 -0.1154
556SOL    HW2 1702   2.919   2.051   0.873  0.4078 -0.6071  0.7623
557SOL     OW 1703   1.253   0.998   1.765  0.3272  0.2665  0.0156
557SOL    HW1 1704   1.343   0.990   1.807  0.2059  2.2376  0.7443
557SOL    HW2 1705   1.218   1.091   1.777 -2.0712 -0.5911  0.2800
558SOL     OW 1706   1.437   1.469   1.269  0.1552  0.1698 -0.3517
558SOL    HW1 1707   1.455   1.456   1.171 -1.0332 -0.7516 -0.4658
558SOL    HW2 1708   1.474   1.392   1.320 -0.0281  0.2090 -0.1623
559SOL     OW 1709   3.049   2.179   0.298 -0.7746  0.4528 -0.5089
559SOL    HW1 1710   3.069   2.147   0.391 -0.3663 -1.6757 -1.2828
559SOL    HW2 1711   2.976   2.123   0.259 -0.5382  0.9453 -1.6845
560SOL     OW 1712   0.996   2.639   1.622  0.1203  0.2521  0.1121
560SOL    HW1 1713   0.944   2.662   1.703 -0.7413  0.3870 -0.4647
560SOL    HW2 1714   1.094   2.642   1.642 -0.0763  0.7742  0.9982
561SOL     OW 1715   0.552   0.903   2.188 -0.5641 -0.3704 -0.7909
561SOL    HW1 1716   0.456   0.924   2.172 -0.6398 -0.0826 -0.0207
561SOL    HW2 1717   0.609   0.969   2.140 -0.7848  0.5619  0.1797
562SOL     OW 1718   1.031   3.093   1.597  0.8594  0.3839  0.4718
562SOL    HW1 1719   1.049   3.134   1.687  0.4717 -1.2821  1.3507
562SOL    HW2 1720   1.117   3.059   1.559  0.8102 -0.3068  0.9512
563SOL     OW 1721   0.729   1.968   1.325 -0.3150 -0.3458 -0.8711
563SOL    HW1 1722   0.794   2.041   1.346 -1.9896  1.0754 -0.3940
563SOL    HW2 1723   0.777   1.881   1.320  1.6505  0.6870 -0.8331
564SOL     OW 1724   0.329   1.299   1.699  0.1771 -0.2517 -0.1491
564SOL    HW1 1725   0.230   1.292   1.689  0.2285  0.5169 -1.5062
564SOL    HW2 1726   0.351   1.374   1.761 -0.0960  0.2266 -0.6165
565SOL     OW 1727   2.809   1.399   1.034  0.0699  0.4196  0.2600
565SOL    HW1 1728   2.812   1.494   1.062  2.7203  0.6806 -0.6357
565SOL    HW2 1729   2.831   1.340   1.112 -1.0446  0.5331  0.6821
566SOL     OW 1730   0.170   2.413   0.237 -0.0347  0.4104  0.0897
566SOL    HW1 1731   0.143   2.321   0.209  0.8087  0.5780 -1.3582
566SOL    HW2 1732   0.118   2.480   0.185  1.0618  0.7277 -0.6361
567SOL     OW 1733   0.823   2.644   0.241 -0.1186  0.2561 -0.2393
567SOL    HW1 1734   0.858   2.649   0.335 -0.3116 -1.4871 -0.0405
567SOL    HW2 1735   0.895   2.608   0.181 -0.1742  0.8474 -0.6654
568SOL     OW 1736   0.018   0.123   1.854  0.3428 -0.6029  0.3900
568SOL    HW1 1737   0.102   0.178   1.853 -0.5766  0.9008  1.5912
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568SOL   HW2 1738  -0.002   0.091   1.761   2.3845 -1.2522  0.1275
569SOL    OW 1739   1.879   1.372   0.499  -0.4294 -0.3201  0.0136
569SOL   HW1 1740   1.928   1.444   0.548  -1.5146  0.4065  0.0525
569SOL   HW2 1741   1.787   1.403   0.477  -0.4680 -1.2035 -1.1578
570SOL    OW 1742   2.365   0.029   0.721  -0.6558  0.9277  0.4886
570SOL   HW1 1743   2.384  -0.064   0.751  -0.4903  0.0853 -1.9883
570SOL   HW2 1744   2.424   0.093   0.771   1.4083 -0.6054  0.1313
571SOL    OW 1745   0.374   1.693   1.559   0.0531 -0.1171  1.2707
571SOL   HW1 1746   0.317   1.775   1.563  -0.6859 -0.5787  0.3793
571SOL   HW2 1747   0.392   1.660   1.652   0.4682  1.1132  1.6494
572SOL    OW 1748   2.196   0.565   1.378   0.2253 -0.4636  0.2214
572SOL   HW1 1749   2.229   0.504   1.450   1.2940 -1.2228 -0.8776
572SOL   HW2 1750   2.263   0.570   1.305  -0.8117  0.3299 -0.7163
573SOL    OW 1751   2.283   2.102   0.634   0.0013 -0.0483  0.0812
573SOL   HW1 1752   2.233   2.025   0.676  -2.3082  1.4183  0.1911
573SOL   HW2 1753   2.236   2.130   0.551   0.3453  1.7390  0.4623
574SOL    OW 1754   0.955   2.102   1.051  -0.0207  0.3331 -0.4544
574SOL   HW1 1755   0.887   2.174   1.040  -1.9930 -1.2307  0.8440
574SOL   HW2 1756   0.913   2.013   1.031   1.8881 -0.6227 -0.4364
575SOL    OW 1757   0.113   3.034   0.685   0.5944 -0.0312 -0.1274
575SOL   HW1 1758   0.130   3.015   0.782   1.7005 -0.9278 -0.4790
575SOL   HW2 1759   0.015   3.038   0.669   0.3995  1.3841  1.2617
576SOL    OW 1760   0.099   2.902   0.339   0.0846  0.9495 -0.2886
576SOL   HW1 1761   0.019   2.941   0.292  -0.3329  1.0786  0.5142
576SOL   HW2 1762   0.116   2.953   0.423   0.8863  0.7771 -0.3411
577SOL    OW 1763   1.139   1.449   1.496   0.0304  0.4785 -0.2262
577SOL   HW1 1764   1.172   1.497   1.577   0.0523  0.9518 -0.5096
577SOL   HW2 1765   1.204   1.461   1.421   0.0742 -0.0637 -0.2809
578SOL    OW 1766   2.616   2.995   1.693  -0.6110  0.9208 -0.4885
578SOL   HW1 1767   2.707   2.955   1.684  -0.5939  1.2285 -1.8289
578SOL   HW2 1768   2.568   2.952   1.771   0.0714 -0.3896 -0.7612
579SOL    OW 1769   0.270   2.039   1.521   0.6561  0.7161  0.0128
579SOL   HW1 1770   0.200   2.044   1.450   0.1728  0.2425  0.4486
579SOL   HW2 1771   0.358   2.012   1.481  -0.1455 -2.0529 -0.0858
580SOL    OW 1772   2.998   1.193   1.467   0.6600  0.1839  0.1545
580SOL   HW1 1773   3.006   1.211   1.565  -1.0128 -0.5968  0.4691
580SOL   HW2 1774   2.909   1.153   1.447   1.6375 -1.3930 -1.4337
581SOL    OW 1775   2.168   0.794   0.671  -0.7347 -0.7491 -0.2409
581SOL   HW1 1776   2.240   0.760   0.732  -0.2239 -1.0828 -1.0140
581SOL   HW2 1777   2.136   0.883   0.704  -2.2263 -2.0058  1.9337
582SOL    OW 1778   0.856   2.113   1.909   0.2796 -0.3369  0.1399
582SOL   HW1 1779   0.929   2.149   1.966   0.8363 -2.0396  0.5427
582SOL   HW2 1780   0.842   2.016   1.928  -2.7356  0.0946  0.7603
583SOL    OW 1781   0.985   0.104   0.064  -0.2187 -0.2474 -0.0346
583SOL   HW1 1782   0.954   0.045   0.139   1.7952 -0.0633  1.0122
583SOL   HW2 1783   0.935   0.191   0.067  -0.3199 -0.3323  0.9641
584SOL    OW 1784   2.066   2.224   1.287  -0.8722  0.1793  0.1004
584SOL   HW1 1785   2.078   2.302   1.348   0.0854 -0.1938  0.4072
584SOL   HW2 1786   1.973   2.224   1.251  -1.0309  1.1874  0.4700
585SOL    OW 1787   0.216   2.049   1.120  -0.0552 -0.3659  0.0302
585SOL   HW1 1788   0.176   2.017   1.206   0.3400 -2.3516 -0.4757
585SOL   HW2 1789   0.312   2.020   1.115  -0.3114 -1.0353 -1.4350
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586SOL    OW 1790   0.770   2.529   0.568   0.4768  0.3135  0.2886
586SOL   HW1 1791   0.693   2.473   0.536   0.8385 -1.0299  1.6304
586SOL   HW2 1792   0.735   2.604   0.623   0.0854 -0.0600  0.5633
587SOL    OW 1793   1.272   0.941   1.497   0.4616 -0.6658  0.3107
587SOL   HW1 1794   1.367   0.922   1.473   0.4308  1.1177 -1.5444
587SOL   HW2 1795   1.269   0.986   1.587   1.3123 -1.1409  0.5899
588SOL    OW 1796   2.253   2.311   2.147   0.3548 -0.2400 -0.2795
588SOL   HW1 1797   2.293   2.378   2.085  -2.6143  2.9767  0.9588
588SOL   HW2 1798   2.191   2.251   2.096   0.0477  0.5637 -0.8639
589SOL    OW 1799   1.070   1.600   0.698   0.7935  0.5580  0.4368
589SOL   HW1 1800   1.091   1.503   0.715   0.2466  0.4059  0.2670
589SOL   HW2 1801   1.036   1.611   0.605   2.9466  1.2642 -0.3052
590SOL    OW 1802   0.697   0.764   1.298  -0.5497 -0.0579  0.1787
590SOL   HW1 1803   0.783   0.737   1.340  -0.2299 -1.0306 -1.0540
590SOL   HW2 1804   0.636   0.802   1.369   1.8701  3.3931  0.6516
591SOL    OW 1805   1.116   0.087   1.164  -0.2716 -0.0164 -1.0736
591SOL   HW1 1806   1.078   0.036   1.087  -0.0928  0.3165 -1.3882
591SOL   HW2 1807   1.043   0.107   1.230  -0.5392  0.1647 -1.4188
592SOL    OW 1808   1.141   0.363   1.915   0.0422 -0.7196  0.3127
592SOL   HW1 1809   1.093   0.434   1.862   0.7079  0.7498  1.5990
592SOL   HW2 1810   1.237   0.359   1.886   0.3816  0.0110  1.2580
593SOL    OW 1811   0.058   1.486   1.505   0.2318 -0.1420  0.9717
593SOL   HW1 1812   0.152   1.495   1.473  -0.0984 -0.4839 -0.1365
593SOL   HW2 1813  -0.005   1.488   1.427  -0.6131 -0.9913  1.6014
594SOL    OW 1814   3.101   0.231   0.100  -0.7072 -0.1234 -0.6325
594SOL   HW1 1815   3.095   0.293   0.022   0.3930 -0.7604 -1.2420
594SOL   HW2 1816   3.186   0.180   0.096  -0.0165  0.7091  1.6588
595SOL    OW 1817   0.014   2.080   1.760   0.0808  0.1794  0.2252
595SOL   HW1 1818  -0.015   2.082   1.664   1.2026  0.7069 -0.1281
595SOL   HW2 1819   0.107   2.043   1.765   0.3971  1.0635  1.0094
596SOL    OW 1820   1.012   1.341   1.020   0.6034  0.1614  0.1023
596SOL   HW1 1821   0.961   1.341   1.106  -0.4609 -0.9305 -0.4989
596SOL   HW2 1822   0.948   1.337   0.943   1.5697 -0.6923 -0.6915
597SOL    OW 1823   0.433   1.337   0.632  -0.2667 -0.1024 -0.1528
597SOL   HW1 1824   0.525   1.376   0.633   0.2055 -1.1735  0.0868
597SOL   HW2 1825   0.438   1.240   0.656  -1.3787 -0.3605 -0.8988
598SOL    OW 1826   0.870   2.130   1.630   0.0915 -0.2579 -0.1194
598SOL   HW1 1827   0.922   2.211   1.602  -0.2159 -0.0975 -0.2337
598SOL   HW2 1828   0.864   2.127   1.730   0.9276 -0.6646 -0.0702
599SOL    OW 1829   0.444   2.197   2.178   0.7932  0.2803 -0.6262
599SOL   HW1 1830   0.363   2.159   2.133   0.4860  1.3206 -0.9681
599SOL   HW2 1831   0.495   2.123   2.222  -1.2151 -0.2167  1.0237
600SOL    OW 1832   1.074   2.647   2.201   0.1578  0.0786  0.1754
600SOL   HW1 1833   1.133   2.567   2.212  -0.7597 -0.4451  1.5652
600SOL   HW2 1834   0.978   2.619   2.208  -0.2627  1.0178 -1.3145
601SOL    OW 1835   1.853   2.758   0.783   0.1944 -0.0759 -0.1427
601SOL   HW1 1836   1.948   2.728   0.789  -0.1224 -0.9088  1.3054
601SOL   HW2 1837   1.829   2.810   0.865  -0.1196  1.6667 -1.2956
602SOL    OW 1838   0.730   0.659   2.155  -0.0114 -0.6249  0.0319
602SOL   HW1 1839   0.762   0.629   2.245  -1.2168 -0.3722  0.5674
602SOL   HW2 1840   0.663   0.733   2.166   0.2201 -0.2191 -1.1004
603SOL    OW 1841   2.988   2.132   1.539   0.8794 -0.3223 -0.7504
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603SOL   HW1 1842   3.032   2.192   1.472  0.1182  1.6382  0.4481
603SOL   HW2 1843   2.957   2.048   1.493 -0.4804  1.3510 -3.0888
604SOL    OW 1844   2.283   0.325   1.500 -0.2729  0.0374 -0.2245
604SOL   HW1 1845   2.210   0.257   1.492  1.9340 -2.3314 -2.6179
604SOL   HW2 1846   2.348   0.313   1.424  1.8905  2.8960  0.9789
605SOL    OW 1847   2.062   2.596   0.982 -0.1235 -0.0754 -0.0914
605SOL   HW1 1848   2.058   2.696   0.975 -0.4163 -0.1751 -2.0640
605SOL   HW2 1849   1.984   2.563   1.034 -1.1904  0.6283 -1.1804
606SOL    OW 1850   0.775   1.624   1.599  0.0853 -0.7858 -0.0379
606SOL   HW1 1851   0.690   1.617   1.548 -0.3112 -1.9601  0.7408
606SOL   HW2 1852   0.818   1.534   1.605  1.1249 -0.3100  0.0364
607SOL    OW 1853   0.347   1.490   0.868 -0.2288  0.8056  0.3282
607SOL   HW1 1854   0.359   1.437   0.785 -0.4823  2.1616 -0.6019
607SOL   HW2 1855   0.249   1.503   0.886 -0.1825  0.3666  0.9590
608SOL    OW 1856   2.302   1.598   0.234 -0.3023 -0.0217  0.6293
608SOL   HW1 1857   2.372   1.611   0.165 -0.0473 -0.3322  0.8275
608SOL   HW2 1858   2.226   1.662   0.218 -0.0150  0.2531  0.3664
609SOL    OW 1859   0.039   3.012   1.390  0.4080  0.2839  0.3213
609SOL   HW1 1860   0.106   2.941   1.368  0.1653 -0.0097  0.5170
609SOL   HW2 1861  -0.054   2.977   1.372  0.1488 -0.2044  2.3683
610SOL    OW 1862   2.112   0.252   1.883 -0.5548  0.0026  0.6060
610SOL   HW1 1863   2.174   0.330   1.893  0.0079 -0.3131 -0.2982
610SOL   HW2 1864   2.051   0.268   1.806 -1.0861 -0.0360  1.0116
611SOL    OW 1865   2.046   1.301   0.159  0.3985  0.0297  0.1914
611SOL   HW1 1866   2.087   1.238   0.093 -2.0197  0.1124 -1.4798
611SOL   HW2 1867   1.950   1.278   0.173 -0.1039  2.2807  0.8695
612SOL    OW 1868   0.989   1.732   1.885 -0.0498  0.2814  0.1872
612SOL   HW1 1869   0.938   1.796   1.826 -0.6735 -2.1435 -2.0845
612SOL   HW2 1870   0.958   1.743   1.979 -0.3500  3.0498 -0.1380
613SOL    OW 1871   0.082   2.682   0.155  0.1085 -0.1418 -0.5660
613SOL   HW1 1872   0.097   2.730   0.068 -2.2304  1.4736 -0.1629
613SOL   HW2 1873   0.107   2.742   0.231  1.1595 -1.1742 -0.0587
614SOL    OW 1874   2.876   2.829   0.238  0.3533 -0.4407 -0.2290
614SOL   HW1 1875   2.844   2.765   0.169 -1.5585  0.3697 -0.1455
614SOL   HW2 1876   2.871   2.787   0.329 -0.3474 -0.3672 -0.2337
615SOL    OW 1877   2.926   0.091   2.175  0.4305 -0.0612 -0.1026
615SOL   HW1 1878   2.930   0.131   2.084  1.9020 -1.1002 -0.5270
615SOL   HW2 1879   3.014   0.050   2.198  0.1061  0.2113  1.8175
616SOL    OW 1880   0.865   0.657   0.607 -0.1557  0.4992 -0.0951
616SOL   HW1 1881   0.881   0.645   0.705 -0.2302 -0.4295 -0.1806
616SOL   HW2 1882   0.838   0.569   0.567  0.0773  0.8211 -0.9887
617SOL    OW 1883   2.872   0.214   1.549 -0.2502 -0.0527  0.4413
617SOL   HW1 1884   2.955   0.268   1.543 -0.1035 -0.1987  1.0256
617SOL   HW2 1885   2.813   0.252   1.621 -0.5500 -0.1286  0.2381
618SOL    OW 1886   2.272   2.858   1.560  0.4747 -0.0515  0.4342
618SOL   HW1 1887   2.313   2.945   1.588 -0.4283  0.1366  1.1953
618SOL   HW2 1888   2.286   2.845   1.461  1.7331  0.3349  0.5437
619SOL    OW 1889   0.562   2.769   1.529 -0.0906  0.2295  0.1128
619SOL   HW1 1890   0.545   2.781   1.626 -1.6207  1.0019 -0.2118
619SOL   HW2 1891   0.660   2.772   1.511  0.1344  3.8942  1.2074
620SOL    OW 1892   2.287   3.147   0.234  0.8567 -0.4137 -0.4152
620SOL   HW1 1893   2.283   3.053   0.269 -0.0447 -0.6100 -1.0280
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620SOL    HW2 1894   2.203   3.168   0.184  1.0041  0.7572 -0.2045
621SOL     OW 1895   0.648   1.575   0.698 -0.3902  0.5068 -0.1191
621SOL    HW1 1896   0.583   1.632   0.748  0.7500  0.6187  1.3172
621SOL    HW2 1897   0.730   1.561   0.755  0.0794 -1.1191 -1.1472
622SOL     OW 1898   1.364   2.561   0.632 -0.6794 -0.1689  0.2966
622SOL    HW1 1899   1.344   2.573   0.535 -0.3819 -0.3246  0.2139
622SOL    HW2 1900   1.457   2.593   0.651 -1.1476  0.9856  0.7637
623SOL     OW 1901   2.316   2.269   1.171 -0.5102  0.0908  0.1947
623SOL    HW1 1902   2.388   2.278   1.240  0.3251  0.6675 -0.7257
623SOL    HW2 1903   2.234   2.233   1.214  0.9314 -2.6665  0.8965
624SOL     OW 1904   2.568   2.781   1.357 -0.3011  0.1245 -0.6175
624SOL    HW1 1905   2.518   2.865   1.378  0.5666  0.9136 -1.6061
624SOL    HW2 1906   2.658   2.785   1.400 -0.1311 -0.1622 -0.9490
625SOL     OW 1907   1.238   1.823   1.998  0.3292  0.1566  0.0172
625SOL    HW1 1908   1.176   1.865   1.931  0.4171  0.8073  0.3400
625SOL    HW2 1909   1.306   1.768   1.950  0.1968  0.3619 -0.4117
626SOL     OW 1910   0.989   0.543   0.848  0.1362 -0.3831 -0.0948
626SOL    HW1 1911   1.075   0.553   0.798  0.5442 -0.5703  0.5581
626SOL    HW2 1912   0.991   0.458   0.901 -0.6629 -0.6538 -0.4800
627SOL     OW 1913   2.954   1.919   1.162  0.5091  0.0498  0.2549
627SOL    HW1 1914   2.966   1.832   1.115 -2.4036 -1.3511  1.8181
627SOL    HW2 1915   2.893   1.978   1.108 -0.3473 -0.3339  0.7736
628SOL     OW 1916   0.058   1.272   1.677 -0.6870  0.5026 -0.3290
628SOL    HW1 1917   0.047   1.345   1.610  0.2630  1.5853  0.6318
628SOL    HW2 1918   0.012   1.298   1.762  0.2647  0.3326  0.2549
629SOL     OW 1919   1.918   1.662   1.955 -0.0400  0.1408  0.1795
629SOL    HW1 1920   1.956   1.599   2.023  0.3625  1.1009  0.8553
629SOL    HW2 1921   1.971   1.747   1.954 -0.0820  0.1873 -1.2831
630SOL     OW 1922   0.036   1.761   1.548 -0.3937 -0.1430  0.3497
630SOL    HW1 1923   0.044   1.661   1.547  1.9407 -0.0001 -0.4851
630SOL    HW2 1924   0.082   1.797   1.630  0.6896  0.3355 -0.4459
631SOL     OW 1925   0.555   1.919   1.859  0.8285  0.3445  0.4513
631SOL    HW1 1926   0.540   1.884   1.951  0.5098 -1.5596 -0.2620
631SOL    HW2 1927   0.642   1.882   1.824 -0.9982 -2.6095 -1.4992
632SOL     OW 1928   2.470   1.849   1.438 -0.7120  0.4367 -0.3697
632SOL    HW1 1929   2.544   1.887   1.493 -0.8896  1.1913 -0.6511
632SOL    HW2 1930   2.483   1.874   1.342 -0.1291 -1.2918 -0.7822
633SOL     OW 1931   2.811   0.347   0.417  0.4576 -0.7763  0.3944
633SOL    HW1 1932   2.878   0.274   0.402 -0.5459 -1.9420  1.4779
633SOL    HW2 1933   2.837   0.400   0.497  0.9902 -0.1304 -0.1857
634SOL     OW 1934   3.033   2.439   1.741 -0.0090 -0.0192 -0.0938
634SOL    HW1 1935   2.952   2.497   1.751 -0.0417  0.0718 -0.8240
634SOL    HW2 1936   3.005   2.347   1.713  0.1356  0.0077 -0.3312
635SOL     OW 1937   0.938   3.003   0.781  0.5327 -0.2011  0.5041
635SOL    HW1 1938   0.921   2.905   0.793  0.4658 -0.0847  1.4375
635SOL    HW2 1939   0.986   3.018   0.695  0.2014 -1.0163  0.1705
636SOL     OW 1940   0.978   0.941   2.008 -0.4570 -0.0759  0.2969
636SOL    HW1 1941   1.018   0.898   2.089 -0.0965  0.7152  0.5545
636SOL    HW2 1942   1.018   1.032   1.996  0.0051 -0.4419 -1.1703
637SOL     OW 1943   1.590   1.359   0.503  0.3797  0.7363 -0.2483
637SOL    HW1 1944   1.537   1.422   0.560  0.5607 -0.1832  0.9785
637SOL    HW2 1945   1.528   1.303   0.448 -0.1145 -1.5593  2.4682
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638SOL    OW 1946   1.179   1.240   1.291  0.0854  0.4007 -0.2558
638SOL   HW1 1947   1.137   1.329   1.278  0.9092  0.9479  0.6703
638SOL   HW2 1948   1.266   1.251   1.339 -0.0169 -0.9420  0.2904
639SOL    OW 1949   2.318   0.890   0.268  0.0339 -0.3383 -0.0196
639SOL   HW1 1950   2.331   0.968   0.330 -1.6672  0.5084 -0.6576
639SOL   HW2 1951   2.240   0.835   0.301  1.5019 -2.0993  0.6968
640SOL    OW 1952   2.224   1.239   1.904 -0.0351 -0.0626 -0.0507
640SOL   HW1 1953   2.307   1.231   1.960  1.4956 -0.2043 -2.2271
640SOL   HW2 1954   2.220   1.330   1.864 -0.8560 -0.1176 -0.0947
641SOL    OW 1955   2.423   0.698   0.784 -0.0673  0.5021  0.1086
641SOL   HW1 1956   2.493   0.677   0.851  0.1263  1.0440  0.0816
641SOL   HW2 1957   2.415   0.797   0.774  1.6373  0.4796 -2.4237
642SOL    OW 1958   2.578   1.328   0.362 -0.5692  0.2087  0.2197
642SOL   HW1 1959   2.614   1.322   0.269 -0.4500  1.5070  0.1712
642SOL   HW2 1960   2.493   1.276   0.368 -0.7419  0.3741 -0.6930
643SOL    OW 1961   1.752   2.854   1.024  0.0825  0.1216  0.4125
643SOL   HW1 1962   1.711   2.945   1.030 -2.2479 -0.7566 -0.9704
643SOL   HW2 1963   1.832   2.850   1.085 -0.1864  2.8146  1.0941
644SOL    OW 1964   0.754   2.352   1.308  0.2489 -0.1850 -0.1958
644SOL   HW1 1965   0.778   2.432   1.363  0.1894 -1.4554  1.7947
644SOL   HW2 1966   0.822   2.280   1.323  0.5384 -0.4062 -2.2753
645SOL    OW 1967   1.310   0.954   0.934 -0.3237 -0.7044 -0.0033
645SOL   HW1 1968   1.345   0.918   0.848  1.8660 -0.3982  0.7031
645SOL   HW2 1969   1.382   1.005   0.981 -1.7551 -0.0098  1.5615
646SOL    OW 1970   2.851   1.170   2.072 -0.4086 -0.0897 -0.4920
646SOL   HW1 1971   2.871   1.235   2.145 -0.1724 -0.0560 -0.5865
646SOL   HW2 1972   2.769   1.199   2.023 -0.2946  0.1431 -0.5443
647SOL    OW 1973   2.872   1.597   1.478  0.5376 -0.4007 -0.3651
647SOL   HW1 1974   2.885   1.544   1.561 -0.7346 -0.9135 -0.4691
647SOL   HW2 1975   2.933   1.563   1.407 -0.0033 -1.4990 -0.3255
648SOL    OW 1976   1.275   0.252   0.259  0.1522  0.8040 -0.8862
648SOL   HW1 1977   1.241   0.345   0.243  2.2932  1.5692 -1.3046
648SOL   HW2 1978   1.304   0.213   0.171 -0.3374 -0.1273 -0.6467
649SOL    OW 1979   2.393   2.545   1.406  0.0901 -0.2612 -0.2578
649SOL   HW1 1980   2.451   2.472   1.370 -1.2495 -0.8187 -1.3672
649SOL   HW2 1981   2.440   2.633   1.395 -0.0700 -0.4419 -3.0421
650SOL    OW 1982   1.658   2.029   0.838  0.5615  0.2518 -0.4393
650SOL   HW1 1983   1.578   2.042   0.895 -0.4321 -0.5680 -1.5927
650SOL   HW2 1984   1.726   2.100   0.859  0.6854 -0.5852  2.4312
651SOL    OW 1985   0.588   0.782   1.556  0.3083  0.4910 -0.2452
651SOL   HW1 1986   0.543   0.729   1.628 -0.8722 -1.2367 -2.1473
651SOL   HW2 1987   0.673   0.821   1.591  0.7704 -1.9062  1.5264
652SOL    OW 1988   2.583   1.727   1.825 -0.2091  0.3528  0.2311
652SOL   HW1 1989   2.654   1.797   1.816  0.6251 -0.4683  0.2973
652SOL   HW2 1990   2.579   1.673   1.741  0.2830 -0.5445  0.7639
653SOL    OW 1991   1.595   1.054   1.963  0.5332 -0.8118  0.3273
653SOL   HW1 1992   1.677   1.068   1.906  1.9353 -1.0881  2.1681
653SOL   HW2 1993   1.577   0.956   1.972 -2.7595 -0.8187 -3.6504
654SOL    OW 1994   2.630   2.189   0.037 -0.4560 -0.4782 -0.2626
654SOL   HW1 1995   2.678   2.105   0.014 -0.2431 -0.2884 -0.5157
654SOL   HW2 1996   2.546   2.196  -0.018 -0.5526 -0.5986 -0.1313
655SOL    OW 1997   2.809   2.113   0.978  0.0749 -0.2190  0.0629
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655SOL   HW1 1998   2.710   2.113   0.989  0.2131  0.9271  1.5451
655SOL   HW2 1999   2.843   2.207   0.986  1.4070 -0.7546  0.9255
656SOL    OW 2000   1.180   1.947   1.372 -0.0560 -0.2088  0.3830
656SOL   HW1 2001   1.095   1.897   1.386 -0.2642  0.2825  0.9147
656SOL   HW2 2002   1.258   1.890   1.398 -0.1632 -0.9238 -0.7799
657SOL    OW 2003   1.035   2.524   1.097  0.5100 -0.0095 -0.3328
657SOL   HW1 2004   1.004   2.509   1.191 -1.9071 -0.6512 -1.1460
657SOL   HW2 2005   1.126   2.485   1.085  1.3404  1.0399  1.9803
658SOL    OW 2006   1.836   2.562   1.151  0.5433  0.4945 -0.0675
658SOL   HW1 2007   1.748   2.535   1.112  0.2467  1.2148  0.0944
658SOL   HW2 2008   1.835   2.548   1.250  0.8851 -0.2085 -0.1505
659SOL    OW 2009   1.363   0.293   1.770 -0.2159 -0.2173  0.2204
659SOL   HW1 2010   1.445   0.338   1.736 -0.9706  1.3225  0.3552
659SOL   HW2 2011   1.384   0.198   1.792  1.5623  0.1852  0.4134
660SOL    OW 2012   2.796   1.551   0.068 -0.0286  0.1008 -0.4912
660SOL   HW1 2013   2.800   1.454   0.092  0.1900  0.5395  1.4316
660SOL   HW2 2014   2.817   1.562  -0.029 -1.1080 -1.8504 -1.0130
661SOL    OW 2015   1.433   1.220   1.409 -0.3203 -0.2759 -0.0857
661SOL   HW1 2016   1.476   1.232   1.499 -1.8590 -0.4900  0.7041
661SOL   HW2 2017   1.456   1.129   1.374  0.4946 -0.0991 -0.0267
662SOL    OW 2018   1.607   0.402   1.000 -0.0401  0.0464  0.6118
662SOL   HW1 2019   1.674   0.451   1.056 -0.2014 -0.2108  1.0261
662SOL   HW2 2020   1.530   0.463   0.979 -1.1313 -0.5343  2.6440
663SOL    OW 2021   0.913   1.160   1.698 -1.0079  0.6889  0.0233
663SOL   HW1 2022   1.009   1.183   1.715 -1.2234  0.9615  0.8894
663SOL   HW2 2023   0.870   1.232   1.644 -0.3884 -0.0647 -1.5601
664SOL    OW 2024   1.997   1.787   1.569  0.4800 -0.3972 -0.2640
664SOL   HW1 2025   1.962   1.876   1.543  2.4451  0.7938  0.8606
664SOL   HW2 2026   2.072   1.761   1.507  1.3971 -0.1807  0.7204
665SOL    OW 2027   0.750   0.406   0.988  0.1667  0.0255 -0.3530
665SOL   HW1 2028   0.837   0.396   1.035  1.5397  0.1240 -2.7027
665SOL   HW2 2029   0.699   0.482   1.028  1.9603  1.1297 -0.0597
666SOL    OW 2030   0.170   2.736   2.164  0.1327  0.1819  0.7704
666SOL   HW1 2031   0.210   2.649   2.132  2.5051  1.1691  0.8417
666SOL   HW2 2032   0.172   2.738   2.264 -0.3180  0.1766  0.7838
667SOL    OW 2033   1.108   0.181   0.532  0.4571 -0.2195 -0.0367
667SOL   HW1 2034   1.106   0.215   0.626  2.1625  2.6501 -0.8975
667SOL   HW2 2035   1.077   0.254   0.470 -2.1695 -2.5372 -1.6764
668SOL    OW 2036   0.017   0.938   1.840  0.1415 -0.3552 -0.2608
668SOL   HW1 2037  -0.006   0.845   1.812  0.3880 -0.1734 -1.0661
668SOL   HW2 2038   0.062   0.985   1.766  0.9661  0.0777  0.4989
669SOL    OW 2039   0.674   2.310   2.073  0.0622 -0.0378  0.1743
669SOL   HW1 2040   0.738   2.234   2.062  0.8224  0.6828 -0.4391
669SOL   HW2 2041   0.584   2.273   2.098  0.5435 -1.0993  0.4405
670SOL    OW 2042   1.310   1.586   2.169  0.1669 -0.9857 -0.1427
670SOL   HW1 2043   1.291   1.682   2.190  1.0358 -0.6556 -0.8094
670SOL   HW2 2044   1.233   1.529   2.198  0.5978 -0.3968  2.4805
671SOL    OW 2045   1.552   2.293   0.513  0.5034  0.3081 -0.1792
671SOL   HW1 2046   1.562   2.309   0.611 -1.5399 -0.6911  0.2492
671SOL   HW2 2047   1.629   2.239   0.480  0.9160  0.1516  0.9964
672SOL    OW 2048   1.605   1.451   1.962 -0.0526 -0.2594  0.3136
672SOL   HW1 2049   1.652   1.429   1.877  1.6567  1.0174  0.8424
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672SOL   HW2 2050   1.652   1.405   2.038 -1.9125 -1.8641  0.5625
673SOL    OW 2051   0.185   1.205   0.113  0.1375  0.3453  0.2633
673SOL   HW1 2052   0.272   1.228   0.069  0.9061 -0.6228  1.2100
673SOL   HW2 2053   0.145   1.125   0.068  1.1116 -0.8803  1.4774
674SOL    OW 2054   2.444   1.814   0.616  0.1874 -0.0079  0.0663
674SOL   HW1 2055   2.470   1.879   0.545  1.3086 -0.5196 -0.0045
674SOL   HW2 2056   2.462   1.855   0.706 -0.6567  0.4014  0.0601
675SOL    OW 2057   1.395   1.221   1.949  0.0474 -0.1660 -0.2509
675SOL   HW1 2058   1.428   1.313   1.970 -0.9351 -0.3224  2.3276
675SOL   HW2 2059   1.470   1.155   1.960  0.1798  0.0786  0.3826
676SOL    OW 2060   0.464   0.976   0.228  0.3669 -0.0774  0.2957
676SOL   HW1 2061   0.555   0.960   0.265  0.2051 -2.6218 -0.2401
676SOL   HW2 2062   0.431   1.065   0.258  2.2418  0.0799  2.0845
677SOL    OW 2063   0.116   1.095   0.788  0.0970  0.1462 -0.2775
677SOL   HW1 2064   0.047   1.092   0.861 -0.2735  1.6145 -0.5480
677SOL   HW2 2065   0.174   1.013   0.794 -0.0655  0.1215  1.5250
678SOL    OW 2066   2.517   0.721   0.146 -0.1473 -0.4003 -0.1244
678SOL   HW1 2067   2.438   0.774   0.179  0.9056  1.0252  0.1997
678SOL   HW2 2068   2.579   0.702   0.222  1.5095  1.5368 -0.8871
679SOL    OW 2069   2.851   2.941   0.576  0.1776  0.0836 -0.3615
679SOL   HW1 2070   2.783   2.983   0.515  0.6929 -1.4864 -2.1027
679SOL   HW2 2071   2.915   3.012   0.607  0.8204  0.7426 -2.9341
680SOL    OW 2072   0.650   1.257   1.043  0.4951 -0.2684  0.0547
680SOL   HW1 2073   0.693   1.286   0.958  0.5091  1.0116  0.4743
680SOL   HW2 2074   0.667   1.159   1.057  1.8578 -0.1576 -0.6091
681SOL    OW 2075   0.083   1.936   1.334 -0.4621  0.5803  0.3415
681SOL   HW1 2076   0.079   1.867   1.407 -0.0532  2.9977  2.8144
681SOL   HW2 2077  -0.009   1.953   1.300 -1.0820  1.2326  2.2085
682SOL    OW 2078   1.636   3.084   1.602 -0.2187  0.2809 -0.1855
682SOL   HW1 2079   1.629   3.026   1.683 -0.5884  0.6826  0.0785
682SOL   HW2 2080   1.568   3.055   1.534 -3.9709  3.3619  1.8607
683SOL    OW 2081   1.626   1.886   1.875 -0.6555  0.1476 -0.2306
683SOL   HW1 2082   1.659   1.803   1.829 -1.6413  0.0576 -0.8021
683SOL   HW2 2083   1.528   1.895   1.861 -0.7594  0.7977  0.8231
684SOL    OW 2084   1.289   0.735   1.115  0.0639 -0.2246 -0.4338
684SOL   HW1 2085   1.196   0.748   1.149  0.5722  1.5034  0.4267
684SOL   HW2 2086   1.308   0.802   1.044  1.1019  0.4258  0.4287
685SOL    OW 2087   0.590   0.899   0.844 -0.5960  0.1462 -0.4585
685SOL   HW1 2088   0.610   0.831   0.774  1.1258 -0.0015  0.1428
685SOL   HW2 2089   0.671   0.956   0.861 -1.8205  2.0267 -0.5678
686SOL    OW 2090   1.597   0.182   1.136 -0.1703  0.9514 -0.2511
686SOL   HW1 2091   1.581   0.265   1.083 -2.9415 -0.1833 -1.3913
686SOL   HW2 2092   1.539   0.182   1.217  0.9857  0.7975  0.6095
687SOL    OW 2093   2.147   2.171   0.381  0.1022  0.1854  0.1622
687SOL   HW1 2094   2.086   2.092   0.377 -1.0578  1.0382  0.5394
687SOL   HW2 2095   2.108   2.246   0.329 -1.4136  2.2138  3.8529
688SOL    OW 2096   1.925   2.067   1.498 -0.2011 -0.0670  0.0497
688SOL   HW1 2097   1.926   2.146   1.559  0.5078 -0.5957  0.7369
688SOL   HW2 2098   1.933   2.099   1.403  0.6137  0.6678  0.3491
689SOL    OW 2099   0.409   1.570   1.786 -0.1907 -0.1467 -0.0274
689SOL   HW1 2100   0.342   1.558   1.859  1.3079  0.4757  1.5100
689SOL   HW2 2101   0.497   1.532   1.815 -0.0397 -1.7648 -2.3432
```

```
690SOL    OW 2102   2.804   0.758   1.881 -0.0843 -0.0650 -0.9271
690SOL   HW1 2103   2.900   0.748   1.856  0.3140 -2.4553  1.1191
690SOL   HW2 2104   2.797   0.803   1.970 -0.9771  1.1522 -1.5786
691SOL    OW 2105   3.153   0.127   1.233 -0.2333  0.0279 -0.2857
691SOL   HW1 2106   3.149   0.047   1.292  0.4183 -0.2008 -0.5370
691SOL   HW2 2107   3.061   0.164   1.220 -0.3323  0.4244  1.3261
692SOL    OW 2108   1.816   2.069   1.830  0.2784  0.1872  0.4123
692SOL   HW1 2109   1.750   1.995   1.840  1.3943 -0.6846  1.7585
692SOL   HW2 2110   1.834   2.110   1.920  1.1090  0.7976 -0.0208
693SOL    OW 2111   2.733   1.486   0.510  0.7267 -0.1696  0.5475
693SOL   HW1 2112   2.664   1.439   0.456  0.0542  0.6876  0.6339
693SOL   HW2 2113   2.821   1.440   0.500  0.5652 -0.1829 -1.0586
694SOL    OW 2114   1.373   1.378   0.105  0.0040 -1.3651  0.1880
694SOL   HW1 2115   1.444   1.448   0.113  1.0823 -2.5948  2.1422
694SOL   HW2 2116   1.339   1.376   0.011 -0.7060  2.3074  0.1947
695SOL    OW 2117   2.385   1.325   2.125  0.1288  0.0170  0.3487
695SOL   HW1 2118   2.408   1.415   2.088  0.5942  0.2030  1.0693
695SOL   HW2 2119   2.338   1.335   2.213 -1.8399 -0.3936 -0.6019
696SOL    OW 2120   1.557   1.222   1.645  0.3261  0.2597  0.1006
696SOL   HW1 2121   1.599   1.133   1.660  1.9487  0.7148 -1.4116
696SOL   HW2 2122   1.618   1.294   1.678 -0.6879  0.8535  0.7391
697SOL    OW 2123   1.982   2.916   1.847  0.5946 -0.1925 -0.3093
697SOL   HW1 2124   2.035   2.832   1.861  1.3644  0.3207 -0.0621
697SOL   HW2 2125   2.021   2.989   1.903  1.0072  0.7716 -1.7872
698SOL    OW 2126   2.941   2.151   1.939 -0.0312  0.5622 -0.2355
698SOL   HW1 2127   3.007   2.130   1.866 -0.1666  1.7024 -0.7051
698SOL   HW2 2128   2.982   2.214   2.004 -0.7664  1.6112 -0.7558
699SOL    OW 2129   2.103   2.528   2.147 -0.1576 -0.1012 -0.1222
699SOL   HW1 2130   2.161   2.447   2.149  0.1042  0.0935  0.0887
699SOL   HW2 2131   2.069   2.548   2.239 -0.8033 -0.3869 -0.2881
700SOL    OW 2132   0.278   0.900   1.116  0.3774 -0.0163 -0.5565
700SOL   HW1 2133   0.277   0.851   1.029  1.9289 -0.8131 -0.1739
700SOL   HW2 2134   0.255   0.836   1.190  1.9684 -0.1204 -0.1010
701SOL    OW 2135   2.760   1.990   0.660 -0.4034 -0.2732  0.0259
701SOL   HW1 2136   2.846   2.035   0.684 -0.2988 -0.5980  0.2610
701SOL   HW2 2137   2.690   2.060   0.642 -0.0916 -0.0089 -0.1760
702SOL    OW 2138   2.841   2.843   1.704 -0.1026  0.0621  0.1826
702SOL   HW1 2139   2.814   2.800   1.618 -0.2965 -2.1927  1.2703
702SOL   HW2 2140   2.856   2.771   1.773 -2.3502  1.8041  2.7276
703SOL    OW 2141   0.254   2.077   2.044 -0.3367  0.3352  0.1022
703SOL   HW1 2142   0.238   1.979   2.058 -0.6473  0.6971  2.8227
703SOL   HW2 2143   0.173   2.117   1.999  0.4511 -0.8413 -2.6099
704SOL    OW 2144   3.086   0.371   1.556 -0.3054 -0.0831  0.2370
704SOL   HW1 2145   3.069   0.451   1.498  0.9167  0.8244  1.0673
704SOL   HW2 2146   3.085   0.400   1.652  0.2891 -1.0541  0.5463
705SOL    OW 2147   3.124   2.608   1.522  0.7911 -0.4414  0.0687
705SOL   HW1 2148   3.126   2.689   1.579 -1.4793  0.1341 -0.5604
705SOL   HW2 2149   3.122   2.526   1.580  0.7059  0.0505  0.7658
706SOL    OW 2150   2.304   0.046   1.851  0.1691  0.5535  0.0298
706SOL   HW1 2151   2.386   0.070   1.798  1.1306  1.4054  1.8261
706SOL   HW2 2152   2.237   0.119   1.844 -0.0861  0.2584 -0.7139
707SOL    OW 2153   1.848   0.750   2.036 -0.1389  0.1652 -0.1315
```

```
707SOL   HW1 2154   1.880   0.844   2.045   0.5599   0.0605 -1.2476
707SOL   HW2 2155   1.751   0.749   2.010  -0.5084   0.5340  1.1837
708SOL    OW 2156   1.138   2.956   1.002  -0.1002  -0.3238 -0.1999
708SOL   HW1 2157   1.236   2.971   1.012   0.2628  -2.7968  0.5981
708SOL   HW2 2158   1.117   2.938   0.906   0.6266  -2.0205 -0.0667
709SOL    OW 2159   2.532   0.125   1.733  -0.5473   0.7757  0.4206
709SOL   HW1 2160   2.587   0.198   1.693  -0.2094   0.5635  0.4971
709SOL   HW2 2161   2.589   0.044   1.747  -0.1589   1.4193  3.0862
710SOL    OW 2162   3.054   2.296   2.110   0.0531   0.3948 -0.0059
710SOL   HW1 2163   3.096   2.277   2.199   0.0080  -1.6929 -0.3881
710SOL   HW2 2164   3.125   2.315   2.043   0.2463  -0.5001 -0.0634
711SOL    OW 2165   1.364   1.528   0.751   0.2156  -0.3889 -0.1157
711SOL   HW1 2166   1.389   1.608   0.697   1.4811  -0.3244  0.5263
711SOL   HW2 2167   1.312   1.464   0.694  -0.8835   0.9061 -0.6166
712SOL    OW 2168   1.260   0.467   0.756  -0.1015   0.1343 -0.7266
712SOL   HW1 2169   1.318   0.499   0.830  -2.0514   0.1355  0.8891
712SOL   HW2 2170   1.207   0.387   0.786  -1.9252   0.9315 -1.6214
 3.13000   3.13000   2.21324   0.00000   0.00000   0.00000   0.00000   1.56500   1.56500
```

4. CARTESIAN COORDINATES OF DASPMI IN S0 STATE (ξ1-ξ2 grid)

The cartesian coordinates are collected following the order:
i-0, i-30, i-60, i-90, i-120, i-150, i-180, i-210, i-240, i-270, i-300
with i=0, 30, 60, 90

The Dalton format has been used (the atoms are separately rported according to their atomic number.)

BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
 c -1.696   1.405 -0.001
 c -0.810   0.296 0.000
 c -1.404 -0.993 0.001
 c -2.768 -1.163 0.001
 c -3.652 -0.042 -0.001
 c -3.063 1.254 -0.001
 c -5.597 -1.553 0.007
 c 0.600   0.541 -0.001
 c 1.589 -0.414 0.001

```
c  3.019  -0.360   0.002
c  5.186   0.702  -0.001
c  5.849  -0.494  -0.002
c  5.090  -1.681  -0.001
c  3.718  -1.600   0.002
c -5.898   0.959  -0.005
c  3.218   2.136   0.007
     1.   19
h -6.931   0.616  -0.009
h -5.746   1.580   0.883
h -5.740   1.576  -0.897
h -6.681  -1.464   0.013
h -5.306  -2.121  -0.882
h -5.295  -2.114   0.898
h -3.169  -2.165   0.001
h -0.781  -1.878   0.002
h  0.851   1.591  -0.002
h  1.248  -1.443   0.002
h  5.706   1.647  -0.001
h  3.123  -2.502   0.001
h  5.581  -2.644  -0.002
h  6.929  -0.510  -0.003
h -3.688   2.134  -0.002
h -1.281   2.407  -0.001
h  4.020   2.871   0.009
h  2.610   2.279  -0.887
h  2.611   2.274   0.902
     7.   2
n -5.005  -0.208  -0.002
n  3.812   0.782   0.003
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.644   1.320  -0.383
c -0.791   0.235  -0.056
c -1.418  -0.990   0.283
c -2.786  -1.123   0.303
c -3.639  -0.026  -0.019
c -3.015   1.207  -0.366
c -5.621  -1.438   0.354
c  0.626   0.428  -0.108
c  1.596  -0.506   0.153
c  3.021  -0.408   0.043
c  5.122   0.772   0.033
c  5.827  -0.359  -0.276
c  5.128  -1.577  -0.390
c  3.763  -1.588  -0.226
c -5.861   0.984  -0.336
c  3.131   2.021   0.669
```

```
   1.  19
h -6.901  0.677 -0.254
h -5.697  1.823  0.349
h -5.685  1.328 -1.362
h -6.702 -1.326  0.319
h -5.335 -2.227 -0.348
h -5.343 -1.749  1.366
h -3.215 -2.077  0.567
h -0.817 -1.856  0.537
h  0.922  1.424 -0.416
h  1.272 -1.523  0.348
h  5.599  1.732  0.162
h  3.206 -2.510 -0.327
h  5.659 -2.493 -0.615
h  6.898 -0.305 -0.409
h -3.616  2.065 -0.623
h -1.202  2.272 -0.656
h  3.887  2.620  1.174
h  2.733  2.585 -0.174
h  2.330  1.789  1.370
   7.   2
n -4.997 -0.155  0.000
n  3.758  0.756  0.213
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6.  16
c -1.610  1.176 -0.673
c -0.779  0.182 -0.101
c -1.427 -0.926  0.499
c -2.799 -1.029  0.537
c -3.630 -0.021 -0.032
c -2.984  1.089 -0.644
c -5.641 -1.277  0.637
c  0.645  0.336 -0.171
c  1.604 -0.514  0.305
c  3.023 -0.406  0.039
c  5.109  0.784  0.152
c  5.796 -0.260 -0.411
c  5.095 -1.437 -0.729
c  3.737 -1.501 -0.494
c -5.831  0.921 -0.600
c  3.123  1.858  1.091
    1.  19
h -6.878  0.664 -0.453
h -5.652  1.897 -0.136
h -5.647  1.006 -1.676
h -6.720 -1.150  0.584
h -5.381 -2.210  0.127
h -5.361 -1.363  1.693
```

```
h  -3.244  -1.894   1.006
h  -0.840  -1.719   0.947
h   0.975   1.243  -0.673
h   1.306  -1.492   0.672
h   5.589   1.708   0.437
h   3.174  -2.388  -0.744
h   5.615  -2.280  -1.164
h   6.857  -0.168  -0.590
h  -3.570   1.877  -1.095
h  -1.150   2.035  -1.150
h   3.871   2.344   1.717
h   2.734   2.574   0.368
h   2.308   1.486   1.708
     7.   2
n  -4.992  -0.120   0.006
n   3.762   0.707   0.400
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c  -1.599   0.826  -1.100
c  -0.779   0.053  -0.252
c  -1.429  -0.752   0.708
c  -2.804  -0.785   0.817
c  -3.629  -0.003  -0.040
c  -2.977   0.807  -1.006
c  -5.645  -0.877   1.073
c   0.657   0.118  -0.407
c   1.605  -0.544   0.297
c   3.045  -0.404   0.019
c   5.111   0.735   0.439
c   5.788  -0.078  -0.448
c   5.085  -1.080  -1.120
c   3.722  -1.233  -0.879
c  -5.826   0.777  -0.829
c   3.098   1.471   1.643
     1.   19
h  -6.874   0.617  -0.581
h  -5.609   1.845  -0.721
h  -5.678   0.496  -1.879
h  -6.723  -0.748   1.002
h  -5.419  -1.938   0.916
h  -5.335  -0.602   2.088
h  -3.252  -1.420   1.566
h  -0.846  -1.370   1.382
h   0.994   0.782  -1.203
h   1.345  -1.238   1.092
h   5.598   1.527   0.986
h   3.148  -1.997  -1.384
h   5.592  -1.730  -1.821
```

```
h  6.845  0.074 -0.606
h -3.554  1.418 -1.682
h -1.135  1.455 -1.853
h  3.838  2.156  2.051
h  2.306  2.025  1.146
h  2.666  0.872  2.444
      7.   2
n -4.995 -0.034  0.066
n  3.776  0.572  0.664
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.  16
c -1.619  0.364 -1.381
c -0.780 -0.082 -0.332
c -1.414 -0.479  0.869
c -2.782 -0.446  1.012
c -3.623 -0.003 -0.050
c -2.991  0.403 -1.256
c -5.615 -0.403  1.342
c  0.641 -0.095 -0.531
c  1.612 -0.472  0.352
c  3.021 -0.343  0.048
c  5.165  0.609  0.572
c  5.741  0.047 -0.541
c  4.940 -0.716 -1.406
c  3.601 -0.902 -1.107
c -5.834  0.497 -1.011
c  3.257  1.121  2.033
      1.  19
h -6.874  0.456 -0.698
h -5.599  1.531 -1.284
h -5.718 -0.133 -1.900
h -6.694 -0.308  1.245
h -5.383 -1.449  1.567
h -5.294  0.217  2.187
h -3.219 -0.765  1.948
h -0.820 -0.830  1.706
h  0.967  0.236 -1.516
h  1.349 -0.705  1.379
h  5.722  1.213  1.272
h  2.971 -1.516 -1.734
h  5.370 -1.170 -2.289
h  6.793  0.200 -0.733
h -3.583  0.745 -2.091
h -1.168  0.681 -2.316
h  3.967  1.861  2.395
h  2.328  1.612  1.743
h  3.055  0.395  2.822
      7.   2
```

n -4.983 0.029 0.089
n 3.834 0.444 0.845
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
 c -1.672 -0.004 -1.475
 c -0.804 -0.079 -0.357
 c -1.411 -0.122 0.924
 c -2.777 -0.100 1.079
 c -3.647 -0.031 -0.051
 c -3.042 0.017 -1.339
 c -5.608 -0.057 1.437
 c 0.607 -0.093 -0.574
 c 1.605 -0.146 0.364
 c 2.997 -0.156 0.028
 c 5.267 0.403 0.611
 c 5.754 -0.107 -0.564
 c 4.843 -0.661 -1.485
 c 3.499 -0.686 -1.184
 c -5.883 0.060 -1.072
 c 3.477 1.013 2.169
      1.   19
 h -6.918 0.070 -0.739
 h -5.702 0.974 -1.651
 h -5.743 -0.805 -1.729
 h -6.690 -0.031 1.337
 h -5.336 -0.975 1.968
 h -5.300 0.803 2.043
 h -3.191 -0.137 2.074
 h -0.794 -0.180 1.813
 h 0.902 -0.043 -1.620
 h 1.342 -0.105 1.414
 h 5.909 0.838 1.363
 h 2.798 -1.156 -1.859
 h 5.200 -1.084 -2.415
 h 6.815 -0.084 -0.762
 h -3.656 0.072 -2.224
 h -1.244 0.038 -2.470
 h 4.324 1.508 2.638
 h 2.700 1.750 1.958
 h 3.088 0.253 2.847
      7.   2
 n -5.002 -0.012 0.100
 n 3.928 0.395 0.899
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom

6. 16
c -1.705 -1.518 -0.070
c -0.814 -0.412 -0.018
c -1.404   0.877   0.042
c -2.767   1.053   0.050
c -3.655 -0.063 -0.002
c -3.070 -1.361 -0.063
c -5.593   1.454   0.067
c   0.591 -0.655 -0.030
c   1.602   0.274   0.014
c   2.994 -0.038 -0.001
c   5.281   0.738   0.036
c   5.778 -0.534 -0.022
c   4.866 -1.609 -0.073
c   3.515 -1.358 -0.062
c -5.905 -1.055 -0.046
c   3.490   2.402   0.110
        1. 19
h -6.936 -0.706 -0.024
h -5.758 -1.630 -0.965
h -5.748 -1.715   0.813
h -6.677   1.370   0.055
h -5.300   1.975   0.984
h -5.289   2.059 -0.794
h -3.165   2.056   0.097
h -0.774   1.758   0.083
h   0.857 -1.706 -0.079
h   1.327   1.317   0.062
h   5.920   1.607   0.076
h   2.820 -2.181 -0.100
h   5.228 -2.626 -0.119
h   6.846 -0.696 -0.029
h -3.699 -2.237 -0.103
h -1.293 -2.520 -0.117
h   4.368   3.042   0.139
h   2.897   2.651 -0.771
h   2.899   2.571   1.013
        7.   2
n -5.007   0.108   0.005
n   3.931   0.989   0.046
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
        6. 16
c -1.672 -0.013   1.475
c -0.803 -0.083   0.357
c -1.412 -0.118 -0.925
c -2.777 -0.094 -1.079
c -3.647 -0.031   0.051
c -3.041   0.009   1.339

```
c  -5.608  -0.053  -1.437
c   0.607  -0.098   0.574
c   1.605  -0.146  -0.366
c   2.997  -0.158  -0.029
c   5.267   0.408  -0.605
c   5.752  -0.103   0.569
c   4.841  -0.665   1.486
c   3.498  -0.693   1.183
c  -5.883   0.059   1.074
c   3.479   1.019  -2.165
     1.  19
h  -6.917   0.071   0.741
h  -5.742  -0.810   1.726
h  -5.701   0.968   1.657
h  -6.692  -0.037  -1.334
h  -5.309   0.811  -2.040
h  -5.330  -0.968  -1.970
h  -3.192  -0.124  -2.075
h  -0.795  -0.171  -1.814
h   0.902  -0.055   1.619
h   1.343  -0.099  -1.414
h   5.909   0.847  -1.354
h   2.798  -1.167   1.853
h   5.198  -1.090   2.414
h   6.813  -0.078   0.769
h  -3.656   0.058   2.226
h  -1.243   0.021   2.471
h   4.327   1.512  -2.634
h   3.087   0.260  -2.844
h   2.704   1.757  -1.953
     7.   2
n  -5.001  -0.007  -0.099
n   3.928   0.399  -0.896
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c  -1.620   0.368   1.379
c  -0.780  -0.079   0.333
c  -1.414  -0.478  -0.869
c  -2.782  -0.445  -1.012
c  -3.624  -0.002   0.049
c  -2.991   0.407   1.255
c  -5.615  -0.395  -1.345
c   0.641  -0.093   0.531
c   1.612  -0.472  -0.351
c   3.021  -0.343  -0.045
c   5.166   0.607  -0.570
c   5.741   0.046   0.544
c   4.939  -0.715   1.409
```

```
c  3.600  -0.902  1.110
c  -5.834  0.482  1.018
c  3.258  1.119  -2.031
     1.  19
h  -6.876  0.409  0.717
h  -5.690  -0.138  1.909
h  -5.625  1.525  1.281
h  -6.694  -0.293  -1.250
h  -5.288  0.224  -2.187
h  -5.391  -1.443  -1.572
h  -3.217  -0.764  -1.948
h  -0.819  -0.830  -1.705
h  0.967  0.238  1.517
h  1.350  -0.705  -1.377
h  5.723  1.209  -1.270
h  2.970  -1.515  1.736
h  5.369  -1.169  2.292
h  6.793  0.198  0.736
h  -3.584  0.754  2.088
h  -1.169  0.688  2.314
h  3.969  1.858  -2.396
h  3.052  0.393  -2.819
h  2.330  1.612  -1.740
     7.   2
n  -4.983  0.029  -0.090
n  3.835  0.442  -0.842
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c  -1.600  0.824  1.102
c  -0.779  0.050  0.254
c  -1.431  -0.754  -0.706
c  -2.806  -0.784  -0.817
c  -3.630  -0.001  0.039
c  -2.978  0.807  1.006
c  -5.644  -0.883  -1.069
c  0.658  0.116  0.410
c  1.607  -0.545  -0.294
c  3.047  -0.405  -0.016
c  5.111  0.736  -0.438
c  5.790  -0.075  0.447
c  5.089  -1.078  1.119
c  3.726  -1.233  0.882
c  -5.825  0.785  0.824
c  3.092  1.466  -1.638
     1.  19
h  -6.873  0.622  0.583
h  -5.671  0.514  1.875
h  -5.610  1.853  0.707
```

```
h -6.723 -0.766 -0.990
h -5.347 -0.606 -2.087
h -5.405 -1.940 -0.913
h -3.256 -1.419 -1.566
h -0.850 -1.374 -1.380
h  0.995  0.780  1.206
h  1.349 -1.239 -1.089
h  5.598  1.528 -0.986
h  3.154 -1.998  1.387
h  5.598 -1.727  1.820
h  6.848  0.078  0.604
h -3.557  1.419  1.682
h -1.137  1.452  1.856
h  3.830  2.140 -2.069
h  2.638  0.865 -2.424
h  2.315  2.037 -1.134
    7.   2
 n -4.996 -0.030 -0.069
 n  3.775  0.572 -0.662
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
 c -1.610  1.180  0.667
 c -0.780  0.185  0.099
 c -1.427 -0.925 -0.499
 c -2.798 -1.029 -0.538
 c -3.630 -0.020  0.031
 c -2.984  1.093  0.638
 c -5.641 -1.271 -0.650
 c  0.644  0.338  0.169
 c  1.604 -0.514 -0.303
 c  3.022 -0.406 -0.036
 c  5.110  0.783 -0.149
 c  5.795 -0.261  0.416
 c  5.093 -1.436  0.736
 c  3.735 -1.500  0.500
 c -5.831  0.907  0.623
 c  3.127  1.855 -1.097
     1.  19
 h -6.876  0.620  0.524
 h -5.604  1.008  1.689
 h -5.697  1.882  0.141
 h -6.719 -1.135 -0.611
 h -5.347 -1.354 -1.701
 h -5.395 -2.208 -0.140
 h -3.243 -1.895 -1.004
 h -0.839 -1.718 -0.945
 h  0.974  1.248  0.668
 h  1.304 -1.493 -0.662
```

```
h  5.591  1.706 -0.436
h  3.170 -2.386  0.752
h  5.611 -2.281  1.172
h  6.857 -0.171  0.595
h -3.570  1.884  1.081
h -1.151  2.041  1.140
h  3.876  2.334 -1.725
h  2.313  1.480 -1.713
h  2.736  2.576 -0.379
      7.   2
n -4.991 -0.121 -0.006
n  3.763  0.707 -0.396
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.  16
c -1.696  1.405 -0.001
c -0.810  0.296  0.000
c -1.404 -0.993  0.001
c -2.768 -1.163  0.001
c -3.652 -0.042 -0.001
c -3.063  1.254 -0.001
c -5.597 -1.553  0.007
c  0.600  0.541 -0.001
c  1.589 -0.414  0.001
c  3.019 -0.360  0.002
c  5.186  0.702 -0.001
c  5.849 -0.494 -0.002
c  5.090 -1.681 -0.001
c  3.718 -1.600  0.002
c -5.898  0.959 -0.005
c  3.218  2.136  0.007
      1.  19
h -6.931  0.616 -0.009
h -5.746  1.580  0.883
h -5.740  1.576 -0.897
h -6.681 -1.464  0.013
h -5.306 -2.121 -0.882
h -5.295 -2.114  0.898
h -3.169 -2.165  0.001
h -0.781 -1.878  0.002
h  0.851  1.591 -0.002
h  1.248 -1.443  0.002
h  5.706  1.647 -0.001
h  3.123 -2.502  0.001
h  5.581 -2.644 -0.002
h  6.929 -0.510 -0.003
h -3.688  2.134 -0.002
h -1.281  2.407 -0.001
h  4.020  2.871  0.009
```

h 2.610 2.279 -0.887
h 2.611 2.274 0.902
     7. 2
n -5.005 -0.208 -0.002
n 3.812 0.782 0.003
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.634 1.233 -0.634
c -0.786 0.259 -0.051
c -1.415 -0.828 0.606
c -2.783 -0.971 0.623
c -3.629 -0.022 -0.021
c -3.003 1.096 -0.643
c -5.614 -1.327 0.628
c 0.631 0.465 -0.038
c 1.584 -0.519 0.046
c 3.011 -0.415 -0.033
c 5.114 0.738 0.182
c 5.814 -0.312 -0.348
c 5.109 -1.481 -0.700
c 3.744 -1.520 -0.536
c -5.845 0.834 -0.666
c 3.134 1.841 1.069
     1. 19
h -6.884 0.528 -0.567
h -5.732 1.816 -0.195
h -5.617 0.928 -1.733
h -6.689 -1.284 0.468
h -5.243 -2.267 0.208
h -5.429 -1.327 1.708
h -3.215 -1.808 1.153
h -0.808 -1.557 1.132
h 0.943 1.483 -0.253
h 1.237 -1.546 0.050
h 5.594 1.652 0.498
h 3.183 -2.401 -0.817
h 5.637 -2.334 -1.104
h 6.884 -0.235 -0.473
h -3.603 1.855 -1.123
h -1.191 2.101 -1.109
h 3.881 2.285 1.724
h 2.786 2.592 0.360
h 2.299 1.486 1.669
     7. 2
n -4.986 -0.170 -0.024
n 3.752 0.691 0.362
BASIS
6-31G*

ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.606 1.036 -0.898
c -0.778 0.214 -0.098
c -1.424 -0.687 0.781
c -2.796 -0.805 0.817
c -3.624 -0.017 -0.033
c -2.979 0.919 -0.888
c -5.633 -1.112 0.879
c 0.646 0.398 -0.116
c 1.592 -0.539 0.193
c 3.014 -0.404 -0.039
c 5.113 0.715 0.302
c 5.789 -0.210 -0.453
c 5.073 -1.294 -0.994
c 3.712 -1.382 -0.776
c -5.823 0.701 -0.874
c 3.139 1.615 1.430
     1. 19
h -6.867 0.437 -0.722
h -5.701 1.764 -0.635
h -5.583 0.551 -1.932
h -6.707 -1.087 0.707
h -5.280 -2.130 0.681
h -5.450 -0.875 1.933
h -3.243 -1.495 1.518
h -0.831 -1.287 1.462
h 0.985 1.352 -0.520
h 1.268 -1.559 0.376
h 5.606 1.559 0.761
h 3.136 -2.197 -1.195
h 5.582 -2.044 -1.584
h 6.851 -0.101 -0.610
h -3.564 1.555 -1.534
h -1.146 1.769 -1.555
h 3.888 1.956 2.142
h 2.766 2.464 0.858
h 2.313 1.144 1.958
     7.   2
n -4.985 -0.142 -0.012
n 3.766 0.609 0.530
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.622 0.631 -1.273
c -0.781 0.130 -0.260
c -1.403 -0.386 0.896

```
c  -2.778  -0.452   1.012
c  -3.625   0.005  -0.035
c  -2.998   0.560  -1.181
c  -5.614  -0.650   1.262
c   0.658   0.240  -0.395
c   1.590  -0.556   0.178
c   3.036  -0.396  -0.059
c   5.121   0.598   0.572
c   5.787  -0.052  -0.445
c   5.068  -0.898  -1.293
c   3.701  -1.062  -1.090
c  -5.844   0.441  -1.007
c   3.113   1.145   1.883
     1.  19
h  -6.887   0.285  -0.737
h  -5.692   1.515  -1.165
h  -5.655  -0.079  -1.952
h  -6.693  -0.669   1.124
h  -5.276  -1.678   1.429
h  -5.396  -0.060   2.159
h  -3.207  -0.842   1.924
h  -0.795  -0.724   1.728
h   1.003   1.002  -1.096
h   1.299  -1.393   0.809
h   5.621   1.263   1.259
h   3.117  -1.709  -1.729
h   5.568  -1.419  -2.099
h   6.849   0.104  -0.569
h  -3.596   0.941  -1.995
h  -1.178   1.070  -2.162
h   3.867   1.702   2.433
h   2.359   1.823   1.488
h   2.633   0.420   2.540
     7.   2
n  -4.991  -0.072   0.068
n   3.782   0.426   0.758
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c  -1.650   0.047  -1.470
c  -0.784  -0.033  -0.355
c  -1.386  -0.017   0.924
c  -2.754  -0.003   1.084
c  -3.623   0.006  -0.043
c  -3.021   0.042  -1.331
c  -5.584  -0.029   1.446
c   0.642   0.004  -0.557
c   1.601  -0.489   0.274
c   3.018  -0.340  -0.003
```

```
c  5.170   0.500   0.652
c  5.751   0.055  -0.511
c  4.949  -0.590  -1.465
c  3.601  -0.780  -1.204
c -5.862   0.056  -1.067
c  3.253   0.875   2.142
     1.  19
h -6.898   0.043  -0.735
h -5.701   0.970  -1.648
h -5.703  -0.807  -1.723
h -6.666  -0.087   1.347
h -5.247  -0.906   2.010
h -5.340   0.871   2.020
h -3.165   0.022   2.082
h -0.761  -0.001   1.810
h  0.965   0.389  -1.524
h  1.322  -0.863   1.255
h  5.730   1.008   1.423
h  2.968  -1.306  -1.904
h  5.382  -0.951  -2.388
h  6.808   0.208  -0.673
h -3.637   0.075  -2.217
h -1.223   0.088  -2.467
h  3.973   1.549   2.599
h  2.339   1.417   1.902
h  3.024   0.064   2.836
     7.   2
n -4.983   0.004   0.108
n  3.834   0.330   0.888
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.684  -1.049  -1.077
c -0.806  -0.244  -0.311
c -1.400   0.724   0.536
c -2.766   0.826   0.675
c -3.644  -0.040  -0.040
c -3.052  -0.976  -0.935
c -5.589   1.019   1.036
c  0.608  -0.337  -0.528
c  1.596   0.001   0.357
c  2.997  -0.139   0.076
c  5.258   0.611   0.433
c  5.766  -0.346  -0.407
c  4.872  -1.233  -1.037
c  3.519  -1.127  -0.791
c -5.889  -0.834  -0.661
c  3.437   1.818   1.544
     1.  19
```

```
h -6.921 -0.621 -0.387
h -5.780 -0.667 -1.738
h -5.690 -1.889 -0.448
h -6.669  0.890  1.044
h -5.219  0.869  2.056
h -5.369  2.047  0.729
h -3.171  1.591  1.320
h -0.770  1.421  1.077
h  0.899 -0.812 -1.463
h  1.315  0.466  1.293
h  5.886  1.321  0.948
h  2.830 -1.830 -1.230
h  5.246 -2.007 -1.694
h  6.832 -0.409 -0.567
h -3.675 -1.635 -1.520
h -1.267 -1.764 -1.777
h  4.274  2.476  1.766
h  2.656  2.383  1.037
h  3.047  1.409  2.478
    7.   2
n -4.998  0.043  0.110
n  3.911  0.727  0.659
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6.  16
c -1.707 -0.146  1.508
c -0.813 -0.155  0.408
c -1.393 -0.177 -0.888
c -2.755 -0.119 -1.072
c -3.645 -0.039  0.038
c -3.071 -0.065  1.341
c -5.571  0.062 -1.493
c  0.592 -0.281  0.637
c  1.592  0.123 -0.212
c  2.990 -0.014  0.045
c  5.263  0.331 -0.691
c  5.779 -0.225  0.447
c  4.884 -0.700  1.427
c  3.529 -0.595  1.221
c -5.901  0.084  1.015
c  3.447  1.058 -2.159
    1.  19
h -6.926  0.155  0.660
h -5.812 -0.821  1.626
h -5.697  0.955  1.646
h -6.651  0.167 -1.416
h -5.185  0.907 -2.073
h -5.355 -0.864 -2.036
h -3.148 -0.160 -2.077
```

```
 h -0.753 -0.271 -1.757
 h  0.859 -0.630  1.631
 h  1.296  0.568 -1.150
 h  5.890  0.713 -1.482
 h  2.844 -0.969  1.968
 h  5.262 -1.148  2.337
 h  6.850 -0.295  0.577
 h -3.705 -0.033  2.214
 h -1.302 -0.179  2.515
 h  4.315  1.338 -2.749
 h  2.845  0.348 -2.728
 h  2.859  1.952 -1.945
     7.   2
 n -4.996  0.039 -0.141
 n  3.910  0.437 -0.895
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
 c -1.663  0.344  1.419
 c -0.801 -0.089  0.382
 c -1.412 -0.556 -0.809
 c -2.778 -0.534 -0.978
 c -3.637 -0.039  0.046
 c -3.029  0.391  1.259
 c -5.602 -0.455 -1.379
 c  0.610 -0.158  0.610
 c  1.594 -0.103 -0.345
 c  2.993 -0.152 -0.038
 c  5.250  0.479 -0.593
 c  5.756 -0.156  0.511
 c  4.863 -0.811  1.381
 c  3.513 -0.810  1.100
 c -5.864  0.489  0.954
 c  3.429  1.247 -2.045
     1.  19
 h -6.897  0.454  0.616
 h -5.775 -0.134  1.850
 h -5.625  1.524  1.220
 h -6.677 -0.302 -1.325
 h -5.220  0.112 -2.234
 h -5.415 -1.520 -1.550
 h -3.197 -0.920 -1.895
 h -0.795 -0.969 -1.599
 h  0.915 -0.133  1.654
 h  1.304  0.051 -1.376
 h  5.877  0.997 -1.302
 h  2.822 -1.353  1.728
 h  5.236 -1.330  2.253
 h  6.820 -0.151  0.692
```

```
 h -3.640  0.751  2.075
 h -1.232  0.667  2.361
 h  4.265  1.796 -2.472
 h  3.031  0.561 -2.795
 h  2.652  1.949 -1.742
     7.   2
 n -4.990  0.003 -0.124
 n  3.905  0.496 -0.858
BASIS
6-31G*
ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
 c -1.589  0.609  1.247
 c -0.776 -0.108  0.340
 c -1.433 -0.820 -0.690
 c -2.802 -0.779 -0.840
 c -3.615 -0.013  0.045
 c -2.959  0.676  1.102
 c -5.632 -0.686 -1.197
 c  0.645 -0.180  0.555
 c  1.601 -0.397 -0.396
 c  3.016 -0.330 -0.102
 c  5.148  0.709 -0.483
 c  5.740 -0.032  0.512
 c  4.953 -0.935  1.243
 c  3.612 -1.075  0.933
 c -5.797  0.796  0.844
 c  3.222  1.450 -1.815
     1.   19
 h -6.844  0.704  0.559
 h -5.686  0.412  1.864
 h -5.536  1.860  0.840
 h -6.699 -0.475 -1.169
 h -5.250 -0.370 -2.174
 h -5.496 -1.770 -1.102
 h -3.260 -1.356 -1.629
 h -0.852 -1.439 -1.366
 h  0.981  0.050  1.565
 h  1.308 -0.446 -1.440
 h  5.695  1.426 -1.077
 h  2.991 -1.789  1.454
 h  5.396 -1.529  2.032
 h  6.794  0.092  0.715
 h -3.534  1.254  1.811
 h -1.123  1.136  2.073
 h  3.934  2.229 -2.075
 h  2.989  0.860 -2.704
 h  2.307  1.897 -1.427
     7.   2
 n -4.973  0.040 -0.105
```

n 3.817 0.585 -0.764
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6. 16
 c -1.591 1.018 0.890
 c -0.779 0.040 0.279
 c -1.435 -1.001 -0.410
 c -2.810 -1.034 -0.536
 c -3.624 -0.018 0.034
 c -2.965 1.007 0.763
 c -5.646 -1.114 -0.847
 c 0.659 0.076 0.461
 c 1.592 -0.438 -0.373
 c 3.038 -0.380 -0.094
 c 5.113 0.795 -0.305
 c 5.790 -0.188 0.386
 c 5.081 -1.299 0.851
 c 3.714 -1.383 0.607
 c -5.812 0.991 0.542
 c 3.095 1.787 -1.301
      1. 19
 h -6.859 0.800 0.317
 h -5.691 0.987 1.631
 h -5.561 1.991 0.169
 h -6.717 -0.923 -0.876
 h -5.280 -1.160 -1.878
 h -5.486 -2.093 -0.378
 h -3.266 -1.862 -1.060
 h -0.854 -1.812 -0.835
 h 1.005 0.633 1.332
 h 1.302 -0.964 -1.280
 h 5.605 1.676 -0.689
 h 3.136 -2.228 0.954
 h 5.588 -2.083 1.397
 h 6.851 -0.084 0.556
 h -3.540 1.790 1.237
 h -1.124 1.810 1.467
 h 3.846 2.510 -1.610
 h 2.603 1.363 -2.174
 h 2.350 2.267 -0.669
      7.   2
 n -4.988 -0.041 -0.096
 n 3.773 0.698 -0.536
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6. 16

```
c -1.623  1.283  0.442
c -0.783  0.185  0.139
c -1.417 -1.047 -0.145
c -2.789 -1.160 -0.203
c -3.629 -0.034  0.029
c -2.996  1.193  0.369
c -5.626 -1.413 -0.389
c  0.644  0.324  0.266
c  1.593 -0.421 -0.370
c  3.020 -0.381 -0.107
c  5.120  0.785 -0.025
c  5.801 -0.358  0.310
c  5.089 -1.565  0.407
c  3.725 -1.565  0.189
c -5.841  1.028  0.239
c  3.132  2.043 -0.697
    1.  19
h -6.883  0.743  0.117
h -5.702  1.382  1.266
h -5.630  1.855 -0.447
h -6.702 -1.266 -0.460
h -5.270 -1.787 -1.354
h -5.435 -2.175  0.375
h -3.226 -2.126 -0.406
h -0.817 -1.935 -0.301
h  0.970  1.169  0.870
h  1.277 -1.300 -0.925
h  5.609  1.741 -0.132
h  3.153 -2.480  0.272
h  5.603 -2.484  0.657
h  6.867 -0.315  0.480
h -3.589  2.069  0.584
h -1.173  2.231  0.720
h  3.883  2.647 -1.201
h  2.325  1.805 -1.386
h  2.732  2.591  0.157
    7.  2
n -4.990 -0.135 -0.048
n  3.768  0.774 -0.252
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6.  16
c -1.656  1.246 -0.562
c -0.809  0.276  0.023
c -1.434 -0.804  0.685
c -2.804 -0.971  0.671
c -3.646 -0.049 -0.008
c -3.023  1.076 -0.617
c -5.628 -1.382  0.588
```

```
c   0.608   0.545   0.174
c   1.580  -0.355  -0.171
c   3.017  -0.332  -0.128
c   5.186   0.637   0.269
c   5.840  -0.464  -0.218
c   5.072  -1.552  -0.674
c   3.699  -1.475  -0.624
c  -5.859   0.772  -0.715
c   3.230   1.942   0.899
      1.   19
h  -6.894   0.442  -0.656
h  -5.784   1.753  -0.233
h  -5.595   0.880  -1.773
h  -6.695  -1.371   0.381
h  -5.215  -2.318   0.196
h  -5.489  -1.368   1.676
h  -3.234  -1.803   1.209
h  -0.824  -1.514   1.233
h   0.852   1.578   0.381
h   1.212  -1.315  -0.517
h   5.713   1.503   0.639
h   3.095  -2.298  -0.975
h   5.556  -2.439  -1.059
h   6.919  -0.480  -0.239
h  -3.621   1.822  -1.118
h  -1.219   2.129  -1.017
h   4.030   2.539   1.330
h   2.732   2.523   0.123
h   2.523   1.678   1.684
      7.    2
n  -5.002  -0.220  -0.052
n   3.815   0.710   0.320
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
c  -1.591   1.014  -0.860
c  -0.788   0.197  -0.031
c  -1.458  -0.658   0.872
c  -2.833  -0.772   0.880
c  -3.634  -0.020  -0.022
c  -2.964   0.889  -0.888
c  -5.668  -1.079   0.871
c   0.638   0.435   0.062
c   1.592  -0.538  -0.036
c   3.024  -0.408  -0.099
c   5.112   0.710   0.315
c   5.818  -0.215  -0.408
c   5.124  -1.303  -0.971
c   3.758  -1.388  -0.807
```

c -5.809   0.665 -0.955
c   3.126   1.611   1.396
      1.   19
h -6.857   0.399 -0.827
h -5.701   1.736 -0.747
h -5.536   0.481 -1.999
h -6.737 -1.065   0.669
h -5.308 -2.103   0.728
h -5.516 -0.799   1.920
h -3.299 -1.427   1.602
h -0.878 -1.231   1.588
h   0.940   1.477 -0.019
h   1.247 -1.556 -0.184
h   5.585   1.555   0.791
h   3.202 -2.206 -1.244
h   5.656 -2.060 -1.531
h   6.886 -0.105 -0.522
h -3.530   1.505 -1.570
h -1.116   1.737 -1.515
h   3.866   1.918   2.134
h   2.791   2.485   0.837
h   2.281   1.153   1.905
      7.   2
n -4.996 -0.146 -0.040
n   3.752   0.613   0.490
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
c -1.567   0.745 -1.093
c -0.782   0.174 -0.068
c -1.463 -0.414   1.017
c -2.842 -0.512   1.040
c -3.629 -0.012 -0.031
c -2.943   0.629 -1.099
c -5.682 -0.778   1.092
c   0.655   0.398 -0.039
c   1.595 -0.572   0.102
c   3.026 -0.396 -0.098
c   5.118   0.654   0.425
c   5.788 -0.108 -0.499
c   5.073 -1.070 -1.229
c   3.714 -1.210 -1.017
c -5.790   0.424 -1.129
c   3.149   1.323   1.714
      1.   19
h -6.843   0.214 -0.946
h -5.668   1.509 -1.213
h -5.514 -0.033 -2.085
h -6.752 -0.793   0.892

```
h -5.345 -1.814  1.216
h -5.519 -0.243  2.035
h -3.317 -0.960  1.900
h -0.895 -0.791  1.860
h  0.986  1.399 -0.322
h  1.270 -1.607  0.162
h  5.611  1.399  1.032
h  3.137 -1.934 -1.575
h  5.580 -1.693 -1.955
h  6.850  0.037 -0.641
h -3.498  1.048 -1.925
h -1.081  1.262 -1.913
h  3.904  1.532  2.470
h  2.772  2.260  1.305
h  2.329  0.764  2.156
     7.   2
n -4.996 -0.124 -0.025
n  3.774  0.499  0.640
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.614  0.257 -1.386
c -0.786  0.145 -0.253
c -1.414  0.036  1.000
c -2.792 -0.035  1.118
c -3.626  0.010 -0.027
c -2.990  0.168 -1.287
c -5.625 -0.220  1.390
c  0.664  0.315 -0.375
c  1.585 -0.555  0.082
c  3.038 -0.379 -0.116
c  5.126  0.490  0.666
c  5.795 -0.017 -0.428
c  5.074 -0.726 -1.393
c  3.703 -0.900 -1.227
c -5.835  0.006 -1.119
c  3.111  0.876  2.022
     1.   19
h -6.878 -0.107 -0.828
h -5.726  0.972 -1.627
h -5.595 -0.790 -1.833
h -6.701 -0.317  1.259
h -5.267 -1.115  1.911
h -5.437  0.651  2.030
h -3.228 -0.108  2.105
h -0.809  0.015  1.900
h  1.006  1.153 -0.986
h  1.277 -1.454  0.612
h  5.628  1.046  1.444
```

h 3.117 -1.443 -1.953
h 5.575 -1.135 -2.261
h 6.859 0.140 -0.521
h -3.581 0.232 -2.189
h -1.166 0.394 -2.364
h 3.868 1.325 2.661
h 2.383 1.626 1.720
h 2.602 0.076 2.559
    7.　2
n -4.994 -0.077 0.077
n 3.783 0.312 0.814
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6.　16
c -1.645 -1.183 -0.845
c -0.791 -0.230 -0.252
c -1.398 0.881 0.364
c -2.772 0.991 0.477
c -3.630 -0.014 -0.042
c -3.018 -1.104 -0.718
c -5.606 1.207 0.780
c 0.648 -0.292 -0.484
c 1.598 -0.234 0.477
c 3.026 -0.279 0.174
c 5.180 0.770 0.256
c 5.762 -0.269 -0.432
c 4.959 -1.341 -0.849
c 3.607 -1.336 -0.542
c -5.858 -0.960 -0.498
c 3.262 1.943 1.248
    1.　19
h -6.896 -0.717 -0.280
h -5.743 -1.017 -1.586
h -5.644 -1.947 -0.073
h -6.683 1.063 0.814
h -5.240 1.286 1.809
h -5.404 2.155 0.266
h -3.188 1.869 0.949
h -0.775 1.680 0.752
h 0.963 -0.542 -1.499
h 1.309 -0.003 1.499
h 5.742 1.624 0.601
h 2.970 -2.162 -0.821
h 5.394 -2.170 -1.391
h 6.822 -0.243 -0.641
h -3.627 -1.881 -1.154
h -1.217 -2.020 -1.388
h 3.999 2.742 1.268
h 2.371 2.275 0.717

h 2.997 1.666 2.269
    7. 2
n -4.994 0.073 0.083
n 3.843 0.774 0.535
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6. 16
c -1.657 -0.430 1.382
c -0.810 -0.247 0.266
c -1.432 -0.072 -0.989
c -2.803 0.028 -1.113
c -3.648 -0.054 0.026
c -3.026 -0.298 1.282
c -5.631 0.300 -1.390
c 0.614 -0.504 0.385
c 1.596 0.327 -0.055
c 3.007 0.080 0.124
c 5.263 0.369 -0.657
c 5.777 -0.323 0.410
c 4.889 -0.839 1.371
c 3.531 -0.631 1.224
c -5.863 -0.046 1.104
c 3.432 1.276 -2.013
    1. 19
h -6.898 0.121 0.813
h -5.793 -1.042 1.557
h -5.598 0.701 1.861
h -6.707 0.402 -1.258
h -5.256 1.220 -1.853
h -5.448 -0.535 -2.076
h -3.231 0.147 -2.098
h -0.819 -0.030 -1.883
h 0.891 -1.352 1.011
h 1.306 1.196 -0.634
h 5.888 0.792 -1.428
h 2.841 -0.986 1.975
h 5.268 -1.379 2.227
h 6.845 -0.454 0.500
h -3.627 -0.399 2.173
h -1.221 -0.643 2.353
h 4.269 1.418 -2.692
h 2.663 0.683 -2.506
h 3.027 2.251 -1.736
    7. 2
n -5.008 0.071 -0.083
n 3.914 0.555 -0.806
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.661 0.220 1.412
c -0.815 -0.154 0.341
c -1.443 -0.578 -0.853
c -2.813 -0.528 -1.011
c -3.653 -0.052 0.033
c -3.028 0.311 1.259
c -5.636 -0.363 -1.391
c 0.598 -0.360 0.573
c 1.597 0.142 -0.211
c 3.002 -0.019 0.038
c 5.273 0.428 -0.634
c 5.785 -0.247 0.443
c 4.888 -0.837 1.354
c 3.532 -0.724 1.145
c -5.863 0.478 0.982
c 3.463 1.294 -2.032
     1.   19
h -6.899 0.487 0.650
h -5.788 -0.192 1.846
h -5.600 1.492 1.302
h -6.706 -0.174 -1.332
h -5.234 0.218 -2.228
h -5.489 -1.429 -1.602
h -3.245 -0.884 -1.935
h -0.835 -0.973 -1.659
h 0.850 -0.774 1.548
h 1.299 0.671 -1.104
h 5.903 0.900 -1.371
h 2.842 -1.187 1.834
h 5.262 -1.380 2.211
h 6.855 -0.319 0.574
h -3.625 0.649 2.093
h -1.222 0.476 2.370
h 4.336 1.639 -2.582
h 2.870 0.646 -2.679
h 2.869 2.156 -1.728
     7.   2
n -5.010 0.028 -0.124
n 3.922 0.541 -0.837
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.612 0.579 1.230
c -0.801 -0.123 0.308
c -1.464 -0.867 -0.695
c -2.836 -0.838 -0.833

```
c -3.643 -0.056  0.038
c -2.981  0.646  1.084
c -5.671 -0.749 -1.176
c  0.617 -0.275  0.554
c  1.601 -0.040 -0.365
c  3.005 -0.140 -0.069
c  5.253  0.600 -0.485
c  5.761 -0.226  0.486
c  4.873 -1.038  1.214
c  3.522 -0.995  0.929
c -5.820  0.781  0.831
c  3.433  1.606 -1.784
     1.  19
h -6.864  0.713  0.532
h -5.733  0.403  1.856
h -5.532  1.838  0.824
h -6.738 -0.543 -1.142
h -5.297 -0.447 -2.160
h -5.527 -1.830 -1.064
h -3.296 -1.440 -1.602
h -0.880 -1.491 -1.362
h  0.910 -0.395  1.596
h  1.307  0.269 -1.359
h  5.880  1.248 -1.079
h  2.832 -1.648  1.442
h  5.247 -1.706  1.977
h  6.825 -0.246  0.671
h -3.553  1.230  1.790
h -1.145  1.104  2.055
h  4.267  2.228 -2.101
h  3.042  1.064 -2.646
h  2.652  2.237 -1.362
     7.   2
n -5.004 -0.002 -0.103
n  3.912  0.654 -0.750
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.537  0.793  1.000
c -0.778 -0.149  0.273
c -1.487 -1.087 -0.505
c -2.863 -1.038 -0.626
c -3.621 -0.040  0.042
c -2.909  0.873  0.868
c -5.703 -0.930 -0.930
c  0.653 -0.280  0.509
c  1.603 -0.293 -0.460
c  3.027 -0.294 -0.164
c  5.150  0.809 -0.324
```

```
c  5.749 -0.126  0.490
c  4.968 -1.168  1.012
c  3.624 -1.243  0.682
c -5.748  1.044  0.649
c  3.218  1.801 -1.474
      1.  19
h -6.802  0.942  0.402
h -5.637  0.925  1.733
h -5.431  2.057  0.376
h -6.761 -0.677 -0.933
h -5.342 -0.897 -1.963
h -5.599 -1.955 -0.556
h -3.360 -1.789 -1.222
h -0.941 -1.876 -1.011
h  0.982 -0.216  1.546
h  1.302 -0.176 -1.497
h  5.693  1.638 -0.751
h  3.006 -2.052  1.042
h  5.415 -1.914  1.653
h  6.802 -0.042  0.713
h -3.443  1.633  1.419
h -1.032  1.489  1.660
h  3.934  2.614 -1.579
h  2.976  1.401 -2.460
h  2.311  2.166 -0.996
      7.   2
n -4.984  0.030 -0.086
n  3.820  0.739 -0.625
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.  16
c -1.551  1.110  0.614
c -0.781 -0.017  0.272
c -1.472 -1.177 -0.119
c -2.851 -1.195 -0.244
c -3.624 -0.038  0.032
c -2.928  1.117  0.477
c -5.689 -1.246 -0.552
c  0.667 -0.027  0.499
c  1.588 -0.346 -0.430
c  3.041 -0.349 -0.166
c  5.111  0.851 -0.149
c  5.796 -0.254  0.311
c  5.093 -1.440  0.538
c  3.723 -1.476  0.297
c -5.770  1.156  0.229
c  3.079  2.024 -0.889
      1.  19
h -6.823  0.959  0.041
```

```
h -5.659   1.431   1.285
h -5.472   2.014  -0.384
h -6.752  -1.029  -0.643
h -5.326  -1.576  -1.532
h -5.569  -2.073   0.158
h -3.336  -2.113  -0.537
h -0.915  -2.086  -0.318
h  1.010   0.345   1.467
h  1.278  -0.666  -1.422
h  5.598   1.794  -0.345
h  3.151  -2.377   0.465
h  5.608  -2.320   0.899
h  6.860  -0.185   0.485
h -3.471   2.015   0.725
h -1.058   2.006   0.977
h  3.827   2.793  -1.066
h  2.562   1.789  -1.818
h  2.354   2.368  -0.154
     7.   2
n -4.991  -0.038  -0.105
n  3.768   0.801  -0.380
BASIS
6-31G*
 ground

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.601   1.297   0.154
c -0.788   0.145   0.148
c -1.442  -1.104   0.179
c -2.819  -1.205   0.113
c -3.633  -0.046   0.023
c -2.977   1.214   0.058
c -5.654  -1.448  -0.097
c  0.651   0.258   0.354
c  1.590  -0.334  -0.423
c  3.028  -0.348  -0.178
c  5.127   0.777   0.110
c  5.809  -0.411   0.206
c  5.095  -1.612   0.076
c  3.726  -1.568  -0.121
c -5.824   1.074  -0.100
c  3.136   2.146  -0.256
     1.   19
h -6.871   0.788  -0.182
h -5.703   1.668   0.814
h -5.576   1.705  -0.960
h -6.723  -1.307  -0.243
h -5.276  -2.061  -0.921
h -5.507  -1.997   0.841
h -3.272  -2.185   0.155
h -0.852  -2.010   0.271
```

```
h  0.968   0.977   1.111
h  1.260  -1.058  -1.164
h  5.619   1.736   0.182
h  3.152  -2.478  -0.214
h  5.608  -2.563   0.137
h  6.878  -0.402   0.367
h -3.553   2.126   0.020
h -1.139   2.277   0.203
h  3.882   2.844  -0.631
h  2.318   2.062  -0.969
h  2.750   2.500   0.701
      7.   2
n -4.998  -0.137  -0.069
n  3.774   0.812  -0.097
```

5. CARTESIAN COORDINATES OF DASPMI IN S0 STATE ($\xi 1$-$\xi 2$ grid)

The cartesian coordinates are collected following the order:
i-0, i-30, i-60, i-90, i-120, i-150, i-180, i-210, i-240, i-270, i-300
with i=0, 30, 60, 90

The Dalton format has been used (the atoms are separately rported according to their atomic number.)

BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
```
      6.   16
c -1.712   1.427  -0.005
c -0.818   0.335  -0.003
c -1.388  -0.958  -0.002
c -2.747  -1.148  -0.002
c -3.641  -0.045  -0.001
c -3.074   1.256  -0.006
c -5.560  -1.572  -0.018
c  0.615   0.602  -0.002
c  1.569  -0.369  -0.001
c  3.013  -0.361   0.001
```

```
c  5.188   0.661   0.002
c  5.815  -0.549   0.007
c  5.041  -1.723   0.009
c  3.666  -1.598   0.005
c -5.897   0.919   0.026
c  3.264   2.143  -0.010
     1.  19
h -6.921   0.562   0.079
h -5.709   1.550   0.900
h -5.791   1.528  -0.876
h -6.644  -1.501  -0.031
h -5.242  -2.123  -0.909
h -5.263  -2.141   0.868
h -3.133  -2.156   0.000
h -0.752  -1.833  -0.000
h  0.866   1.649  -0.002
h  1.205  -1.390   0.001
h  5.738   1.589  -0.002
h  3.048  -2.485   0.007
h  5.508  -2.697   0.013
h  6.894  -0.585   0.010
h -3.712   2.127  -0.012
h -1.310   2.433  -0.010
h  4.086   2.854  -0.021
h  2.660   2.307  -0.903
h  2.666   2.323   0.884
     7.   2
n -4.991  -0.227   0.002
n  3.820   0.785  -0.001
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.630   1.296  -0.479
c -0.787   0.232  -0.094
c -1.410  -0.958   0.344
c -2.776  -1.086   0.378
c -3.620  -0.017  -0.024
c -2.998   1.186  -0.453
c -5.601  -1.393   0.419
c  0.657   0.406  -0.180
c  1.574  -0.537   0.145
c  3.025  -0.452   0.084
c  5.074   0.793   0.004
c  5.780  -0.317  -0.357
c  5.123  -1.557  -0.456
c  3.753  -1.588  -0.235
c -5.833   0.983  -0.370
c  3.111   1.948   0.851
     1.  19
h -6.872   0.700  -0.231
```

h -5.632 1.859 0.252
h -5.690 1.258 -1.419
h -6.679 -1.303 0.322
h -5.268 -2.223 -0.211
h -5.367 -1.629 1.462
h -3.205 -2.013 0.723
h -0.809 -1.796 0.668
h 0.981 1.373 -0.541
h 1.222 -1.525 0.425
h 5.544 1.757 0.134
h 3.211 -2.519 -0.338
h 5.668 -2.457 -0.701
h 6.841 -0.230 -0.541
h -3.598 2.023 -0.773
h -1.183 2.222 -0.817
h 3.857 2.460 1.455
h 2.749 2.636 0.081
h 2.284 1.664 1.496
      7.   2
n -4.975 -0.138 0.006
n 3.721 0.752 0.255
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
c -1.572 1.005 -0.921
c -0.766 0.074 -0.226
c -1.426 -0.874 0.595
c -2.788 -0.913 0.690
c -3.598 0.012 -0.033
c -2.936 0.980 -0.843
c -5.618 -1.034 0.879
c 0.672 0.136 -0.383
c 1.571 -0.669 0.208
c 3.044 -0.508 0.067
c 5.014 0.859 0.263
c 5.742 -0.059 -0.427
c 5.141 -1.237 -0.910
c 3.775 -1.415 -0.647
c -5.773 0.942 -0.675
c 3.015 1.563 1.482
      1.   19
h -6.818 0.748 -0.457
h -5.541 1.964 -0.366
h -5.621 0.850 -1.753
h -6.692 -0.913 0.780
h -5.354 -2.041 0.552
h -5.352 -0.917 1.931
h -3.249 -1.651 1.327
h -0.847 -1.587 1.162
h 1.037 0.910 -1.050

```
h  1.232 -1.432  0.905
h  5.446  1.757  0.675
h  3.273 -2.303 -1.007
h  5.712 -1.988 -1.430
h  6.794  0.128 -0.586
h -3.510  1.699 -1.406
h -1.091  1.745 -1.547
h  3.499  2.539  1.451
h  1.960  1.692  1.255
h  3.109  1.161  2.496
     7.   2
n -4.944 -0.025  0.053
n  3.648  0.695  0.494
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.609  0.793 -1.158
c -0.779  0.062 -0.269
c -1.420 -0.702  0.742
c -2.777 -0.738  0.859
c -3.609 -0.003 -0.043
c -2.969  0.771 -1.060
c -5.601 -0.812  1.130
c  0.647  0.130 -0.435
c  1.572 -0.500  0.317
c  3.024 -0.405  0.041
c  5.100  0.779  0.335
c  5.715 -0.054 -0.539
c  5.004 -1.118 -1.151
c  3.650 -1.248 -0.838
c -5.803  0.696 -0.879
c  3.218  1.339  1.821
     1.  19
h -6.841  0.457 -0.674
h -5.664  1.773 -0.768
h -5.581  0.406 -1.907
h -6.677 -0.692  1.045
h -5.364 -1.874  1.038
h -5.290 -0.455  2.112
h -3.223 -1.333  1.639
h -0.825 -1.276  1.437
h  1.000  0.739 -1.261
h  1.255 -1.113  1.157
h  5.606  1.598  0.821
h  3.063 -2.027 -1.306
h  5.487 -1.792 -1.838
h  6.758  0.109 -0.766
h -3.560  1.347 -1.753
h -1.144  1.385 -1.933
h  3.826  2.224  2.006
```

```
h  2.196   1.670   1.641
h  3.239   0.716   2.722
     7.   2
n -4.948  -0.040   0.064
n  3.746   0.637   0.661
BASIS
6-31G*


Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.676   0.704  -1.256
c -0.810   0.127  -0.298
c -1.407  -0.558   0.789
c -2.763  -0.639   0.927
c -3.633  -0.042  -0.036
c -3.035   0.634  -1.140
c -5.582  -0.794   1.245
c  0.619   0.266  -0.471
c  1.570  -0.217   0.345
c  3.009  -0.214  -0.013
c  5.255   0.459   0.521
c  5.740  -0.309  -0.490
c  4.875  -1.080  -1.292
c  3.500  -1.010  -1.010
c -5.861   0.461  -0.921
c  3.405   1.473   1.779
     1.   19
h -6.891   0.243  -0.656
h -5.737   1.545  -0.968
h -5.661   0.034  -1.905
h -6.661  -0.695   1.182
h -5.331  -1.856   1.255
h -5.248  -0.337   2.178
h -3.176  -1.173   1.768
h -0.783  -1.036   1.530
h  0.937   0.789  -1.366
h  1.290  -0.769   1.241
h  5.883   1.078   1.143
h  2.799  -1.587  -1.597
h  5.246  -1.676  -2.109
h  6.806  -0.312  -0.673
h -3.654   1.102  -1.888
h -1.244   1.227  -2.100
h  4.174   1.646   2.530
h  3.158   2.429   1.305
h  2.518   1.096   2.287
     7.   2
n -4.972  -0.123   0.090
n  3.893   0.493   0.818
BASIS
6-31G*
```

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.711   0.207 -1.491
c -0.821   0.040 -0.409
c -1.387 -0.190   0.865
c -2.745 -0.223   1.053
c -3.638 -0.040 -0.037
c -3.071   0.173 -1.323
c -5.558 -0.285   1.471
c 0.612   0.124 -0.651
c 1.578 -0.001   0.287
c 3.000 -0.101 -0.021
c 5.272   0.306   0.641
c 5.743 -0.279 -0.498
c 4.840 -0.812 -1.436
c 3.478 -0.709 -1.168
c -5.895   0.092 -0.991
c 3.477   1.061   2.131
     1. 19
h -6.920   0.031 -0.637
h -5.755   1.065 -1.470
h -5.742 -0.693 -1.737
h -6.641 -0.243   1.403
h -5.274 -1.262   1.871
h -5.226   0.490   2.168
h -3.132 -0.401   2.045
h -0.745 -0.354   1.720
h 0.902   0.281 -1.684
h 1.298 -0.090   1.330
h 5.927   0.732   1.385
h 2.758 -1.129 -1.855
h 5.191 -1.295 -2.335
h 6.809 -0.325 -0.664
h -3.710   0.316 -2.180
h -1.306   0.376 -2.480
h 4.334   1.527   2.613
h 2.745   1.836   1.900
h 3.038   0.345   2.831
     7.   2
n -4.986 -0.073   0.143
n 3.926   0.395   0.907
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.745 -1.552   0.059
c -0.825 -0.479   0.018
c -1.367   0.828 -0.031
c -2.722   1.048 -0.040
c -3.639 -0.034   0.002
c -3.101 -1.349   0.051

```
c -5.523  1.534 -0.049
c  0.594 -0.766  0.029
c  1.584  0.176 -0.008
c  2.997 -0.084  0.002
c  5.245  0.773 -0.029
c  5.775 -0.482  0.020
c  4.907 -1.592  0.063
c  3.546 -1.371  0.053
c -5.917 -0.948  0.026
c  3.407  2.376 -0.094
     1.  19
h -6.934 -0.570 -0.001
h -5.773 -1.606 -0.836
h -5.794 -1.538  0.940
h -6.609  1.487 -0.038
h -5.195  2.116  0.817
h -5.211  2.056 -0.959
h -3.086  2.063 -0.079
h -0.709  1.686 -0.065
h  0.849 -1.818  0.068
h  1.284  1.212 -0.048
h  5.865  1.655 -0.063
h  2.871 -2.212  0.085
h  5.300 -2.596  0.102
h  6.847 -0.608  0.027
h -3.759 -2.202  0.086
h -1.364 -2.564  0.099
h  4.261  3.049 -0.121
h  2.808  2.539 -0.992
h  2.809  2.610  0.790
     7.  2
n -4.985  0.177 -0.007
n  3.896  0.995 -0.039
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.711  0.215  1.489
c -0.821  0.043  0.409
c -1.387 -0.194 -0.865
c -2.745 -0.228 -1.053
c -3.638 -0.038  0.035
c -3.071  0.181  1.321
c -5.559 -0.288 -1.471
c  0.611  0.128  0.651
c  1.580 -0.001 -0.286
c  3.000 -0.101  0.023
c  5.272  0.302 -0.642
c  5.743 -0.276  0.502
c  4.839 -0.807  1.441
c  3.478 -0.703  1.172
```

```
c -5.895  0.089  0.991
c  3.477  1.049 -2.136
     1.  19
h -6.919  0.009  0.640
h -5.727 -0.687  1.743
h -5.767  1.068  1.461
h -6.641 -0.242 -1.403
h -5.225  0.483 -2.171
h -5.279 -1.268 -1.868
h -3.131 -0.412 -2.043
h -0.745 -0.360 -1.718
h  0.902  0.291  1.683
h  1.299 -0.097 -1.329
h  5.929  0.726 -1.387
h  2.757 -1.121  1.861
h  5.192 -1.285  2.342
h  6.809 -0.321  0.667
h -3.710  0.330  2.177
h -1.306  0.391  2.478
h  4.332  1.518 -2.617
h  3.045  0.327 -2.835
h  2.740  1.819 -1.911
     7.   2
n -4.986 -0.074 -0.143
n  3.926  0.392 -0.907
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.673  0.700  1.258
c -0.809  0.125  0.296
c -1.407 -0.557 -0.791
c -2.764 -0.637 -0.928
c -3.632 -0.044  0.037
c -3.033  0.628  1.143
c -5.583 -0.788 -1.245
c  0.620  0.264  0.469
c  1.570 -0.216 -0.351
c  3.008 -0.220  0.008
c  5.254  0.469 -0.511
c  5.737 -0.297  0.505
c  4.870 -1.076  1.297
c  3.497 -1.011  1.008
c -5.859  0.463  0.923
c  3.408  1.461 -1.793
     1.  19
h -6.889  0.242  0.661
h -5.656  0.039  1.908
h -5.737  1.548  0.966
h -6.662 -0.702 -1.173
h -5.261 -0.318 -2.177
```

```
h -5.321 -1.848 -1.268
h -3.177 -1.168 -1.770
h -0.784 -1.033 -1.534
h  0.940  0.780  1.367
h  1.288 -0.758 -1.252
h  5.881  1.096 -1.124
h  2.794 -1.590  1.592
h  5.240 -1.672  2.115
h  6.800 -0.291  0.697
h -3.652  1.094  1.893
h -1.240  1.218  2.103
h  4.183  1.635 -2.538
h  2.529  1.073 -2.308
h  3.148  2.418 -1.329
     7.   2
n -4.972 -0.122 -0.089
n  3.894  0.492 -0.820
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.610  0.826  1.131
c -0.776  0.068  0.269
c -1.415 -0.727 -0.721
c -2.771 -0.766 -0.841
c -3.606 -0.001  0.034
c -2.969  0.801  1.029
c -5.596 -0.862 -1.106
c  0.649  0.137  0.440
c  1.574 -0.521 -0.288
c  3.026 -0.415 -0.023
c  5.114  0.728 -0.406
c  5.738 -0.092  0.473
c  5.026 -1.119  1.146
c  3.663 -1.240  0.866
c -5.799  0.741  0.831
c  3.124  1.450 -1.683
     1.   19
h -6.838  0.551  0.588
h -5.627  0.450  1.869
h -5.606  1.810  0.719
h -6.671 -0.741 -1.028
h -5.284 -0.550 -2.104
h -5.355 -1.918 -0.966
h -3.215 -1.385 -1.604
h -0.818 -1.321 -1.397
h  0.999  0.772  1.246
h  1.254 -1.161 -1.108
h  5.622  1.515 -0.937
h  3.079 -2.005  1.361
h  5.515 -1.777  1.842
```

```
 h  6.794  0.051  0.655
 h -3.562  1.393  1.707
 h -1.147  1.438  1.893
 h  3.882  2.095 -2.123
 h  2.680  0.862 -2.491
 h  2.352  2.088 -1.244
      7.   2
 n -4.943 -0.039 -0.075
 n  3.750  0.599 -0.687
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
 c -1.572  1.001  0.924
 c -0.766  0.074  0.224
 c -1.425 -0.869 -0.600
 c -2.787 -0.909 -0.695
 c -3.599  0.013  0.032
 c -2.937  0.977  0.846
 c -5.620 -1.056 -0.851
 c  0.671  0.136  0.381
 c  1.571 -0.666 -0.214
 c  3.044 -0.506 -0.071
 c  5.016  0.860 -0.255
 c  5.742 -0.064  0.430
 c  5.139 -1.244  0.906
 c  3.773 -1.419  0.640
 c -5.775  0.959  0.648
 c  3.019  1.574 -1.471
      1.   19
 h -6.814  0.804  0.376
 h -5.680  0.849  1.731
 h -5.494  1.974  0.365
 h -6.692 -0.971 -0.705
 h -5.403 -0.928 -1.915
 h -5.307 -2.054 -0.540
 h -3.249 -1.641 -1.338
 h -0.847 -1.579 -1.173
 h  1.037  0.906  1.053
 h  1.234 -1.424 -0.917
 h  5.450  1.758 -0.662
 h  3.270 -2.309  0.993
 h  5.709 -1.999  1.422
 h  6.795  0.121  0.593
 h -3.511  1.690  1.416
 h -1.092  1.738  1.554
 h  3.502  2.549 -1.433
 h  3.112  1.179 -2.488
 h  1.964  1.704 -1.244
      7.   2
 n -4.944 -0.027 -0.053
```

n 3.650 0.698 -0.488
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
 c -1.719 1.431 -0.271
 c -0.824 0.422 0.130
 c -1.367 -0.829 0.479
 c -2.719 -1.072 0.408
 c -3.620 -0.053 0.004
 c -3.075 1.214 -0.327
 c -5.512 -1.591 0.285
 c 0.623 0.692 0.151
 c 1.537 -0.279 -0.084
 c 2.984 -0.327 -0.101
 c 5.196 0.581 0.139
 c 5.775 -0.621 -0.132
 c 4.956 -1.735 -0.401
 c 3.588 -1.556 -0.378
 c -5.879 0.775 -0.479
 c 3.325 2.102 0.447
     1. 19
 h -6.898 0.402 -0.436
 h -5.803 1.643 0.184
 h -5.674 1.098 -1.504
 h -6.589 -1.569 0.157
 h -5.105 -2.375 -0.361
 h -5.292 -1.846 1.325
 h -3.091 -2.048 0.677
 h -0.712 -1.614 0.831
 h 0.893 1.716 0.351
 h 1.127 -1.257 -0.318
 h 5.780 1.461 0.353
 h 2.936 -2.395 -0.580
 h 5.386 -2.699 -0.623
 h 6.851 -0.701 -0.134
 h -3.724 2.022 -0.629
 h -1.329 2.403 -0.545
 h 4.172 2.774 0.572
 h 2.719 2.472 -0.382
 h 2.741 2.108 1.367
     7. 2
 n -4.962 -0.284 -0.066
 n 3.832 0.757 0.157
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
 c -1.662 1.252 -0.706
 c -0.799 0.372 -0.025

c -1.382 -0.693   0.689
c -2.741 -0.899   0.691
c -3.608 -0.022 -0.012
c -3.023   1.071 -0.705
c -5.549 -1.347   0.698
c   0.654   0.578 -0.082
c   1.541 -0.437 -0.007
c   2.995 -0.413 -0.059
c   5.123   0.660   0.216
c   5.774 -0.391 -0.356
c   5.042 -1.523 -0.763
c   3.667 -1.503 -0.598
c -5.841   0.703 -0.729
c   3.176   1.780   1.158
       1.   19
h -6.870   0.377 -0.606
h -5.754   1.720 -0.332
h -5.611   0.723 -1.797
h -6.623 -1.343   0.545
h -5.151 -2.295   0.328
h -5.353 -1.280   1.773
h -3.144 -1.732   1.245
h -0.750 -1.356   1.265
h   0.980   1.599 -0.230
h   1.137 -1.445   0.027
h   5.647   1.534   0.576
h   3.071 -2.348 -0.916
h   5.537 -2.381 -1.192
h   6.847 -0.347 -0.473
h -3.646   1.769 -1.242
h -1.241   2.085 -1.253
h   3.956   2.231   1.766
h   2.761   2.547   0.500
h   2.393   1.413   1.817
       7.   2
n -4.957 -0.216 -0.016
n   3.758   0.672   0.393
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
       6.   16
c -1.627   0.941 -1.088
c -0.777   0.241 -0.205
c -1.378 -0.532   0.812
c -2.739 -0.659   0.904
c -3.595   0.010 -0.017
c -2.989   0.828 -1.014
c -5.559 -0.982   1.068
c   0.669   0.367 -0.343
c   1.542 -0.582   0.017
c   3.020 -0.467 -0.086

```
c   5.071   0.651   0.484
c   5.772  -0.167  -0.344
c   5.116  -1.171  -1.085
c   3.730  -1.287  -0.922
c  -5.818   0.632  -0.846
c   3.012   1.372   1.615
     1.  19
h  -6.852   0.428  -0.588
h  -5.646   1.707  -0.758
h  -5.653   0.328  -1.883
h  -6.629  -1.024   0.888
h  -5.160  -1.994   1.001
h  -5.390  -0.595   2.076
h  -3.159  -1.254   1.699
h  -0.754  -1.022   1.544
h   1.028   1.262  -0.840
h   1.160  -1.498   0.465
h   5.543   1.411   1.088
h   3.188  -2.053  -1.461
h   5.661  -1.840  -1.730
h   6.843  -0.041  -0.413
h  -3.602   1.358  -1.725
h  -1.189   1.564  -1.855
h   3.720   2.098   2.010
h   2.174   1.916   1.177
h   2.639   0.768   2.446
     7.   2
n  -4.940  -0.113   0.062
n   3.689   0.557   0.615
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c  -1.630   0.660  -1.275
c  -0.784   0.193  -0.239
c  -1.398  -0.332   0.926
c  -2.754  -0.430   1.035
c  -3.603   0.002  -0.030
c  -2.988   0.561  -1.192
c  -5.571  -0.673   1.263
c   0.649   0.321  -0.379
c   1.552  -0.484   0.205
c   3.008  -0.388  -0.053
c   5.148   0.557   0.521
c   5.739  -0.131  -0.485
c   4.979  -0.985  -1.326
c   3.609  -1.081  -1.070
c  -5.811   0.340  -1.034
c   3.181   1.185   1.881
     1.  19
h  -6.844   0.145  -0.767
```

```
h -5.693  1.411 -1.210
h -5.582 -0.203 -1.952
h -6.648 -0.665  1.134
h -5.248 -1.705  1.417
h -5.323 -0.081  2.145
h -3.183 -0.827  1.940
h -0.780 -0.647  1.754
h  0.997  1.042 -1.110
h  1.208 -1.251  0.896
h  5.693  1.212  1.183
h  2.992 -1.723 -1.685
h  5.441 -1.538 -2.126
h  6.803 -0.020 -0.634
h -3.595  0.911 -2.010
h -1.182  1.094 -2.158
h  3.954  1.767  2.379
h  2.406  1.877  1.543
h  2.750  0.505  2.622
     7.   2
n -4.940 -0.106  0.062
n  3.776  0.464  0.771
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.656  0.393 -1.391
c -0.810  0.226 -0.273
c -1.416 -0.059  0.972
c -2.772 -0.184  1.096
c -3.623 -0.032 -0.038
c -3.014  0.267 -1.292
c -5.587 -0.453  1.369
c  0.625  0.391 -0.430
c  1.557 -0.219  0.320
c  2.996 -0.224 -0.032
c  5.257  0.350  0.558
c  5.719 -0.263 -0.565
c  4.834 -0.903 -1.456
c  3.464 -0.858 -1.147
c -5.833 -0.025 -1.099
c  3.442  1.143  2.010
     1.  19
h -6.862 -0.196 -0.800
h -5.756  0.978 -1.523
h -5.571 -0.759 -1.865
h -6.664 -0.489  1.244
h -5.251 -1.419  1.755
h -5.350  0.325  2.096
h -3.195 -0.394  2.065
h -0.796 -0.164  1.852
h  0.950  0.965 -1.290
```

```
h  1.245  -0.864   1.140
h  5.899   0.868   1.251
h  2.747  -1.328  -1.806
h  5.188  -1.383  -2.352
h  6.781  -0.244  -0.765
h -3.623   0.401  -2.171
h -1.215   0.626  -2.350
h  4.236   1.193   2.754
h  3.176   2.163   1.714
h  2.574   0.678   2.478
     7.   2
n -4.962  -0.164   0.073
n  3.899   0.345   0.882
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.   16
c -1.697  -0.758  -1.309
c -0.823  -0.038  -0.473
c -1.392   0.686   0.593
c -2.748   0.694   0.817
c -3.627  -0.029  -0.031
c -3.056  -0.753  -1.111
c -5.554   0.724   1.292
c  0.620  -0.064  -0.731
c  1.563   0.057   0.226
c  2.992  -0.131   0.004
c  5.251   0.448   0.585
c  5.748  -0.398  -0.360
c  4.863  -1.157  -1.153
c  3.499  -0.999  -0.948
c -5.866  -0.791  -0.690
c  3.422   1.520   1.818
     1.   19
h -6.890  -0.655  -0.357
h -5.792  -0.446  -1.724
h -5.632  -1.858  -0.657
h -6.633   0.601   1.278
h -5.177   0.362   2.253
h -5.328   1.791   1.204
h -3.139   1.262   1.646
h -0.752   1.269   1.242
h  0.919  -0.238  -1.759
h  1.248   0.243   1.247
h  5.889   1.054   1.210
h  2.795  -1.582  -1.526
h  5.236  -1.849  -1.892
h  6.817  -0.476  -0.489
h -3.688  -1.307  -1.788
h -1.287  -1.324  -2.136
h  4.269   2.082   2.205
```

h 2.706 2.224 1.391
h 2.955 0.988 2.650
     7. 2
n -4.972 -0.029 0.183
n 3.898 0.588 0.795
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
c -1.741 -0.029 1.560
c -0.829 -0.238 0.506
c -1.356 -0.351 -0.797
c -2.704 -0.234 -1.041
c -3.619 -0.023 0.022
c -3.092 0.068 1.337
c -5.488 0.002 -1.569
c 0.606 -0.327 0.784
c 1.562 0.058 -0.102
c 2.987 -0.024 0.092
c 5.204 0.318 -0.779
c 5.776 -0.202 0.343
c 4.946 -0.660 1.387
c 3.580 -0.563 1.239
c -5.894 0.284 0.896
c 3.310 1.003 -2.157
     1. 19
h -6.906 0.310 0.506
h -5.826 -0.534 1.619
h -5.699 1.226 1.415
h -6.563 0.149 -1.543
h -5.051 0.773 -2.210
h -5.285 -0.978 -2.012
h -3.062 -0.320 -2.055
h -0.689 -0.556 -1.623
h 0.874 -0.695 1.768
h 1.220 0.466 -1.042
h 5.793 0.678 -1.609
h 2.932 -0.914 2.028
h 5.374 -1.080 2.285
h 6.852 -0.258 0.414
h -3.753 0.220 2.177
h -1.364 0.059 2.571
h 4.139 1.307 -2.791
h 2.707 0.274 -2.702
h 2.703 1.883 -1.935
     7. 2
n -4.959 0.087 -0.210
n 3.846 0.419 -0.925
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
 c -1.720 0.557 1.416
 c -0.822 -0.043 0.511
 c -1.365 -0.673 -0.626
 c -2.716 -0.666 -0.876
 c -3.617 -0.046 0.027
 c -3.074 0.561 1.192
 c -5.508 -0.662 -1.410
 c 0.621 0.003 0.767
 c 1.552 0.015 -0.203
 c 2.989 -0.097 0.034
 c 5.230 0.396 -0.679
 c 5.750 -0.339 0.344
 c 4.889 -0.996 1.245
 c 3.518 -0.858 1.060
 c -5.880 0.582 0.743
 c 3.366 1.373 -1.940
     1. 19
 h -6.896 0.475 0.375
 h -5.817 0.101 1.722
 h -5.666 1.648 0.860
 h -6.583 -0.516 -1.428
 h -5.083 -0.214 -2.313
 h -5.305 -1.738 -1.422
 h -3.088 -1.155 -1.764
 h -0.705 -1.191 -1.310
 h 0.926 0.052 1.807
 h 1.225 0.060 -1.238
 h 5.849 0.915 -1.394
 h 2.828 -1.372 1.714
 h 5.283 -1.596 2.052
 h 6.823 -0.412 0.445
 h -3.724 1.035 1.911
 h -1.329 1.033 2.306
 h 4.197 1.929 -2.370
 h 2.908 0.774 -2.730
 h 2.633 2.087 -1.560
     7.   2
 n -4.958 -0.038 -0.208
 n 3.870 0.530 -0.857
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6. 16
 c -1.670 0.906 1.123
 c -0.807 0.055 0.396
 c -1.396 -0.884 -0.482
 c -2.750 -0.931 -0.675
 c -3.616 -0.045 0.031
 c -3.025 0.874 0.947

```
c -5.553 -0.973 -1.156
c  0.631  0.132  0.604
c  1.550 -0.185 -0.313
c  3.002 -0.226 -0.017
c  5.222  0.558 -0.510
c  5.748 -0.351  0.353
c  4.918 -1.248  1.056
c  3.534 -1.155  0.832
c -5.857  0.748  0.647
c  3.317  1.735 -1.525
     1.  19
h -6.880  0.429  0.471
h -5.643  0.638  1.711
h -5.768  1.801  0.368
h -6.606 -0.730 -1.259
h -5.074 -0.838 -2.126
h -5.465 -2.019 -0.853
h -3.161 -1.670 -1.343
h -0.765 -1.594 -0.996
h  0.964  0.518  1.563
h  1.229 -0.533 -1.295
h  5.822  1.270 -1.054
h  2.858 -1.827  1.342
h  5.324 -1.961  1.753
h  6.820 -0.371  0.492
h -3.644  1.562  1.499
h -1.241  1.610  1.822
h  4.072  2.060 -2.239
h  2.437  1.422 -2.086
h  3.046  2.589 -0.895
     7.   2
n -4.953 -0.085 -0.155
n  3.847  0.627 -0.744
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.589  0.994  0.951
c -0.776  0.011  0.333
c -1.426 -1.010 -0.406
c -2.781 -1.029 -0.556
c -3.596 -0.013  0.033
c -2.945  1.001  0.801
c -5.601 -1.063 -0.907
c  0.653  0.030  0.541
c  1.560 -0.473 -0.316
c  3.021 -0.402 -0.083
c  5.094  0.805 -0.323
c  5.749 -0.159  0.365
c  5.062 -1.296  0.861
c  3.689 -1.372  0.613
```

c -5.770 1.018 0.501
c 3.056 1.746 -1.361
    1. 19
h -6.808 0.832 0.244
h -5.672 0.992 1.587
h -5.495 2.008 0.135
h -6.668 -0.862 -0.929
h -5.230 -1.072 -1.932
h -5.443 -2.045 -0.457
h -3.238 -1.830 -1.113
h -0.836 -1.804 -0.839
h 1.010 0.571 1.411
h 1.211 -0.953 -1.228
h 5.582 1.680 -0.719
h 3.124 -2.219 0.979
h 5.577 -2.069 1.408
h 6.811 -0.046 0.531
h -3.525 1.776 1.275
h -1.115 1.763 1.546
h 3.801 2.454 -1.719
h 2.557 1.319 -2.234
h 2.321 2.299 -0.770
    7.   2
n -4.932 -0.017 -0.121
n 3.720 0.721 -0.575
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6. 16
c -1.548 1.128 0.706
c -0.765 0.028 0.292
c -1.438 -1.094 -0.242
c -2.800 -1.118 -0.367
c -3.589 -0.003 0.042
c -2.911 1.125 0.590
c -5.623 -1.190 -0.639
c 0.679 0.062 0.459
c 1.555 -0.593 -0.319
c 3.031 -0.471 -0.184
c 4.997 0.913 -0.068
c 5.729 -0.133 0.398
c 5.135 -1.397 0.594
c 3.768 -1.515 0.305
c -5.743 1.131 0.330
c 3.018 1.827 -1.176
    1. 19
h -6.788 0.919 0.132
h -5.626 1.324 1.399
h -5.459 2.025 -0.228
h -6.691 -1.000 -0.648
h -5.296 -1.382 -1.662

```
h -5.435 -2.076 -0.029
h -3.275 -1.998 -0.771
h -0.867 -1.962 -0.538
h  1.061  0.724  1.231
h  1.185 -1.193 -1.146
h  5.420  1.887 -0.255
h  3.268 -2.460  0.468
h  5.711 -2.243  0.928
h  6.778  0.021  0.608
h -3.471  1.984  0.923
h -1.055  1.992  1.130
h  3.484  2.785 -0.948
h  3.150  1.622 -2.245
h  1.955  1.899 -0.965
     7.  2
n -4.933 -0.021 -0.082
n  3.633  0.794 -0.348
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.  16
c -1.671  1.311 -0.539
c -0.826  0.541  0.289
c -1.391 -0.585  0.921
c -2.716 -0.905  0.781
c -3.581 -0.072  0.015
c -3.012  1.055 -0.645
c -5.486 -1.513  0.582
c  0.640  0.783  0.298
c  1.502 -0.122 -0.246
c  2.924 -0.221 -0.275
c  5.161  0.388  0.402
c  5.690 -0.747 -0.110
c  4.832 -1.663 -0.778
c  3.497 -1.386 -0.838
c -5.784  0.498 -0.901
c  3.400  2.023  0.752
      1.  19
h -6.796  0.109 -0.848
h -5.786  1.522 -0.522
h -5.470  0.505 -1.947
h -6.549 -1.551  0.368
h -5.027 -2.439  0.230
h -5.350 -1.435  1.663
h -3.095 -1.804  1.240
h -0.749 -1.222  1.513
h  0.974  1.488  1.047
h  1.045 -0.922 -0.822
h  5.765  1.130  0.901
h  2.822 -2.080 -1.321
h  5.232 -2.561 -1.224
```

h 6.748 -0.936 -0.016
h -3.632 1.704 -1.242
h -1.243 2.145 -1.080
h 4.267 2.681 0.750
h 2.664 2.428 0.060
h 2.983 2.002 1.760
    7.   2
n -4.900 -0.353 -0.099
n 3.817 0.689 0.313
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6.   16
c -1.641 1.062 -0.947
c -0.823 0.569 0.089
c -1.415 -0.279 1.042
c -2.749 -0.599 0.994
c -3.588 -0.040 -0.010
c -2.989 0.809 -0.983
c -5.518 -1.219 0.942
c 0.650 0.790 0.052
c 1.508 -0.237 -0.142
c 2.944 -0.299 -0.190
c 5.165 0.449 0.378
c 5.741 -0.510 -0.386
c 4.912 -1.453 -1.051
c 3.553 -1.330 -0.925
c -5.788 0.278 -1.059
c 3.283 1.550 1.463
    1.   19
h -6.817 0.003 -0.847
h -5.711 1.366 -1.043
h -5.529 -0.084 -2.056
h -6.569 -1.351 0.708
h -5.034 -2.198 0.918
h -5.433 -0.805 1.949
h -3.153 -1.290 1.717
h -0.793 -0.703 1.818
h 0.983 1.758 0.403
h 1.056 -1.177 -0.449
h 5.747 1.172 0.930
h 2.899 -2.027 -1.431
h 5.346 -2.240 -1.647
h 6.816 -0.555 -0.468
h -3.587 1.240 -1.770
h -1.193 1.674 -1.717
h 4.097 1.882 2.103
h 2.870 2.423 0.950
h 2.510 1.105 2.087
    7.   2
n -4.915 -0.319 -0.044

n 3.797 0.563 0.520
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
 c -1.615 0.741 -1.201
 c -0.797 0.403 -0.104
 c -1.413 -0.129 1.042
 c -2.767 -0.345 1.094
 c -3.594 -0.002 -0.012
 c -2.972 0.556 -1.166
 c -5.575 -0.769 1.220
 c 0.672 0.586 -0.183
 c 1.521 -0.432 -0.069
 c 2.991 -0.367 -0.187
 c 5.124 0.473 0.552
 c 5.769 -0.261 -0.389
 c 5.040 -1.111 -1.255
 c 3.657 -1.145 -1.108
 c -5.786 0.154 -1.110
 c 3.112 1.169 1.780
      1.   19
 h -6.818 -0.081 -0.870
 h -5.714 1.222 -1.328
 h -5.498 -0.412 -1.998
 h -6.643 -0.848 1.046
 h -5.182 -1.766 1.431
 h -5.411 -0.129 2.090
 h -3.200 -0.777 1.982
 h -0.799 -0.381 1.895
 h 1.028 1.597 -0.361
 h 1.104 -1.432 0.050
 h 5.644 1.114 1.246
 h 3.063 -1.786 -1.746
 h 5.539 -1.710 -1.998
 h 6.845 -0.193 -0.457
 h -3.565 0.831 -2.023
 h -1.156 1.153 -2.089
 h 3.885 1.647 2.377
 h 2.432 1.941 1.411
 h 2.546 0.494 2.427
      7.   2
 n -4.934 -0.201 0.030
 n 3.742 0.441 0.690
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
 c -1.599 0.259 -1.371
 c -0.794 0.252 -0.212

```
c -1.431  0.158  1.043
c -2.789  0.033  1.144
c -3.601  0.003 -0.028
c -2.957  0.125 -1.296
c -5.607 -0.247  1.362
c  0.660  0.420 -0.329
c  1.540 -0.457  0.150
c  3.000 -0.365 -0.099
c  5.164  0.453  0.582
c  5.740 -0.131 -0.496
c  4.964 -0.860 -1.431
c  3.587 -0.949 -1.186
c -5.775 -0.165 -1.150
c  3.208  0.973  2.002
     1.  19
h -6.812 -0.299 -0.863
h -5.686  0.770 -1.705
h -5.482 -0.996 -1.795
h -6.676 -0.337  1.208
h -5.257 -1.133  1.895
h -5.417  0.639  1.970
h -3.243 -0.034  2.120
h -0.828  0.192  1.939
h  1.004  1.220 -0.976
h  1.177 -1.287  0.755
h  5.723  1.011  1.316
h  2.955 -1.500 -1.870
h  5.413 -1.330 -2.289
h  6.808 -0.032 -0.630
h -3.540  0.116 -2.203
h -1.126  0.360 -2.337
h  3.996  1.471  2.565
h  2.454  1.719  1.744
h  2.754  0.225  2.658
     7.   2
n -4.940 -0.132  0.058
n  3.787  0.367  0.817
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
     6.  16
c -1.612 -1.034 -0.983
c -0.809 -0.007 -0.447
c -1.437  0.996  0.313
c -2.792  0.992  0.523
c -3.607 -0.032 -0.038
c -2.970 -1.050 -0.805
c -5.599  0.992  0.971
c  0.653 -0.009 -0.662
c  1.538 -0.074  0.337
c  2.984 -0.247  0.122
```

```
c  5.214  0.639  0.338
c  5.722 -0.411 -0.356
c  4.869 -1.432 -0.838
c  3.501 -1.302 -0.590
c -5.791 -1.079 -0.446
c  3.359  1.848  1.418
      1.  19
h -6.831 -0.862 -0.229
h -5.659 -1.102 -1.529
h -5.546 -2.061 -0.034
h -6.660  0.774  1.038
h -5.183  1.003  1.980
h -5.473  1.977  0.519
h -3.239  1.780  1.109
h -0.836  1.790  0.731
h  0.997 -0.025 -1.690
h  1.183 -0.032  1.364
h  5.827  1.443  0.715
h  2.813 -2.052 -0.950
h  5.261 -2.280 -1.375
h  6.786 -0.452 -0.534
h -3.552 -1.844 -1.244
h -1.142 -1.820 -1.557
h  4.133  2.609  1.497
h  2.480  2.302  0.961
h  3.104  1.515  2.430
      7.   2
n -4.948 -0.040  0.154
n  3.853  0.751  0.599
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.  16
c -1.655 -0.127  1.473
c -0.822 -0.509  0.400
c -1.402 -0.578 -0.881
c -2.736 -0.334 -1.084
c -3.591 -0.037  0.016
c -3.002  0.061  1.310
c -5.516  0.070 -1.503
c  0.641 -0.643  0.593
c  1.536  0.208  0.026
c  2.958  0.104  0.169
c  5.165  0.372 -0.771
c  5.744 -0.246  0.287
c  4.921 -0.714  1.348
c  3.566 -0.536  1.263
c -5.803  0.462  0.963
c  3.243  1.218 -2.030
      1.  19
h -6.827  0.505  0.610
```

```
h -5.732 -0.314  1.726
h -5.547  1.426  1.409
h -6.581  0.263 -1.429
h -5.075  0.809 -2.175
h -5.372 -0.927 -1.924
h -3.133 -0.359 -2.087
h -0.770 -0.818 -1.726
h  0.988 -1.579  1.018
h  1.154  1.026 -0.574
h  5.738  0.752 -1.603
h  2.924 -0.853  2.071
h  5.364 -1.182  2.215
h  6.815 -0.367  0.316
h -3.612  0.298  2.167
h -1.215 -0.011  2.453
h  4.030  1.381 -2.761
h  2.469  0.594 -2.483
h  2.809  2.186 -1.766
      7.   2
n -4.918  0.161 -0.167
n  3.805  0.553 -0.861
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
c -1.675  0.451  1.422
c -0.836 -0.372  0.638
c -1.398 -0.960 -0.515
c -2.719 -0.789 -0.842
c -3.582 -0.039  0.008
c -3.012  0.581  1.158
c -5.475 -0.520 -1.477
c  0.623 -0.415  0.896
c  1.536  0.132  0.040
c  2.949 -0.006  0.116
c  5.135  0.442 -0.815
c  5.752 -0.311  0.127
c  4.958 -0.944  1.124
c  3.605 -0.779  1.101
c -5.791  0.843  0.614
c  3.189  1.463 -1.876
      1.   19
h -6.813  0.739  0.261
h -5.736  0.452  1.631
h -5.532  1.904  0.623
h -6.524 -0.249 -1.545
h -4.969 -0.162 -2.375
h -5.397 -1.608 -1.432
h -3.096 -1.215 -1.758
h -0.760 -1.544 -1.162
h  0.940 -1.198  1.577
```

```
h   1.148   0.766  -0.747
h   5.681   0.950  -1.595
h   2.998  -1.247   1.862
h   5.427  -1.541   1.891
h   6.824  -0.418   0.113
h  -3.629   1.174   1.816
h  -1.245   0.961   2.272
h   3.986   1.877  -2.489
h   2.520   0.886  -2.517
h   2.631   2.289  -1.428
     7.   2
n  -4.898   0.094  -0.277
n   3.772   0.617  -0.840
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
      6.   16
c  -1.669   0.821   1.184
c  -0.833  -0.162   0.617
c  -1.411  -1.070  -0.291
c  -2.746  -1.018  -0.608
c  -3.598  -0.064   0.015
c  -3.014   0.858   0.928
c  -5.524  -0.986  -1.197
c   0.633  -0.138   0.859
c   1.536   0.103  -0.111
c   2.960  -0.080   0.018
c   5.199   0.519  -0.655
c   5.739  -0.438   0.138
c   4.882  -1.266   0.913
c   3.526  -1.065   0.833
c  -5.800   0.953   0.386
c   3.325   1.828  -1.536
      1.   19
h  -6.821   0.795   0.054
h  -5.768   0.846   1.472
h  -5.502   1.970   0.121
h  -6.586  -0.782  -1.282
h  -5.071  -0.892  -2.186
h  -5.393  -2.009  -0.841
h  -3.140  -1.700  -1.345
h  -0.779  -1.809  -0.761
h   0.964  -0.553   1.807
h   1.174   0.497  -1.058
h   5.801   1.170  -1.270
h   2.851  -1.705   1.384
h   5.291  -2.050   1.531
h   6.810  -0.567   0.163
h  -3.627   1.601   1.414
h  -1.233   1.548   1.856
h   4.152   2.466  -1.835
```

h 2.828 1.460 -2.437
h 2.617 2.424 -0.957
    7. 2
n -4.924 -0.030 -0.259
n 3.838 0.732 -0.720
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6. 16
c -1.603 0.982 0.918
c -0.813 -0.089 0.451
c -1.454 -1.148 -0.217
c -2.807 -1.136 -0.441
c -3.606 -0.055 0.027
c -2.958 1.007 0.722
c -5.610 -1.098 -0.943
c 0.651 -0.093 0.673
c 1.543 -0.134 -0.311
c 2.996 -0.222 -0.075
c 5.196 0.704 -0.403
c 5.754 -0.346 0.253
c 4.947 -1.379 0.780
c 3.563 -1.278 0.589
c -5.781 1.031 0.381
c 3.259 1.949 -1.277
    1. 19
h -6.826 0.796 0.200
h -5.627 1.118 1.456
h -5.553 1.989 -0.093
h -6.641 -0.811 -1.125
h -5.117 -1.244 -1.904
h -5.601 -2.039 -0.387
h -3.264 -1.962 -0.963
h -0.863 -1.984 -0.556
h 0.989 -0.067 1.706
h 1.197 -0.111 -1.345
h 5.776 1.509 -0.824
h 2.907 -2.056 0.952
h 5.379 -2.217 1.300
h 6.829 -0.379 0.362
h -3.529 1.846 1.087
h -1.124 1.798 1.438
h 3.981 2.763 -1.263
h 3.033 1.710 -2.321
h 2.349 2.294 -0.787
    7. 2
n -4.945 -0.037 -0.178
n 3.816 0.807 -0.567
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6. 16
c -1.529 1.080 0.664
c -0.782 -0.078 0.350
c -1.482 -1.222 -0.088
c -2.842 -1.209 -0.248
c -3.592 -0.029 0.034
c -2.885 1.119 0.503
c -5.660 -1.185 -0.603
c 0.667 -0.111 0.575
c 1.553 -0.404 -0.375
c 3.020 -0.371 -0.159
c 5.083 0.880 -0.166
c 5.758 -0.207 0.284
c 5.089 -1.430 0.526
c 3.706 -1.463 0.291
c -5.705 1.212 0.165
c 3.022 2.001 -0.941
    1. 19
h -6.752 1.024 -0.047
h -5.605 1.486 1.217
h -5.368 2.042 -0.458
h -6.718 -0.950 -0.662
h -5.313 -1.478 -1.595
h -5.529 -2.020 0.087
h -3.343 -2.105 -0.577
h -0.928 -2.126 -0.289
h 1.015 0.232 1.545
h 1.188 -0.686 -1.362
h 5.560 1.826 -0.365
h 3.153 -2.373 0.472
h 5.616 -2.300 0.881
h 6.821 -0.122 0.452
h -3.420 2.026 0.738
h -1.011 1.954 1.031
h 3.760 2.767 -1.175
h 2.490 1.761 -1.865
h 2.312 2.422 -0.225
    7. 2
n -4.931 -0.001 -0.129
n 3.704 0.837 -0.408
BASIS
6-31G*

Atomtypes=3 Charge=1 Nosymmetry Angstrom
    6. 16
c -1.532 1.230 0.313
c -0.778 0.041 0.359
c -1.461 -1.182 0.227
c -2.822 -1.229 0.064
c -3.587 -0.028 0.039
c -2.894 1.210 0.172

```
c -5.638 -1.338 -0.284
c  0.688  0.076  0.528
c  1.538 -0.424 -0.375
c  3.009 -0.389 -0.252
c  5.035  0.855  0.137
c  5.740 -0.296  0.278
c  5.105 -1.551  0.117
c  3.735 -1.550 -0.138
c -5.725  1.170 -0.106
c  3.037  2.079 -0.614
     1.  19
h -6.779  0.915 -0.148
h -5.544  1.739  0.807
h -5.481  1.790 -0.971
h -6.694 -1.142 -0.436
h -5.257 -1.875 -1.154
h -5.524 -1.965  0.602
h -3.309 -2.186 -0.032
h -0.895 -2.102  0.264
h  1.068  0.564  1.419
h  1.137 -0.929 -1.250
h  5.484  1.830  0.239
h  3.204 -2.489 -0.228
h  5.659 -2.471  0.192
h  6.792 -0.236  0.511
h -3.438  2.141  0.151
h -1.023  2.179  0.401
h  3.754  2.894 -0.537
h  2.726  1.991 -1.659
h  2.164  2.328 -0.011
     7.   2
n -4.931 -0.063 -0.112
n  3.672  0.851 -0.155
```