

Supplementary Information

Appropriate Clusterset Selection for the Prediction of Thermodynamic Properties of Liquid Water with QCE Theory

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1 Cluster Gibbs free energy Details

Eqns. 1 - 5 are based on standard physical chemistry formulae where R is the gas constant, T is temperature in Kelvin, h is Planck's constant, ν is the vibrational frequency in cm^{-1} , m refers to the mass of the molecule, k_b is the Boltzmann's constant, $zpve$ is the zero point vibrational energy and Θ^{rot} refers to the moments of inertia.¹

$$TC = TC_{trans} + TC_{vib} + TC_{rot} = \frac{5}{2}RT + R \sum_i^N \left(\frac{\theta^{vib,i}}{2} + \frac{\theta^{vib,i} e^{-\theta^{vib,i}/T}}{1 - e^{-\theta^{vib,i}/T}} \right) + \frac{3}{2}RT \quad (1)$$

where $\theta^{vib,i} = \frac{h\nu}{k}$

$$S_{trans} = R \log \left(\frac{2\pi m k_b T}{h^2} \right)^{\frac{3}{2}} V + \frac{5}{2} \quad (2)$$

$$S_{rot} = R \log \frac{1}{\sigma} \sqrt{\frac{\pi T^3}{\Theta_1^{rot} \Theta_2^{rot} \Theta_3^{rot}}} + \frac{3}{2} \quad (3)$$

$$S_{vib} = R \sum_i \left(\frac{\theta^{vib,i}/T}{e^{\theta^{vib,i}/T} - 1} - \ln(1 - e^{-\theta^{vib,i}/T}) \right) \quad (4)$$

$$S = S_{trans} + S_{vib} + S_{rot} \quad (5)$$

$$G_n^{cluster} = E_{cluster} + zpve + TC - TS \quad (6)$$

2 Quantum Cluster Equilibrium (QCE) Details

$$q_i = q_i^{trans} q_i^{rot} q_i^{elec} q_i^{vib} \quad (7)$$

To calculate the partition function of cluster size i (q_i), the individual translational (q_i^{trans}), rotational (q_i^{rot}), electronic (q_i^{elec}) and vibrational (q_i^{vib}) components must first be computed.

$$q_i^{trans} = \frac{V - V^{ex}}{\Lambda^3} \quad \text{where } \Lambda = \frac{h}{\sqrt{2\pi m_i k_B T}} \quad (8)$$

where h refers to Planck's constant, m_i is the mass of cluster size i , k_B is Boltzmann's constant, T refers to the temperature and V refers to the phase volume. Since cluster volumes (v_i) are computed using Bondi's radii and assumed to be non-penetrable, an excluded volume term, V^{ex} is subtracted from V to account for inaccessibility of other particles.

$$V^{ex} = b_{xv} \sum N_i v_i \quad (9)$$

where N_i refers to the populations of cluster i . A volume scaling parameter, b_{xv} is determined by fixing the experimental density at ambient conditions. To calculate q_i^{rot} at temperature T , a symmetry number, σ and the rotational temperature, Θ is required.

$$q_i^{rot} = \frac{1}{\sigma} \left(\frac{\pi T^3}{\Theta_A \Theta_B \Theta_C} \right)^{1/2} \quad \text{where } \Theta = \frac{\hbar}{2Ik} \quad (10)$$

where \hbar refers to $h/2\pi$ and I is the moment of inertia around the principal rotational axes. Calculation of q_i^{elec} requires an empirical mean field parameter, a_{mf} to account for inter-cluster interactions and the binding energy, $E_{BIND,i}$ of cluster i to describe intra-cluster interactions. The a_{mf} term is fitted to eq. 12 to minimize the difference between the experimental and predicted boiling point at standard pressure.

$$q_i^{elec} = e^{(E_{BIND,i} - a_{mf} n_i \frac{N^{tot}}{V})} \quad (11)$$

where n_i refers to the number of monomers in cluster size i and N^{tot} is the total number of molecules. To compute q_i^{vib} , a harmonic approximation is assumed and calculated as follows:

$$q_i^{vib} = \prod_{m=1}^{3N-6} \frac{e^{-\theta_m^{vib}/2T}}{1 - e^{-\theta_m^{vib}/T}} \quad \text{where } \theta^{vib} = \frac{h\nu_m}{k_B} \quad (12)$$

where ν_m is the vibrational frequency of the m^{th} mode. Since QCE theory describes a liquid as a NVT ensemble, clusters of varying sizes are treated according to

$$A_1 = \frac{A_2}{2} = \frac{A_3}{3} = \dots = \frac{A_n}{n} \quad (13)$$

Therefore, the populations of cluster size i can be calculated using the monomer population (N_1) and monomer partition function (q_1) based on eq. 15.

$$N_i = q_i \left[\frac{N_1}{q_1} \right]^i \quad (14)$$

The overall system partition function, Q is calculated as a product of the individual cluster partition functions.

$$Q = \prod_{i=1} Q(N_i, V, T) = \prod_{i=1} \frac{q_i^{N_i}}{N_i!} \quad (15)$$

The system partition function, Q is then implemented in standard thermodynamic equations based on eqns. 17 - 20 for the prediction of internal energy (U), Helmholtz energy (A), Gibbs free energy (G) and entropy (S).²

$$U = k_B T^2 \left(\frac{\delta \ln Q}{\delta T} \right)_{N,V} \quad (16)$$

$$A = -k_B T \ln Q \quad (17)$$

$$G = -k_B T \ln Q + PV \quad (18)$$

$$S = k_B T \left(\frac{\delta \ln Q}{\delta T} \right)_{N,V} + k_B T \ln Q \quad (19)$$

References

- [1] McQuarrie, D. A. *Statistical Mechanics*; University Science Books, 2000.
- [2] Von Domaros, M.; Perl, E. Anharmonic Effects in the Quantum Cluster Equilibrium Method. *J. Chem. Phys.* **2017**, *146*.

3 No. of structures within $\Delta G_{BIND/molecule} < 10\text{kJ mol}^{-1}$ criteria for all W_n

Table S1: Number of W_n clusters where $n = 3$ to 10 within $\Delta G_{BIND/mol} < 10\text{kJ mol}^{-1}$

| W_n | No. of molecular graph groups | No. of structures with $\Delta G_{BIND/molecule} < 10\text{kJ mol}^{-1}$ |
|-----------------|-------------------------------|--|
| w ₃ | 3 | 3 |
| w ₄ | 3 | 3 |
| w ₅ | 14 | 12 |
| w ₆ | 46 | 42 |
| w ₇ | 116 | 110 |
| w ₈ | 204 | 197 |
| w ₉ | 304 | 301 |
| w ₁₀ | 367 | 366 |

4 Errors of two-, three-, four- and five-combinations clustersets

Table S2: Errors of all two-combination clustersets tested

| 2-combination clustersets | | | | | Mean Absolute Error | | | |
|---------------------------|---|------|------|-----------|------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| Set | Clusterset | amf | bxv | QCE error | Volume (dm ³) | ΔS (JmolK ⁻¹) | ΔH (kJmol ⁻¹) | ΔU (kJmol ⁻¹) |
| 2a | w ₁ , w ₂ | 0.60 | 1.00 | 3.79E-03 | 1.16E-04 (0.9%) | 5.83 (47.7%) | 1.77 (47.8%) | 1.77 (47.7%) |
| 2b | w ₁ , w ₃ -86_25 | 0.46 | 1.00 | 3.45E-03 | 1.47E-04 (0.8%) | 5.90 (48.6%) | 1.80 (48.6%) | 1.80 (48.5%) |
| 2c | w ₁ w ₄ -100_40 | 0.40 | 1.00 | 3.47E-03 | 2.07E-04 (0.9%) | 5.83 (48.0%) | 1.78 (48.0%) | 1.78 (47.9%) |
| 2d | w ₁ , w ₅ -5_40 | 0.44 | 1.01 | 3.46E-03 | 1.58E-04 (0.8%) | 5.48 (45.6%) | 1.67 (45.6%) | 1.66 (45.5%) |
| 2e | w ₁ , w ₆ -13_80 | 0.42 | 1.01 | 3.48E-03 | 1.77E-04 (0.9%) | 5.57 (46.2%) | 1.69 (46.2%) | 1.69 (46.1%) |
| 2f | w ₁ , w ₇ -26_40 | 0.54 | 1.02 | 3.50E-03 | 1.81E-04 (0.9%) | 5.68 (47.0%) | 1.73 (47.0%) | 1.73 (46.9%) |
| 2g | w ₁ , w ₈ -23_25 | 0.44 | 1.01 | 3.49E-03 | 1.70E-04 (0.9%) | 5.44 (45.3%) | 1.65 (45.3%) | 1.73 (45.2%) |
| 2h | w ₁ , w ₉ -66_25 | 0.48 | 1.02 | 3.48E-03 | 1.70E-04 (0.9%) | 4.33 (44.8%) | 1.61 (44.7%) | 1.65 (44.7%) |
| 2i | w ₁ , w ₁₀ -10_80 | 0.48 | 1.02 | 3.49E-03 | 1.78E-04 (0.9%) | 5.33 (44.8%) | 1.62 (44.7%) | 1.61 (44.7%) |

Table S3: Errors of all three-combination clustersets tested

| 3-combination clustersets | | | | | Mean Absolute Error | | | |
|---------------------------|--|------|------|-----------|------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| Set | Clusterset | amf | bxv | QCE error | Volume (dm ³) | ΔS (JmolK ⁻¹) | ΔH (kJmol ⁻¹) | ΔU (kJmol ⁻¹) |
| 3a | w ₁ , w ₂ , w ₉ -66_25 | 0.48 | 1.02 | 3.41E-03 | 1.66E-04 (0.9%) | 5.90 (31.5%) | 0.89 (30.8%) | 0.89 (30.7%) |
| 3b | w ₁ , w ₃ -86_25, w ₉ -66_25 | 0.46 | 1.00 | 3.45E-03 | 1.47E-04 (0.8%) | 5.83 (48.6%) | 1.80 (48.6%) | 1.80 (48.5%) |
| 3c | w ₁ , w ₄ -100_40, w ₉ -66_25 | 0.40 | 1.00 | 3.47E-03 | 1.66E-04 (0.9%) | 5.48 (47.9%) | 1.77 (47.9%) | 1.77 (47.8%) |
| 3d | w ₁ , w ₅ -5_40, w ₉ -66_25 | 0.44 | 1.01 | 3.45E-03 | 1.57E-04 (0.8%) | 5.48 (43.9%) | 1.62 (43.9%) | 1.62 (43.9%) |
| 3e | w ₁ , w ₆ -13_80, w ₉ -66_25 | 0.42 | 1.01 | 3.48E-03 | 1.76E-04 (0.9%) | 5.57 (44.5%) | 1.65 (44.5%) | 1.65 (44.5%) |
| 3f | w ₁ , w ₇ -26_40, w ₉ -66_25 | 0.54 | 1.02 | 3.50E-03 | 1.81E-04 (0.9%) | 5.68 (46.9%) | 1.73 (46.9%) | 1.72 (46.8%) |
| 3g | w ₁ , w ₈ -23_25, w ₉ -66_25 | 0.46 | 1.02 | 3.48E-03 | 1.66E-04 (0.9%) | 5.44 (25.2%) | 0.96 (25.4%) | 0.96 (25.3%) |
| 3h | w ₁ w ₉ -66_25, w ₁₀ -10_80 | 0.48 | 1.02 | 3.48E-03 | 1.76E-04 (0.9%) | 5.83 (45.1%) | 1.63 (45.0%) | 0.89 (45.1%) |

Table S4: Errors of all four-combination clustersets tested

| 4-combination clustersets | | | | | Mean Absolute Error | | | |
|---------------------------|--|------|------|-----------|------------------------------|--|---------------------------------------|---------------------------------------|
| Set | Clusterset | amf | bxv | QCE error | Volume (dm ³) | ΔS (J mol K ⁻¹) | ΔH (kJ mol ⁻¹) | ΔU (kJ mol ⁻¹) |
| 4a | w ₁ , w ₂ , w _{8-23_25} , w _{9-66_25} | 0.48 | 1.02 | 3.45E-03 | 1.47E-04 (0.8%) | 5.90 (18.1%) | 0.60 (18.0%) | 0.60 (17.9%) |
| 4b | w ₁ , w _{3-86_25} , w _{8-23_25} , w _{9-66_25} | 0.46 | 1.00 | 3.45E-03 | 1.47E-04 (0.8%) | 5.83 (48.6%) | 1.80 (48.6%) | 1.80 (48.5%) |
| 4c | w ₁ , w _{4-100_40} , w _{8-23_25} , w _{9-66_25} | 0.40 | 1.00 | 3.47E-03 | 1.66E-04 (0.9%) | 5.48 (47.7%) | 1.77 (47.9%) | 1.77 (47.8%) |
| 4d | w ₁ , w _{5-5_40} , w _{8-23_25} , w _{9-66_25} | 0.44 | 1.01 | 3.46E-03 | 1.58E-04 (0.8%) | 5.48 (44.0%) | 1.62 (44.1%) | 1.62 (44.0%) |
| 4e | w ₁ , w _{6-13_80} , w _{8-23_25} , w _{9-66_25} | 0.42 | 1.01 | 3.48E-03 | 1.77E-04 (0.9%) | 5.57 (44.3%) | 1.64 (44.4%) | 1.64 (44.3%) |
| 4f | w ₁ , w _{7-26_40} , w _{8-23_25} , w _{9-66_25} | 0.54 | 1.02 | 3.50E-03 | 1.81E-04 (0.9%) | 5.68 (46.8%) | 1.73 (46.9%) | 1.72 (46.8%) |
| 4g | w ₁ , w _{8-23_25} , w _{9-66_25} , w _{10-10_80} | 0.48 | 1.02 | 3.45E-03 | 1.64E-04 (0.9%) | 5.44 (24.4%) | 0.87 (24.4%) | 0.87 (24.3%) |

Table S5: Errors of all five-combination clustersets tested

| 5-combination clustersets | | | | | Mean Absolute Error | | | |
|---------------------------|---|------|------|-----------|------------------------------|--|---------------------------------------|---------------------------------------|
| Set | Clusterset | amf | bxv | QCE error | Volume (dm ³) | ΔS (J mol K ⁻¹) | ΔH (kJ mol ⁻¹) | ΔU (kJ mol ⁻¹) |
| 5a | w ₁ , w ₂ , w _{3-86_25} , w _{8-23_25} , w _{9-66_25} | 0.48 | 1.02 | 3.45E-03 | 1.47E-04 (0.8%) | 5.90 (48.5%) | 1.80 (48.5%) | 1.79 (48.4%) |
| 5b | w ₁ , w ₂ , w _{4-100_40} , w _{8-23_25} , w _{9-66_25} | 0.46 | 1.00 | 3.45E-03 | 1.47E-04 (0.8%) | 5.83 (47.4%) | 1.75 (47.4%) | 1.75 (47.3%) |
| 5c | w ₁ , w ₂ , w _{5-5_40} , w _{8-23_25} , w _{9-66_25} | 0.44 | 1.01 | 3.46E-03 | 1.58E-04 (0.8%) | 5.48 (40.0%) | 1.43 (39.9%) | 1.43 (39.8%) |
| 5d | w ₁ , w ₂ , w _{6-13_80} , w _{8-23_25} , w _{9-66_25} | 0.42 | 1.01 | 3.48E-03 | 1.77E-04 (0.9%) | 5.57 (41.8%) | 1.52 (41.8%) | 1.52 (41.7%) |
| 5e | w ₁ , w ₂ , w _{7-26_40} , w _{8-23_25} , w _{9-66_25} | 0.40 | 1.00 | 3.47E-03 | 1.66E-04 (0.9%) | 5.48 (45.7%) | 1.67 (45.6%) | 1.67 (45.6%) |
| 5f | w ₁ , w ₂ , w _{8-23_25} , w _{9-66_25} , w _{10-10_80} | 0.54 | 1.02 | 3.50E-03 | 1.81E-04 (0.9%) | 5.68 (16.9%) | 0.49 (16.7%) | 0.49 (16.6%) |

5 Errors of best 37 complete sets

Table S6: Error of best 37 complete full sets.

| Best 37 full sets | | | | Mean Absolute Error | | | |
|-------------------|------|------|-----------|------------------------------|--|---------------------------------------|---------------------------------------|
| Set | amf | bxv | QCE error | Volume (dm ³) | ΔS (J mol K ⁻¹) | ΔH (kJ mol ⁻¹) | ΔU (kJ mol ⁻¹) |
| set346 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.21 (2.9%) | 0.07 (3.1%) | 0.07 (3.0%) |
| set345 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.24 (3.1%) | 0.08 (3.3%) | 0.08 (3.2%) |
| set347 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.27 (3.1%) | 0.08 (3.2%) | 0.08 (3.1%) |
| set349 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.30 (3.4%) | 0.10 (3.6%) | 0.10 (3.5%) |
| set363 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.29 (3.4%) | 0.09 (3.6%) | 0.09 (3.6%) |
| set352 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.31 (3.4%) | 0.10 (3.6%) | 0.10 (3.6%) |
| set350 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.31 (3.4%) | 0.10 (3.6%) | 0.10 (3.6%) |
| set351 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.31 (3.5%) | 0.10 (3.6%) | 0.10 (3.6%) |
| set348 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.32 (3.4%) | 0.10 (3.5%) | 0.10 (3.5%) |
| set353 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.32 (3.5%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set357 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.33 (3.5%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set354 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.33 (3.6%) | 0.10 (3.7%) | 0.11 (3.7%) |
| set355 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.34 (3.6%) | 0.11 (3.7%) | 0.11 (3.7%) |
| set362 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.33 (3.6%) | 0.10 (3.8%) | 0.10 (3.8%) |
| set364 | 0.44 | 1.01 | 3.41E-03 | 1.36E-04 (0.7%) | 0.36 (3.6%) | 0.11 (3.8%) | 0.11 (3.7%) |
| set366 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.39 (3.9%) | 0.12 (4.1%) | 0.12 (4.1%) |

| | | | | | | | |
|--------|------|------|----------|-----------------|-------------|-------------|-------------|
| set369 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.1%) |
| set367 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.1%) |
| set368 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.1%) |
| set365 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.41 (4.0%) | 0.13 (4.1%) | 0.13 (4.1%) |
| set370 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.41 (4.0%) | 0.13 (4.2%) | 0.13 (4.2%) |
| set374 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.41 (4.0%) | 0.13 (4.2%) | 0.13 (4.2%) |
| set371 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.42 (4.1%) | 0.13 (4.3%) | 0.13 (4.2%) |
| set372 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.42 (4.1%) | 0.13 (4.3%) | 0.13 (4.3%) |
| set356 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.46 (4.2%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set448 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.34 (3.6%) | 0.11 (3.7%) | 0.11 (3.7%) |
| set447 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.37 (3.8%) | 0.12 (3.9%) | 0.12 (3.9%) |
| set449 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.41 (3.9%) | 0.12 (4.0%) | 0.13 (4.0%) |
| set451 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.44 (4.1%) | 0.14 (4.3%) | 0.14 (4.3%) |
| set452 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set454 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set453 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set455 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.46 (4.3%) | 0.14 (4.4%) | 0.14 (4.4%) |
| set450 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.46 (4.2%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set459 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.46 (4.3%) | 0.14 (4.4%) | 0.15 (4.4%) |
| set456 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.47 (4.3%) | 0.15 (4.5%) | 0.15 (4.4%) |
| set457 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.47 (4.3%) | 0.15 (4.5%) | 0.15 (4.5%) |

6 Population Plots of sets A to E.

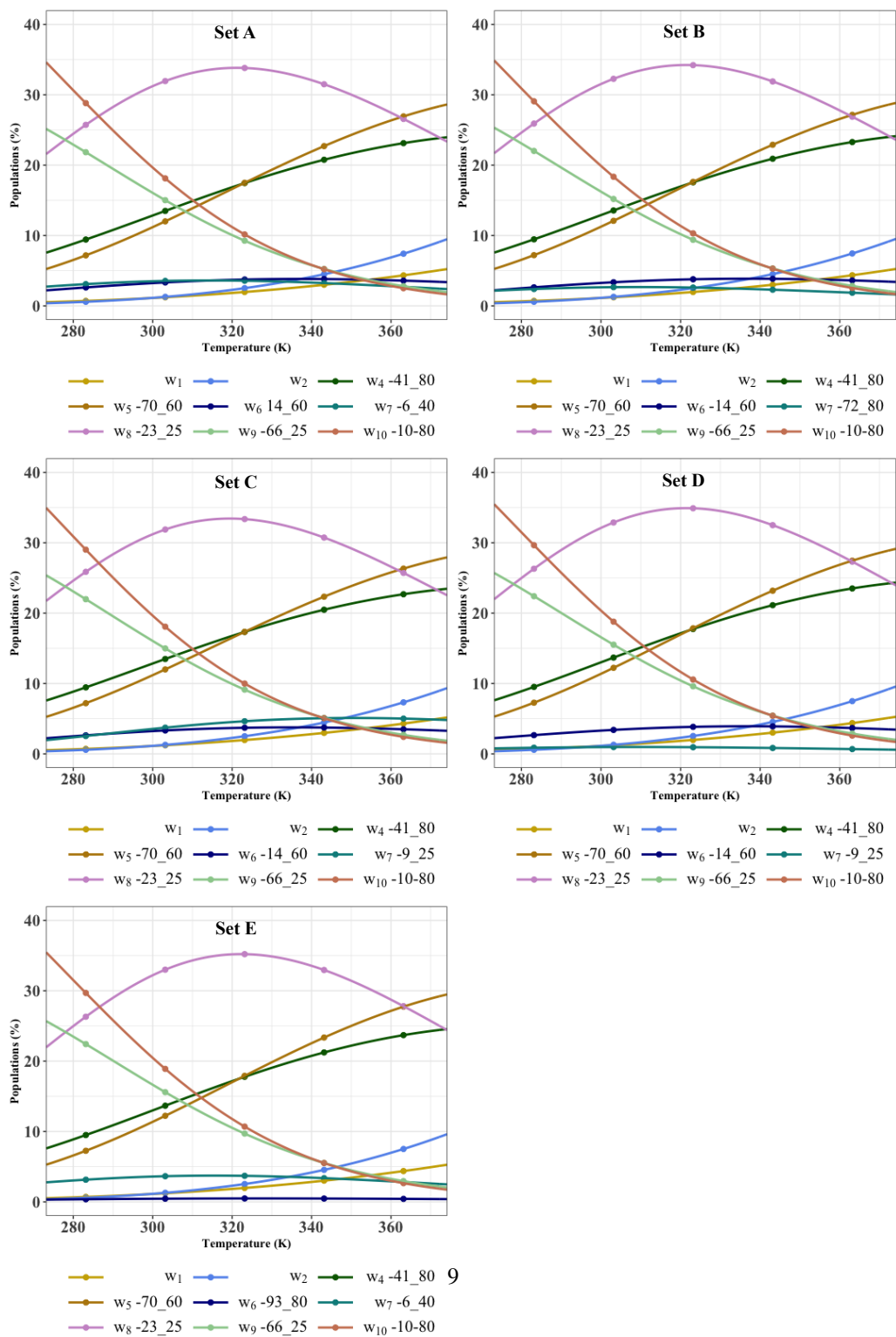


Figure S1: Population plots of set A, B, C, D and E.

7 Errors of all complete 459 clustersets

Note: Sets 346, 347, 345, 348 and 349 correspond to sets A, B, C, D and E in the text.

Table S7: Error of all 459 complete sets tested throughout this work

| 459 complete sets | | | | Mean Absolute Error | | | |
|-------------------|------|------|-----------|------------------------------|--|---------------------------------------|---------------------------------------|
| Set | amf | bxv | QCE error | Volume (dm ³) | ΔS (J mol K ⁻¹) | ΔH (kJ mol ⁻¹) | ΔU (kJ mol ⁻¹) |
| set346 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.22 (2.9%) | 0.07 (3.1%) | 0.07 (3.1%) |
| set347 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.27 (3.1%) | 0.09 (3.2%) | 0.09 (3.2%) |
| set345 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.25 (3.1%) | 0.08 (3.3%) | 0.08 (3.3%) |
| set348 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.33 (3.4%) | 0.10 (3.6%) | 0.11 (3.5%) |
| set349 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.31 (3.4%) | 0.10 (3.6%) | 0.10 (3.6%) |
| set363 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.30 (3.4%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set352 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.32 (3.4%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set350 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.32 (3.4%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set351 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.32 (3.5%) | 0.10 (3.7%) | 0.10 (3.6%) |
| set357 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.33 (3.5%) | 0.11 (3.7%) | 0.11 (3.6%) |
| set353 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.33 (3.5%) | 0.11 (3.7%) | 0.11 (3.7%) |
| set354 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.34 (3.6%) | 0.11 (3.8%) | 0.11 (3.7%) |
| set448 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.34 (3.6%) | 0.11 (3.8%) | 0.11 (3.7%) |
| set355 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.34 (3.6%) | 0.11 (3.8%) | 0.11 (3.7%) |
| set364 | 0.44 | 1.01 | 3.41E-03 | 1.36E-04 (0.7%) | 0.36 (3.6%) | 0.12 (3.8%) | 0.12 (3.8%) |
| set362 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.33 (3.6%) | 0.11 (3.9%) | 0.11 (3.8%) |
| set447 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.37 (3.8%) | 0.12 (4.0%) | 0.12 (3.9%) |
| set449 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.41 (3.9%) | 0.13 (4.0%) | 0.13 (4.0%) |
| set366 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.39 (3.9%) | 0.13 (4.2%) | 0.13 (4.1%) |
| set365 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.42 (4.0%) | 0.13 (4.2%) | 0.13 (4.1%) |
| set367 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.2%) |
| set369 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.2%) |
| set368 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.40 (4.0%) | 0.13 (4.2%) | 0.13 (4.2%) |
| set374 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.42 (4.0%) | 0.14 (4.3%) | 0.14 (4.2%) |
| set370 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.41 (4.0%) | 0.13 (4.3%) | 0.14 (4.2%) |
| set371 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.42 (4.1%) | 0.14 (4.3%) | 0.14 (4.3%) |
| set326 | 0.44 | 1.01 | 3.43E-03 | 1.45E-04 (0.8%) | 0.52 (4.1%) | 0.17 (4.4%) | 0.17 (4.3%) |
| set372 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.43 (4.1%) | 0.14 (4.4%) | 0.14 (4.3%) |
| set451 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.44 (4.1%) | 0.14 (4.3%) | 0.14 (4.3%) |
| set454 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.14 (4.4%) | 0.15 (4.4%) |
| set452 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.14 (4.4%) | 0.15 (4.4%) |
| set453 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.45 (4.2%) | 0.15 (4.4%) | 0.15 (4.4%) |
| set450 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.47 (4.2%) | 0.15 (4.4%) | 0.15 (4.4%) |
| set356 | 0.44 | 1.01 | 3.41E-03 | 1.35E-04 (0.7%) | 0.47 (4.2%) | 0.15 (4.4%) | 0.15 (4.4%) |
| set455 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.46 (4.3%) | 0.15 (4.5%) | 0.15 (4.4%) |
| set459 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.47 (4.3%) | 0.15 (4.5%) | 0.15 (4.4%) |
| set456 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.47 (4.3%) | 0.15 (4.5%) | 0.15 (4.5%) |

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|--------|------|------|----------|-----------------|-------------|-------------|-------------|
| set329 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.47 (4.3%) | 0.14 (4.4%) | 0.14 (4.4%) |
| set457 | 0.44 | 1.01 | 3.41E-03 | 1.34E-04 (0.7%) | 0.48 (4.3%) | 0.15 (4.6%) | 0.15 (4.5%) |
| set312 | 0.44 | 1.01 | 3.42E-03 | 1.36E-04 (0.7%) | 0.32 (4.6%) | 0.10 (4.6%) | 0.10 (4.7%) |
| set328 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.51 (4.6%) | 0.15 (4.6%) | 0.16 (4.6%) |
| set311 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.32 (4.7%) | 0.10 (4.7%) | 0.10 (4.8%) |
| set373 | 0.44 | 1.01 | 3.41E-03 | 1.36E-04 (0.7%) | 0.56 (4.8%) | 0.18 (5.0%) | 0.18 (5.0%) |
| set315 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.33 (5.0%) | 0.10 (5.0%) | 0.11 (5.1%) |
| set330 | 0.44 | 1.01 | 3.42E-03 | 1.34E-04 (0.7%) | 0.54 (5.0%) | 0.16 (5.0%) | 0.16 (5.0%) |
| set316 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.34 (5.0%) | 0.10 (5.0%) | 0.11 (5.1%) |
| set318 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.34 (5.0%) | 0.11 (5.0%) | 0.11 (5.1%) |
| set317 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.34 (5.0%) | 0.11 (5.0%) | 0.11 (5.1%) |
| set332 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.58 (5.1%) | 0.18 (5.2%) | 0.18 (5.2%) |
| set313 | 0.44 | 1.01 | 3.42E-03 | 1.36E-04 (0.7%) | 0.35 (5.1%) | 0.11 (5.1%) | 0.11 (5.2%) |
| set319 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.34 (5.1%) | 0.11 (5.1%) | 0.11 (5.2%) |
| set320 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.34 (5.1%) | 0.11 (5.1%) | 0.11 (5.2%) |
| set333 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.59 (5.1%) | 0.18 (5.2%) | 0.18 (5.2%) |
| set335 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.59 (5.1%) | 0.18 (5.2%) | 0.18 (5.2%) |
| set458 | 0.44 | 1.01 | 3.42E-03 | 1.36E-04 (0.7%) | 0.61 (5.1%) | 0.19 (5.3%) | 0.19 (5.3%) |
| set334 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.59 (5.2%) | 0.18 (5.2%) | 0.18 (5.2%) |
| set323 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.35 (5.2%) | 0.11 (5.1%) | 0.11 (5.2%) |
| set321 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.35 (5.2%) | 0.11 (5.1%) | 0.11 (5.2%) |
| set445 | 0.44 | 1.01 | 3.43E-03 | 1.46E-04 (0.8%) | 0.60 (5.2%) | 0.19 (5.4%) | 0.19 (5.3%) |
| set314 | 0.44 | 1.01 | 3.42E-03 | 1.36E-04 (0.7%) | 0.35 (5.2%) | 0.11 (5.2%) | 0.11 (5.3%) |
| set336 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.60 (5.2%) | 0.18 (5.3%) | 0.19 (5.3%) |
| set308 | 0.44 | 1.01 | 3.43E-03 | 1.42E-04 (0.8%) | 0.67 (5.3%) | 0.21 (5.6%) | 0.21 (5.5%) |
| set340 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.61 (5.3%) | 0.18 (5.4%) | 0.19 (5.4%) |
| set337 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.62 (5.3%) | 0.19 (5.4%) | 0.19 (5.4%) |
| set338 | 0.44 | 1.01 | 3.41E-03 | 1.33E-04 (0.7%) | 0.62 (5.3%) | 0.19 (5.4%) | 0.19 (5.4%) |
| set331 | 0.44 | 1.01 | 3.42E-03 | 1.34E-04 (0.7%) | 0.60 (5.4%) | 0.18 (5.4%) | 0.18 (5.4%) |
| set325 | 0.44 | 1.01 | 3.42E-03 | 1.40E-04 (0.8%) | 0.48 (5.4%) | 0.14 (5.5%) | 0.14 (5.4%) |
| set360 | 0.44 | 1.01 | 3.43E-03 | 1.46E-04 (0.8%) | 0.64 (5.6%) | 0.20 (5.8%) | 0.20 (5.7%) |
| set322 | 0.44 | 1.01 | 3.42E-03 | 1.36E-04 (0.7%) | 0.38 (5.7%) | 0.12 (5.6%) | 0.12 (5.8%) |
| set343 | 0.44 | 1.01 | 3.43E-03 | 1.46E-04 (0.8%) | 0.71 (6.1%) | 0.22 (6.3%) | 0.22 (6.2%) |
| set309 | 0.44 | 1.01 | 3.44E-03 | 1.46E-04 (0.8%) | 0.85 (6.1%) | 0.28 (6.4%) | 0.28 (6.4%) |
| set339 | 0.44 | 1.01 | 3.42E-03 | 1.35E-04 (0.7%) | 0.73 (6.4%) | 0.22 (6.4%) | 0.22 (6.4%) |
| set444 | 0.44 | 1.01 | 3.42E-03 | 1.40E-04 (0.8%) | 0.64 (7.2%) | 0.19 (7.2%) | 0.19 (7.1%) |
| set327 | 0.44 | 1.01 | 3.44E-03 | 1.49E-04 (0.8%) | 0.98 (7.7%) | 0.31 (8.0%) | 0.31 (7.8%) |
| set359 | 0.44 | 1.01 | 3.42E-03 | 1.40E-04 (0.8%) | 0.70 (7.7%) | 0.20 (7.7%) | 0.20 (7.6%) |
| set342 | 0.44 | 1.01 | 3.42E-03 | 1.40E-04 (0.8%) | 0.75 (8.0%) | 0.22 (8.1%) | 0.22 (8.0%) |
| set35 | 0.42 | 1.01 | 3.41E-03 | 1.27E-04 (0.7%) | 0.98 (8.3%) | 0.33 (8.7%) | 0.33 (8.8%) |
| set52 | 0.42 | 1.01 | 3.41E-03 | 1.26E-04 (0.7%) | 0.96 (8.4%) | 0.32 (8.7%) | 0.32 (8.8%) |
| set137 | 0.42 | 1.01 | 3.41E-03 | 1.27E-04 (0.7%) | 0.97 (8.4%) | 0.32 (8.8%) | 0.32 (8.9%) |
| set307 | 0.44 | 1.01 | 3.43E-03 | 1.45E-04 (0.8%) | 1.05 (8.6%) | 0.33 (8.8%) | 0.33 (8.7%) |
| set446 | 0.44 | 1.01 | 3.44E-03 | 1.50E-04 (0.8%) | 1.06 (8.6%) | 0.33 (8.8%) | 0.33 (8.7%) |
| set18 | 0.42 | 1.01 | 3.41E-03 | 1.28E-04 (0.7%) | 1.03 (8.7%) | 0.34 (9.0%) | 0.34 (9.1%) |

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|--------|------|------|----------|-----------------|--------------|--------------|--------------|
| set324 | 0.44 | 1.01 | 3.43E-03 | 1.44E-04 (0.8%) | 0.91 (8.7%) | 0.28 (8.8%) | 0.27 (8.7%) |
| set310 | 0.44 | 1.01 | 3.44E-03 | 1.50E-04 (0.8%) | 1.24 (8.9%) | 0.39 (9.3%) | 0.39 (9.2%) |
| set361 | 0.44 | 1.01 | 3.44E-03 | 1.50E-04 (0.8%) | 1.09 (8.9%) | 0.34 (9.2%) | 0.34 (9.1%) |
| set36 | 0.42 | 1.01 | 3.41E-03 | 1.26E-04 (0.7%) | 0.93 (9.1%) | 0.31 (9.4%) | 0.31 (9.5%) |
| set53 | 0.42 | 1.01 | 3.41E-03 | 1.26E-04 (0.7%) | 0.92 (9.2%) | 0.31 (9.6%) | 0.31 (9.7%) |
| set138 | 0.42 | 1.01 | 3.41E-03 | 1.26E-04 (0.7%) | 0.92 (9.2%) | 0.31 (9.6%) | 0.31 (9.7%) |
| set19 | 0.42 | 1.01 | 3.41E-03 | 1.27E-04 (0.7%) | 0.98 (9.4%) | 0.33 (9.7%) | 0.33 (9.8%) |
| set344 | 0.44 | 1.01 | 3.44E-03 | 1.50E-04 (0.8%) | 1.15 (9.4%) | 0.36 (9.6%) | 0.36 (9.5%) |
| set55 | 0.42 | 1.01 | 3.41E-03 | 1.29E-04 (0.7%) | 1.25 (9.7%) | 0.41 (10.1%) | 0.41 (10.2%) |
| set38 | 0.42 | 1.01 | 3.41E-03 | 1.29E-04 (0.7%) | 1.29 (9.8%) | 0.42 (10.2%) | 0.42 (10.3%) |
| set140 | 0.42 | 1.01 | 3.41E-03 | 1.29E-04 (0.7%) | 1.26 (9.8%) | 0.42 (10.2%) | 0.42 (10.3%) |
| set1 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.36 (9.8%) | 0.45 (10.2%) | 0.45 (10.3%) |
| set37 | 0.42 | 1.01 | 3.41E-03 | 1.28E-04 (0.7%) | 1.18 (10.0%) | 0.39 (10.4%) | 0.39 (10.5%) |
| set2 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.29 (10.0%) | 0.43 (10.4%) | 0.43 (10.5%) |
| set54 | 0.42 | 1.01 | 3.41E-03 | 1.28E-04 (0.7%) | 1.15 (10.0%) | 0.38 (10.4%) | 0.38 (10.5%) |
| set139 | 0.42 | 1.01 | 3.41E-03 | 1.28E-04 (0.7%) | 1.16 (10.1%) | 0.39 (10.5%) | 0.39 (10.6%) |
| set21 | 0.42 | 1.01 | 3.41E-03 | 1.30E-04 (0.7%) | 1.34 (10.1%) | 0.44 (10.5%) | 0.44 (10.6%) |
| set20 | 0.42 | 1.01 | 3.41E-03 | 1.29E-04 (0.7%) | 1.23 (10.3%) | 0.41 (10.7%) | 0.41 (10.8%) |
| set443 | 0.44 | 1.01 | 3.43E-03 | 1.44E-04 (0.8%) | 1.07 (10.3%) | 0.32 (10.3%) | 0.32 (10.2%) |
| set358 | 0.44 | 1.01 | 3.43E-03 | 1.44E-04 (0.8%) | 1.11 (10.7%) | 0.33 (10.8%) | 0.33 (10.7%) |
| set341 | 0.44 | 1.01 | 3.43E-03 | 1.44E-04 (0.8%) | 1.17 (11.1%) | 0.35 (11.1%) | 0.35 (11.0%) |
| set157 | 0.42 | 1.01 | 3.42E-03 | 1.30E-04 (0.7%) | 0.78 (11.3%) | 0.25 (11.4%) | 0.25 (11.5%) |
| set6 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.33 (11.4%) | 0.44 (11.9%) | 0.44 (12.0%) |
| set40 | 0.44 | 1.05 | 7.37E-03 | 7.35E-04 (4.0%) | 1.01 (11.4%) | 0.34 (11.8%) | 0.34 (11.9%) |
| set3 | 0.42 | 1.01 | 3.42E-03 | 1.32E-04 (0.7%) | 1.58 (11.4%) | 0.51 (11.9%) | 0.51 (11.9%) |
| set5 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.4%) | 0.44 (11.9%) | 0.44 (12.0%) |
| set39 | 0.44 | 1.05 | 7.37E-03 | 7.35E-04 (4.0%) | 1.00 (11.5%) | 0.34 (11.9%) | 0.34 (12.0%) |
| set9 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.5%) | 0.44 (12.0%) | 0.44 (12.1%) |
| set11 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set12 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set10 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set7 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.35 (11.6%) | 0.45 (12.1%) | 0.45 (12.2%) |
| set41 | 0.44 | 1.05 | 7.36E-03 | 7.35E-04 (4.0%) | 1.03 (11.6%) | 0.34 (12.0%) | 0.34 (12.1%) |
| set13 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set14 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set15 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.32 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set17 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.33 (11.6%) | 0.44 (12.1%) | 0.44 (12.2%) |
| set8 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.34 (11.6%) | 0.45 (12.1%) | 0.45 (12.2%) |
| set23 | 0.44 | 1.05 | 7.36E-03 | 7.33E-04 (4.0%) | 1.06 (11.6%) | 0.35 (12.0%) | 0.35 (12.2%) |
| set43 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.2%) | 1.01 (11.7%) | 0.34 (12.0%) | 0.34 (12.2%) |
| set16 | 0.42 | 1.01 | 3.42E-03 | 1.31E-04 (0.7%) | 1.34 (11.7%) | 0.45 (12.2%) | 0.45 (12.3%) |
| set42 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.03 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set22 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.06 (11.7%) | 0.35 (12.1%) | 0.35 (12.2%) |
| set46 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set44 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |

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|--------|------|------|----------|-----------------|--------------|--------------|--------------|
| set45 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set142 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set57 | 0.44 | 1.05 | 7.37E-03 | 7.35E-04 (4.0%) | 1.00 (11.7%) | 0.33 (12.1%) | 0.33 (12.2%) |
| set47 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set49 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.02 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set51 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.2%) | 1.02 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set4 | 0.42 | 1.01 | 3.42E-03 | 1.33E-04 (0.7%) | 1.69 (11.7%) | 0.55 (12.2%) | 0.54 (12.2%) |
| set48 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.01 (11.7%) | 0.34 (12.1%) | 0.34 (12.2%) |
| set56 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.3%) | 1.00 (11.8%) | 0.33 (12.1%) | 0.33 (12.2%) |
| set24 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.08 (11.8%) | 0.36 (12.2%) | 0.36 (12.3%) |
| set50 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.03 (11.8%) | 0.34 (12.2%) | 0.34 (12.3%) |
| set141 | 0.46 | 1.09 | 1.52E-02 | 1.33E-03 (7.2%) | 1.01 (11.8%) | 0.34 (12.2%) | 0.34 (12.3%) |
| set26 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.06 (11.8%) | 0.36 (12.2%) | 0.36 (12.3%) |
| set143 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.03 (11.8%) | 0.35 (12.2%) | 0.35 (12.3%) |
| set58 | 0.46 | 1.09 | 1.52E-02 | 1.32E-03 (7.2%) | 1.02 (11.8%) | 0.34 (12.2%) | 0.34 (12.3%) |
| set25 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.08 (11.8%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set28 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set27 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set29 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set30 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set34 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set31 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set60 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.00 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set32 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.07 (11.9%) | 0.36 (12.3%) | 0.36 (12.4%) |
| set59 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.02 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set33 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.08 (11.9%) | 0.36 (12.4%) | 0.36 (12.5%) |
| set63 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set62 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set145 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set61 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (11.9%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set144 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.03 (12.0%) | 0.34 (12.3%) | 0.34 (12.4%) |
| set146 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set147 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set66 | 0.46 | 1.11 | 2.31E-02 | 1.74E-03 (9.5%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set64 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set148 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set68 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.3%) | 0.34 (12.5%) |
| set150 | 0.46 | 1.11 | 2.31E-02 | 1.74E-03 (9.5%) | 1.02 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set149 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.02 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set151 | 0.46 | 1.11 | 2.31E-02 | 1.74E-03 (9.5%) | 1.02 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set65 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.01 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set152 | 0.46 | 1.11 | 2.31E-02 | 1.73E-03 (9.5%) | 1.03 (12.0%) | 0.35 (12.4%) | 0.35 (12.5%) |
| set153 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.02 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set67 | 0.46 | 1.10 | 1.89E-02 | 1.53E-03 (8.4%) | 1.02 (12.0%) | 0.34 (12.4%) | 0.34 (12.5%) |
| set154 | 0.42 | 1.01 | 3.41E-03 | 1.29E-04 (0.7%) | 0.87 (13.1%) | 0.26 (12.9%) | 0.26 (13.1%) |

| | | | | | | | |
|--------|------|------|----------|-----------------|--------------|--------------|--------------|
| set156 | 0.60 | 1.01 | 6.91E-02 | 2.28E-04 (1.2%) | 0.95 (14.3%) | 0.29 (14.3%) | 0.29 (14.4%) |
| set174 | 0.46 | 1.11 | 2.27E-02 | 1.71E-03 (9.4%) | 0.95 (14.7%) | 0.28 (14.5%) | 0.28 (14.6%) |
| set191 | 0.46 | 1.11 | 2.27E-02 | 1.72E-03 (9.4%) | 1.00 (15.1%) | 0.29 (14.8%) | 0.29 (15.0%) |
| set155 | 0.60 | 1.02 | 6.49E-02 | 1.56E-04 (0.8%) | 1.11 (16.1%) | 0.32 (15.8%) | 0.32 (16.0%) |
| set293 | 0.60 | 1.00 | 6.17E-02 | 4.28E-04 (2.3%) | 1.17 (16.6%) | 0.33 (16.1%) | 0.33 (16.3%) |
| set208 | 0.60 | 1.01 | 6.11E-02 | 2.28E-04 (1.2%) | 1.18 (16.6%) | 0.33 (16.1%) | 0.33 (16.3%) |
| set171 | 0.60 | 1.00 | 5.79E-02 | 4.27E-04 (2.3%) | 1.43 (18.4%) | 0.39 (17.7%) | 0.39 (17.9%) |
| set188 | 0.60 | 1.01 | 5.61E-02 | 2.25E-04 (1.2%) | 1.51 (18.9%) | 0.41 (18.1%) | 0.41 (18.2%) |
| set173 | 0.60 | 1.02 | 6.36E-02 | 1.55E-04 (0.8%) | 1.34 (19.1%) | 0.38 (18.5%) | 0.38 (18.7%) |
| set290 | 0.60 | 1.01 | 5.61E-02 | 2.25E-04 (1.2%) | 1.57 (19.5%) | 0.43 (18.7%) | 0.43 (18.8%) |
| set190 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 1.42 (19.6%) | 0.39 (18.9%) | 0.39 (19.1%) |
| set205 | 0.60 | 1.02 | 5.60E-02 | 1.54E-04 (0.8%) | 1.58 (19.6%) | 0.43 (18.7%) | 0.43 (18.9%) |
| set292 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 1.48 (20.2%) | 0.41 (19.5%) | 0.41 (19.7%) |
| set207 | 0.60 | 1.00 | 6.17E-02 | 4.26E-04 (2.3%) | 1.51 (20.4%) | 0.42 (19.7%) | 0.42 (19.8%) |
| set160 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.39 (20.6%) | 0.40 (20.1%) | 0.40 (20.3%) |
| set159 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.40 (20.6%) | 0.40 (20.1%) | 0.40 (20.3%) |
| set161 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.42 (21.0%) | 0.40 (20.5%) | 0.40 (20.6%) |
| set158 | 0.60 | 1.00 | 6.69E-02 | 4.24E-04 (2.3%) | 1.45 (21.1%) | 0.41 (20.5%) | 0.41 (20.7%) |
| set169 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.43 (21.1%) | 0.41 (20.6%) | 0.41 (20.8%) |
| set162 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.44 (21.2%) | 0.41 (20.7%) | 0.41 (20.8%) |
| set163 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.45 (21.3%) | 0.41 (20.7%) | 0.41 (20.9%) |
| set165 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.45 (21.3%) | 0.41 (20.7%) | 0.41 (20.9%) |
| set170 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.44 (21.3%) | 0.41 (20.7%) | 0.41 (20.9%) |
| set164 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.45 (21.3%) | 0.41 (20.7%) | 0.41 (20.9%) |
| set166 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.45 (21.3%) | 0.41 (20.8%) | 0.41 (20.9%) |
| set167 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.46 (21.4%) | 0.41 (20.8%) | 0.41 (21.0%) |
| set168 | 0.60 | 1.02 | 6.76E-02 | 1.57E-04 (0.8%) | 1.46 (21.4%) | 0.41 (20.9%) | 0.41 (21.0%) |
| set172 | 0.60 | 1.00 | 5.91E-02 | 4.25E-04 (2.3%) | 1.75 (22.0%) | 0.47 (21.0%) | 0.47 (21.2%) |
| set189 | 0.60 | 1.00 | 5.79E-02 | 4.24E-04 (2.3%) | 1.85 (22.5%) | 0.50 (21.5%) | 0.50 (21.7%) |
| set291 | 0.60 | 1.01 | 5.73E-02 | 2.23E-04 (1.2%) | 1.91 (23.2%) | 0.52 (22.2%) | 0.52 (22.4%) |
| set206 | 0.60 | 1.01 | 5.73E-02 | 2.23E-04 (1.2%) | 1.93 (23.3%) | 0.52 (22.3%) | 0.52 (22.5%) |
| set177 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 2.18 (28.1%) | 0.58 (26.9%) | 0.58 (27.0%) |
| set176 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.24 (28.3%) | 0.60 (27.1%) | 0.60 (27.2%) |
| set178 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 2.23 (28.6%) | 0.59 (27.3%) | 0.60 (27.5%) |
| set175 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.27 (28.6%) | 0.61 (27.3%) | 0.61 (27.5%) |
| set186 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 2.24 (28.8%) | 0.60 (27.5%) | 0.60 (27.7%) |
| set194 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.31 (28.9%) | 0.62 (27.6%) | 0.62 (27.8%) |
| set187 | 0.60 | 1.02 | 6.23E-02 | 1.55E-04 (0.8%) | 2.27 (29.0%) | 0.61 (27.7%) | 0.61 (27.9%) |
| set193 | 0.60 | 1.00 | 6.04E-02 | 4.21E-04 (2.3%) | 2.37 (29.1%) | 0.64 (27.8%) | 0.64 (28.0%) |
| set179 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.31 (29.1%) | 0.62 (27.8%) | 0.62 (28.0%) |
| set182 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.32 (29.2%) | 0.62 (27.9%) | 0.62 (28.1%) |
| set180 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.32 (29.2%) | 0.62 (27.9%) | 0.62 (28.1%) |
| set181 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.32 (29.2%) | 0.62 (27.9%) | 0.62 (28.1%) |
| set183 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.32 (29.3%) | 0.62 (28.0%) | 0.62 (28.1%) |
| set192 | 0.60 | 1.00 | 6.04E-02 | 4.21E-04 (2.3%) | 2.40 (29.4%) | 0.65 (28.1%) | 0.65 (28.3%) |

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|--------|------|------|----------|-----------------|--------------|--------------|--------------|
| set184 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.33 (29.4%) | 0.62 (28.1%) | 0.63 (28.2%) |
| set195 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.36 (29.4%) | 0.63 (28.1%) | 0.63 (28.3%) |
| set185 | 0.60 | 1.00 | 6.16E-02 | 4.21E-04 (2.3%) | 2.33 (29.4%) | 0.62 (28.1%) | 0.63 (28.2%) |
| set203 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.37 (29.6%) | 0.64 (28.3%) | 0.64 (28.4%) |
| set196 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.40 (29.7%) | 0.65 (28.4%) | 0.65 (28.6%) |
| set197 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.41 (29.8%) | 0.65 (28.5%) | 0.65 (28.6%) |
| set199 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.41 (29.8%) | 0.65 (28.5%) | 0.65 (28.6%) |
| set296 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.39 (29.8%) | 0.64 (28.5%) | 0.64 (28.6%) |
| set198 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.41 (29.8%) | 0.65 (28.5%) | 0.65 (28.7%) |
| set204 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.41 (29.8%) | 0.65 (28.5%) | 0.65 (28.7%) |
| set200 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.42 (29.9%) | 0.65 (28.6%) | 0.65 (28.7%) |
| set211 | 0.60 | 1.02 | 6.10E-02 | 1.54E-04 (0.8%) | 2.41 (29.9%) | 0.65 (28.6%) | 0.65 (28.8%) |
| set295 | 0.60 | 1.00 | 6.04E-02 | 4.21E-04 (2.3%) | 2.45 (30.0%) | 0.66 (28.6%) | 0.66 (28.8%) |
| set201 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.42 (30.0%) | 0.65 (28.6%) | 0.65 (28.8%) |
| set202 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.43 (30.0%) | 0.65 (28.7%) | 0.65 (28.9%) |
| set210 | 0.60 | 1.01 | 5.98E-02 | 2.20E-04 (1.2%) | 2.46 (30.0%) | 0.66 (28.7%) | 0.66 (28.9%) |
| set294 | 0.60 | 1.00 | 6.04E-02 | 4.21E-04 (2.3%) | 2.48 (30.3%) | 0.67 (28.9%) | 0.67 (29.1%) |
| set297 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.44 (30.3%) | 0.65 (28.9%) | 0.66 (29.1%) |
| set209 | 0.60 | 1.01 | 5.98E-02 | 2.20E-04 (1.2%) | 2.49 (30.3%) | 0.67 (29.0%) | 0.67 (29.2%) |
| set305 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.45 (30.5%) | 0.66 (29.1%) | 0.66 (29.3%) |
| set212 | 0.60 | 1.00 | 6.04E-02 | 4.21E-04 (2.3%) | 2.50 (30.6%) | 0.67 (29.3%) | 0.68 (29.5%) |
| set220 | 0.60 | 1.02 | 6.10E-02 | 1.55E-04 (0.8%) | 2.48 (30.7%) | 0.67 (29.3%) | 0.67 (29.5%) |
| set298 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.52 (30.8%) | 0.68 (29.5%) | 0.68 (29.6%) |
| set213 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.53 (30.9%) | 0.68 (29.5%) | 0.68 (29.7%) |
| set301 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.53 (30.9%) | 0.68 (29.5%) | 0.68 (29.7%) |
| set299 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.53 (30.9%) | 0.68 (29.5%) | 0.68 (29.7%) |
| set300 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.53 (30.9%) | 0.68 (29.5%) | 0.68 (29.7%) |
| set306 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.53 (30.9%) | 0.68 (29.6%) | 0.68 (29.7%) |
| set216 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.53 (30.9%) | 0.68 (29.6%) | 0.69 (29.8%) |
| set214 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.54 (30.9%) | 0.68 (29.6%) | 0.69 (29.8%) |
| set215 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.54 (30.9%) | 0.68 (29.6%) | 0.69 (29.8%) |
| set302 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.54 (31.0%) | 0.68 (29.6%) | 0.69 (29.8%) |
| set217 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.54 (31.0%) | 0.69 (29.7%) | 0.69 (29.9%) |
| set221 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.55 (31.0%) | 0.69 (29.7%) | 0.69 (29.9%) |
| set303 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.55 (31.1%) | 0.69 (29.7%) | 0.69 (29.9%) |
| set304 | 0.60 | 1.00 | 6.04E-02 | 4.20E-04 (2.3%) | 2.55 (31.1%) | 0.69 (29.7%) | 0.69 (29.9%) |
| set218 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.55 (31.1%) | 0.69 (29.8%) | 0.69 (29.9%) |
| set219 | 0.60 | 1.01 | 5.98E-02 | 2.19E-04 (1.2%) | 2.55 (31.2%) | 0.69 (29.8%) | 0.69 (30.0%) |
| set104 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set103 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set105 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set106 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set409 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set422 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |
| set425 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.52 (37.5%) | 1.38 (37.6%) | 1.37 (37.5%) |

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|--------|------|------|----------|-----------------|--------------|--------------|--------------|
| set433 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set434 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set123 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set124 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set125 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set122 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set273 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set136 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set130 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set129 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set127 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set120 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set121 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set126 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set128 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set132 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |
| set131 | 0.40 | 1.01 | 3.51E-03 | 1.88E-04 (1.0%) | 4.59 (38.2%) | 1.40 (38.2%) | 1.40 (38.1%) |

8 Unscaled and scaled frequencies of top 5 full sets

w1 (scaling factor 0.998)

Table S8: Scaled and Unscaled Frequencies of w1 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 1639.629 | 1636.349742 |
| Mode 2 | 3774.932 | 3767.382136 |
| Mode 3 | 3902.493 | 3894.688014 |

w2 (scaling factor 0.997)

Table S9: Scaled and Unscaled Frequencies of w2 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 121.700 | 121.334900 |
| Mode 2 | 136.530 | 136.120410 |
| Mode 3 | 141.013 | 140.589961 |
| Mode 4 | 169.969 | 169.459093 |
| Mode 5 | 335.067 | 334.061799 |
| Mode 6 | 603.654 | 601.843038 |
| Mode 7 | 1641.623 | 1636.698131 |
| Mode 8 | 1658.867 | 1653.890399 |
| Mode 9 | 3709.639 | 3698.510083 |
| Mode 10 | 3771.710 | 3760.394870 |
| Mode 11 | 3875.069 | 3863.443793 |

| | | |
|---------|----------|-------------|
| Mode 4 | 119.996 | 118.676044 |
| Mode 5 | 143.608 | 142.028312 |
| Mode 6 | 159.606 | 157.850334 |
| Mode 7 | 176.548 | 174.605972 |
| Mode 8 | 180.503 | 178.517467 |
| Mode 9 | 184.981 | 182.946209 |
| Mode 10 | 191.532 | 189.425148 |
| Mode 11 | 211.727 | 209.398003 |
| Mode 12 | 227.387 | 224.885743 |
| Mode 13 | 243.570 | 240.890730 |
| Mode 14 | 296.166 | 292.908174 |
| Mode 15 | 328.598 | 324.983422 |
| Mode 16 | 366.738 | 362.703882 |
| Mode 17 | 414.846 | 410.282694 |
| Mode 18 | 444.089 | 439.204021 |
| Mode 19 | 489.673 | 484.286597 |
| Mode 20 | 565.927 | 559.701803 |
| Mode 21 | 623.815 | 616.953035 |
| Mode 22 | 637.707 | 630.692223 |
| Mode 23 | 760.341 | 751.977249 |
| Mode 24 | 877.956 | 868.298484 |
| Mode 25 | 1648.057 | 1629.928373 |
| Mode 26 | 1655.761 | 1637.547629 |
| Mode 27 | 1661.924 | 1643.642836 |
| Mode 28 | 1673.388 | 1654.980732 |
| Mode 29 | 1687.270 | 1668.710030 |
| Mode 30 | 3544.495 | 3505.505555 |
| Mode 31 | 3641.238 | 3601.184382 |
| Mode 32 | 3663.643 | 3623.342927 |
| Mode 33 | 3674.362 | 3633.944018 |
| Mode 34 | 3724.518 | 3683.548302 |
| Mode 35 | 3771.051 | 3729.569439 |
| Mode 36 | 3859.782 | 3817.324398 |
| Mode 37 | 3862.676 | 3820.186564 |
| Mode 38 | 3867.626 | 3825.082114 |
| Mode 39 | 3868.487 | 3825.933643 |

w6-14_60 (scaling factor 0.986)

Table S12: Scaled and Unscaled Frequencies of w6-14_60 cluster

| Vibrational Modes | Unscaled Frequencies (cm⁻¹) | Scaled Frequencies (cm⁻¹) |
|--------------------------|---|---|
| Mode 1 | 20.078 | 19.796908 |
| Mode 2 | 24.667 | 24.321662 |
| Mode 3 | 36.181 | 35.674466 |
| Mode 4 | 49.848 | 49.150128 |

| | | |
|---------|----------|-------------|
| Mode 5 | 53.845 | 53.091170 |
| Mode 6 | 111.624 | 110.061264 |
| Mode 7 | 125.459 | 123.702574 |
| Mode 8 | 144.326 | 142.305436 |
| Mode 9 | 159.294 | 157.063884 |
| Mode 10 | 168.909 | 166.544274 |
| Mode 11 | 186.056 | 183.451216 |
| Mode 12 | 197.091 | 194.331726 |
| Mode 13 | 207.921 | 205.010106 |
| Mode 14 | 238.027 | 234.694622 |
| Mode 15 | 242.915 | 239.514190 |
| Mode 16 | 248.035 | 244.562510 |
| Mode 17 | 255.899 | 252.316414 |
| Mode 18 | 312.782 | 308.403052 |
| Mode 19 | 334.695 | 330.009270 |
| Mode 20 | 358.433 | 353.414938 |
| Mode 21 | 374.401 | 369.159386 |
| Mode 22 | 383.996 | 378.620056 |
| Mode 23 | 437.867 | 431.736862 |
| Mode 24 | 489.011 | 482.164846 |
| Mode 25 | 563.713 | 555.821018 |
| Mode 26 | 663.317 | 654.030562 |
| Mode 27 | 669.676 | 660.300536 |
| Mode 28 | 708.313 | 698.396618 |
| Mode 29 | 747.876 | 737.405736 |
| Mode 30 | 835.120 | 823.428320 |
| Mode 31 | 1645.002 | 1621.971972 |
| Mode 32 | 1659.409 | 1636.177274 |
| Mode 33 | 1666.893 | 1643.556498 |
| Mode 34 | 1675.180 | 1651.727480 |
| Mode 35 | 1686.516 | 1662.904776 |
| Mode 36 | 1709.935 | 1685.995910 |
| Mode 37 | 3558.293 | 3508.476898 |
| Mode 38 | 3598.212 | 3547.837032 |
| Mode 39 | 3619.200 | 3568.531200 |
| Mode 40 | 3636.600 | 3585.687600 |
| Mode 41 | 3691.123 | 3639.447278 |
| Mode 42 | 3716.518 | 3664.486748 |
| Mode 43 | 3797.834 | 3744.664324 |
| Mode 44 | 3859.044 | 3805.017384 |
| Mode 45 | 3859.836 | 3805.798296 |
| Mode 46 | 3860.423 | 3806.377078 |
| Mode 47 | 3863.439 | 3809.350854 |
| Mode 48 | 3872.714 | 3818.496004 |

w6-93_80 (scaling factor 0.995)

Table S13: Scaled and Unscaled Frequencies of w6-93_80 cluster

| Vibrational Modes | Unscaled Frequencies (cm⁻¹) | Scaled Frequencies (cm⁻¹) |
|--------------------------|---|---|
| Mode 1 | 4.263 | 4.241685 |
| Mode 2 | 45.675 | 45.446625 |
| Mode 3 | 60.879 | 60.574605 |
| Mode 4 | 68.144 | 67.803280 |
| Mode 5 | 100.711 | 100.207445 |
| Mode 6 | 135.772 | 135.093140 |
| Mode 7 | 157.896 | 157.106520 |
| Mode 8 | 175.285 | 174.408575 |
| Mode 9 | 186.947 | 186.012265 |
| Mode 10 | 201.956 | 200.946220 |
| Mode 11 | 204.747 | 203.723265 |
| Mode 12 | 213.000 | 211.935000 |
| Mode 13 | 227.617 | 226.478915 |
| Mode 14 | 232.877 | 231.712615 |
| Mode 15 | 249.741 | 248.492295 |
| Mode 16 | 271.287 | 269.930565 |
| Mode 17 | 313.252 | 311.685740 |
| Mode 18 | 340.122 | 338.421390 |
| Mode 19 | 364.744 | 362.920280 |
| Mode 20 | 386.202 | 384.270990 |
| Mode 21 | 414.079 | 412.008605 |
| Mode 22 | 438.355 | 436.163225 |
| Mode 23 | 491.754 | 489.295230 |
| Mode 24 | 544.391 | 541.669045 |
| Mode 25 | 599.225 | 596.228875 |
| Mode 26 | 631.211 | 628.054945 |
| Mode 27 | 676.609 | 673.225955 |
| Mode 28 | 746.588 | 742.855060 |
| Mode 29 | 779.878 | 775.978610 |
| Mode 30 | 840.180 | 835.979100 |
| Mode 31 | 1645.963 | 1637.733185 |
| Mode 32 | 1657.982 | 1649.692090 |
| Mode 33 | 1663.440 | 1655.122800 |
| Mode 34 | 1688.917 | 1680.472415 |
| Mode 35 | 1695.804 | 1687.324980 |
| Mode 36 | 1702.312 | 1693.800440 |
| Mode 37 | 3535.991 | 3518.311045 |
| Mode 38 | 3599.085 | 3581.089575 |
| Mode 39 | 3615.121 | 3597.045395 |
| Mode 40 | 3666.272 | 3647.940640 |
| Mode 41 | 3673.530 | 3655.162350 |
| Mode 42 | 3719.499 | 3700.901505 |
| Mode 43 | 3768.562 | 3749.719190 |

| | | |
|---------|----------|-------------|
| Mode 44 | 3813.670 | 3794.601650 |
| Mode 45 | 3843.056 | 3823.840720 |
| Mode 46 | 3856.425 | 3837.142875 |
| Mode 47 | 3862.446 | 3843.133770 |
| Mode 48 | 3865.347 | 3846.020265 |

w7-40_40 (scaling factor 0.983)

Table S14: Scaled and Unscaled Frequencies of w7-40_40 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 15.753 | 15.485199 |
| Mode 2 | 21.433 | 21.068639 |
| Mode 3 | 32.481 | 31.928823 |
| Mode 4 | 45.879 | 45.099057 |
| Mode 5 | 50.167 | 49.314161 |
| Mode 6 | 62.348 | 61.288084 |
| Mode 7 | 91.622 | 90.064426 |
| Mode 8 | 138.985 | 136.622255 |
| Mode 9 | 141.704 | 139.295032 |
| Mode 10 | 164.681 | 161.881423 |
| Mode 11 | 184.125 | 180.994875 |
| Mode 12 | 189.544 | 186.321752 |
| Mode 13 | 190.703 | 187.461049 |
| Mode 14 | 197.137 | 193.785671 |
| Mode 15 | 207.717 | 204.185811 |
| Mode 16 | 215.374 | 211.712642 |
| Mode 17 | 222.413 | 218.631979 |
| Mode 18 | 228.427 | 224.543741 |
| Mode 19 | 243.180 | 239.045940 |
| Mode 20 | 253.561 | 249.250463 |
| Mode 21 | 293.872 | 288.876176 |
| Mode 22 | 333.873 | 328.197159 |
| Mode 23 | 347.700 | 341.789100 |
| Mode 24 | 352.340 | 346.350220 |
| Mode 25 | 360.883 | 354.747989 |
| Mode 26 | 428.154 | 420.875382 |
| Mode 27 | 465.511 | 457.597313 |
| Mode 28 | 492.539 | 484.165837 |
| Mode 29 | 569.682 | 559.997406 |
| Mode 30 | 634.066 | 623.286878 |
| Mode 31 | 658.358 | 647.165914 |
| Mode 32 | 671.080 | 659.671640 |
| Mode 33 | 689.546 | 677.823718 |
| Mode 34 | 737.120 | 724.588960 |
| Mode 35 | 804.847 | 791.164601 |

| | | |
|---------|----------|-------------|
| Mode 36 | 831.734 | 817.594522 |
| Mode 37 | 1656.267 | 1628.110461 |
| Mode 38 | 1660.265 | 1632.040495 |
| Mode 39 | 1665.016 | 1636.710728 |
| Mode 40 | 1669.257 | 1640.879631 |
| Mode 41 | 1677.658 | 1649.137814 |
| Mode 42 | 1689.538 | 1660.815854 |
| Mode 43 | 1700.962 | 1672.045646 |
| Mode 44 | 3572.126 | 3511.399858 |
| Mode 45 | 3589.682 | 3528.657406 |
| Mode 46 | 3620.953 | 3559.396799 |
| Mode 47 | 3631.239 | 3569.507937 |
| Mode 48 | 3643.440 | 3581.501520 |
| Mode 49 | 3653.884 | 3591.767972 |
| Mode 50 | 3714.469 | 3651.323027 |
| Mode 51 | 3744.436 | 3680.780588 |
| Mode 52 | 3802.101 | 3737.465283 |
| Mode 53 | 3858.080 | 3792.492640 |
| Mode 54 | 3859.662 | 3794.047746 |
| Mode 55 | 3860.965 | 3795.328595 |
| Mode 56 | 3863.942 | 3798.254986 |
| Mode 57 | 3865.300 | 3799.589900 |

w7-6_40 (scaling factor 0.989)

Table S15: Scaled and Unscaled Frequencies of w7-6_40 cluster

| Vibrational Modes | Unscaled Frequencies cm^{-1} | Scaled Frequencies (cm^{-1}) |
|-------------------|---------------------------------------|---|
| Mode 1 | 14.797 | 14.634233 |
| Mode 2 | 23.672 | 23.411608 |
| Mode 3 | 30.801 | 30.462189 |
| Mode 4 | 34.115 | 33.739735 |
| Mode 5 | 43.322 | 42.845458 |
| Mode 6 | 66.340 | 65.610260 |
| Mode 7 | 91.787 | 90.777343 |
| Mode 8 | 103.528 | 102.389192 |
| Mode 9 | 108.872 | 107.674408 |
| Mode 10 | 131.880 | 130.429320 |
| Mode 11 | 153.947 | 152.253583 |
| Mode 12 | 166.365 | 164.534985 |
| Mode 13 | 176.222 | 174.283558 |
| Mode 14 | 181.236 | 179.242404 |
| Mode 15 | 190.594 | 188.497466 |
| Mode 16 | 193.856 | 191.723584 |
| Mode 17 | 209.860 | 207.551540 |
| Mode 18 | 217.991 | 215.593099 |

| | | |
|---------|----------|-------------|
| Mode 19 | 228.452 | 225.939028 |
| Mode 20 | 250.127 | 247.375603 |
| Mode 21 | 316.040 | 312.563560 |
| Mode 22 | 339.122 | 335.391658 |
| Mode 23 | 344.605 | 340.814345 |
| Mode 24 | 358.925 | 354.976825 |
| Mode 25 | 392.028 | 387.715692 |
| Mode 26 | 414.697 | 410.135333 |
| Mode 27 | 428.945 | 424.226605 |
| Mode 28 | 497.393 | 491.921677 |
| Mode 29 | 566.270 | 560.041030 |
| Mode 30 | 598.565 | 591.980785 |
| Mode 31 | 642.930 | 635.857770 |
| Mode 32 | 669.527 | 662.162203 |
| Mode 33 | 705.005 | 697.249945 |
| Mode 34 | 726.241 | 718.252349 |
| Mode 35 | 773.002 | 764.498978 |
| Mode 36 | 928.453 | 918.240017 |
| Mode 37 | 1639.456 | 1621.421984 |
| Mode 38 | 1655.478 | 1637.267742 |
| Mode 39 | 1659.891 | 1641.632199 |
| Mode 40 | 1663.978 | 1645.674242 |
| Mode 41 | 1666.832 | 1648.496848 |
| Mode 42 | 1672.101 | 1653.707889 |
| Mode 43 | 1712.497 | 1693.659533 |
| Mode 44 | 3542.936 | 3503.963704 |
| Mode 45 | 3617.160 | 3577.371240 |
| Mode 46 | 3622.850 | 3582.998650 |
| Mode 47 | 3651.192 | 3611.028888 |
| Mode 48 | 3662.196 | 3621.911844 |
| Mode 49 | 3673.620 | 3633.210180 |
| Mode 50 | 3704.703 | 3663.951267 |
| Mode 51 | 3726.586 | 3685.593554 |
| Mode 52 | 3773.909 | 3732.396001 |
| Mode 53 | 3858.781 | 3816.334409 |
| Mode 54 | 3863.927 | 3821.423803 |
| Mode 55 | 3865.960 | 3823.434440 |
| Mode 56 | 3872.748 | 3830.147772 |
| Mode 57 | 3876.144 | 3833.506416 |

w7-72_80 (scaling factor 0.986)

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 1.404 | 1.384344 |
| Mode 2 | 33.874 | 33.399764 |

| | | |
|---------|----------|-------------|
| Mode 3 | 35.883 | 35.380638 |
| Mode 4 | 46.851 | 46.195086 |
| Mode 5 | 56.668 | 55.874648 |
| Mode 6 | 71.496 | 70.495056 |
| Mode 7 | 116.672 | 115.038592 |
| Mode 8 | 135.338 | 133.443268 |
| Mode 9 | 167.026 | 164.687636 |
| Mode 10 | 171.852 | 169.446072 |
| Mode 11 | 175.025 | 172.574650 |
| Mode 12 | 180.528 | 178.000608 |
| Mode 13 | 186.673 | 184.059578 |
| Mode 14 | 194.426 | 191.704036 |
| Mode 15 | 200.455 | 197.648630 |
| Mode 16 | 208.023 | 205.110678 |
| Mode 17 | 216.748 | 213.713528 |
| Mode 18 | 234.746 | 231.459556 |
| Mode 19 | 239.100 | 235.752600 |
| Mode 20 | 252.652 | 249.114872 |
| Mode 21 | 318.687 | 314.225382 |
| Mode 22 | 338.837 | 334.093282 |
| Mode 23 | 359.258 | 354.228388 |
| Mode 24 | 384.472 | 379.089392 |
| Mode 25 | 400.370 | 394.764820 |
| Mode 26 | 411.557 | 405.795202 |
| Mode 27 | 456.848 | 450.452128 |
| Mode 28 | 541.381 | 533.801666 |
| Mode 29 | 570.425 | 562.439050 |
| Mode 30 | 593.929 | 585.613994 |
| Mode 31 | 605.878 | 597.395708 |
| Mode 32 | 663.941 | 654.645826 |
| Mode 33 | 693.841 | 684.127226 |
| Mode 34 | 731.515 | 721.273790 |
| Mode 35 | 787.896 | 776.865456 |
| Mode 36 | 804.732 | 793.465752 |
| Mode 37 | 1656.156 | 1632.969816 |
| Mode 38 | 1660.315 | 1637.070590 |
| Mode 39 | 1664.628 | 1641.323208 |
| Mode 40 | 1668.447 | 1645.088742 |
| Mode 41 | 1676.894 | 1653.417484 |
| Mode 42 | 1693.451 | 1669.742686 |
| Mode 43 | 1710.913 | 1686.960218 |
| Mode 44 | 3580.430 | 3530.303980 |
| Mode 45 | 3592.651 | 3542.353886 |
| Mode 46 | 3622.877 | 3572.156722 |
| Mode 47 | 3648.219 | 3597.143934 |
| Mode 48 | 3655.176 | 3604.003536 |

| | | |
|---------|----------|-------------|
| Mode 49 | 3671.907 | 3620.500302 |
| Mode 50 | 3681.703 | 3630.159158 |
| Mode 51 | 3726.686 | 3674.512396 |
| Mode 52 | 3797.350 | 3744.187100 |
| Mode 53 | 3853.663 | 3799.711718 |
| Mode 54 | 3858.014 | 3804.001804 |
| Mode 55 | 3859.895 | 3805.856470 |
| Mode 56 | 3864.775 | 3810.668150 |
| Mode 57 | 3866.107 | 3811.981502 |

w7-9_25 (scaling factor 0.989)

Table S17: Scaled and Unscaled Frequencies of w7-9_25 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 2.267 | 2.242063 |
| Mode 2 | 23.135 | 22.880515 |
| Mode 3 | 28.262 | 27.951118 |
| Mode 4 | 36.043 | 35.646527 |
| Mode 5 | 40.151 | 39.709339 |
| Mode 6 | 44.249 | 43.762261 |
| Mode 7 | 51.195 | 50.631855 |
| Mode 8 | 64.788 | 64.075332 |
| Mode 9 | 123.835 | 122.472815 |
| Mode 10 | 143.936 | 142.352704 |
| Mode 11 | 166.150 | 164.322350 |
| Mode 12 | 173.818 | 171.906002 |
| Mode 13 | 176.363 | 174.423007 |
| Mode 14 | 185.750 | 183.706750 |
| Mode 15 | 195.133 | 192.986537 |
| Mode 16 | 199.707 | 197.510223 |
| Mode 17 | 213.807 | 211.455123 |
| Mode 18 | 217.911 | 215.513979 |
| Mode 19 | 225.727 | 223.244003 |
| Mode 20 | 231.664 | 229.115696 |
| Mode 21 | 247.542 | 244.819038 |
| Mode 22 | 254.346 | 251.548194 |
| Mode 23 | 327.279 | 323.678931 |
| Mode 24 | 355.745 | 351.831805 |
| Mode 25 | 365.370 | 361.350930 |
| Mode 26 | 396.270 | 391.911030 |
| Mode 27 | 498.270 | 492.789030 |
| Mode 28 | 518.590 | 512.885510 |
| Mode 29 | 543.245 | 537.269305 |
| Mode 30 | 619.758 | 612.940662 |
| Mode 31 | 629.269 | 622.347041 |

| | | |
|---------|----------|-------------|
| Mode 32 | 677.637 | 670.182993 |
| Mode 33 | 721.902 | 713.961078 |
| Mode 34 | 750.891 | 742.631199 |
| Mode 35 | 838.117 | 828.897713 |
| Mode 36 | 853.539 | 844.150071 |
| Mode 37 | 1639.689 | 1621.652421 |
| Mode 38 | 1655.348 | 1637.139172 |
| Mode 39 | 1659.555 | 1641.299895 |
| Mode 40 | 1666.734 | 1648.399926 |
| Mode 41 | 1680.222 | 1661.739558 |
| Mode 42 | 1690.371 | 1671.776919 |
| Mode 43 | 1702.273 | 1683.547997 |
| Mode 44 | 3534.124 | 3495.248636 |
| Mode 45 | 3601.223 | 3561.609547 |
| Mode 46 | 3615.584 | 3575.812576 |
| Mode 47 | 3640.588 | 3600.541532 |
| Mode 48 | 3653.944 | 3613.750616 |
| Mode 49 | 3668.795 | 3628.438255 |
| Mode 50 | 3735.557 | 3694.465873 |
| Mode 51 | 3749.914 | 3708.664946 |
| Mode 52 | 3776.256 | 3734.717184 |
| Mode 53 | 3857.280 | 3814.849920 |
| Mode 54 | 3858.757 | 3816.310673 |
| Mode 55 | 3862.207 | 3819.722723 |
| Mode 56 | 3864.039 | 3821.534571 |
| Mode 57 | 3898.778 | 3855.891442 |

w8-23_25 (scaling factor 0.993)

Table S18: Scaled and Unscaled Frequencies of w8-23_25 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 0.257 | 0.255201 |
| Mode 2 | 2.200 | 2.184600 |
| Mode 3 | 15.947 | 15.835371 |
| Mode 4 | 29.911 | 29.701623 |
| Mode 5 | 47.501 | 47.168493 |
| Mode 6 | 51.243 | 50.884299 |
| Mode 7 | 59.310 | 58.894830 |
| Mode 8 | 76.129 | 75.596097 |
| Mode 9 | 93.248 | 92.595264 |
| Mode 10 | 117.434 | 116.611962 |
| Mode 11 | 134.990 | 134.045070 |
| Mode 12 | 143.097 | 142.095321 |
| Mode 13 | 178.900 | 177.647700 |
| Mode 14 | 182.624 | 181.345632 |

| | | |
|---------|----------|-------------|
| Mode 15 | 188.915 | 187.592595 |
| Mode 16 | 193.027 | 191.675811 |
| Mode 17 | 193.855 | 192.498015 |
| Mode 18 | 200.980 | 199.573140 |
| Mode 19 | 216.014 | 214.501902 |
| Mode 20 | 217.088 | 215.568384 |
| Mode 21 | 244.068 | 242.359524 |
| Mode 22 | 250.733 | 248.977869 |
| Mode 23 | 258.215 | 256.407495 |
| Mode 24 | 292.548 | 290.500164 |
| Mode 25 | 334.099 | 331.760307 |
| Mode 26 | 354.928 | 352.443504 |
| Mode 27 | 368.814 | 366.232302 |
| Mode 28 | 389.549 | 386.822157 |
| Mode 29 | 408.989 | 406.126077 |
| Mode 30 | 423.426 | 420.462018 |
| Mode 31 | 449.620 | 446.472660 |
| Mode 32 | 480.225 | 476.863425 |
| Mode 33 | 520.430 | 516.786990 |
| Mode 34 | 553.215 | 549.342495 |
| Mode 35 | 582.027 | 577.952811 |
| Mode 36 | 613.209 | 608.916537 |
| Mode 37 | 644.237 | 639.727341 |
| Mode 38 | 699.597 | 694.699821 |
| Mode 39 | 716.734 | 711.716862 |
| Mode 40 | 784.285 | 778.795005 |
| Mode 41 | 848.634 | 842.693562 |
| Mode 42 | 876.440 | 870.304920 |
| Mode 43 | 1641.158 | 1629.669894 |
| Mode 44 | 1648.581 | 1637.040933 |
| Mode 45 | 1658.859 | 1647.246987 |
| Mode 46 | 1661.809 | 1650.176337 |
| Mode 47 | 1667.157 | 1655.486901 |
| Mode 48 | 1678.184 | 1666.436712 |
| Mode 49 | 1689.420 | 1677.594060 |
| Mode 50 | 1694.585 | 1682.722905 |
| Mode 51 | 3565.399 | 3540.441207 |
| Mode 52 | 3574.088 | 3549.069384 |
| Mode 53 | 3615.062 | 3589.756566 |
| Mode 54 | 3629.595 | 3604.187835 |
| Mode 55 | 3651.435 | 3625.874955 |
| Mode 56 | 3666.012 | 3640.349916 |
| Mode 57 | 3701.081 | 3675.173433 |
| Mode 58 | 3709.150 | 3683.185950 |
| Mode 59 | 3729.842 | 3703.733106 |

| | | |
|---------|----------|-------------|
| Mode 60 | 3795.671 | 3769.101303 |
| Mode 61 | 3812.037 | 3785.352741 |
| Mode 62 | 3854.886 | 3827.901798 |
| Mode 63 | 3858.210 | 3831.202530 |
| Mode 64 | 3863.547 | 3836.502171 |
| Mode 65 | 3870.002 | 3842.911986 |
| Mode 66 | 3880.171 | 3853.009803 |

w9-66_25 (scaling factor 0.987)

Table S19: Scaled and Unscaled Frequencies of w9-66_25 cluster

| Vibrational Modes | Unscaled Frequencies (cm ⁻¹) | Scaled Frequencies (cm ⁻¹) |
|-------------------|--|--|
| Mode 1 | 0.270 | 0.266490 |
| Mode 2 | 26.732 | 26.384484 |
| Mode 3 | 29.874 | 29.485638 |
| Mode 4 | 36.300 | 35.828100 |
| Mode 5 | 45.687 | 45.093069 |
| Mode 6 | 50.302 | 49.648074 |
| Mode 7 | 58.465 | 57.704955 |
| Mode 8 | 65.277 | 64.428399 |
| Mode 9 | 74.908 | 73.934196 |
| Mode 10 | 130.617 | 128.918979 |
| Mode 11 | 137.548 | 135.759876 |
| Mode 12 | 154.214 | 152.209218 |
| Mode 13 | 169.121 | 166.922427 |
| Mode 14 | 171.937 | 169.701819 |
| Mode 15 | 180.819 | 178.468353 |
| Mode 16 | 193.364 | 190.850268 |
| Mode 17 | 201.740 | 199.117380 |
| Mode 18 | 203.785 | 201.135795 |
| Mode 19 | 216.497 | 213.682539 |
| Mode 20 | 218.205 | 215.368335 |
| Mode 21 | 222.801 | 219.904587 |
| Mode 22 | 227.186 | 224.232582 |
| Mode 23 | 228.048 | 225.083376 |
| Mode 24 | 236.487 | 233.412669 |
| Mode 25 | 241.707 | 238.564809 |
| Mode 26 | 264.050 | 260.617350 |
| Mode 27 | 292.002 | 288.205974 |
| Mode 28 | 339.721 | 335.304627 |
| Mode 29 | 345.583 | 341.090421 |
| Mode 30 | 364.021 | 359.288727 |
| Mode 31 | 367.235 | 362.460945 |
| Mode 32 | 375.915 | 371.028105 |
| Mode 33 | 419.193 | 413.743491 |

| | | |
|---------|----------|-------------|
| Mode 34 | 450.474 | 444.617838 |
| Mode 35 | 478.442 | 472.222254 |
| Mode 36 | 524.372 | 517.555164 |
| Mode 37 | 551.464 | 544.294968 |
| Mode 38 | 590.911 | 583.229157 |
| Mode 39 | 614.727 | 606.735549 |
| Mode 40 | 649.589 | 641.144343 |
| Mode 41 | 666.722 | 658.054614 |
| Mode 42 | 670.637 | 661.918719 |
| Mode 43 | 700.318 | 691.213866 |
| Mode 44 | 761.091 | 751.196817 |
| Mode 45 | 775.387 | 765.306969 |
| Mode 46 | 809.799 | 799.271613 |
| Mode 47 | 849.899 | 838.850313 |
| Mode 48 | 938.160 | 925.963920 |
| Mode 49 | 1651.318 | 1629.850866 |
| Mode 50 | 1653.994 | 1632.492078 |
| Mode 51 | 1657.030 | 1635.488610 |
| Mode 52 | 1658.605 | 1637.043135 |
| Mode 53 | 1672.493 | 1650.750591 |
| Mode 54 | 1673.738 | 1651.979406 |
| Mode 55 | 1683.922 | 1662.031014 |
| Mode 56 | 1701.884 | 1679.759508 |
| Mode 57 | 1709.584 | 1687.359408 |
| Mode 58 | 3534.789 | 3488.836743 |
| Mode 59 | 3559.185 | 3512.915595 |
| Mode 60 | 3585.908 | 3539.291196 |
| Mode 61 | 3605.414 | 3558.543618 |
| Mode 62 | 3613.646 | 3566.668602 |
| Mode 63 | 3638.994 | 3591.687078 |
| Mode 64 | 3651.571 | 3604.100577 |
| Mode 65 | 3665.410 | 3617.759670 |
| Mode 66 | 3672.885 | 3625.137495 |
| Mode 67 | 3687.569 | 3639.630603 |
| Mode 68 | 3727.920 | 3679.457040 |
| Mode 69 | 3770.365 | 3721.350255 |
| Mode 70 | 3841.944 | 3791.998728 |
| Mode 71 | 3853.090 | 3802.999830 |
| Mode 72 | 3860.871 | 3810.679677 |
| Mode 73 | 3861.109 | 3810.914583 |
| Mode 74 | 3862.376 | 3812.165112 |
| Mode 75 | 3863.788 | 3813.558756 |

w10-10_80 (scaling factor 0.987)

Table S20: Scaled and Unscaled Frequencies of w10-10_80 cluster

| Vibrational Modes | Unscaled Frequencies (cm⁻¹) | Scaled Frequencies (cm⁻¹) |
|--------------------------|---|---|
| Mode 1 | 1.390 | 1.371930 |
| Mode 2 | 17.375 | 17.149125 |
| Mode 3 | 20.533 | 20.266071 |
| Mode 4 | 31.579 | 31.168473 |
| Mode 5 | 35.589 | 35.126343 |
| Mode 6 | 42.295 | 41.745165 |
| Mode 7 | 45.110 | 44.523570 |
| Mode 8 | 58.686 | 57.923082 |
| Mode 9 | 60.887 | 60.095469 |
| Mode 10 | 71.169 | 70.243803 |
| Mode 11 | 80.187 | 79.144569 |
| Mode 12 | 116.465 | 114.950955 |
| Mode 13 | 128.484 | 126.813708 |
| Mode 14 | 131.669 | 129.957303 |
| Mode 15 | 139.509 | 137.695383 |
| Mode 16 | 145.216 | 143.328192 |
| Mode 17 | 156.626 | 154.589862 |
| Mode 18 | 170.601 | 168.383187 |
| Mode 19 | 172.771 | 170.524977 |
| Mode 20 | 176.798 | 174.499626 |
| Mode 21 | 180.716 | 178.366692 |
| Mode 22 | 188.659 | 186.206433 |
| Mode 23 | 192.632 | 190.127784 |
| Mode 24 | 199.985 | 197.385195 |
| Mode 25 | 218.712 | 215.868744 |
| Mode 26 | 227.177 | 224.223699 |
| Mode 27 | 237.389 | 234.302943 |
| Mode 28 | 251.157 | 247.891959 |
| Mode 29 | 257.921 | 254.568027 |
| Mode 30 | 282.800 | 279.123600 |
| Mode 31 | 327.145 | 322.892115 |
| Mode 32 | 328.880 | 324.604560 |
| Mode 33 | 352.855 | 348.267885 |
| Mode 34 | 362.159 | 357.450933 |
| Mode 35 | 375.139 | 370.262193 |
| Mode 36 | 407.782 | 402.480834 |
| Mode 37 | 424.924 | 419.399988 |
| Mode 38 | 445.596 | 439.803252 |
| Mode 39 | 461.090 | 455.095830 |
| Mode 40 | 519.618 | 512.862966 |
| Mode 41 | 541.678 | 534.636186 |
| Mode 42 | 560.791 | 553.500717 |
| Mode 43 | 591.309 | 583.621983 |

| | | |
|---------|----------|-------------|
| Mode 44 | 598.317 | 590.538879 |
| Mode 45 | 615.809 | 607.803483 |
| Mode 46 | 623.825 | 615.715275 |
| Mode 47 | 641.563 | 633.222681 |
| Mode 48 | 692.559 | 683.555733 |
| Mode 49 | 699.166 | 690.076842 |
| Mode 50 | 723.452 | 714.047124 |
| Mode 51 | 733.389 | 723.854943 |
| Mode 52 | 762.894 | 752.976378 |
| Mode 53 | 819.101 | 808.452687 |
| Mode 54 | 888.380 | 876.831060 |
| Mode 55 | 1651.373 | 1629.905151 |
| Mode 56 | 1657.148 | 1635.605076 |
| Mode 57 | 1658.974 | 1637.407338 |
| Mode 58 | 1660.410 | 1638.824670 |
| Mode 59 | 1663.558 | 1641.931746 |
| Mode 60 | 1677.170 | 1655.366790 |
| Mode 61 | 1690.970 | 1668.987390 |
| Mode 62 | 1706.237 | 1684.055919 |
| Mode 63 | 1711.010 | 1688.766870 |
| Mode 64 | 1719.531 | 1697.177097 |
| Mode 65 | 3554.025 | 3507.822675 |
| Mode 66 | 3600.410 | 3553.604670 |
| Mode 67 | 3610.169 | 3563.236803 |
| Mode 68 | 3616.905 | 3569.885235 |
| Mode 69 | 3638.977 | 3591.670299 |
| Mode 70 | 3655.580 | 3608.057460 |
| Mode 71 | 3656.753 | 3609.215211 |
| Mode 72 | 3665.814 | 3618.158418 |
| Mode 73 | 3681.308 | 3633.450996 |
| Mode 74 | 3687.204 | 3639.270348 |
| Mode 75 | 3705.195 | 3657.027465 |
| Mode 76 | 3722.881 | 3674.483547 |
| Mode 77 | 3728.790 | 3680.315730 |
| Mode 78 | 3780.397 | 3731.251839 |
| Mode 79 | 3859.060 | 3808.892220 |
| Mode 80 | 3860.219 | 3810.036153 |
| Mode 81 | 3864.677 | 3814.436199 |
| Mode 82 | 3866.580 | 3816.314460 |
| Mode 83 | 3870.667 | 3820.348329 |
| Mode 84 | 3878.407 | 3827.987709 |

9 List of all 459 clustersets tested

Table S21: List of W_n clusters making up all the 459 clustersets tested in this work.

| Set | Clusters | | | | | | | | |
|-------|----------|------|----------|----------|----------|----------|----------|----------|-----------|
| set1 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set2 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set3 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set4 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set5 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set6 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set7 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set8 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set9 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set10 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set11 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set12 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set13 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set14 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set15 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set16 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set17 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-28_60 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set18 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set19 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set20 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set21 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set22 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set23 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set24 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set25 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set26 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set27 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set28 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set29 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set30 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set31 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set32 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set33 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set34 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-59_25 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set35 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set36 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set37 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set38 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set39 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set40 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-14_60 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |

| | | | | | | | | | |
|---------------|----|------|----------|----------|----------|----------|----------|----------|-----------|
| set87 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set88 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set89 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set90 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set91 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set92 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set93 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set94 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set95 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set96 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set97 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set98 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set99 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set100 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set101 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set102 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-65_40 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set103 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set104 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set105 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set106 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set107 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set108 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set109 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set110 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set111 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set112 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set113 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set114 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set115 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set116 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set117 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set118 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set119 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-13_40 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set120 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set121 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set122 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set123 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set124 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set125 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set126 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set127 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set128 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set129 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set130 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set131 | w1 | 2-w2 | w4-41_80 | w5-59_80 | w6-47_40 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |

| | | | | | | | | | |
|---------------|----|------|----------|----------|----------|----------|----------|----------|-----------|
| set267 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set268 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set269 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set270 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set271 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set272 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-13_40 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set273 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set274 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set275 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set276 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set277 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set278 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set279 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set280 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set281 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set282 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set283 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set284 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set285 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set286 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set287 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set288 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set289 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-47_40 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set290 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set291 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set292 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set293 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set294 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set295 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set296 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set297 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set298 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set299 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set300 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set301 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set302 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set303 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set304 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set305 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set306 | w1 | 2-w2 | w4-41_80 | w5-76_80 | w6-32_80 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set307 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-28_60 | w7-97_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set308 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-28_60 | w7-76_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set309 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-28_60 | w7-95_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set310 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-28_60 | w7-33_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set311 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-28_60 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |

| | | | | | | | | | |
|---------------|----|------|----------|----------|----------|----------|----------|----------|-----------|
| set447 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-72_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set448 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-6_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set449 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-9_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set450 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-92_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set451 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-40_40 | w8-23_25 | w9-66_25 | w10-10_80 |
| set452 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-17_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set453 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-47_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set454 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-67_25 | w8-23_25 | w9-66_25 | w10-10_80 |
| set455 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-86_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set456 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-1_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set457 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-35_60 | w8-23_25 | w9-66_25 | w10-10_80 |
| set458 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-40_80 | w8-23_25 | w9-66_25 | w10-10_80 |
| set459 | w1 | 2-w2 | w4-41_80 | w5-70_60 | w6-32_80 | w7-56_40 | w8-23_25 | w9-66_25 | w10-10_80 |

10 Cartesian coordinates of W_n for all 459 sets

w1-w1

| | | | |
|---|--------------|-------------|--------------|
| O | -4.373887254 | 2.199597294 | -4.092304572 |
| H | -4.562108491 | 1.250724812 | -4.106033927 |
| H | -5.222714255 | 2.600477894 | -3.858291501 |

w2

| | | | |
|---|--------------|-------------|--------------|
| O | -1.705990148 | 2.09296745 | -2.983665308 |
| H | -2.55489867 | 2.153994512 | -3.454606039 |
| H | -1.096812019 | 2.610267667 | -3.526978388 |
| O | -4.405188256 | 2.119243589 | -4.219588082 |
| H | -4.703655563 | 1.214373176 | -4.389475285 |
| H | -5.056025344 | 2.469463605 | -3.594626897 |

w4-41_80

12

| | | | |
|---|--------------|--------------|--------------|
| O | -0.216710815 | 1.630595376 | -0.383144575 |
| H | -0.854986048 | 2.030599211 | -0.988463023 |
| H | 0.083867714 | 0.82008447 | -0.838581103 |
| O | -1.02559137 | 0.513419352 | 2.119164804 |
| H | -0.782354678 | 1.013595959 | 1.315350911 |
| H | -0.648835958 | 1.025518468 | 2.846761312 |
| O | -0.241044493 | -2.086148388 | 1.198628114 |
| H | -0.506141967 | -1.272949437 | 1.670872953 |
| H | 0.327598977 | -2.559131678 | 1.820253548 |

| | | | |
|---|-------------|--------------|--------------|
| O | 0.668472908 | -0.953020433 | -1.261619121 |
| H | 0.337523972 | -1.470905029 | -2.007228907 |
| H | 0.400591759 | -1.461817871 | -0.471294915 |

w5-59_80

15

| | | | |
|---|--------------|--------------|--------------|
| O | -0.654135222 | 0.920246474 | 1.676642093 |
| H | -0.344544556 | 1.046090956 | 2.583557376 |
| H | 0.105929463 | 0.511580859 | 1.212384447 |
| O | 2.382959184 | 0.908391146 | -2.125890825 |
| H | 2.792402865 | 1.7601998 | -1.917215169 |
| H | 1.656520469 | 1.135978683 | -2.723778433 |
| O | -0.606937314 | -2.544137726 | -0.457934289 |
| H | -1.356334613 | -2.168846018 | 0.044385642 |
| H | -0.538936918 | -3.45710373 | -0.148276389 |
| O | -2.562718996 | -1.122694617 | 1.087563714 |
| H | -3.343109751 | -0.725050201 | 0.679136145 |
| H | -2.009225899 | -0.361611255 | 1.353303378 |
| O | 1.31583054 | -0.508351494 | 0.250323686 |
| H | 1.70141907 | -0.118471704 | -0.552575313 |
| H | 0.796131678 | -1.271671174 | -0.063276061 |

w5-70_60

15

| | | | |
|---|--------------|--------------|--------------|
| O | -0.195367053 | 0.898983601 | -1.53335214 |
| H | 0.335314025 | 0.118069403 | -1.28734317 |
| H | -0.158804688 | 0.926803707 | -2.498796298 |
| O | 1.532203449 | 0.821712057 | 1.886914942 |
| H | 1.453622399 | 1.720857094 | 1.53867609 |
| H | 1.75268023 | 0.285727364 | 1.106380521 |
| O | 1.198931891 | -1.249626621 | -0.233886436 |
| H | 1.592105922 | -2.093579766 | -0.490693312 |
| H | 0.502407556 | -1.467692613 | 0.421781374 |
| O | -2.576003252 | 0.245414119 | -0.026776767 |
| H | -1.879515967 | 0.594083926 | -0.614209027 |
| H | -3.142236221 | 1.003904987 | 0.166748195 |
| O | -0.738065178 | -1.114675207 | 1.770095886 |
| H | -0.220757201 | -0.376760901 | 2.1370549 |
| H | -1.48151591 | -0.67507115 | 1.317055242 |

w5-76_80

15

| | | | |
|---|--------------|-------------|--------------|
| O | -1.090964138 | 0.609218725 | -2.459081001 |
|---|--------------|-------------|--------------|

| | | | |
|---|--------------|--------------|--------------|
| H | -1.614387351 | 1.009415414 | -3.164690824 |
| H | -0.16636585 | 0.65756922 | -2.760503838 |
| O | 1.781396572 | 0.539917247 | -2.191834978 |
| H | 1.49665088 | 0.633998089 | -1.263678408 |
| H | 2.510812339 | 1.165477743 | -2.292264433 |
| O | -0.257826354 | 1.527829966 | 2.831998474 |
| H | -0.170818887 | 0.579195425 | 3.036438635 |
| H | 0.260528011 | 1.980569961 | 3.509654364 |
| O | -0.179143041 | -1.299770552 | 2.307526778 |
| H | -0.066299361 | -0.960707232 | 1.400154262 |
| H | 0.37451075 | -2.089931174 | 2.351387055 |
| O | 0.089381745 | 0.579912772 | 0.135436311 |
| H | -0.06537008 | 1.199569156 | 0.870089908 |
| H | -0.617625236 | 0.74183524 | -0.513672303 |

w6-13_40

18

| | | | |
|---|--------------|--------------|--------------|
| O | -1.446711504 | 2.148750304 | -1.889912863 |
| H | -0.533093926 | 1.812104361 | -1.994423055 |
| H | -1.776467154 | 2.249541933 | -2.792386143 |
| O | -2.405230771 | 0.457927547 | 0.149845306 |
| H | -2.870794688 | 0.974870999 | 0.820540161 |
| H | -2.204962729 | 1.093239947 | -0.567324185 |
| O | -2.309810285 | -2.459421706 | -0.145732011 |
| H | -2.625907007 | -1.540710972 | -0.191842083 |
| H | -2.89864652 | -2.955640343 | -0.729034692 |
| O | 2.492140905 | 0.823683033 | 0.68501363 |
| H | 3.198983681 | 0.675868357 | 1.326467576 |
| H | 1.877938236 | 0.08011093 | 0.810550396 |
| O | 1.061353545 | 0.840774373 | -1.950009612 |
| H | 0.799482377 | 0.069574843 | -1.416078781 |
| H | 1.78576929 | 1.209047114 | -1.418528776 |
| O | 0.195214459 | -0.898431955 | 0.265821225 |
| H | -0.593626732 | -0.352669848 | 0.434692177 |
| H | -0.188791176 | -1.782138918 | 0.150571729 |

w6-14_60

18

| | | | |
|---|--------------|--------------|--------------|
| O | -2.232446696 | -1.031536571 | -1.622016728 |
| H | -3.147789254 | -0.722826678 | -1.613366024 |
| H | -1.985487547 | -1.10537753 | -0.677746576 |
| O | -0.161281221 | 0.228653241 | -3.09615916 |
| H | 0.104112637 | -0.423747914 | -3.757895697 |
| H | -0.904257039 | -0.194919308 | -2.622182047 |

| | | | |
|---|--------------|--------------|--------------|
| O | 1.804566141 | 1.319789404 | -1.366145383 |
| H | 1.141174629 | 0.953799565 | -1.985130712 |
| H | 1.843141758 | 2.259643447 | -1.587206613 |
| O | 1.234172989 | -2.675014217 | 1.408231657 |
| H | 1.518928059 | -1.758128928 | 1.245725646 |
| H | 1.790693945 | -3.21259924 | 0.829350468 |
| O | 1.285539714 | 0.243183657 | 1.20178247 |
| H | 1.508935908 | 0.701046385 | 0.366734076 |
| H | 1.698981534 | 0.770199519 | 1.898119765 |
| O | -1.331274868 | -1.180584483 | 1.059080912 |
| H | -0.661164073 | -0.486918004 | 1.182633141 |
| H | -0.804656617 | -1.986102346 | 1.197390805 |

w6-28_60

18

| | | | |
|---|--------------|--------------|--------------|
| O | 0.626629316 | 2.100446744 | -0.326369701 |
| H | 1.4816524 | 1.958052378 | 0.115504839 |
| H | 0.714082312 | 1.510995636 | -1.094901498 |
| O | -0.795290775 | -1.880047387 | -3.299457815 |
| H | -1.570402947 | -1.38033272 | -2.981378121 |
| H | -0.921560014 | -1.965881858 | -4.252846077 |
| O | -1.18606543 | 0.10662737 | 0.533367548 |
| H | -0.631234904 | 0.911475905 | 0.485062148 |
| H | -1.461136904 | 0.030992255 | 1.456203516 |
| O | 2.95300522 | 0.429617621 | 0.394193215 |
| H | 3.902732184 | 0.258778436 | 0.352927394 |
| H | 2.56093816 | -0.154066373 | -0.27955327 |
| O | -2.789848969 | -0.36966025 | -1.84162872 |
| H | -2.346341218 | -0.135454024 | -1.00549299 |
| H | -3.234906399 | 0.444326747 | -2.112571264 |
| O | 0.962230281 | -0.699758314 | -1.334203854 |
| H | 0.276436199 | -0.818648046 | -0.656154617 |
| H | 0.602301488 | -1.16660412 | -2.108630733 |

w6-32_80

18

| | | | |
|---|--------------|--------------|--------------|
| O | 0.84392654 | -3.639803694 | 0.402301919 |
| H | 1.507916396 | -4.222170026 | 0.010898896 |
| H | 1.348209597 | -2.867533355 | 0.729495623 |
| O | 1.990817304 | -1.14948465 | 1.173591283 |
| H | 1.539399167 | -0.848850343 | 1.980148443 |
| H | 1.542399032 | -0.615853689 | 0.493260045 |
| O | -1.267272821 | -2.27475235 | -0.955568964 |
| H | -2.072418676 | -2.466517046 | -0.455514048 |

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|---|--------------|--------------|--------------|
| H | -0.590050703 | -2.846559539 | -0.542797448 |
| O | 0.087178731 | 2.300159581 | -2.463419101 |
| H | 0.959917356 | 2.407889932 | -2.867056695 |
| H | -0.221865736 | 3.204250427 | -2.31265218 |
| O | -0.344987397 | 0.200265164 | 2.489210706 |
| H | -0.430519298 | 0.43183049 | 1.546239678 |
| H | -0.598362696 | 1.000905459 | 2.966612781 |
| O | -0.068494244 | 0.242669597 | -0.387027445 |
| H | -0.557911632 | -0.537246826 | -0.714306858 |
| H | -0.08294092 | 0.893690868 | -1.108166635 |

w6-38_40

18

| | | | |
|---|--------------|--------------|--------------|
| O | -0.366700441 | -1.466840739 | 3.134960989 |
| H | -0.880727699 | -0.843686464 | 2.586938996 |
| H | -1.002099944 | -2.149114147 | 3.390236052 |
| O | 0.760845218 | 2.421120792 | 0.666465086 |
| H | 0.91041719 | 3.296739994 | 1.044923251 |
| H | -0.08257302 | 2.115844461 | 1.041497181 |
| O | 1.82154665 | -2.089709228 | 1.365799489 |
| H | 2.66075508 | -2.06465127 | 1.844208357 |
| H | 1.140713741 | -1.953732714 | 2.052808682 |
| O | -1.329694145 | 0.424056223 | 1.185008533 |
| H | -0.657304296 | 0.094282165 | 0.556480565 |
| H | -2.14259252 | 0.371385998 | 0.659313356 |
| O | -1.816830126 | -0.449445466 | -1.696351291 |
| H | -0.847023605 | -0.465448005 | -1.625747683 |
| H | -1.999327562 | -0.656248283 | -2.62217843 |
| O | 0.870147335 | -0.204875362 | -0.571340912 |
| H | 1.366346296 | -0.832405105 | -0.012180141 |
| H | 1.238621848 | 0.67007715 | -0.364102081 |

w6-47_40

18

| | | | |
|---|--------------|--------------|--------------|
| O | -2.644997876 | -1.71455351 | -1.356158492 |
| H | -1.790922029 | -2.097572262 | -1.637440921 |
| H | -2.827704728 | -2.107960187 | -0.493308105 |
| O | -0.10181788 | -2.016789371 | -2.599969927 |
| H | 0.682033057 | -1.9498076 | -2.025743774 |
| H | -0.251090711 | -1.102792002 | -2.891534921 |
| O | 0.818247393 | -0.815978885 | 1.675979361 |
| H | 0.554098761 | -0.019289621 | 1.176397262 |
| H | 0.16804483 | -0.91455692 | 2.38209445 |
| O | -1.447578803 | 0.688895507 | -2.293937968 |

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|---|--------------|--------------|--------------|
| H | -1.987135639 | 1.35215022 | -2.7438493 |
| H | -2.08142086 | 0.05061756 | -1.914781457 |
| O | 2.113084168 | -1.543900735 | -0.742727465 |
| H | 2.978337723 | -1.973733641 | -0.730347346 |
| H | 1.791536261 | -1.583579127 | 0.176808006 |
| O | 0.720385597 | 1.131498532 | -0.377310456 |
| H | 1.397092528 | 0.564471524 | -0.781676317 |
| H | -0.02159179 | 1.088900518 | -1.006912631 |

w6-59_25

18

| | | | |
|---|--------------|--------------|--------------|
| O | 1.710372389 | -2.737773681 | -2.019592285 |
| H | 1.036955465 | -2.942673541 | -1.339420084 |
| H | 2.410386975 | -3.388644723 | -1.879347428 |
| O | -2.335173815 | -0.960835406 | -0.889909145 |
| H | -3.208160878 | -0.62191299 | -0.65272258 |
| H | -1.708043584 | -0.415783527 | -0.380438863 |
| O | -0.253953516 | -2.912645783 | 0.03185466 |
| H | -1.127384686 | -2.728876624 | -0.35307566 |
| H | -0.047751252 | -2.05909576 | 0.45272382 |
| O | 0.597439231 | 1.660792833 | 2.817843069 |
| H | 0.969032068 | 1.172860874 | 3.56646184 |
| H | 1.175311087 | 2.431333901 | 2.725298785 |
| O | 1.849735939 | 0.094568035 | -1.70323861 |
| H | 1.484226315 | 0.467537424 | -2.517190531 |
| H | 1.907175512 | -0.864084494 | -1.887389883 |
| O | 0.028688265 | -0.027525472 | 0.486834178 |
| H | 0.692883007 | 0.14606694 | -0.208407668 |
| H | 0.245431478 | 0.574351993 | 1.218616385 |

w6-65_40

18

| | | | |
|---|--------------|--------------|--------------|
| O | 0.573749965 | 0.237365766 | -2.974898083 |
| H | -0.355950254 | 0.509316724 | -2.90849971 |
| H | 0.968254714 | 0.689082863 | -2.210891059 |
| O | -2.651369016 | -1.674134931 | -0.979845285 |
| H | -3.303840919 | -1.873135347 | -0.29541951 |
| H | -2.608438228 | -0.700989401 | -1.009576548 |
| O | 1.967881902 | 1.604209319 | 2.461485998 |
| H | 1.735119111 | 2.364033774 | 3.01272433 |
| H | 2.931452271 | 1.647600305 | 2.385049154 |
| O | -1.912202764 | 1.110965369 | -1.2698935 |
| H | -2.374928969 | 1.956469098 | -1.206895441 |
| H | -1.134506391 | 1.194299187 | -0.683077171 |

| | | | |
|---|--------------|--------------|--------------|
| O | 0.27284322 | -1.882010547 | -0.861342472 |
| H | 0.427242293 | -1.529090959 | -1.7554 |
| H | -0.689574063 | -2.033996984 | -0.84883679 |
| O | 0.584049182 | 0.796091822 | 0.003843028 |
| H | 1.011309946 | 1.029534238 | 0.844504611 |
| H | 0.565088002 | -0.181320296 | -0.032091553 |

w6-93_80

18

| | | | |
|---|--------------|--------------|--------------|
| O | -0.997721434 | -0.594295534 | -2.721705079 |
| H | -1.462981146 | -0.368611534 | -3.537789783 |
| H | -0.836427288 | 0.262163725 | -2.278577183 |
| O | -1.574180326 | -2.075183707 | -0.290136328 |
| H | -1.622514202 | -1.641830317 | -1.161709049 |
| H | -1.74509511 | -1.350018473 | 0.335569786 |
| O | 1.283063201 | -2.172020842 | -0.26521167 |
| H | 1.525291839 | -2.201511039 | -1.201528612 |
| H | 0.310337073 | -2.287059671 | -0.276501336 |
| O | -1.519509347 | 0.295592389 | 1.504311791 |
| H | -1.895282103 | 0.368111482 | 2.391845285 |
| H | -0.55272618 | 0.304360054 | 1.631136972 |
| O | -0.529051341 | 1.659092337 | -1.015304191 |
| H | 0.279857589 | 1.423115964 | -0.529264029 |
| H | -1.209884225 | 1.549048903 | -0.331808389 |
| O | 1.299484364 | 0.35555512 | 0.942762648 |
| H | 1.439501382 | -0.53095686 | 0.547065886 |
| H | 2.120657252 | 0.559708003 | 1.40890328 |

w7-17_60

21

| | | | |
|---|--------------|--------------|--------------|
| O | 0.591446065 | 2.424105752 | -2.598023905 |
| H | 1.150371396 | 1.663550285 | -2.349782261 |
| H | 0.106816125 | 2.123744151 | -3.378988495 |
| O | 2.252904141 | 0.214261339 | -1.742770367 |
| H | 3.176321881 | 0.260472217 | -2.02602468 |
| H | 2.29195797 | 0.178950292 | -0.767254285 |
| O | 0.754003724 | -2.356081088 | -0.742456521 |
| H | 1.186343896 | -1.947196287 | 0.027379162 |
| H | 1.082579405 | -1.805227105 | -1.470382162 |
| O | 1.856763699 | -0.26157136 | 1.042427847 |
| H | 0.98591751 | 0.152463629 | 1.238563574 |
| H | 2.367505191 | -0.177851611 | 1.857975799 |
| O | -1.830542121 | -1.687261999 | 0.316873452 |
| H | -2.616237631 | -2.03688297 | -0.12128769 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.072132155 | -2.030232413 | -0.192391151 |
| O | -1.144335665 | 3.014179588 | -0.389633601 |
| H | -0.539915466 | 2.908703538 | -1.149173507 |
| H | -1.02827894 | 3.930183616 | -0.105181218 |
| O | -0.692730828 | 0.748731815 | 1.350091451 |
| H | -1.27104128 | 0.037606694 | 1.019986616 |
| H | -0.906796922 | 1.523791919 | 0.798981944 |

w7-1_80

21

| | | | |
|---|--------------|--------------|--------------|
| O | 2.481108659 | -0.041791943 | 0.678241037 |
| H | 1.80852804 | 0.556226866 | 1.07242488 |
| H | 3.177583523 | -0.121195967 | 1.342946635 |
| O | -1.660714451 | 0.339180699 | 2.944923789 |
| H | -1.626087386 | 0.357901843 | 3.910372405 |
| H | -1.59469962 | -0.607364134 | 2.711975153 |
| O | 0.259697354 | -1.741627167 | -0.341941045 |
| H | 1.091785183 | -1.392922772 | 0.022327052 |
| H | -0.100767606 | -0.973814216 | -0.817965618 |
| O | 0.332793356 | 1.607135096 | 1.282828966 |
| H | -0.075868089 | 1.564389397 | 0.400840917 |
| H | -0.348650225 | 1.243783934 | 1.879503302 |
| O | -1.25808088 | -2.324954781 | 1.99879787 |
| H | -1.948650305 | -2.968016903 | 1.791897767 |
| H | -0.775922822 | -2.198674532 | 1.156803766 |
| O | 2.47404103 | 1.037577033 | -1.992603452 |
| H | 2.901579132 | 0.432008863 | -2.613457619 |
| H | 2.68402461 | 0.672173215 | -1.112121348 |
| O | -0.313709545 | 0.961564282 | -1.509615801 |
| H | 0.5804934 | 1.089796823 | -1.884400349 |
| H | -0.919103355 | 1.380854366 | -2.134998304 |

w7-33_40

21

| | | | |
|---|--------------|--------------|--------------|
| O | -0.402794793 | 3.236302091 | 1.697158111 |
| H | 0.357348662 | 2.712429542 | 1.368528181 |
| H | -0.159043375 | 3.480452898 | 2.59956195 |
| O | 2.453463839 | 1.821134583 | -2.038418185 |
| H | 3.309924152 | 1.468955271 | -2.31548423 |
| H | 1.801986354 | 1.203616109 | -2.423009603 |
| O | -0.711735479 | -3.017476043 | 1.14548714 |
| H | 0.105756847 | -3.164218831 | 1.642826988 |
| H | -1.414879992 | -3.227059906 | 1.776576697 |
| O | 0.412706268 | -0.071235983 | -2.773832338 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.068652055 | -0.23357352 | -1.940016959 |
| H | -0.278749525 | 0.062481078 | -3.435103501 |
| O | -2.500041758 | 1.462874987 | 0.973430179 |
| H | -3.142992249 | 1.954541987 | 0.445333911 |
| H | -1.868858447 | 2.142966722 | 1.284153179 |
| O | 1.50282151 | 1.408225637 | 0.697866528 |
| H | 0.882927153 | 0.694791645 | 0.461006636 |
| H | 1.932324664 | 1.62289053 | -0.150907017 |
| O | -0.647663186 | -0.396444682 | -0.137553633 |
| H | -1.372950299 | 0.159951837 | 0.20643725 |
| H | -0.763038293 | -1.267625951 | 0.280308716 |

w7-35_60

21

| | | | |
|---|--------------|--------------|--------------|
| O | 0.240677944 | -0.518798197 | 2.719373569 |
| H | -0.274309687 | 0.236981868 | 3.058773935 |
| H | 0.966898443 | -0.098581734 | 2.226172734 |
| O | -1.421754643 | 1.794529847 | 3.203140384 |
| H | -1.394096986 | 2.490407647 | 3.872613398 |
| H | -1.123685314 | 2.224643429 | 2.376472617 |
| O | -1.873043286 | 0.586996753 | -0.958053553 |
| H | -1.940745632 | -0.178068621 | -0.356696941 |
| H | -2.778709786 | 0.765663775 | -1.244820852 |
| O | -0.397186284 | 2.56478323 | 0.661739021 |
| H | 0.480977234 | 2.146370072 | 0.645509694 |
| H | -0.92161719 | 2.005585839 | 0.060802511 |
| O | 1.983739905 | 0.77364658 | 0.720046998 |
| H | 2.936374051 | 0.917714563 | 0.646422516 |
| H | 1.744708392 | 0.214997995 | -0.048223055 |
| O | -1.212501783 | -1.700449416 | 0.659162559 |
| H | -1.643653484 | -2.521308061 | 0.930550532 |
| H | -0.770681256 | -1.361296192 | 1.468593396 |
| O | 0.797794112 | -0.810251219 | -1.295288795 |
| H | 0.127437842 | -0.23632778 | -1.700032146 |
| H | 0.25264741 | -1.389380378 | -0.733738522 |

w7-40_40

21

| | | | |
|---|--------------|--------------|-------------|
| O | -0.607422597 | 1.294363849 | 3.713617296 |
| H | -1.005989641 | 1.91879677 | 4.333633407 |
| H | 0.056968339 | 1.819695518 | 3.224580312 |
| O | -1.754148896 | -0.254152737 | 1.636624848 |
| H | -1.518006344 | 0.244708839 | 2.444326885 |
| H | -2.72015192 | -0.266609947 | 1.619904088 |

| | | | |
|---|--------------|--------------|--------------|
| O | -0.659370874 | -2.321890643 | -2.265878584 |
| H | -0.352139345 | -2.385335978 | -1.339040994 |
| H | -0.293646763 | -3.105177691 | -2.697709699 |
| O | 0.077973337 | 0.383971122 | -2.855432598 |
| H | -0.196981117 | -0.552311191 | -2.80673403 |
| H | -0.536432052 | 0.791158472 | -3.47995277 |
| O | 0.301229227 | -2.105988721 | 0.417185866 |
| H | -0.43605207 | -1.881626986 | 1.009241767 |
| H | 0.713918116 | -1.234452179 | 0.287177387 |
| O | 1.24026902 | 2.623066026 | 1.992189969 |
| H | 1.053847881 | 2.132724473 | 1.167819631 |
| H | 2.189832855 | 2.506667848 | 2.131568667 |
| O | 0.343113143 | 0.868439876 | -0.042587961 |
| H | -0.532731105 | 0.625972766 | 0.306673102 |
| H | 0.235430806 | 0.868010513 | -1.01229659 |

w7-40_80

21

| | | | |
|---|--------------|--------------|--------------|
| O | 2.310453465 | 1.923735378 | 2.047511913 |
| H | 2.780071136 | 1.154885674 | 1.676732949 |
| H | 1.64599058 | 2.11177631 | 1.363585777 |
| O | -0.08059753 | 1.53027615 | 3.58489637 |
| H | -0.182967036 | 2.096619204 | 4.360889982 |
| H | 0.856547817 | 1.626026788 | 3.325728389 |
| O | 3.208926469 | -0.39676935 | 0.48710709 |
| H | 2.36892178 | -0.683767111 | 0.083841663 |
| H | 3.684732417 | -1.215106502 | 0.67875599 |
| O | -0.48056055 | 1.399923854 | -2.179209216 |
| H | -0.630475738 | 1.841617141 | -1.324335821 |
| H | 0.004045289 | 2.048991787 | -2.706993135 |
| O | -0.396033713 | 1.651582435 | 0.678078084 |
| H | -0.14651615 | 0.7177976 | 0.55500275 |
| H | -0.623720684 | 1.718031202 | 1.621238114 |
| O | -1.125656712 | -3.12973317 | -0.269255378 |
| H | -1.743990666 | -3.452786762 | -0.93976923 |
| H | -1.669908955 | -3.020133505 | 0.523804571 |
| O | 0.552455379 | -0.770528038 | -0.583808426 |
| H | -0.003496144 | -1.568564867 | -0.612125573 |
| H | 0.292199546 | -0.237514219 | -1.357136864 |

w7-47_80

21

| | | | |
|---|--------------|--------------|--------------|
| O | -2.919796935 | -1.322022861 | -1.035034515 |
| H | -2.280960085 | -1.328999798 | -0.299420684 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.516839354 | -2.059180616 | -0.852490325 |
| O | 1.858640881 | 1.481125293 | 2.516444849 |
| H | 2.717709729 | 1.873706178 | 2.312741759 |
| H | 1.26209433 | 1.812007863 | 1.820261299 |
| O | 0.029565557 | 2.092352659 | -2.19647967 |
| H | -0.093126539 | 1.143460358 | -2.407400447 |
| H | 0.758035978 | 2.38150892 | -2.760939931 |
| O | 1.327174367 | -1.349257426 | 2.671580554 |
| H | 1.611105274 | -0.417426196 | 2.73424659 |
| H | 1.094784793 | -1.59482538 | 3.577023627 |
| O | -0.220836967 | 2.089698255 | 0.597369897 |
| H | -0.948493198 | 2.68058229 | 0.83393286 |
| H | -0.102291625 | 2.209541192 | -0.367395945 |
| O | -0.327607616 | -0.701136529 | -2.394091226 |
| H | -1.26708712 | -0.948687617 | -2.427911133 |
| H | -0.105724481 | -0.919113054 | -1.471228448 |
| O | -0.547372483 | -0.822955051 | 0.528085176 |
| H | 0.01162415 | -1.158289611 | 1.252590572 |
| H | -0.529008655 | 0.143451133 | 0.64833514 |

w7-56_40

21

| | | | |
|---|--------------|--------------|--------------|
| O | -2.415662676 | 1.42677242 | 1.901444529 |
| H | -2.0539014 | 2.282002584 | 2.169917307 |
| H | -1.935849292 | 0.774041398 | 2.447854094 |
| O | -1.036153925 | -0.638762434 | 3.309751877 |
| H | -0.755867059 | -0.613723949 | 4.233840922 |
| H | -0.294942645 | -1.063555174 | 2.835922056 |
| O | -0.484730859 | -0.943710568 | -3.728470978 |
| H | -0.223776045 | -1.607239916 | -4.380606115 |
| H | -0.159174004 | -1.285089623 | -2.87703183 |
| O | 0.401689677 | 1.61386159 | -2.431607719 |
| H | -0.446681587 | 1.674121564 | -1.961389333 |
| H | 0.184018424 | 1.031237838 | -3.178984175 |
| O | 1.065797963 | -1.814657542 | 1.757563944 |
| H | 0.912653644 | -1.55618151 | 0.827521943 |
| H | 1.169289409 | -2.775106826 | 1.726381384 |
| O | -2.003847938 | 0.679234529 | -0.783410326 |
| H | -2.837660426 | 0.458725114 | -1.220026237 |
| H | -2.251434804 | 0.968152552 | 0.118267812 |
| O | 0.359293788 | -0.950699357 | -0.881747866 |
| H | 0.842208751 | -0.169202079 | -1.205913777 |
| H | -0.528888996 | -0.570520607 | -0.735757512 |

w7-67_25

21

| | | | |
|---|--------------|--------------|--------------|
| O | -3.403838319 | 1.312750393 | 0.463513892 |
| H | -3.946017816 | 1.994183818 | 0.882289295 |
| H | -2.898187092 | 1.781484768 | -0.232146609 |
| O | -3.862361005 | -1.578145053 | 0.32324819 |
| H | -3.948411906 | -0.625697633 | 0.143435532 |
| H | -4.23337917 | -2.013983107 | -0.455288539 |
| O | 1.041686681 | -0.389741689 | 3.02545802 |
| H | 0.847903502 | -0.172167776 | 3.946537467 |
| H | 0.16773551 | -0.500548472 | 2.607785154 |
| O | -1.327094898 | -0.541103056 | 1.402365436 |
| H | -1.90286141 | -1.285032339 | 1.15791631 |
| H | -1.936937061 | 0.215078729 | 1.338014355 |
| O | -1.643810628 | 2.441817513 | -1.413190167 |
| H | -0.848789737 | 1.892853318 | -1.248076589 |
| H | -1.739848047 | 2.44880258 | -2.374471896 |
| O | 2.565882761 | 1.135339205 | 1.10896792 |
| H | 2.162839879 | 0.64530416 | 1.850927285 |
| H | 3.412972132 | 0.692958283 | 0.96267635 |
| O | 0.358889015 | 0.59640715 | -0.730861135 |
| H | -0.132546009 | 0.048492642 | -0.093679993 |
| H | 1.164083617 | 0.843066565 | -0.239320276 |

w7-6_40

21

| | | | |
|---|--------------|--------------|--------------|
| O | 2.268017604 | -2.20207442 | 0.35994838 |
| H | 2.237305066 | -3.168151447 | 0.377463329 |
| H | 2.284492524 | -1.975430438 | -0.590076821 |
| O | 0.030330514 | 1.892051077 | 2.273913662 |
| H | -0.033080611 | 2.438017377 | 1.467955822 |
| H | 0.743164037 | 2.293593972 | 2.788074816 |
| O | -0.31699462 | 3.047140462 | -0.350600893 |
| H | -0.265486471 | 2.289274439 | -0.963078131 |
| H | -0.031876131 | 3.811976845 | -0.866396898 |
| O | -2.386881448 | -1.234469566 | -0.653117103 |
| H | -3.27478131 | -1.309230775 | -0.279855583 |
| H | -1.796866633 | -1.168011068 | 0.118141912 |
| O | 2.028148883 | -1.284935522 | -2.359795301 |
| H | 1.293093971 | -0.644937299 | -2.302776799 |
| H | 2.722431309 | -0.82106041 | -2.846013372 |
| O | -0.038890024 | -0.636562068 | 0.959946934 |
| H | 0.766542641 | -1.186392156 | 0.980248405 |
| H | 0.102519873 | 0.101050484 | 1.582187865 |
| O | -0.155586624 | 0.467988156 | -1.642372827 |

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|---|--------------|-------------|--------------|
| H | -0.047230107 | 0.119607985 | -0.732283605 |
| H | -1.033902444 | 0.121094371 | -1.873963792 |

w7-72_80

21

| | | | |
|---|--------------|--------------|--------------|
| O | 2.427161919 | -2.241078707 | 0.952265938 |
| H | 1.980002269 | -2.182456876 | 1.821198762 |
| H | 3.154139939 | -2.863528364 | 1.085431787 |
| O | -2.329189033 | 1.351152218 | -0.252250633 |
| H | -1.569200614 | 1.615683347 | -0.805463152 |
| H | -2.704857062 | 2.18209016 | 0.067051422 |
| O | 1.603784363 | 0.620586274 | 0.443734078 |
| H | 0.780080307 | 0.226799444 | 0.789693484 |
| H | 2.214762826 | -0.133279541 | 0.451695953 |
| O | 0.123387394 | 1.671898468 | -1.737974945 |
| H | 0.521619846 | 2.433983494 | -2.178031479 |
| H | 0.795715751 | 1.372667755 | -1.094762389 |
| O | 0.734794864 | -1.839220597 | 3.201930651 |
| H | 0.952241251 | -1.249200505 | 3.936275494 |
| H | 0.01465705 | -1.382091899 | 2.728473474 |
| O | -0.001198347 | -2.754940821 | -0.582419489 |
| H | 0.080335093 | -2.495166665 | -1.510784638 |
| H | 0.904754613 | -2.684217759 | -0.228440627 |
| O | -0.893115109 | -0.681934745 | 1.177417934 |
| H | -0.833302906 | -1.386030434 | 0.503781214 |
| H | -1.549784414 | -0.050194248 | 0.83187716 |

w7-76_40

21

| | | | |
|---|--------------|--------------|--------------|
| O | -3.042722143 | 1.763004052 | -1.712936016 |
| H | -2.154375739 | 1.604658081 | -2.087011452 |
| H | -3.292433036 | 2.640328723 | -2.031791397 |
| O | 2.93554631 | -1.943600983 | 2.104413363 |
| H | 2.196799809 | -2.305534595 | 1.57742972 |
| H | 3.722312357 | -2.391126071 | 1.766563507 |
| O | 0.558171298 | -2.526710888 | 0.617136802 |
| H | 0.42693207 | -2.986303693 | -0.222590914 |
| H | 0.282896131 | -1.60509335 | 0.440975513 |
| O | -2.523733282 | 1.181368582 | 1.037209691 |
| H | -3.165795768 | 0.53565644 | 1.361825346 |
| H | -2.837029429 | 1.411567479 | 0.140472656 |
| O | -0.35170798 | 1.017266287 | -2.37501213 |
| H | 0.365500882 | 1.528806686 | -2.771645104 |
| H | -0.039419598 | 0.807141702 | -1.472554373 |

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|---|--------------|--------------|-------------|
| O | 2.446055503 | 0.851054907 | 1.781427882 |
| H | 2.473503489 | 1.296022188 | 2.638908797 |
| H | 2.725163145 | -0.066459873 | 1.970380107 |
| O | 0.069534177 | 0.268208393 | 0.332715491 |
| H | 0.794788727 | 0.609394586 | 0.891019692 |
| H | -0.761236925 | 0.600281341 | 0.72557282 |

w7-86_60

21

| | | | |
|---|--------------|--------------|--------------|
| O | 1.732964438 | 0.855578169 | 2.437141543 |
| H | 1.238601485 | 0.015654476 | 2.374621025 |
| H | 1.125077421 | 1.462915049 | 2.880646963 |
| O | -1.495418961 | 0.510534172 | 0.162062095 |
| H | -0.793329891 | -0.098978975 | -0.127714494 |
| H | -1.720152336 | 0.197949134 | 1.048717739 |
| O | -0.123823043 | 2.350113534 | -1.656597826 |
| H | 0.745003556 | 2.249378913 | -1.23109532 |
| H | -0.734332588 | 2.031916938 | -0.969235236 |
| O | 2.35526056 | 1.346777575 | -0.279433603 |
| H | 3.287398407 | 1.555708072 | -0.426124634 |
| H | 2.250908677 | 1.296560926 | 0.692165997 |
| O | 0.340124399 | -1.617571564 | 1.900196035 |
| H | 0.510678864 | -1.724960856 | 0.946536787 |
| H | 0.595305832 | -2.461534668 | 2.296351774 |
| O | -0.021677118 | 0.01955364 | -3.352961662 |
| H | -0.753326686 | -0.069135007 | -3.977357573 |
| H | -0.160125892 | 0.886354475 | -2.921854209 |
| O | 0.828901919 | -1.053911511 | -0.831690703 |
| H | 1.481313198 | -0.332713105 | -0.769089096 |
| H | 0.52585776 | -1.002449386 | -1.756365602 |

w7-92_60

21

| | | | |
|---|--------------|--------------|--------------|
| O | 1.740597281 | 1.680156251 | 2.670524846 |
| H | 1.565489224 | 2.363187059 | 2.001528281 |
| H | 1.139342398 | 1.878965866 | 3.399862871 |
| O | -3.729392857 | -0.664400531 | -1.703888003 |
| H | -4.518970538 | -0.192563079 | -2.000618756 |
| H | -3.038070193 | -0.420564501 | -2.350430964 |
| O | -1.467718395 | 0.142483414 | -3.253048655 |
| H | -0.862695995 | 0.379352208 | -2.522658789 |
| H | -0.959507905 | -0.467676095 | -3.804005146 |
| O | 1.787690567 | 2.883393096 | -0.012401064 |
| H | 2.258350586 | 3.621456737 | -0.421323949 |

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|---|--------------|--------------|--------------|
| H | 2.392646065 | 2.116872249 | -0.072366725 |
| O | 2.689453664 | 0.21454193 | 0.26746548 |
| H | 1.810401251 | 0.008840304 | -0.097553547 |
| H | 2.517362878 | 0.287077835 | 1.221679606 |
| O | -2.321065375 | 0.007683421 | 0.685090943 |
| H | -2.916536629 | -0.261320822 | -0.042277926 |
| H | -2.284894628 | -0.762695456 | 1.267929965 |
| O | -0.032739263 | 0.719090943 | -0.848611422 |
| H | 0.271851559 | 1.619800045 | -0.646075031 |
| H | -0.766733693 | 0.545799124 | -0.226192018 |

w7-95_40

21

| | | | |
|---|--------------|--------------|--------------|
| O | -1.6691687 | 1.130177588 | -2.24909164 |
| H | -1.989036723 | 0.673516241 | -1.449347544 |
| H | -2.222357765 | 0.789897748 | -2.964456762 |
| O | -0.899956422 | 0.240174961 | 2.801838813 |
| H | -0.112257137 | 0.221979363 | 2.22688437 |
| H | -0.683271359 | 0.864426135 | 3.506904608 |
| O | -1.006395394 | -2.605748517 | 1.287587208 |
| H | -1.124895675 | -2.339350469 | 2.212357302 |
| H | -0.169962088 | -2.169974477 | 1.047604047 |
| O | -2.305135018 | -0.187043156 | 0.207249209 |
| H | -2.204280481 | 0.248589607 | 1.069830328 |
| H | -2.106462449 | -1.116794168 | 0.422586999 |
| O | 2.84319534 | 0.75104074 | -1.015198774 |
| H | 2.312066947 | 1.2220215 | -1.686712811 |
| H | 3.446311879 | 0.195004449 | -1.526377537 |
| O | 1.003941501 | 2.046022305 | -2.771361693 |
| H | 0.945249227 | 3.01060127 | -2.783828804 |
| H | 0.090295505 | 1.750018331 | -2.59952362 |
| O | 0.704572051 | -0.348850629 | 0.527511803 |
| H | -0.053752893 | -0.095934643 | -0.023032498 |
| H | 1.486629654 | -0.027954174 | 0.039106994 |

w7-97_25

21

| | | | |
|---|--------------|--------------|--------------|
| O | -0.163385513 | 3.350291467 | -0.43915292 |
| H | 0.443998868 | 2.601936964 | -0.585656008 |
| H | 0.416924098 | 4.108122666 | -0.288459124 |
| O | -1.479481519 | -2.07446365 | -0.954817431 |
| H | -1.538543826 | -2.958961095 | -0.569518457 |
| H | -1.410137986 | -1.473821731 | -0.186907989 |
| O | 1.914669475 | -0.029194946 | 2.000648493 |

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|---|--------------|--------------|--------------|
| H | 0.957392789 | -0.191276896 | 2.066830534 |
| H | 2.308112547 | -0.483015312 | 2.756362384 |
| O | 0.79810743 | -1.237150472 | -2.499594378 |
| H | 0.555997462 | -1.116983685 | -3.427432796 |
| H | -0.004374456 | -1.603128327 | -2.07914014 |
| O | 1.307058911 | 0.880612931 | -0.658571647 |
| H | 1.913899534 | 0.54990899 | 0.025156124 |
| H | 1.302535878 | 0.205873119 | -1.363966637 |
| O | -2.221436501 | 2.416669735 | 1.352799425 |
| H | -3.085156701 | 2.603415584 | 0.960893426 |
| H | -1.585092158 | 2.867150447 | 0.764346107 |
| O | -0.830948231 | -0.096721163 | 1.008409547 |
| H | -1.442089007 | 0.62833364 | 1.239251354 |
| H | -0.226791094 | 0.320801734 | 0.363770132 |

w7-9_25

21

| | | | |
|---|--------------|--------------|--------------|
| O | 3.033471185 | 1.853655056 | -1.601553471 |
| H | 3.25379475 | 1.782003926 | -2.540164102 |
| H | 2.829194877 | 0.937880799 | -1.329707857 |
| O | 0.490618534 | 3.126802822 | -0.973983177 |
| H | 1.367055732 | 2.791935243 | -1.240941236 |
| H | -0.128935154 | 2.546260709 | -1.452724994 |
| O | 2.288229018 | -0.755715282 | -0.633558461 |
| H | 2.84831671 | -1.099617399 | 0.075309506 |
| H | 1.404873775 | -0.671814995 | -0.225211398 |
| O | -1.913689427 | -2.488068257 | 1.551062542 |
| H | -1.789747896 | -3.348185268 | 1.125681797 |
| H | -2.078352 | -2.699213629 | 2.480610866 |
| O | -0.086091238 | 2.243886852 | 1.636097913 |
| H | 0.532894062 | 2.591520522 | 2.290922572 |
| H | 0.170827437 | 2.676430998 | 0.793795303 |
| O | -1.261515811 | 1.007169503 | -1.965678946 |
| H | -1.097285039 | 0.465073894 | -1.170914711 |
| H | -2.22207659 | 1.110854234 | -1.995615235 |
| O | -0.33244304 | -0.297092652 | 0.443651231 |
| H | -0.283675199 | 0.48628111 | 1.02601194 |
| H | -0.856414685 | -0.962278185 | 0.921139918 |

w8-23_25

24

| | | | |
|---|-------------|--------------|--------------|
| O | 3.3232648 | -1.440686771 | -3.298482569 |
| H | 3.926394097 | -1.838518832 | -3.940582499 |
| H | 3.340777465 | -0.486384731 | -3.489336116 |

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|---|--------------|--------------|--------------|
| O | 2.521242794 | 1.279945862 | -2.809911172 |
| H | 2.736475692 | 1.00381896 | -1.894841653 |
| H | 2.666379403 | 2.234423902 | -2.836775823 |
| O | -2.931917636 | 0.446003355 | 2.108744219 |
| H | -2.237893098 | 1.015245978 | 1.720694689 |
| H | -3.726293904 | 0.658940842 | 1.600808482 |
| O | 0.356205891 | -0.776911341 | -2.965941563 |
| H | 1.091518928 | -1.368633359 | -3.195563855 |
| H | 0.773237636 | 0.097817138 | -3.05100257 |
| O | 3.113226852 | -0.241870375 | -0.519443414 |
| H | 2.232358209 | -0.521608822 | -0.205685697 |
| H | 3.385608265 | -0.964714252 | -1.107847001 |
| O | -1.420427924 | -1.951222779 | 1.725563083 |
| H | -2.075092521 | -1.257352159 | 1.932404424 |
| H | -1.820486728 | -2.782230641 | 2.009082176 |
| O | -0.712011961 | 1.785701414 | 0.890004985 |
| H | -0.276181983 | 1.002559714 | 0.498196077 |
| H | -0.040107941 | 2.172842823 | 1.467424641 |
| O | 0.3138713 | -0.684331222 | -0.116968812 |
| H | -0.250382088 | -1.296382478 | 0.390044538 |
| H | 0.133964453 | -0.852172227 | -1.06199457 |

w9-66_25

27

| | | | |
|---|--------------|--------------|--------------|
| O | 2.49921747 | 0.234719651 | 2.989872184 |
| H | 3.366201091 | 0.237719702 | 3.416984827 |
| H | 2.544169917 | 0.939533005 | 2.309466384 |
| O | -0.9809234 | -0.290911929 | 1.334345217 |
| H | -1.900165863 | -0.245174087 | 1.009956264 |
| H | -0.939652778 | 0.240286493 | 2.1504203 |
| O | -0.14683138 | 1.160977843 | 3.664223661 |
| H | -0.493536591 | 0.995779298 | 4.551326262 |
| H | 0.766358943 | 0.819418184 | 3.685581577 |
| O | -3.403412694 | -0.028449914 | -0.128400448 |
| H | -3.924443765 | -0.78584558 | -0.426676041 |
| H | -3.001737557 | 0.330433563 | -0.943694293 |
| O | 1.358760861 | -2.056674453 | 1.493077568 |
| H | 0.453337189 | -1.699800189 | 1.474063908 |
| H | 1.829296083 | -1.412170139 | 2.050972968 |
| O | 2.153413147 | 2.277714633 | 1.096301069 |
| H | 1.539916536 | 2.91895186 | 1.482395879 |
| H | 1.647095719 | 1.880253075 | 0.360274631 |
| O | -1.876388092 | 0.999492382 | -2.32938384 |
| H | -1.99154888 | 1.871317838 | -2.729731736 |
| H | -0.977604283 | 1.017062193 | -1.945345801 |

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|---|-------------|--------------|--------------|
| O | 2.317866734 | -1.41215387 | -1.110547204 |
| H | 2.054507492 | -1.801088471 | -0.251919799 |
| H | 2.303634746 | -2.149183696 | -1.73504449 |
| O | 0.538011687 | 0.811286329 | -0.797929087 |
| H | 1.137085544 | 0.092756201 | -1.081652717 |
| H | 0.034652123 | 0.40877008 | -0.060607238 |

w10-10_80

30

| | | | |
|---|--------------|--------------|--------------|
| O | 2.522998298 | 2.858228189 | 1.064143573 |
| H | 2.421247272 | 2.108675925 | 0.446706542 |
| H | 2.997171907 | 3.531476821 | 0.559329945 |
| O | 0.510196018 | 2.957927459 | 3.098729788 |
| H | 1.191380209 | 3.083325497 | 2.410681942 |
| H | -0.02815007 | 3.759508889 | 3.062495201 |
| O | 2.041055888 | -1.263541413 | 1.71556991 |
| H | 2.390699507 | -0.747748298 | 0.963547961 |
| H | 2.800600678 | -1.4341578 | 2.288305732 |
| O | 2.661130743 | 0.604667414 | -3.315348895 |
| H | 1.70281731 | 0.621295042 | -3.498738824 |
| H | 2.994295278 | -0.130583349 | -3.847454013 |
| O | -1.791854206 | -2.043529079 | 2.885900733 |
| H | -2.737665045 | -1.996268692 | 3.076855894 |
| H | -1.494429018 | -1.115630366 | 2.845842923 |
| O | -0.342092281 | 0.349214419 | 2.266988986 |
| H | -0.147924531 | 1.226725254 | 2.646801932 |
| H | 0.519325523 | -0.107205428 | 2.253291042 |
| O | 2.175895117 | 0.473480777 | -0.489173318 |
| H | 1.225184632 | 0.277464484 | -0.60624924 |
| H | 2.523413968 | 0.463724615 | -1.400977317 |
| O | -0.223668268 | -2.803767502 | 0.524611676 |
| H | 0.630754549 | -2.58608854 | 0.934707279 |
| H | -0.840246159 | -2.771427011 | 1.278930447 |
| O | -0.216060343 | 0.552235772 | -3.317533638 |
| H | -0.970533352 | 0.923328608 | -3.791944091 |
| H | -0.548554725 | 0.3527253 | -2.424126665 |
| O | -0.614616777 | -0.188192984 | -0.569809213 |
| H | -0.583711823 | -1.141209093 | -0.347468489 |
| H | -0.770160299 | 0.220445091 | 0.301042197 |