An improved generalized AMBER force field (GAFF) for urea

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Abstract: We describe an improved force field parameter set for urea for the Generalized Amber Force Field (GAFF) force field. Quantum chemical computations were used to obtain geometrical and energetic parameters of urea dimers and larger oligomers using AM1 semiempirical MO theory, density functional theory at the B3LYP/6-31G(d,p) level, MP2 and CCSD ab initio calculations with the 6-311++G(d,p), aug-cc-pVDZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets and with the CBS-QB3 and CBS-APNO complete basis set methods. Seven different urea dimer structures were optimized at the MP2/aug-cc-pVDZ level to obtain accurate interaction energies. Atomic partial charges were calculated at the MP2/aug-cc-pVDZ level with the restrained electrostatic potential (RESP) fitting approach. The interaction energies computed with these new RESP charges in the force field are consistent with those obtained from CCSD and MP2 calculations. The linear dimer structure calculated using the force field with modified geometrical parameters and the new RESP charge set agrees well with available experimental data.

Response to Reviewers: We have added a sentence to emphasise the importance of the fact that urea's carbonyl oxygen can accept four hydrogen bonds and have cited Margaret Etter's Acc. Chem. Res. article.

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Abstract

We describe an improved force field parameter set for urea for the Generalized Amber Force Field (GAFF) force field. Quantum chemical computations were used to obtain geometrical and energetic parameters of urea dimers and larger oligomers using AM1 semiempirical MO theory, density functional theory at the B3LYP/6-31G(d,p) level, MP2 and CCSD *ab initio* calculations with the 6-311++G(d,p), aug-cc-pVDZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets and with the CBS-QB3 and CBS-APNO complete basis set methods. Seven different urea dimer structures were optimized at the MP2/aug-cc-pVDZ level to obtain accurate interaction energies. Atomic partial charges were calculated at the MP2/aug-cc-pVDZ level with the restrained electrostatic potential (RESP) fitting approach. The interaction energies computed with these new RESP charges in the force field are consistent with those obtained from CCSD and MP2 calculations. The linear dimer structure calculated using the force field with modified geometrical parameters and the new RESP charge set agrees well with available experimental data.

Keywords GAFF · Force Field Parameters · Urea · Urea Dimers · Urea crystal

Introduction

Urea and substituted ureas are an important class of organic molecules since they are used in many areas such as the agricultural, pharmaceutical, chemical, and medical industries. Urea has been used as a powerful protein denaturant, stabilizer in nitrocellulose explosive, cloud-seeding agent, flame-proofing agent, and nitrogen source [1]. Its interesting non-linear optical properties [2], ability to form clathrates [3] and transition-metal complexes [4], and the relative simplicity of its crystal structure make urea one of the most interesting crystalline materials. X-ray and neutron diffraction studies of its crystal structure have been performed by several authors [5-13]. These early studies agreed on the space group, unit cell, and that its oxygen atom accepts four hydrogen bonds N-H…O in the crystal structure. Fig. 1 shows the unit cell structure of crystalline urea.

<Figure 1>

There have been many theoretical studies of the electronic [14-19] and energetic [20, 21] properties of urea. Molecular dynamics simulations [22-25] of its interactions with water and organic molecules have also been used in order to understand the growth of urea crystals from aqueous solution. However, the reported data on interactions and hydrogen bond formation differ significantly because of the different empirical force fields used [26, 27], which emphasizes the importance of an accurate and consistent set of parameters for urea. This is important because urea is quite unusual in that it contains four hydrogen-bond donors and that its carbonyl oxygen accepts four hydrogen bonds in the crystal structure. Etter [28] reviewed hydrogen-bond patterns of organic compounds, especially ureas, and was able to establish rules for hydrogen bonding in crystals, co-crystals and clathrates. Hence, in this work, we present a refined force field based on the generalized AMBER force field [29] (GAFF). Geometrical parameters were produced for urea systems using semiempirical, density functional and high level *ab initio* calculations. Since an accurate description of urea dimer formation is essential in order to be able to describe urea nucleation, aggregation and behavior as a clathrate host, we have investigated the structures and energies of different urea oligomers. In order to fit urea-urea interactions obtained from high level *ab initio* calculations, we have generated a set of charges for each dimer and compared the interaction energies after energy minimization with force fields using these charge sets.

Computational methods

Semiempirical computations were carried out using the VAMP 10.0 [30] program and all other calculations were performed using the Gaussian 03 [31] suite of programs. The geometry optimizations of the urea monomer were performed with CCSD [32-34], CCSD(T), MP2 [35], B3LYP [36, 37], AM1 [38] and complete basis set [39-41] (CBS) methods. The aug-cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ [42-46], 6–311++G(d,p) [47-49], and 6–31G(d,p) [50, 51] basis sets were used. Urea clusters were built by repeating the unit cell in the A, B, and C directions. For the cluster optimizations, AM1 and B3LYP/6–31G(d,p) were chosen as compromises between accuracy and computational cost.

The different urea dimer structures were optimized at the MP2/aug-cc-pVDZ level and frequency calculations at the same level were carried out within the harmonic approximation to characterize the dimeric stationary points. The counterpoise (CP) correction method of Boys and Bernardi [52] was used in order to correct for basis set superposition error (BSSE) in the dimers. Single-point calculations at the MP2/aug-cc-pVTZ and CCSD/aug-cc-pVDZ levels were also performed.

The AMBER [53] program was used for energy minimizations with GAFF and the modified force field. Atom types were assigned using the default GAFF parameters. A set of restrained electrostatic potential (RESP) atomic charges [54] were calculated at the MP2/aug-cc-pVDZ level using Gaussian 03. The RESP charges for hydrogen atoms on the NH_2 groups were constrained to be equal. The fitting procedure was performed using the single-conformation, two-stage RESP fitting approach. Dimer geometries were optimized with 1,000 steps of steepest-descent minimization.

Results

Urea monomer

The urea molecule exhibits C_{2v} symmetry in the solid state. Therefore, the experimental values for its geometrical parameters in the literature refer to the C_{2v} structure. However, the most stable conformation in gas phase has C_2 symmetry. Microwave spectra [55] of urea have confirmed that the hydrogen atoms bonded each nitrogen atom are located in *anti-*

configurations to each other in the gas phase. Fig. 2 shows the calculated potential energy surface of urea. Relative energies for the urea conformers are listed in Table 1, which shows that the stabilities of urea conformers depend strongly on the computational method used. Increasing the size of the basis set decreases the relative energy of the C_{2v} structure by 0.2 – 1.1 kcal mol^{-1}. Interestingly, AM1 gives relative energies very close to those obtained with CCSD/aug-cc-pVDZ and CCSD(T)/aug-cc-pVDZ.

< Table 1 here>

< Figure 2 here>

Geometrical parameters of the two urea conformers are shown in Table 2. The change of symmetry from C_2 to C_{2v} causes the C-N and N-H bonds to shorten and the C=O bond to lengthen. The N-C-N, H-N-C, and H-N-H bond angles increase and the N-C-O bond angle narrows. Remarkably, the AM1-calculated C=O bond length and N-C-N bond angle agree best with experiment. All methods overestimate the C-N bond length. The H-N bond lengths are shorter than those of Andrew *et al*. [8], but the AM1 bond length is close to the experimental one published by Worsham *et al*. [7] The H_5-N-C bond angles are underestimated and the H_4-N-C bond angles overestimated by all the methods investigated. In the existing GAFF parameters [29], the C-N bond length and the H-C-N bond angle agree with the experimental data and the C=O distance is consistent with the data obtained from high level calculations. However, the N-C-N angle is quiet narrow compared to both the experimental and high level theoretical values. In an alternative force field parameter set generated by Cornell *et al*. [57], the C=O distance is close to the AM1 and experimental values and the C-N distance agrees with those obtained from the computations with CCSD/aug-cc-pVDZ and MP2/aug-cc-pVDZ. Generally, the bond angles in this parameterization agree better with the experimental data than either the original GAFF force field or our quantum mechanically calculated values.

<Table 2 here>

The experimental dipole moment of urea has been estimated to be 3.83 D [55] in the gas phase, 4.2 D [58] in aqueous solution and 4.66 D [59] in the solid state. Fig. 3 shows comparisons of computed urea dipole moments with experimental data. The AM1 and B3LYP dipole moments for the C_{2v} structure are very close to the experimental one found in solution.

The CCSD/aug-cc-pvtz and CBS-APNO methods agree best with the experimental value in the solid state.

<Figure 3 here>

Urea dimers

In order to be able to describe the formation of the urea dimer correctly, we have optimized seven different urea dimer structures at the MP2/aug-cc-pVDZ level. The optimized geometries are shown in Fig. 4. **D1** is the linear "head-to-tail" dimer found in the crystal structure and **D6** is cyclic dimer that is most stable in the gas phase. The C=O bond distance lengthens from 1.23 to 1.24 Å because of C=O…N-H hydrogen bonding, whereas the C-N single bond shortens from 1.39 to 1.37 Å, in agreement with experiment. Relative energies are listed in Table 3.

<Figure 4 here>

<Table 3 here>

All methods agree on the stability order **D6**>**D3**≈**D7**>**D5**~**D2**>**D1**>**D4**. The BSSE correction does not affect the relative MP2/aug-cc-pVDZ energies significantly, as might be expected for urea, which is relatively polar [60-62].

Urea oligomers

In order to see how the bond distances change as the number of urea molecules increases, we built urea clusters containing up to 160 urea molecules and optimized their geometries with AM1 and at the B3LYP/6-31G(d,p) level. The optimized urea clusters are shown in Figs. 5 and 6. As the number of molecules in the cluster increases, the length of the single bond C-N shortens and the C=O double bond lengthens (Table 4) because of the hydrogen bonding. This explains the differences between the bond distances and angles calculated experimentally and theoretically. As the size of the system increases, AM1 begins to overestimate the C=O and C-N distances. However, B3LYP gives more reasonable values for these distances. The N-H bond distances did not change on increasing the size of the clusters. The deviations of the mean C-N and C=O bond lengths from the experimental values are +0.046 and +0.020 Å, respectively, for AM1 (160 molecules) and +0.020 and +0.001 Å for B3LYP (24 molecules).

The O-C-N bond angle shrinks and the N-C-N, C-N-H and H-N-H bond angles widen as the size of the cluster increases (Table 5).

<Table 4 here>

<Figure 5 here>

<Figure 6 here>

A plot of the calculated binding energies of the urea clusters is shown in Fig. 7. The results can be fitted to the following linear equations to allow us to estimate the lattice energy of the urea crystal at AM1 and B3LYP/6-31G(d,p).

$$E_{AM1} = 35.3 - 11.25n \quad (1)$$

$$E_{B3LYP} = 32.2 - 19.48n \quad (2)$$

The predicted lattice energies (−11.3 and −19.5 kcal mol^{-1} for AM1 and B3LYP/6-31G(d,p), respectively) are smaller than the experimental values (taken here to be minus the sublimation energy) of −20.95 ± 0.21 [63] and −23.6 kcal mol^{-1} [64]. These deviations can be expected because neither AM1 nor B3LYP can reproduce the stabilizing dispersion interaction, although the magnitude of the deviation for AM1 also suggests that it underestimates the strength of the intermolecular hydrogen bonds and Coulomb interactions. The relatively good B3LYP result suggests that dispersion does not play a major role.

<Figure 7 here>

The calculated and experimental lattice constants are listed in Table 6. Swaminathan *et al*. [13] investigated the crystal structure and molecular thermal motion of urea and observed that the lattice parameters, especially the lattice parameter *a*, are change significantly with increasing temperature because of the hydrogen bonding. One can see that AM1 agrees better with experiment for the *c* lattice vector than for the *a* lattice vector. Very satisfactory performance is observed for B3LYP with an acceptable mean deviation.

< Table 6 here>

The force field

The computed RESP charges for each dimer are listed in Table 7. Bertran *et al*. [65] also computed a charge set for non-planar urea that is similar to ours. The OPLS (Optimized Potentials for Liquid Simulations) urea charge set developed by Jorgensen *et al*. [66] and a modification to the OPLS charges by Nilsson *et al*. [27] are also shown.

<Table 7 here>

Interaction energies

The geometry of each urea dimer was optimized using force fields based on each RESP charge set. Dimer stability orders were found to agree with that of the CCSD method. The interaction energies computed using the RESP-**D3** charge set agrees best with the MP2/aug-cc-pVTZ energies (Table 8). Therefore, we used this charge set for the further calculations. Nonbonding interaction parameters from both GAFF and OPLS (Table 9) were tested for energy minimizations of the linear dimer that is found in the crystal structure. Fig. 8 shows the linear dimer geometries obtained and Table 10 shows the parameters used in the energy minimization for each structure.

<Table 8 here>

<Table 9 here>

The linear dimer **a** (Fig. 8) is the geometry obtained from MP2 optimization. The dimer **b** was obtained from energy minimization with unmodified GAFF [29] parameters. The C=O and C-N bond distances are far smaller than the diffraction results (1.243 [7] and 1.335 Å [6]). Changing only the bond and angle parameters to those given by Cornell *et al*. [57] gave structure **c**, in which the bond distances are in a very good agreement with the neutron diffraction results. The deviations from experiment are only 0.012, 0.004, and 0.004 Å for the C=O, C-N, and N-H bonds, respectively. Using the nonbonding interaction parameters from OPLS led to a large change in the hydrogen-bond distances (Fig. 8, **d-f**). The experimental hydrogen bond length [5] varies between 2.014 and 2.071 Å. The GAFF nonbonding parameters underestimate these limits by 0.045 and 0.102 Å whereas OPLS parameters overestimate them seriously (by 2.478 and 2. 421 Å, respectively).

<Table 10 here>

<Fig. 8 here>

We therefore decided to use parameter set **c** for further work. The complete parameter set is defined in Table 11.

<Table 11 here>

The calculated lattice energy for urea using this force field is 23.9 kcal mol^{-1}. This agrees well with the experimental sublimation energies of –20.95 ± 0.21 [64] and –23.6 kcal mol^{-1} [65]. The calculated lattice constants (a = 5.488, c = 4.611, and c/a = 0.8402) tend to be slightly shorter than the experimental values [13] (a = 5.565, c = 4.684, and c/a = 0.8417), but the mean deviations of -1.40 and -1.58 %, respectively, are acceptable considering that the force field was constructed from data for dimers.

Summary and conclusions

We have optimized the force field for urea to reproduce the observed molecular geometries and structures of urea dimers. The resulting force field gives good results for the urea crystal and the force field should thus be well suited for calculations of the nucleation and dissolution of urea crystals and clathrates. We will report such studies using the new force field for molecular-dynamics simulations.

The quantum mechanical calculations show that B3LYP gives a reasonable lattice energy for urea, whereas AM1 underestimates it significantly. The former suggests that dispersion is not very important for crystalline urea.

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Supplementary material

Supplementary material available

References

1. Bonin M, Marshall WG, Weber HP, Tolendo P (1999) Ploymorphysim in urea. IOP Publishing ISIS. http://www.isis.rl.ac.uk/archive/isis99/highlights/urea4.htm. Accessed August 1999
2. Mathews CK, van Holde KE (1996) Biochemistry 2nd edn. Benjamin/Cummings, Menlo Park, CA, p 4
3. Bhatnagar VM (1968) Clathrates of urea nad thiourea. J Struct Chem 8:513-529. doi:10.1007/BF00751656
4. Theophanides T, Harvey PD (1987) Structural and spectroscopic properties of metal-urea complexes. Coord Chem Rev 76:237-264. doi:10.1016/0010-8545(87)85005-1
5. Zavodnik V, Stash A, Tsirelson V, De Vires R, Feil D (1999) Electron density study of urea using TDS-corrected X-ray diffraction data: quantitative comparison of experimental and theoretical results. Acta Crystallogr Sect B 55:45-54. doi:10.1107/S0108768198005746
6. Vaughan P, Donohue J (1952) The structure of urea. Interatomic distances and resonance in urea and related compounds. Acta Crystallogr 5:530-535. doi:10.1107/S0365110X52001477
7. Worsham JE, Levy HA, Peterson SE (1957) The positions of hydrogen atoms in urea by neutron diffraction. Acta Crystallogr 10:319-323. doi:10.1107/S0365110X57000924
8. Andrew ER, Hyndman D (1953) Proton magnetic resonance evidence for the planar structure of the urea molecule. Proc Phys Soc A66:1187-1188. doi:10.1088/0370-1298/66/12/119
9. Wyckoff RWG (1930) Z Kristallogr 75:529-537
10. Hendriks SB (1928) The crystal structure of urea and the molecular symmetry of thiourea. J Am Chem Soc 50:2455-2464. doi:10.1021/ja01396a019
11. Mark H, Weissenberg K (1923) Röntgenographische Bestimmung der Struktur des Harnstoffs und des Zinntetrajodids. Z Phys 16:1-22. doi:10.1007/BF01327372
12. Sklar N, Senko ME, Post B (1961) Thermal effects in urea: the crystal structure at -140°C and at room temperature. Acta Crystallogr 14:716-722. doi:10.1107/S0365110X61002187
13. Swaminathan S, Craven BM (1984) The crystal structure and molecular thermal motion of urea at 12, 60 and 123 K from neutron diffraction. Acta Crystallogr Sect B 40:300-306. doi:10.1107/S0108768184002135

14. Pluta T, Sadlej AJ (2001) Electric properties of urea and thiourea. J Chem Phys 114:136-146. doi:10.1063/1.1328398
15. Alparone A, Millefiori S (2005) Gas and solution phase electronic and vibrational (hyper)polarizabilities in the series formaldehyde, formamide and urea: CCSD(T) and DFT theoretical study. Chem Phys Lett 416:282-288
16. Olah GA, Surya Prakash GK, Rasul G (2008) ^{13}C and ^{15}N NMR and Ab Initio/GIAO-CCSD(T) Study of the Structure of Mono-, Di-, and Triprotonated Guanidine, Urea, and Thiourea. J Phys Chem C 112:7895-7899. doi:10.1021/jp711727c
17. Benková Z, Černušák I, Zahradník P (2007) Electric properties of formaldehyde, thioformaldehyde, urea, formamide, and thioformamide - Post-HF and DFT study. Int J Quantum Chem 107:2133-2152. doi:10.1002/qua.21399
18. Masunov A, Dannenberg JJ (1999) Theoretical Study of Urea. I. Monomers and Dimers. J Phys Chem A 103:178-184. doi:10.1021/jp9835871
19. Spoliti M, Perrone G, Bencivenni L, Pieretti A, Grandi A, Ramondo F (2005) Computational and vibrational spectroscopy study of the microclusters of C_2 symmetry urea molecule in the ^1A electronic ground state. J Mol Struct THEOCHEM 756:113-126. doi:10.1016/j.theochem.2005.07.021
20. Singh A, Chakraborty S, Ganguly B (2007) Computational Study of Urea and Its Homologue Glycinamide: Conformations, Rotational Barriers, and Relative Interactions with Sodium Chloride. Langmuir 23:5406-5411. doi:10.1021/la062405o
21. Civalleri B, Doll K, Zicovich-Wilson CM (2007) Ab initio investigation of structure and cohesive energy of crystalline urea. J Phys Chem B 111:26-33. doi:10.1021/jp065757c
22. Boek ES, Briels WJ (1993) Molecular dynamics simulations of aqueous urea solutions: Study of dimer stability and solution structure, and calculation of the total nitrogen radial distribution function $G_N(r)$. J Chem Phys 98:1422-1427. doi:10.1063/1.464306
23. Astrand PO, Wallqvist A, Karlström G (1994) Molecular dynamics simulations of 2 m aqueous urea solutions. J Phys Chem 98:8224-8233. doi:10.1021/j100084a046
24. Boek ES, Briels WJ, van Eerden J, Feil D (1992) Molecular-dynamics simulations of interfaces between water and crystalline urea. J Chem Phys 96:7010-7018. doi:10.1063/1.462560
25. Liu XY, Boek ES, Briels WJ, Bennema P (1995) Analysis of morphology of crystals based on identification of interfacial structure. J Chem Phys 103:3747-3754. doi:10.1063/1.470053

26. Kallies B (2002) Coupling of solvent and solute dynamics—molecular dynamics simulations of aqueous urea solutions with different intramolecular potentials. Phys Chem Chem Phys 4:86-95. doi:10.1039/b105836n
27. Caballo-Herrera A, Nilsson L (2006) Urea parametrization for molecular dynamics simulations. J Mol Struct THEOCHEM 758:139-148. doi:10.1016/j.theochem.2005.10.018
28. Etter M (1990) Encoding and decoding Hydrogen-Bond Patterns of Organic Compounds. Acc Chem Res 23:120-126. doi 10.1021/ar00172a005
29. Wang J, Wolf RM, Caldwell JW, Kollman PA, Case DA (2004) Development and testing of a general amber force field. J Comput Chem 25:1157-1174. doi:10.1002/jcc.20035
30. Clark T, Alex A, Beck B, Burkhardt F, Chandrasekhar J, Gedeck P, Horn A, Hutter M, Martin B, Rauhut G, Sauer W, Schindler T, Steinke T, Version (2003) VAMP 10.0, Erlangen
31. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA, Jr., Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Gonzalez C, Pople JA (2004) Gaussian 03, Revision D.02. Gaussian, Inc, Wallingford CT
32. Čízek J (1969) In: Lefebre R, Moser C (eds) Correlation Effects in Atoms & Molecules. Advances in chemical physics 14. Interscience, New York, p 35
33. Purvis GD, Bartlett RJ (1982) A full coupled-cluster singles and doubles model: The inclusion of disconnected triples. J Chem Phys 76:1910-1918. doi:10.1063/1.443164
34. Scuseria GE, Janssen CL, Schaefer III HF (1988) An efficient reformulation of the closed-shell coupled cluster single and double excitation (CCSD) equations. J Chem Phys 89:7382-7387. doi:10.1063/1.455269

35. Moller C, Plesset MS (1934) Note on an Approximation Treatment for Many-Electron Systems. Phys Rev 46:618-622. doi:10.1103/PhysRev.46.618
36. Becke AD (1993) Density-functional thermochemistry. III. The role of exact exchange. J Chem Phys 98:5648-5652. doi:10.1063/1.464913
37. Lee C, Yang W, Parr RG (1988) Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Phys Rev B 37:785-789. doi:10.1103/PhysRevB.37.785
38. Dewar M, Thiel W (1977) Ground states of molecules. 38. The MNDO method. Approximations and parameters. J Am Chem Soc 99:4899-4907. doi:10.1021/ja00457a004
39. Nyden MR, Petersson GA (1981) Complete basis set correlation energies. I. The asymptotic convergence of pair natural orbital expansions. J Chem Phys 75:1843-1862. doi:10.1063/1.442208
40. Petersson GA, Al-Laham MA (1991) A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms. J Chem Phys 94:6081-6090. doi:10.1063/1.460447
41. Petersson GA, Tensfeldt TG, Montgomery JA Jr (1991) A complete basis set model chemistry. III. The complete basis set-quadratic configuration interaction family of methods. J Chem Phys 94:6091-6101. doi:10.1063/1.460448
42. Dunning TH Jr (1989) Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. J Chem Phys 90:1007-1023. doi:10.1063/1.456153
43. Kendall RA, Dunning TH Jr, Harrison RJ (1992) Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. J Chem Phys 96:6796-6806. doi:10.1063/1.462569
44. Woon DE, Dunning TH Jr (1993) Gaussian-basis sets for use in correlated molecular calculations. 3. The atoms aluminum through argon. J Chem Phys 98:1358-1371. doi:10.1063/1.464303
45. Peterson KA, Woon DE, Dunning TH Jr (1994) Benchmark calculations with correlated molecular wave functions. IV. The classical barrier height of the $H+H_2 \rightarrow H_2+H$ reaction. J Chem Phys 100:7410-7415. doi:10.1063/1.466884
46. Wilson AK, van Mourik T, Dunning TH Jr (1996) Gaussian Basis Sets for use in Correlated Molecular Calculations. VI. Sextuple zeta correlation consistent basis sets for

boron through neon. J Mol Struct THEOCHEM 388:339-349. doi:10.1016/S0166-1280(96)80048-0

47. McLean AD, Chandler GS (1980) Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18. J Chem Phys 72:5639-5648. doi:10.1063/1.438980
48. Raghavachari K, Binkley JS, Seeger R, Pople JA (1980) Self-Consistent Molecular Orbital Methods. 20. Basis set for correlated wave-functions. J Chem Phys 72:650-654. doi:10.1063/1.438955
49. Clark T, Chandrasekhar J, Spitznagel GW, Schleyer PvR (1983) Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F. J Comput Chem 4:294-301. doi:10.1002/jcc.540040303
50. Ditchfield R, Hehre WJ, Pople JA (1971) Self-Consistent Molecular Orbital Methods. 9. Extended Gaussian-type basis for molecular-orbital studies of organic molecules. J Chem Phys 54:724-728. doi:10.1063/1.1674902
51. Frisch MJ, Pople JA, Binkley JS (1984) Self-Consistent Molecular Orbital Methods. 25. Supplementary Functions for Gaussian Basis Sets. J Chem Phys 80:3265-3269. doi:10.1063/1.447079
52. Boys SF, Bernardi F (1970) The calculation of small molecular interactions by the differences of separate total energies. Some procedures with reduced errors. Mol Phys 19:553-566. doi:10.1080/00268977000101561
53. Case DA, Darden TA, Cheatham TE III, Simmerling CL, Wang J, Duke RE, Luo R, Crowley M, Walker RC, W Zhang, Merz KM, Wang B, Hayik S, Roitberg A, Seabra G, Kolossváry I, Wong KF, Paesani F, Vanicek J, Wu X, Brozell SR, Steinbrecher T, Gohlke H, Yang L, Tan C, Mongan J, Hornak V, Cui G, Mathews DH, Seetin MG, Sagui C, Babin V, Kollman PA (2008) AMBER 10. University of California, San Francisco
54. Bayly CI, Cieplak P, Cornell WD, Kollman PA (1993) A well-behaved electrostatic potential based method using charge restraints for deriving atomic charges: the RESP model. J Phys Chem 97:10269-10280. doi:10.1021/j100142a004
55. Brown RD, Godfrey PD, Story J (1975) The microwave spectrum of urea. J Mol Spectrosc 58:445-450. doi:10.1016/0022-2852(75)90224-6
56. Strassner T (1996) Ab Initio and Molecular Mechanics Calculations of Various Substituted Ureas - Rotational Barriers and a New Parametrization for Ureas. J Mol Model 2:217-226. doi:10.1007/s0089460020217

57. Cornell WD, Cieplak P, Bayly CI, Gould IR, Merz KM Jr, Ferguson DM, Spellmeyer DC, Fox T, Caldwell JW, Kollman PA (1995) A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. J Am Chem Soc 117:5179-5197. doi:10.1021/ja00124a002
58. Gilkerson W, Srivastava K (1960) The dipole moment of urea. J Phys Chem 64:1485-1487. doi:10.1021/j100839a032
59. Lefebvre J (1973) Longitudinal phonons of translation along the 4 axis on urea. Solid State Commun 13:1873-1875. doi:10.1016/0038-1098(73)90748-5
60. Lee JS (1999) On the Effectiveness of Function Counterpoise Method in the Calculation of He-He Interaction Energies. Bull Korean Chem Soc 20:241-243
61. Schwenke DW, Truhlar DG (1985) Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules. J Chem Phys 85:2418-2426. doi:10.1063/1.448335
62. Åstrand PO, Wallqvist A, Karlström G (1994) Nonempirical intermolecular potentials for urea–water systems. J Chem Phys 100:1262-1273. doi:10.1063/1.466655
63. Suzuki K, Onishi S, Koide T, Seki S (1956) Vapor pressures of molecular crystals. xi. vapor pressures of crystalline urea and diformylhydrazine. Energies of hydrogen bonds in these crystals. Bull Chem Soc Jpn 29:127-131. doi:10.1246/bcsj.29.127
64. Dewit HGM, Van Miltenburg JC, DeKruif CG (1983) Thermodynamic properties of molecular organic crystals containing nitrogen, oxygen, and sulphur 1. Vapour pressures and enthalpies of sublimation. J Chem Thermodyn 15:651-663. doi:10.1016/002-9614(83)90079-4
65. Bertran CA, Cirino JJV, Freitas LCG (2002) Theoretical Studies of Concentrated Aqueous Urea Solutions Using Computacional Monte Carlo Simulation. J Braz Chem Soc 13:238-244. doi:10.1590/S0103-50532002000200016
66. Duffy EM, Severance DL, Jorgensen WL (1993) Urea: Potential Functions, log P, and free energy of hydration. Isr J Chem 33:323-330

Tables

Table 1 Relative total energies (kcal $mol^{-1)}$ for urea conformers

Computational Method	$\Delta E(C_{2v}\text{-}C_2)$
AM1	0.87
HF/6-31G(d)	1.57[a]
HF/D95**	1.29[a]
HF/6-311+G(3df,2p)	0.58[a]
B3PW91/D95**	1.46[a]
B3PW91/6-311+G(3df,2p)	0.59[a]
B3LYP/6-31G(d,p)	1.63
B3LYP/6-311+G*	1.20[b]
MP2/D95**	2.49[a]
MP2/6-31G*	1.32[c]
MP2/6-311++G(d,p)	2.75
MP2/6-311+G(3df,2p)	1.19[a]
MP2/aug-cc-pVDZ	1.58
MP2/aug-cc-pVTZ	1.42
MP2/aug-cc-pVQZ	1.22
CCSD/aug-cc-pVDZ	0.94
CCSD/aug-cc-pVTZ	0.70
CCSD(T)/aug-cc-pVDZ	0.94[d]
CCSD(T)/aug-cc-pVTZ	0.56[e]
CBS-QB3	1.29
CBS-APNO	1.12

[a] taken from Ref. [20]
[b] taken from Ref. [18]
[c] taken from Ref. [57]
[d] Single point energy at CCSD/aug-cc-pVDZ geometry
[e] Single point energy at CCSD/aug-cc-pVTZ geometry

Table 2 Geometrical parameters (bond distances (Å) and angles (°)) for urea

	C=O		C-N		N-H4		N-H5		∠N-C-N		∠N-C-O		∠H4-N-C		∠H5-N-C		∠H-N-H	
	C2	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*	*C2*	*C2v*
AM1	1.256	1.258	1.403	1.389	0.994	0.988	0.991	0.984	120.1	120.3	120.0	119.8	118.6	122.9	114.8	117.3	115.7	119.8
B3LYP/6-31G**	1.221	1.224	1.390	1.377	1.011	1.006	1.010	1.005	113.7	114.9	123.1	122.5	117.4	124.3	112.3	116.6	113.7	119.1
CCSD/aug-cc-pvdz	1.223	1.228	1.395	1.380	1.014	1.008	1.014	1.008	113.6	114.9	123.2	122.5	116.0	123.4	112.2	117.1	113.7	119.5
CCSD/aug-cc-pvtz	1.212	1.216	1.384	1.369	1.006	1.000	1.006	1.001	113.8	115.0	123.1	122.5	116.7	123.4	112.7	117.0	114.2	119.5
CBS-QB3	1.214	1.217	1.389	1.376	1.009	1.004	1.009	1.004	113.6	114.8	123.2	122.6	117.6	124.1	112.9	116.8	114.4	119.1
CBS-APNO	1.212	1.216	1.394	1.377	1.010	1.003	1.009	1.003	112.7	114.3	123.6	122.9	115.0	123.7	111.7	117.0	113.0	119.3
MP2/aug-cc-pvdz	1.230	1.233	1.394	1.381	1.014	1.008	1.014	1.009	113.5	114.8	123.2	122.6	116.5	123.6	112.4	117.0	114.0	119.4
MP2/aug-cc-pvtz	1.219	1.222	1.384	1.371	1.007	1.001	1.007	1.002	113.6	114.8	123.2	122.6	117.1	123.6	112.8	117.0	114.5	119.5
MP2/aug-cc-pvqz	1.216	1.219	1.381	1.368	1.005	1.000	1.005	1.001	113.7	114.8	123.1	122.6	117.5	123.5	113.1	117.0	114.8	119.5
MP2/6-311++G**	1.218	1.221	1.391	1.377	1.010	1.004	1.010	1.005	113.1	114.5	123.4	122.8	116.2	123.8	112.4	117.0	113.8	119.2
GAFF Parameters	-	1.214	-	1.345	-	1.009	-	1.009	-	111.7	-	122.0	-	118.5	-	118.5	-	117.8
Cornell et al. [58]	-	1.250	-	1.383	-	1.010	-	1.010	-	118.6	-	120.9	-	120.0	-	120.0	-	120.0
Exp.	-	1.262[a]	-	1.335[a]	-	0.988[b]	-	0.995[b]	-	118.0[a]	-	121.0[a]	-	119.8[b]	-	118.1[b]	-	122.0[b]
		1.243[b]		1.351[b]		1.046[c]		1.046[c]		117.0[b]		121.5[b]		120.0[c]		120.0[c]		119.0[c]

[a] taken from Ref. [7]
[b] taken from Ref. [8]
[c] taken from Ref. [9]

Table 3 Relative energies (kcal mol^{-1}) (E: total energy, E_{ZPE}: Zero point corrected energy, and E_{BSSE}: Counterpoise corrected energy) and the number of imaginary frequencies (NIMAG) of urea dimers optimized with MP2/aug-cc-pVDZ. All single point energies are corrected with the MP2/aug-cc-pVDZ zero-point vibrational energy

	E	**E_{ZPE}**	**E_{BSSE}**	**E^a**	**E^b**	**E^c**	**E^d**	**E^e**	**E^f**	**NIMAG**
D1	7.56	5.18	6.74	7.39	7.50	7.94	5.01	5.12	5.56	5
D2	5.85	4.51	6.00	6.18	5.72	6.23	4.83	4.37	4.89	2
D3	1.75	1.92	2.10	2.22	2.06	2.43	2.39	2.22	2.60	0
D4	7.47	7.54	7.57	8.25	7.63	8.37	8.32	7.70	8.44	0
D5	5.06	5.55	5.72	6.16	5.50	6.37	6.65	5.99	6.86	0
D6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0
D7	1.81	1.99	2.15	2.25	2.09	2.43	2.43	2.27	2.62	0

[a] MP2/aug-cc-pVTZ// MP2/aug-cc-pVDZ energy
[b] CCSD/ aug-cc-pVDZ// MP2/aug-cc-pVDZ energy
[c] CCSD(T)/ aug-cc-pVTZ// MP2/aug-cc-pVDZ energy
[d] MP2/aug-cc-pVTZ// MP2/aug-cc-pVDZ energy corrected with the MP2/aug-cc-pVDZ zero-point vibrational energy
[e] CCSD/ aug-cc-pVDZ// MP2/aug-cc-pVDZ energy corrected with the MP2/aug-cc-pVDZ zero-point vibrational energy
[f] CCSD(T)/ aug-cc-pVTZ// MP2/aug-cc-pVDZ energy corrected with the MP2/aug-cc-pVDZ zero-point vibrational energy

Table 4 Mean values of optimized bond distances (Å) for some urea clusters. Maximum and minimum values are given in parenthesis

Number of	C-N		C=O		N-H	
molecules	**AM1**	**B3LYP**	**AM1**	**B3LYP**	**AM1**	**B3LYP**
4	1.398 1.394	1.359 1.390	1.264 1.269	1.242	0.995 (1.003-0.986)	1.014 1.012 1.008 1.021
7	1.394 (1.403-1.384)	1.368 (1.395-1.357)	1.267 (1.270-1.264)	1.238 1.258 1.247 1.243	0.995 (1.003-0.986)	1.014 (1.027-1.007)
12	1.393 (1.403-1.377)	1.364 (1.376-1.356)	1.269 (1.277-1.264)	1.253 (1.262-1.237)	0.995 (1.003-0.988)	1.016 (1.028-1.008)
24	1.391 (1.401-1.377)	1.363 (1.388-1.349)	1.270 (1.274-1.266)	1.254 (1.262-1.234)	0.995 (1.003-0.988)	1.015 (1.030-1.007)
34	1.391 (1.408-1.379)	-	1.271 (1.275-1.266)	-	0.995 (1.003-0.987)	-
48	1.391 (1.406-1.379)	-	1.271 (1.276-1.266)	-	0.995 (1.003-0.988)	-
72	1.390 (1.408-1.377)	-	1.272 (1.276-1.267)	-	0.995 (1.001-0.986)	-
93	1.389 (1.407-1.375)	-	1.272 (1.277-1.267)	-	0.995 (1.001-0.987)	-
120	1.389 (1.407-1.379)	-	1.272 (1.277-1.267)	-	0.995 (1.003-0.987)	-
160	1.389 (1.408-1.374)	-	1.273 (1.276-1.267)	-	0.995 (1.001-0.987)	-
Exp.	1.335 or 1.351		1.262 or 1.243		0.988 or 0.995 or 1.046	

Table 5 Mean values of optimized bond angles (^{o}) for urea clusters. Maximum and minimum values are given in parenthesis

Number of molecules	O-C-N		N-C-N		C-N-H		H-N-H	
	AM1	**B3LYP**	**AM1**	**B3LYP**	**AM1**	**B3LYP**	**AM1**	**B3LYP**
4	119.59 (120.3-118.9)	121.7 122.7	120.58 120.81	115.5	116.8 (119.4-114.8)	119.5 117.7 113.6 110.3	115.95 (117.1-114.7)	118.2 110.6
7	119.50 (120.5-118.9)	122.5 (125.0-120.5)	120.94 (121.6-120.2)	115.9 114.5	117.03 (121.5-113.6)	117.03 (121.3-112.6)	115.87 (119.0-113.5)	117.41 (120.0-114.4)
12	119.43 (120.3-118.4)	121.5 (123.5-120.1)	121.06 (121.9-120.2)	116.9 (118.8-115.4)	117.18 (122.3-113.4)	117.1 (119.5-112.9)	116.22 (118.8-113.8)	116.6 (119.4-113.6)
24	119.48 (120.4-118.6)	121.7 (123.6-120.6)	120.95 (121.6-120.5)	116.5 (118.4-114.4)	117.43 (121.9-113.9)	117.8 (121.3-113.7)	116.64 (119.4-113.2)	116.6 (119.2-113.6)
34	119.48 (120.6-118.5)	-	120.94 (121.7-120.3)	-	117.48 (121.4-112.7)	-	116.78 (119.3-112.5)	-
48	119.44 (120.5-118.4)	-	121.03 (121.6-120.3)	-	117.36 (121.8-112.7)	-	116.56 (119.8-112.5)	-
72	119.43 (120.6-118.4)	-	121.08 (121.9-120.2)	-	117.64 (122.1-113.4)	-	116.98 (120.1-113.0)	-
93	119.43 (120.6-118.4)	-	121.08 (121.8-120.5)	-	117.67 (122.0-112.7)	-	117.07 (120.1-112.6)	-
120	119.43 (120.5-118.5)	-	121.08 (121.9-120.4)	-	117.66 (122.1-112.5)	-	117.04 (120.1-112.9)	-
160	119.39 (120.5-118.4)	-	121.16 (121.9-120.5)	-	117.73 (122.1-113.3)	-	117.14 (120.0-113.0)	-
Exp.	121.0 or 121.5		118.0 or 117.0		119.8 or 118.1 or 120.0		122.0 or 119.0	

Table 6 A comparison of the lattice constants (Å) calculated by B3LYP and AM1 with experimental data. Percentage deviations with respect to experiment carried out by Zavodnik *et al.* [5] are reported in parentheses

	12K [13]	30K [13]	60K [13]	90K [13]	123K [13]	150K [13]	173K [13]	293K [5]	298K [12]	AM1	B3LYP
a	5.565	5.565	5.570	5.576	5.584	5.590	5.598	5.660	5.662	5.481 (-3.27)	5.606 (-0.96)
c	4.684	4.685	4.688	4.689	4.689	4.692	4.694	4.711	4.716	4.683 (-0.60)	4.747 (0.76)
c/a	0.8417	0.8419	0.8417	0.8409	0.8397	0.8394	0.8385	0.8323	0.8329	0.8544	0.8468

Table 7 RESP charges calculated with MP2/aug-cc-pVDZ for each dimer structure

	RESP-**D1**	RESP-**D2**	RESP-**D3**	RESP-**D4**	RESP-**D5**	RESP-**D6**	RESP-**D7**	Bertran et al. [66]	Nilsson et al. [29]	OPLS [67]
C	1.172	0.675	0.884	0.783	0.893	0.866	0.871	0.963	0.142	0.142
O	-0.795	-0.571	-0.660	-0.600	-0.622	-0.614	-0.653	-0.578	-0.502	-0.390
N	-1.098	-0.735	-0.888	-0.777	-0.888	-0.880	-0.873	-1.004	-0.569	-0.542
H	0.454	0.342	0.388	0.343	0.376	0.377	0.382	0.406	0.333	0.333

Table 8 Interaction energies (kcal mol^{-1}) of urea dimers

	MP2		CCSD	Force Field[c], RESP charge set						
	aug-cc-pVDZ[a]	**aug-cc-pVTZ[b]**	**aug-cc-pVDZ[b]**	**D1**	**D2**	**D3**	**D4**	**D5**	**D6**	**D7**
D1	-10.33	-9.58	-9.93	-16.07	-9.86	-11.99	-9.83	-10.38	1.62	-11.76
D2	-12.04	-10.79	-11.71	-11.7	-7.79	-8.86	-7.51	-7.54	4.44	-8.73
D3	-16.14	-14.75	-15.37	-17.33	-11.12	-13.12	-10.77	-11.41	0.49	-12.86
D4	-10.42	-8.72	-9.80	-6.47	-4.45	-4.77	-4.12	-4.35	7.56	-4.76
D5	-12.83	-10.81	-11.93	-6.86	-2.74	-3.03	-2.58	-2.61	9.39	-2.85
D6	-17.89	-16.97	-17.43	-19.37	-12.18	-14.62	-11.95	-12.62	-0.68	-14.34
D7	-16.09	-14.72	-15.34	-17.36	-11.18	-13.16	-10.8	-11.44	0.45	-12.9

[a] Basis set corrected energy.
[b] Single point energy at the MP2/aug-cc-pVDZ geometry.
[c] Total interaction energy.

Table 9 Non-bonding interaction parameters. (ε (kcal mol^{-1}) is the depth of the potential well and σ (Å) is the distance at which the *inter*-particle potential is zero.)

	GAFF		OPLS	
	σ	ε	σ	ε
C	1.908	0.086	3.750	0.105
O	1.661	0.210	2.960	0.210
N	1.824	0.170	3.250	0.170
H	0.600	0.016	0.000	0.000

Table 10 The parameters used for energy minimization of the linear dimer

	Bond & Angle Parameters	**Nonbonding Interaction Parameters**	**Charge**
b	GAFF	GAFF	Resp-**D3**
c	Cornell et al.	GAFF	Resp-**D3**
d	GAFF	OPLS	Resp-**D3**
e	Cornell et al.	OPLS	Resp-**D3**
f	Cornell et al.	OPLS	OPLS

Table 11 Improved general AMBER force field parameters

Bond Parameters				
bond	K_r[a]	r[b]		
c –o	656	1.250		
c -n	424	1.383		
hn-n	434	1.010		
Angle Parametres				
angle	K_θ[c]	θ[d]		
n –c –o	80	120.9		
c –n –hn	30	120.0		
hn –n –hn	35	120.0		
n –c –n	70	118.6		
Dihedral Parameters				
torsion	no. of paths[e]	$V_n/2$[f]	γ[g]	n[h]
hn –n –c –o	1	2.5	180	-2
hn –n –c –o	1	2.0	0	1
Improper Dihedral Parameters				
torsion		$V_n/2$[f]	γ[g]	n[h]
n –n –c –o		10.5	180	2
c –hn –n –hn		1.1	180	2
Nonbonding Parameters				
atom type	σ[i]	ε[j]		
hn	0.6000	0.0157		
o	1.6612	0.2100		
c	1.9080	0.0860		
n	1.8240	0.1700		

[a] Force constant (kcal mol^{-1} Å^{-2}). [b] Bond distance (Å).
[c] Force constant (kcal mol^{-1} radian^{-2}). [d] Angle (deg.).
[e] Number of bond paths that the total $\frac{V_n}{2}$ is divided into.
[f] Magnitude of torsion (kcal mol^{-1}).
[g] Phase offset (°).
[h] The periodicity of the torsion. A negative value is not used in the computation but signifies more than one component around a given bond.
[i] Å.
[j] kcal mol^{-1}.

Figure captions

Fig. 1 The unit cell of urea crystal. (I) and (II) are projections of the structure down the a-axis and along c-axis, respectively. The space group is $P\bar{4}2_1m$ and unit cell dimensions are a=b=5.565 and c=4.684 Å [12]

Fig. 2 Potential energy surface of urea. Relative energies at the B3LYP/6-31G**, B3PW95/D95** [20] (bold), MP2/D95** [18] (in parentheses), and MP2/6-31G* [56] (italics) levels

Fig . 3 Comparison of computed urea dipole moments (Debye) with experimental data

Fig. 4 Urea dimer structures optimized at the MP2/aug-cc-pVDZ level. (Red = O, Grey = C, Blue = N, and White = H, distances in Ångstrøm). The exact geometries are given in the Supporting Information

Fig. 5 AM1 (left column) and B3LYP (right column) optimized geometries of urea clusters (n=4, 7, 12, and 24). Dash lines show hydrogen bonding. (Red = O, Grey = C, Blue = N, and White = H). The exact geometries are given in the Supporting Information

Fig. 6 AM1 optimization results for urea clusters. Dashed lines show hydrogen bonds. (Red = O, Grey = C, Blue = N, and White = H). The exact geometries are given in the Supporting Information

Fig. 7 Calculated AM1 (above) and B3LYP (below) binding energies (kcal mol^{-1}) of urea clusters

Fig. 8 Linear dimer geometries (distances in Å) after energy minimization with the different force-field parameter sets defined in Table 10. The distances given in italic form are the C…C distances

colour figure 1

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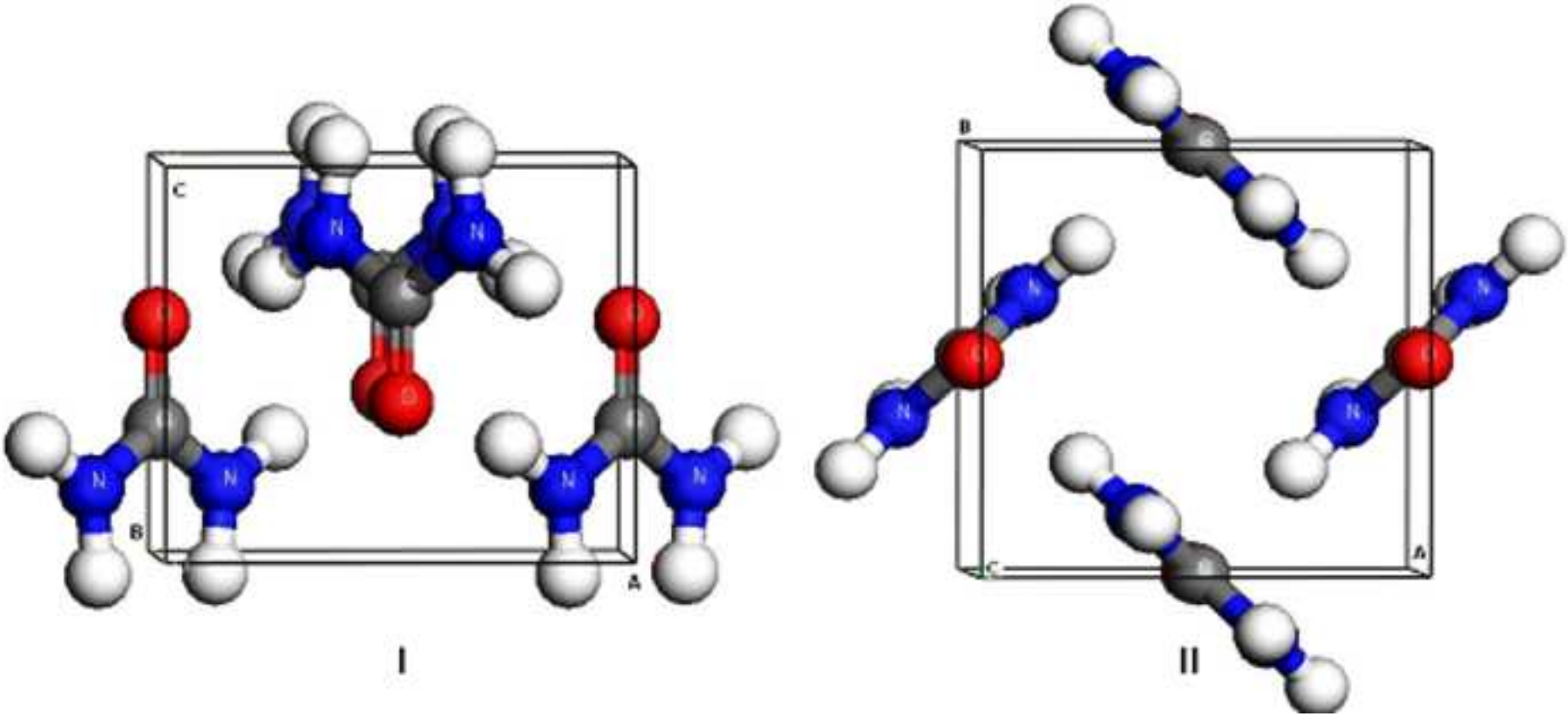

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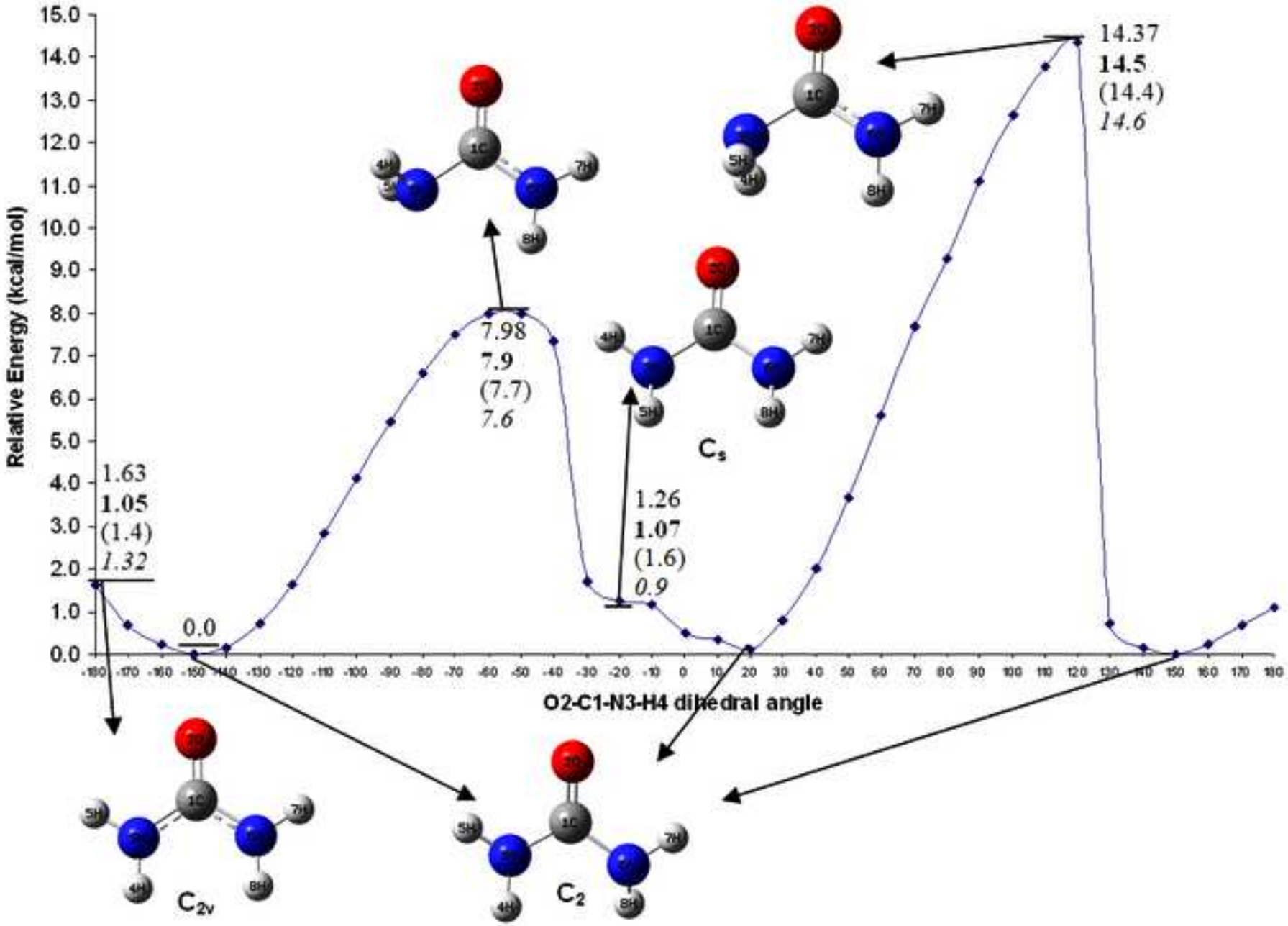

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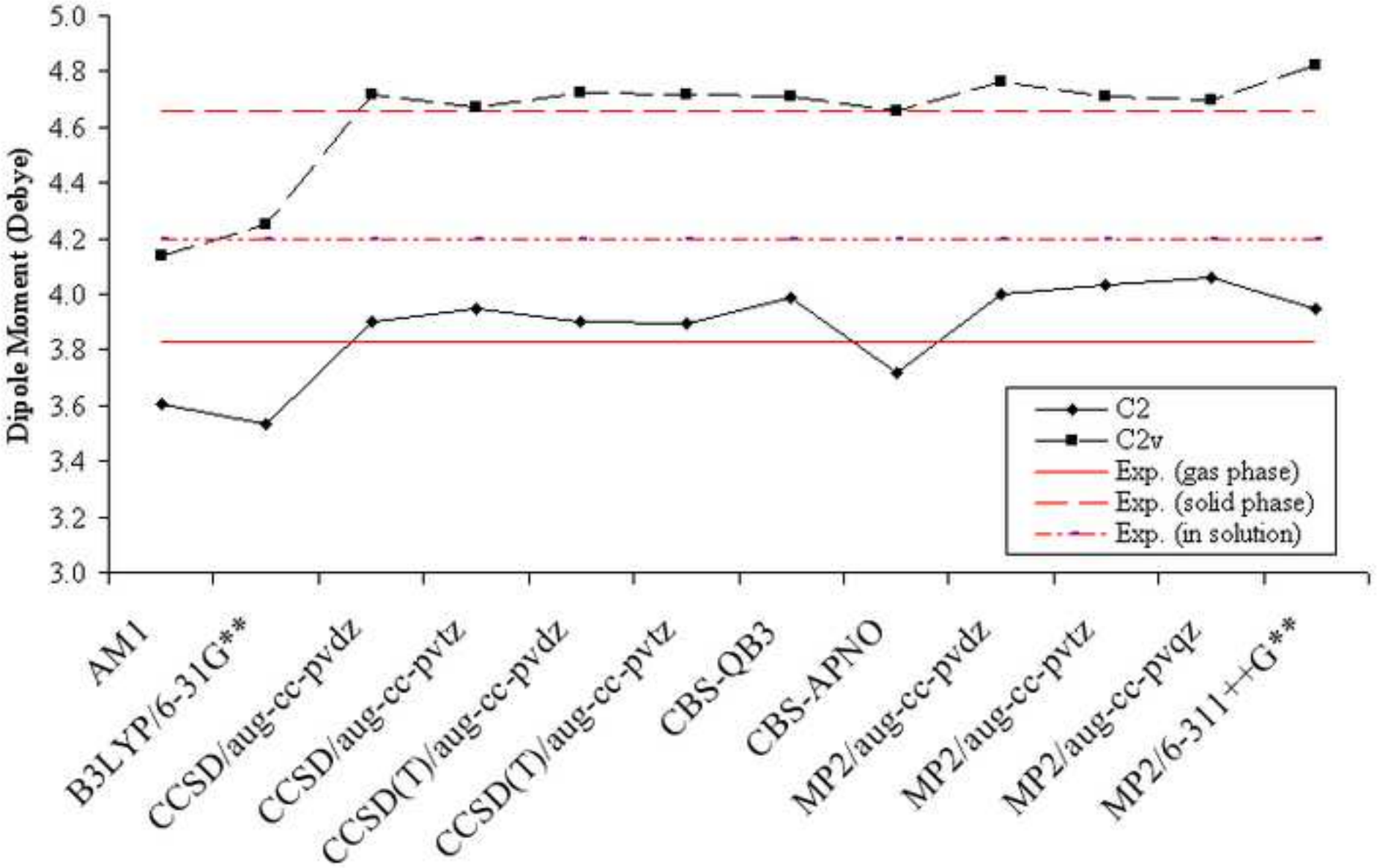

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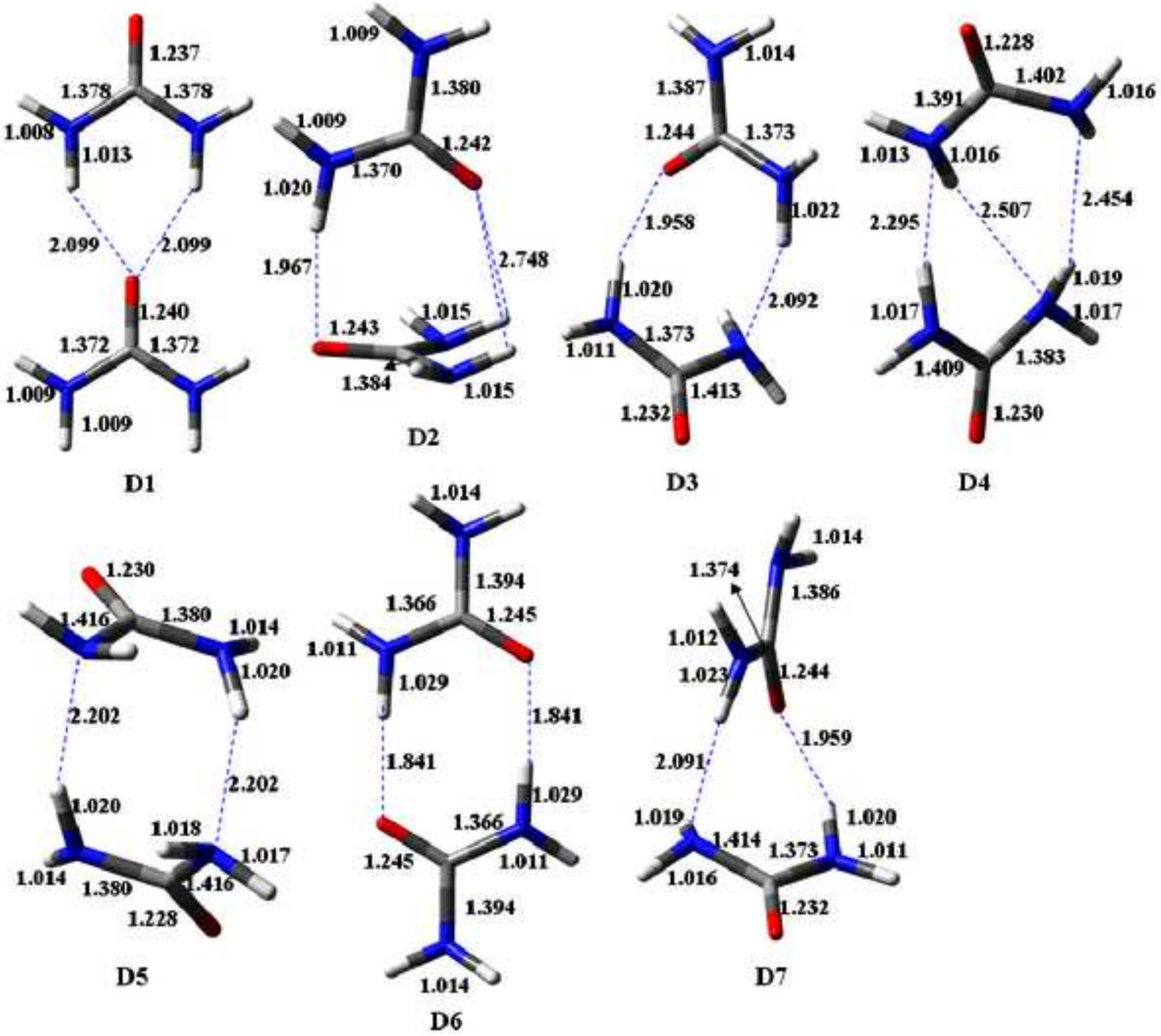

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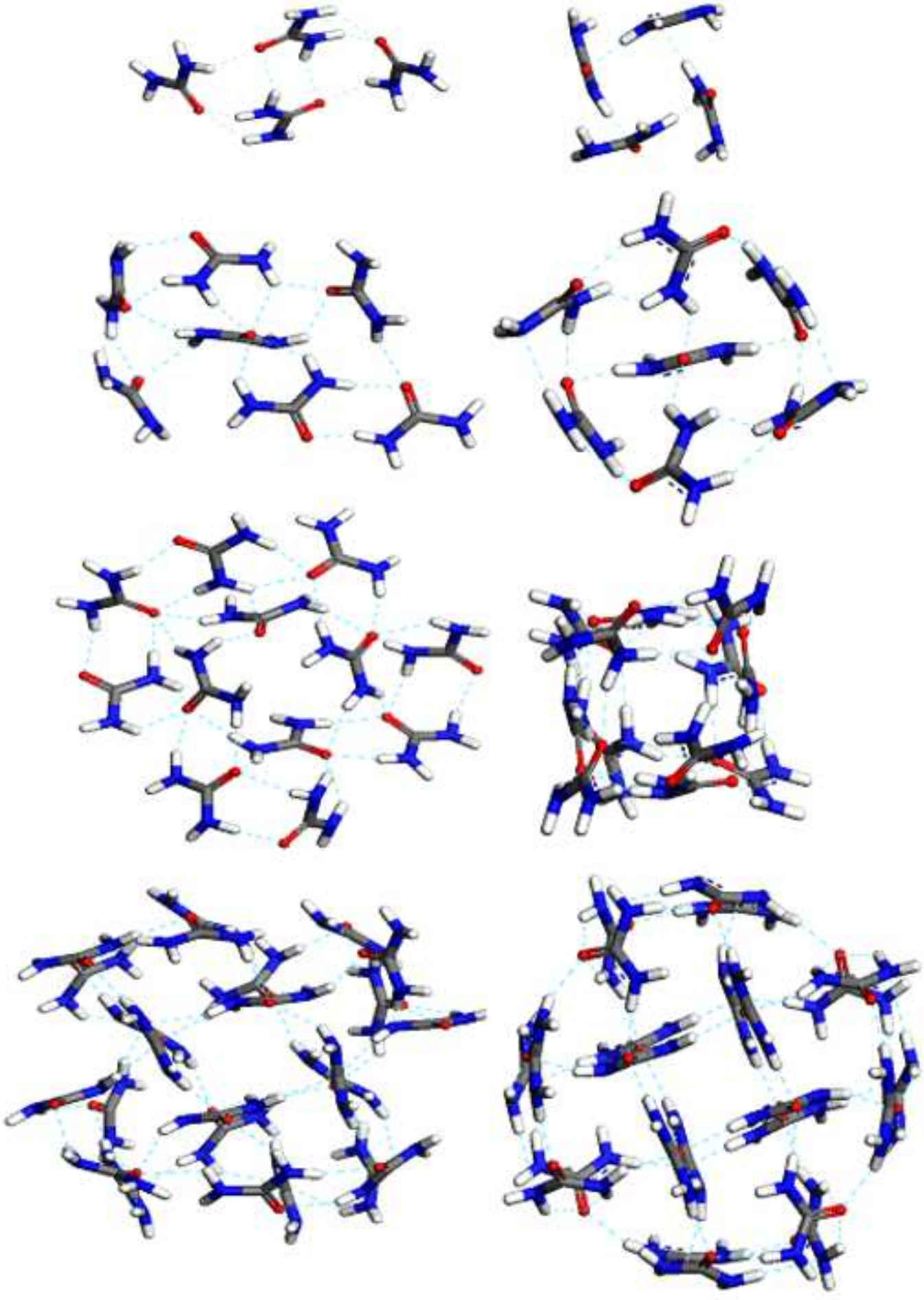

colour figure 6

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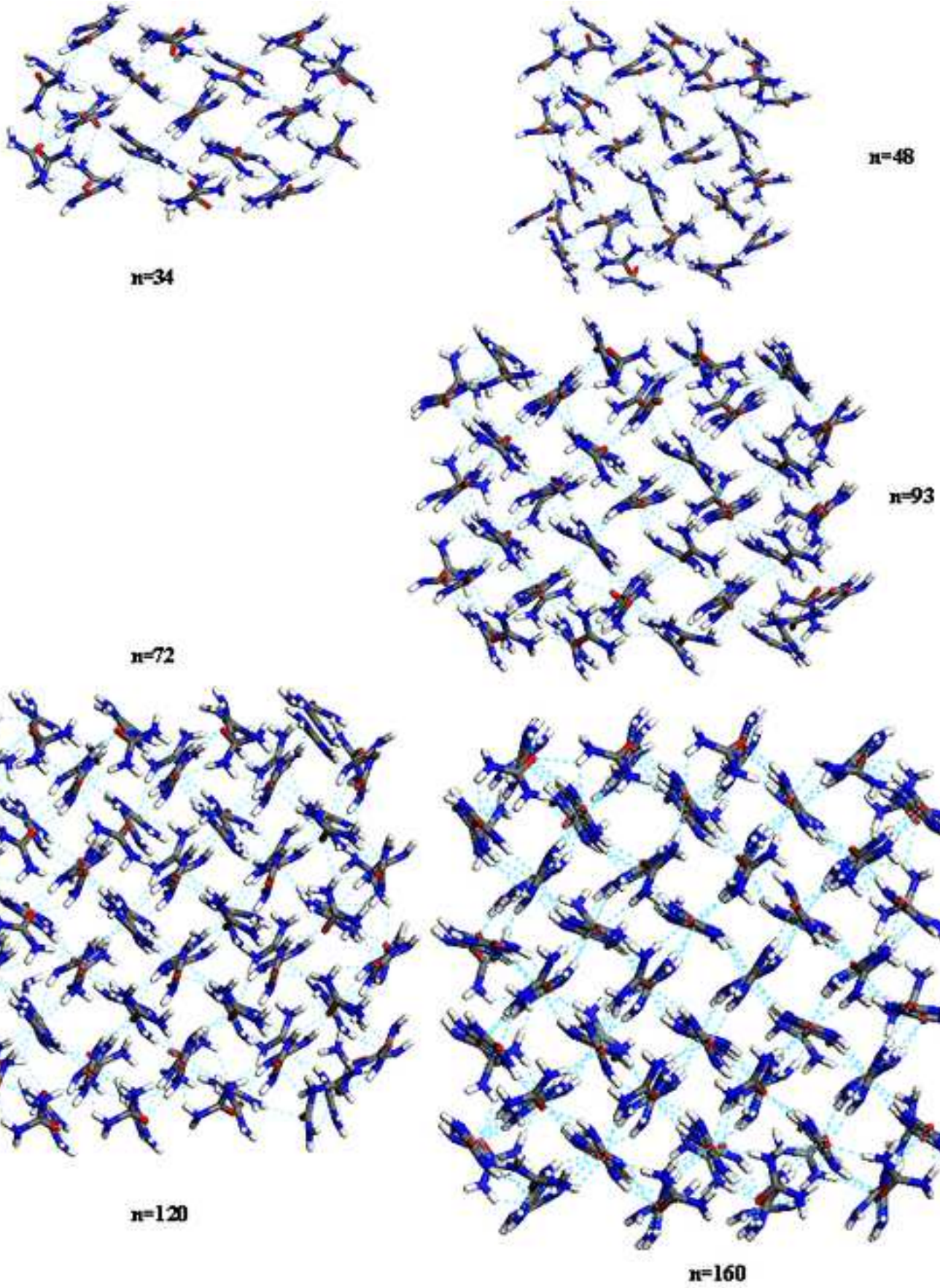

bw figure 7

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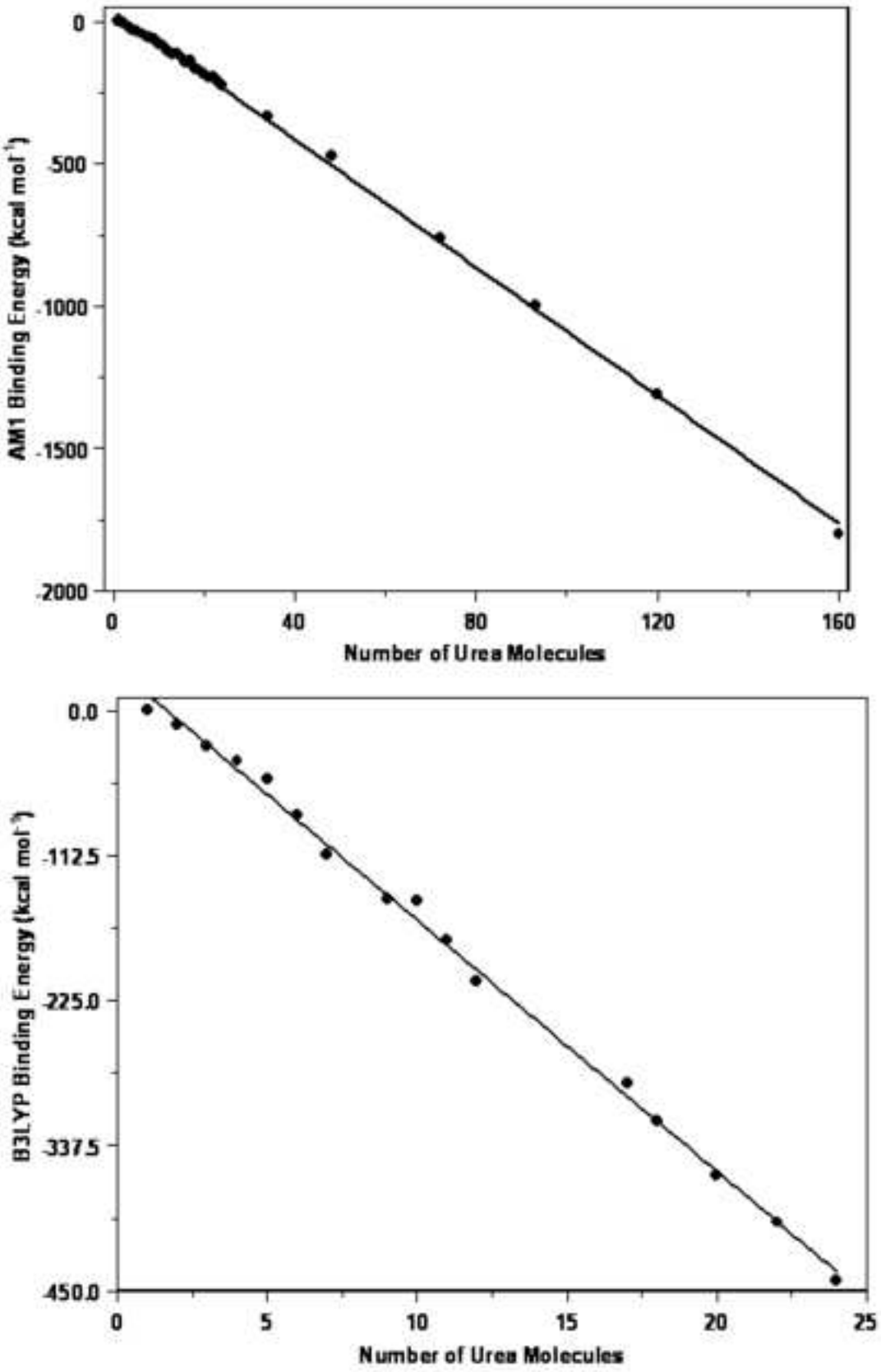

colour figure 8

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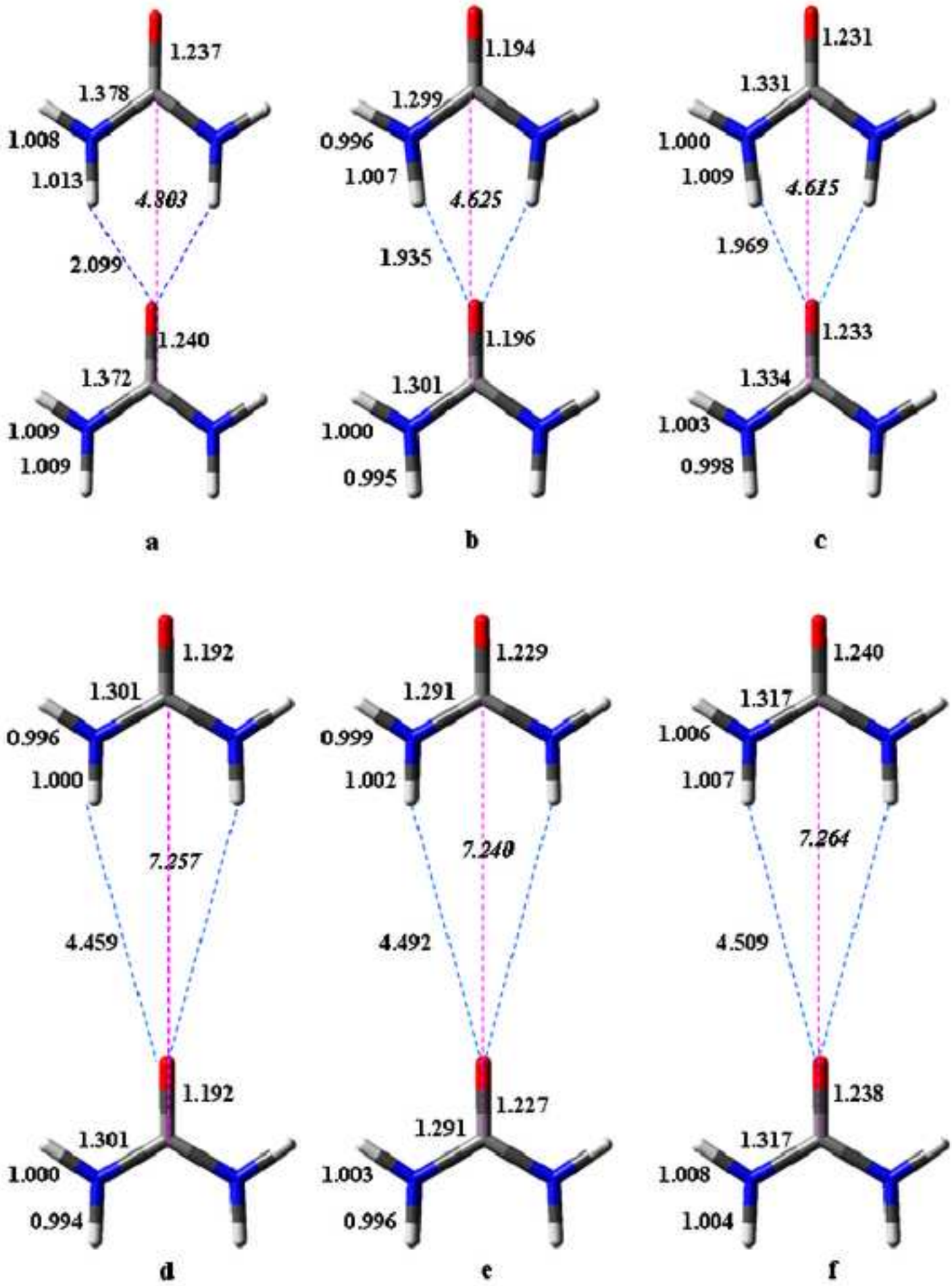

An Improved General AMBER Force Field (GAFF) for Urea

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Table of Contents

1. Absolute energies of monourea conformers

Table S1. Absolute energy (au) of urea conformers.

Computational Method	C_2	C_{2v}
AM1	-0.071744	-0.070351
B3LYP/6-31G(d,p)	-225.273788	-225.271187
MP2/6-311++G(d,p)	-224.756496	-224.752121
MP2/aug-cc-pVDZ	-224.715357	-224.712843
MP2/aug-cc-pVTZ	-224.910610	-224.908342
MP2/aug-cc-pVQZ	-224.975090	-224.973151
CCSD/aug-cc-pVDZ	-224.029296	-224.027793
CCSD/aug-cc-pVTZ	-224.084910	-224.083793
CCSD(T)/aug-cc-pVDZ	-224.029296	-224.027793
CCSD(T)/aug-cc-pVTZ	-224.081943	-224.081048
CBS-QB3	-224.877690	-224.875638
CBS-APNO	-224.940220	-224.938441

2. Absolute energies of urea dimers

Table S2. Absolute energies (au) of urea dimers. (E: total energy, E_{ZPE}: Zero point corrected energy, and E_{BSSE}: Counterpoise corrected energy)

	E	**E_{ZPE}**	**E_{BSSE}**	**E^a**	**E^b**	**E^c**
D1	-449.442419	-449.316880	-449.439881	-449.831950	-449.482423	-449.926744
D2	-449.444876	-449.317956	-449.441057	-449.833881	-449.485255	-449.929471
D3	-449.451412	-449.322082	-449.447280	-449.840186	-449.491094	-449.935527
D4	-449.442291	-449.313123	-449.438564	-449.830577	-449.482206	-449.926058
D5	-449.446134	-449.316288	-449.441510	-449.833909	-449.485601	-449.929250
D6	-449.454201	-449.325138	-449.450619	-449.843729	-449.494370	-449.939402
D7	-449.451323	-449.321965	-449.447199	-449.840144	-449.491044	-449.935524

[a] Single point MP2/aug-cc-pVTZ energy.
[b] Single point CCSD/ aug-cc-pVDZ energy.
[c] Single point CCSD(T)/ aug-cc-pVTZ energy.

3. Absolute energies of urea oligomers

Table S3. Absolute total energies (au) of urea oligomers computed with B3LYP/6-31G(d,p).

Number of urea molecules	Energy
1	-225.271187
2	-450.560071
3	-675.858482
4	-901.148609
5	-1126.440385
6	-1351.756500
7	-1577.076498
9	-2027.673714
10	-2252.946881
11	-2478.266919
12	-2703.589885
17	-3830.070226
24	-5407.213376

Table S4. Heat of formation (kcal/mol) of urea oligomers computed with AM1 using VAMP package.

Number of urea molecules	H_f
1	-44.935479
2	-98.426810
3	-151.622430
4	-207.956352
5	-261.222524
6	-312.408307
7	-364.237858
8	-416.687723
9	-468.393196
10	-527.792471
11	-580.304880
12	-641.124508
13	-699.006176
14	-741.710929
15	-802.092222
16	-865.270104
17	-903.268358
18	-975.244274
19	-1026.583651
20	-1081.325890
21	-1142.150271
22	-1185.900689
23	-1247.053746
24	-1302.952958
34	-1859.712696
48	-2630.278461
72	-3999.049297
93	-5175.379461
120	-6701.410152
160	-8990.672564

4. Total energies of urea dimers calculated with RESP charges

Table S5. Total energies of urea dimers calculated with RESP charges.

	RESP D1	RESP D2	RESP D3	RESP D4	RESP D5	RESP D6	RESP D7
Di1	-5.23E+02	-2.53E+02	-3.52E+02	-2.73E+02	-3.32E+02	-3.28E+02	-3.42E+02
Di2	-5.19E+02	-2.51E+02	-3.49E+02	-2.71E+02	-3.29E+02	-3.25E+02	-3.39E+02
Di3	-5.25E+02	-2.54E+02	-3.53E+02	-2.74E+02	-3.33E+02	-3.29E+02	-3.43E+02
Di4	-5.14E+02	-2.48E+02	-3.45E+02	-2.68E+02	-3.26E+02	-3.22E+02	-3.35E+02
Di5	-5.14E+02	-2.46E+02	-3.43E+02	-2.66E+02	-3.24E+02	-3.20E+02	-3.33E+02
Di6	-5.27E+02	-2.55E+02	-3.55E+02	-2.75E+02	-3.34E+02	-3.30E+02	-3.44E+02
Di7	-5.25E+02	-2.54E+02	-3.53E+02	-2.74E+02	-3.33E+02	-3.29E+02	-3.43E+02

5. Total energy of the dimer D1 calculated with RESP-D3 using different force fields

Table S6. Total energies of the dimer D1 calculated with RESP-D3 charges using GAFF

Total Energy of the dimer D1	Bond & Angle Parameters	Nonbonding Interaction Parameters	Charge
-3.52E+02	GAFF	GAFF	Resp-**D3**
-3.44E+02	Cornell et al.	GAFF	Resp-**D3**
-3.43E+02	GAFF	OPLS	Resp-**D3**
-3.44E+02	Cornell et al.	OPLS	Resp-**D3**
-1.42E+02	Cornell et al.	OPLS	OPLS

6. Total energy of urea clusters minimized with improved force field

Table S7. Total energies of the urea clusters calculated with RESP-D3 charges using improved force field.

Number of urea molecules	Energy
1	-170.01
4	-697.95
7	-1218.8
12	-1998.1
24	-4372.6
34	-6126
48	-8948.3
93	-17419
120	-23120
160	-32008
196	-38335
240	-47800
420	-80177

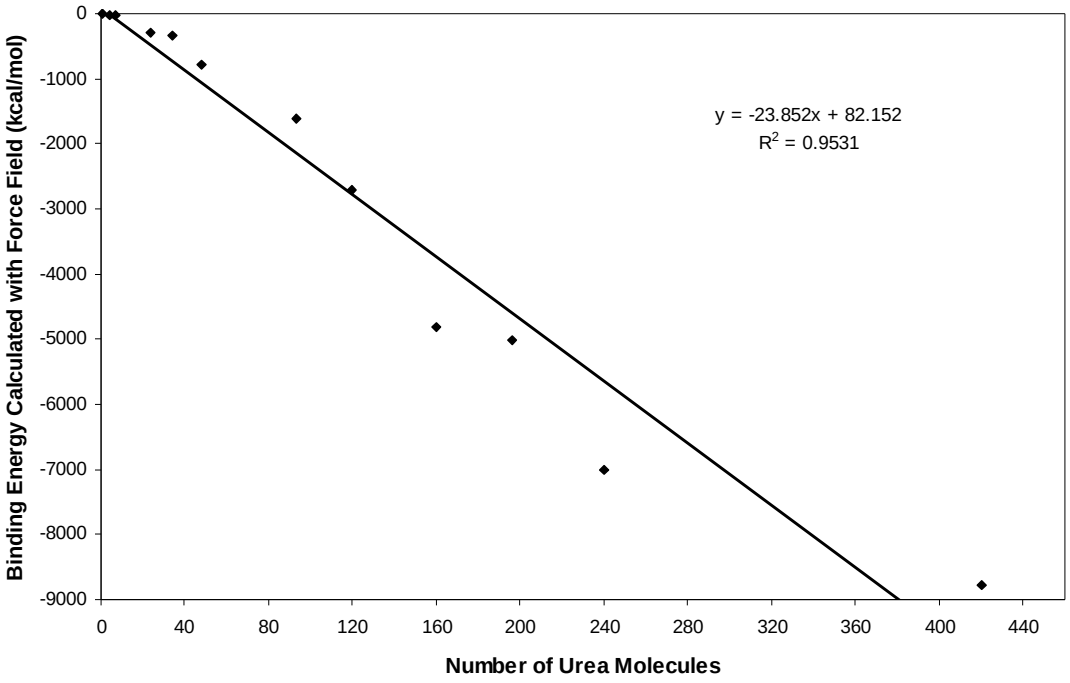

Figure S1. Binding energy calculated with improved force filed.

7. Cartesian Coordinates of the optimized monourea confomers

AM1 optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000071	0.102791	0.000040
2	8	0	0.000263	1.358425	0.000113
3	7	0	-1.213550	-0.597584	-0.068420
4	1	0	-1.248876	-1.520792	0.290433
5	1	0	-2.015300	-0.036415	0.108005
6	7	0	1.213273	-0.597794	0.068032
7	1	0	2.015419	-0.037387	-0.108546
8	1	0	1.248171	-1.521905	-0.288316

B3LYP/6-31G(d,p) optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000011	0.143741	-0.000568
2	8	0	-0.000365	1.364263	0.000153
3	7	0	-1.161010	-0.616020	-0.076532
4	1	0	-1.160836	-1.512933	0.389947
5	1	0	-1.992523	-0.065777	0.085710
6	7	0	1.161260	-0.615472	0.076670
7	1	0	1.992677	-0.064889	-0.084882
8	1	0	1.161918	-1.512510	-0.389556

MP2/6-311++G(d,p) optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000031	0.148185	-0.000039
2	8	0	0.000035	1.366039	0.000018
3	7	0	1.157823	-0.618682	0.079346
4	1	0	1.142220	-1.502822	-0.408537
5	1	0	1.992445	-0.075404	-0.088487
6	7	0	-1.157892	-0.618664	-0.079424
7	1	0	-1.992352	-0.075209	0.088720
8	1	0	-1.142306	-1.502566	0.408931

MP2/aug-cc-pVDZ optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000040	0.144188	-0.000125
2	8	0	0.000000	1.373891	0.000064
3	7	0	1.163303	-0.620206	0.078616
4	1	0	1.151425	-1.514957	-0.398996
5	1	0	1.999618	-0.071783	-0.090254
6	7	0	-1.163371	-0.620301	-0.078801
7	1	0	-1.999386	-0.071550	0.090698
8	1	0	-1.151424	-1.514419	0.400088

MP2/aug-cc-pVTZ optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000032	0.143887	-0.000006
2	8	0	0.000073	1.362954	0.000013
3	7	0	1.155555	-0.613505	0.075546
4	1	0	1.143661	-1.515556	-0.370921
5	1	0	1.988592	-0.073934	-0.093930
6	7	0	-1.155663	-0.613444	-0.075679
7	1	0	-1.988473	-0.073634	0.094255
8	1	0	-1.143809	-1.515191	0.371462

MP2/aug-cc-pVQZ optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000010	0.143378	-0.000002
2	8	0	0.000007	1.359719	0.000012
3	7	0	1.153802	-0.611099	0.073371
4	1	0	1.144126	-1.517751	-0.359657
5	1	0	1.987159	-0.073639	-0.091149
6	7	0	-1.153820	-0.611112	-0.073429
7	1	0	-1.987096	-0.073543	0.091180
8	1	0	-1.144186	-1.517608	0.359947

CCSD/aug-cc-pVDZ optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000037	0.145248	-0.000120
2	8	0	-0.000009	1.368492	0.000046
3	7	0	1.164905	-0.619275	0.081288
4	1	0	1.150281	-1.505977	-0.411260
5	1	0	1.998251	-0.068795	-0.094791
6	7	0	-1.164966	-0.619356	-0.081422
7	1	0	-1.998057	-0.068645	0.095300
8	1	0	-1.150206	-1.505595	0.412034

CCSD/aug-cc-pVTZ optimization for C_2 conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000121	0.144490	-0.000029
2	8	0	0.000144	1.356313	0.000087
3	7	0	1.155945	-0.611525	0.077024
4	1	0	1.142534	-1.507673	-0.378603
5	1	0	1.986409	-0.071580	-0.095993
6	7	0	-1.156212	-0.611531	-0.077573
7	1	0	-1.985864	-0.070581	0.096749
8	1	0	-1.143086	-1.506216	0.381166

CBS-QB3 optimization for C_2 conformer:

```
C,0,0.0001549839,-0.0003079753,0.0034874245
O,0,0.0006596704,0.0033155389,1.21734233260
N,0,1.1616455147,0.003203214,-0.7570191217
H,0,1.1292024782,0.4499031242,-1.6613906558
H,0,1.9857204389,0.2154710363,-0.2155617267
N,0,-1.162518013,-0.0079240021,-0.7560601624
H,0,-1.9852338537,-0.2181291878,-0.2115747185
H,0,-1.1309106295,-0.4635313585,-1.6561240053
```

CBS-APNO optimization for C_2 conformer:

```
C,0,0.0001470609,-0.000445763,0.0019675891
O,0,0.000882041,0.0038665738,1.2134723575
N,0,1.1603298882,-0.0252681047,-0.7710668913
H,0,1.107228367,0.4929777959,-1.6360877006
H,0,1.9775564389,0.2018494253,-0.2240151242
N,0,-1.160973212,0.0188782244,-0.7698159751
H,0,-1.9775321834,-0.2043401594,-0.2201685375
H,0,-1.1089178107,-0.5055176025,-1.6311863513
```

AM1 optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.102270
2	8	0	0.000000	0.000000	1.360160
3	7	0	0.000000	1.205128	-0.589050
4	1	0	0.000000	1.258231	-1.571632
5	1	0	0.000000	2.034616	-0.052465
6	7	0	0.000000	-1.205128	-0.589050
7	1	0	0.000000	-2.034616	-0.052465
8	1	0	0.000000	-1.258231	-1.571632

B3LYP/6-31G(d,p) optimization for C_{2v} conformer:

```
C,0.,0.,-0.1412639375
O,0.,0.,-1.3649939375
N,0.,1.160564,0.5993100625
H,0.,1.191025,1.6043220625
H,0.,2.023926,0.0842750625
N,0.,-1.160564,0.5993100625
H,0.,-2.023926,0.0842750625
H,0.,-1.191025,1.6043220625
```

MP2/6-311++G(d,p) optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.144909
2	8	0	0.000000	0.000000	1.366029
3	7	0	0.000000	1.157715	-0.600094
4	1	0	0.000000	1.175131	-1.604139
5	1	0	0.000000	2.025953	-0.094044
6	7	0	0.000000	-1.157715	-0.600094
7	1	0	0.000000	-2.025953	-0.094044
8	1	0	0.000000	-1.175131	-1.604139

MP2/aug-cc-pVDZ optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.141647
2	8	0	0.000000	0.000000	1.374267
3	7	0	0.000000	1.162795	-0.602625
4	1	0	0.000000	1.179445	-1.610819
5	1	0	0.000000	2.033541	-0.092812
6	7	0	0.000000	-1.162795	-0.602625
7	1	0	0.000000	-2.033541	-0.092812
8	1	0	0.000000	-1.179445	-1.610819

MP2/aug-cc-pVTZ optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.140455
2	8	0	0.000000	0.000000	1.362388
3	7	0	0.000000	1.155040	-0.597545
4	1	0	0.000000	1.172554	-1.598527
5	1	0	0.000000	2.018897	-0.089578
6	7	0	0.000000	-1.155040	-0.597545
7	1	0	0.000000	-2.018897	-0.089578
8	1	0	0.000000	-1.172554	-1.598527

MP2/aug-cc-pVQZ optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.140484
2	8	0	0.000000	0.000000	1.359762
3	7	0	0.000000	1.153036	-0.596408
4	1	0	0.000000	1.169725	-1.596244
5	1	0	0.000000	2.016010	-0.089399
6	7	0	0.000000	-1.153036	-0.596408
7	1	0	0.000000	-2.016010	-0.089399
8	1	0	0.000000	-1.169725	-1.596244

CCSD/aug-cc-pVDZ optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.141719
2	8	0	0.000000	0.000000	1.369411
3	7	0	0.000000	1.163157	-0.600467
4	1	0	0.000000	1.178446	-1.608137
5	1	0	0.000000	2.033543	-0.091396
6	7	0	0.000000	-1.163157	-0.600467
7	1	0	0.000000	-2.033543	-0.091396
8	1	0	0.000000	-1.178446	-1.608137

CCSD/aug-cc-pVTZ optimization for C_{2v} conformer:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.140643
2	8	0	0.000000	0.000000	1.356618
3	7	0	0.000000	1.154441	-0.594997
4	1	0	0.000000	1.170050	-1.594557
5	1	0	0.000000	2.017478	-0.088867
6	7	0	0.000000	-1.154441	-0.594997
7	1	0	0.000000	-2.017478	-0.088867
8	1	0	0.000000	-1.170050	-1.594557

CBS-QB3 optimization for C_{2v} conformer:

```
C,0,0.,0.,0.0017723807
O,0,0.,0.,1.2192277861
N,0,1.1595845409,0.,-0.7393824282
H,0,1.1867494925,0.,-1.7432416007
H,0,2.0236996615,0.,-0.227710058
N,0,-1.1595845409,0.,-0.7393824282
H,0,-2.0236996615,0.,-0.227710058
H,0,-1.1867494925,0.,-1.7432416007
```

CBS-APNO optimization for C_{2v} conformer:

```
C,0,0.,0.,0.0080277814
O,0,0.,0.,1.2239296851
N,0,1.1562192924,0.,-0.7389785348
H,0,1.1709698508,0.,-1.74162829
H,0,2.0237566693,0.,-0.2352059122
N,0,-1.1562192924,0.,-0.7389785348
H,0,-2.0237566693,0.,-0.2352059122
H,0,-1.1709698508,0.,-1.74162829
```

8. Cartesian Coordinates of the optimized urea dimers

D1 optimized with MP2/aug-cc-pVDZ

C	0.00000000	0.00000000	2.52904900
O	0.00000000	0.00000000	3.76637800
C	0.00000000	0.00000000	-2.24997600
O	0.00000000	0.00000000	-1.00950400
N	0.00000000	1.15405800	1.77555100
H	0.00000000	2.02905500	2.27600800
H	0.00000000	1.12389100	0.76323800
N	0.00000000	1.16117900	-2.98142900
H	0.00000000	2.03283300	-2.47291800
H	0.00000000	1.17901500	-3.98989300
N	0.00000000	-1.15405800	1.77555100
H	0.00000000	-2.02905500	2.27600800
H	0.00000000	-1.12389100	0.76323800
N	0.00000000	-1.16117900	-2.98142900
H	0.00000000	-2.03283300	-2.47291800
H	0.00000000	-1.17901500	-3.98989300

D2 optimized with MP2/aug-cc-pVDZ

C	0.21180500	1.69308900	0.00000000
O	1.12837600	0.85544500	0.00000000
C	-0.24529600	-1.78587400	0.00000000
O	-1.47369100	-1.59635700	0.00000000
N	-1.11609500	1.35475700	0.00000000
H	-1.37575600	0.36845300	0.00000000
H	-1.84284300	2.05451700	0.00000000
N	0.47605600	3.04799400	0.00000000
H	1.44489700	3.32906000	0.00000000
H	-0.24474500	3.75335300	0.00000000
N	0.47605600	-1.95357300	1.16885000
H	-0.03713300	-1.62109000	1.97835100
H	1.43583200	-1.62421500	1.14367900
N	0.47605600	-1.95357300	-1.16885000
H	-0.03713300	-1.62109000	-1.97835100
H	1.43583200	-1.62421500	-1.14367900

D3 optimized with MP2/aug-cc-pVDZ

C	-1.89196400	-0.01889400	0.05372700
O	-1.30157100	0.79556700	0.78530600
N	-3.16887100	0.22647500	-0.42893500
H	-3.75695500	-0.57315500	-0.63345400
H	-3.63628100	0.99135300	0.04415300
N	-1.33465700	-1.21028300	-0.34185000
H	-0.34099700	-1.31654500	-0.12694000

H	-1.68244900	-1.65721900	-1.18062700
H	1.73288800	1.83656100	-0.99949400
N	1.41189800	1.26075400	-0.23282600
C	2.08468000	0.07704000	-0.05789300
H	0.44225300	1.33280900	0.07547700
O	3.13188400	-0.22541800	-0.63260200
N	1.44205200	-0.80422100	0.83994600
H	0.89069400	-0.34576200	1.56379400
H	2.09909300	-1.48719200	1.20610400

D4 optimized with MP2/aug-cc-pVDZ

C	2.16543800	-0.06808100	0.07380500
O	3.14552200	-0.66379000	-0.36598200
N	1.85878100	1.25494500	-0.27388700
H	1.41873700	1.81551500	0.45030700
H	2.65395500	1.71365100	-0.70857300
N	1.19546700	-0.68435000	0.85789000
H	1.52229500	-1.51467500	1.33842200
H	0.52092400	-0.10704200	1.35175000
H	-1.81741000	1.93512500	0.20494800
N	-1.30136600	1.06652000	0.09186200
C	-2.19362400	-0.00829900	-0.08954100
H	-0.56826900	1.13397400	-0.61301100
O	-3.38489500	0.06114200	0.21018000
N	-1.59276800	-1.13284700	-0.62565700
H	-0.59880900	-1.26130100	-0.45194000
H	-2.16811400	-1.96565700	-0.58251800

D5 optimized with MP2/aug-cc-pVDZ

C	1.86146700	-0.11086900	0.15263400
O	2.63990800	-0.95539800	-0.28647300
N	1.59272100	1.09360700	-0.54122600
H	1.42940100	1.89199800	0.06805200
H	2.32950400	1.27861400	-1.21777300
N	1.15369400	-0.22898600	1.33094300
H	1.17234500	-1.16310200	1.72471300
H	0.25996900	0.25898800	1.38381600
H	-1.17307000	-1.16991400	-1.72032700
N	-1.15380800	-0.23435100	-1.33004100
C	-1.86148900	-0.11134900	-0.15217400
H	-0.25990100	0.25303700	-1.38495800
O	-2.64033000	-0.95380200	0.29017800
N	-1.59219400	1.09572500	0.53700600
H	-1.42866800	1.89164100	-0.07545900
H	-2.32896600	1.28368400	1.21275700

D6 optimized with MP2/aug-cc-pVDZ

C	2.04190100	0.07263100	-0.00509500
O	1.41837100	1.14756600	-0.07272300
N	3.41751400	0.05318100	0.21672000
H	3.93402800	-0.72335500	-0.18138700
H	3.84847700	0.95866700	0.06666500
N	1.45061700	-1.15332400	-0.12626900
H	0.42232900	-1.18049400	-0.11761500
H	1.94300400	-1.96474400	0.22313700
H	-0.42283000	1.18082400	-0.12183200
N	-1.45104400	1.15341900	-0.12775600
C	-2.04190200	-0.07258000	-0.00598800
H	-1.94297300	1.96494000	0.22198700
O	-1.41825800	-1.14739500	-0.07497100
N	-3.41712900	-0.05345400	0.21831800
H	-3.93457300	0.72283100	-0.17907900
H	-3.84806400	-0.95909300	0.06908800

D7 optimized with MP2/aug-cc-pVDZ

C	1.90830900	0.00664200	0.01923900
O	1.29112300	0.90181600	0.62305800
N	3.28219600	0.06283600	-0.15850800
H	3.67731700	-0.42092300	-0.95648100
H	3.67515800	0.97868500	0.02579000
N	1.28887300	-1.10048800	-0.50853900
H	0.33445900	-1.25618600	-0.17591000
H	1.84609300	-1.92236400	-0.70483100
H	-1.84413600	1.74936800	-1.09936700
N	-1.47548600	1.23885000	-0.30793700
C	-2.10690500	0.05208100	-0.02889300
H	-0.48906100	1.34026800	-0.06710000
O	-3.17378300	-0.31029300	-0.52716500
N	-1.39574500	-0.75640900	0.88732800
H	-0.82907500	-0.23652600	1.55596900
H	-2.01676400	-1.43035400	1.32630800

9. Cartesian Coordinates of the optimized urea oligomers

n=4 urea cluster optimized with B3LYP/6-31G(d,p)

C	0.189900	-2.433300	0.581200
O	0.527400	-2.307100	-0.607800
N	0.846100	-1.818300	1.600000
H	1.408700	-0.996800	1.375100
H	0.501100	-1.915300	2.541700
N	-0.846100	-3.278900	0.960500
H	-1.341600	-3.614300	0.144300
H	-1.490600	-2.859700	1.621100
C	-0.189900	2.433300	0.581200
O	-0.527400	2.307100	-0.607800
N	0.846100	3.278900	0.960500
H	1.341600	3.614300	0.144300
H	1.490600	2.859700	1.621100
N	-0.846100	1.818300	1.600000
H	-1.408700	0.996800	1.375100
H	-0.501100	1.915300	2.541700
C	-2.433300	-0.189900	-0.581200
O	-2.307100	-0.527400	0.607800

N	-3.278900	0.846100	-0.960500
H	-3.614300	1.341600	-0.144300
H	-2.859700	1.490600	-1.621100
N	-1.818300	-0.846100	-1.600000
H	-0.996800	-1.408700	-1.375100
H	-1.915300	-0.501100	-2.541700
C	2.433300	0.189900	-0.581200
O	2.307100	0.527400	0.607800
N	1.818300	0.846100	-1.600000
H	0.996800	1.408700	-1.375100
H	1.915300	0.501100	-2.541700
N	3.278900	-0.846100	-0.960500
H	3.614300	-1.341600	-0.144300
H	2.859700	-1.490600	-1.621100

n=7 urea cluster optimized with B3LYP/6-31G(d,p)

C	3.733200	1.402600	-1.043400
O	3.197600	1.996700	-1.988600
N	3.341900	1.492300	0.256200
H	2.450300	1.954800	0.385000
H	3.506000	0.678900	0.861300
N	4.801000	0.532900	-1.267500
H	5.226200	0.665400	-2.175100
H	5.461100	0.424300	-0.507600
C	0.000000	0.000000	2.534200
O	0.000000	0.000000	1.291300
N	-1.097100	0.386400	3.261900
H	-1.984400	0.470700	2.753600
H	-1.160600	0.107700	4.230000
N	1.097100	-0.386400	3.261900
H	1.984400	-0.470700	2.753600
H	1.160600	-0.107700	4.230000
C	-3.733200	-1.402600	-1.043400
O	-3.197600	-1.996700	-1.988600
N	-4.801000	-0.532900	-1.267500
H	-5.226200	-0.665400	-2.175100
H	-5.461100	-0.424300	-0.507600
N	-3.341900	-1.492300	0.256200
H	-2.450300	-1.954800	0.385000
H	-3.506000	-0.678900	0.861300
C	3.012800	-1.958600	1.008200
O	3.443600	-0.988600	1.683300
N	2.230000	-2.928500	1.562300
H	1.812400	-2.694000	2.450100
H	1.699500	-3.516900	0.920700
N	3.326000	-2.137200	-0.299800
H	3.819200	-1.390400	-0.774100
H	2.779600	-2.805800	-0.834600
C	0.000000	-3.308500	-1.272300
O	1.020800	-3.908500	-0.880100
N	-0.832300	-3.838100	-2.214600
H	-0.670800	-4.805400	-2.443000
H	-1.767000	-3.452200	-2.312800
N	-0.380500	-2.083600	-0.803900
H	0.198100	-1.565500	-0.155100
H	-1.104600	-1.583900	-1.301400
C	0.000000	3.308500	-1.272300
O	-1.020800	3.908500	-0.880100
N	0.380500	2.083600	-0.803900
H	-0.198100	1.565500	-0.155100
H	1.104600	1.583900	-1.301400

N	0.832300	3.838100	-2.214600
H	0.670800	4.805400	-2.443000
H	1.767000	3.452200	-2.312800
C	-3.012800	1.958600	1.008200
O	-3.443600	0.988600	1.683300
N	-3.326000	2.137200	-0.299800
H	-3.819200	1.390400	-0.774100
H	-2.779600	2.805800	-0.834600
N	-2.230000	2.928500	1.562300
H	-1.812400	2.694000	2.450100
H	-1.699500	3.516900	0.920700

n=12 urea cluster optimized with B3LYP/6-31G(d,p)

C	2.495200	2.408000	3.674000
O	1.853400	1.354700	3.410100
N	3.428400	2.874700	2.802100
H	3.347100	2.533700	1.837000
H	3.808800	3.799900	2.929300
N	2.308300	3.067400	4.845400
H	1.429500	2.878000	5.344200
H	2.670900	4.004300	4.939700
C	-0.682400	2.728300	0.005900
O	-1.932700	2.699800	-0.161400
N	0.177200	2.849200	-1.035500
H	-0.209900	2.600700	-1.942200
H	1.168100	2.696000	-0.856400
N	-0.132500	2.686600	1.248000
H	-0.746000	2.501100	2.029000
H	0.839300	2.418100	1.345200
C	-2.053700	-1.175700	-5.456200
O	-2.794700	-0.323800	-5.962300
N	-1.853400	-2.393000	-6.063100
H	-2.489600	-2.601300	-6.816800
H	-1.528500	-3.174600	-5.514500
N	-1.385300	-0.991800	-4.268100
H	-1.345200	-0.012300	-3.982300
H	-0.507100	-1.490600	-4.137300
C	2.053700	1.175700	-5.456200
O	2.794700	0.323800	-5.962300
N	1.385300	0.991800	-4.268100
H	1.345200	0.012300	-3.982300
H	0.507100	1.490600	-4.137300
N	1.853400	2.393000	-6.063100
H	2.489600	2.601300	-6.816800
H	1.528500	3.174600	-5.514500
C	0.682400	-2.728300	0.005900
O	1.932700	-2.699800	-0.161400
N	0.132500	-2.686600	1.248000
H	0.746000	-2.501100	2.029000
H	-0.839300	-2.418100	1.345200
N	-0.177200	-2.849200	-1.035500
H	0.209900	-2.600700	-1.942200
H	-1.168100	-2.696000	-0.856400
C	-2.495200	-2.408000	3.674000
O	-1.853400	-1.354700	3.410100
N	-2.308300	-3.067400	4.845400
H	-1.429500	-2.878000	5.344200
H	-2.670900	-4.004300	4.939700
N	-3.428400	-2.874700	2.802100
H	-3.347100	-2.533700	1.837000
H	-3.808800	-3.799900	2.929300

C	-1.175700	2.053700	5.456200
O	-0.323800	2.794700	5.962300
N	-2.393000	1.853400	6.063100
H	-2.601300	2.489600	6.816800
H	-3.174600	1.528500	5.514500
N	-0.991800	1.385300	4.268100
H	-0.012300	1.345200	3.982300
H	-1.490600	0.507100	4.137300
C	-2.408000	2.495200	-3.674000
O	-1.354700	1.853400	-3.410100
N	-3.067400	2.308300	-4.845400
H	-2.878000	1.429500	-5.344200
H	-4.004300	2.670900	-4.939700
N	-2.874700	3.428400	-2.802100
H	-2.533700	3.347100	-1.837000
H	-3.799900	3.808800	-2.929300
C	2.728300	0.682400	-0.005900
O	2.699800	1.932700	0.161400
N	2.849200	-0.177200	1.035500
H	2.600700	0.209900	1.942200
H	2.696000	-1.168100	0.856400
N	2.686600	0.132500	-1.248000
H	2.501100	0.746000	-2.029000
H	2.418100	-0.839300	-1.345200
C	-2.728300	-0.682400	-0.005900
O	-2.699800	-1.932700	0.161400
N	-2.686600	-0.132500	-1.248000
H	-2.501100	-0.746000	-2.029000
H	-2.418100	0.839300	-1.345200
N	-2.849200	0.177200	1.035500
H	-2.600700	-0.209900	1.942200
H	-2.696000	1.168100	0.856400
C	2.408000	-2.495200	-3.674000
O	1.354700	-1.853400	-3.410100
N	2.874700	-3.428400	-2.802100
H	2.533700	-3.347100	-1.837000
H	3.799900	-3.808800	-2.929300
N	3.067400	-2.308300	-4.845400
H	2.878000	-1.429500	-5.344200
H	4.004300	-2.670900	-4.939700
C	1.175700	-2.053700	5.456200
O	0.323800	-2.794700	5.962300
N	0.991800	-1.385300	4.268100
H	0.012300	-1.345200	3.982300
H	1.490600	-0.507100	4.137300
N	2.393000	-1.853400	6.063100
H	2.601300	-2.489600	6.816800
H	3.174600	-1.528500	5.514500

n=24 urea cluster optimized with B3LYP/6-31G(d,p)

C	-3.283300	4.544100	2.972400
O	-4.346800	4.333400	2.334900
N	-2.559300	3.541300	3.527200
H	-2.742600	2.579900	3.231700
H	-1.638800	3.732100	3.901300
N	-2.826400	5.815200	3.206300
H	-3.353300	6.532500	2.732000
H	-1.813900	5.967500	3.244200
C	1.268300	2.465200	3.315100
O	1.133800	2.404100	2.065700
N	1.793500	1.438400	4.014300

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H       2.156600    0.618300    3.513800
H       1.894200    1.486700    5.014800
N       0.835100    3.558000    4.018300
H       0.654400    4.417400    3.480800
H       1.202700    3.702600    4.948000
C       5.993900   -0.862600    2.910600
O       6.252600   -0.888300    1.684700
N       5.812300   -2.017300    3.611600
H       5.520800   -2.825600    3.060100
H       5.359600   -1.958200    4.512000
N       5.964900    0.318000    3.589700
H       5.839800    1.152600    3.016200
H       5.496900    0.344000    4.482800
C      -5.993900    0.862600    2.910600
O      -6.252600    0.888300    1.684700
N      -5.964900   -0.318000    3.589700
H      -5.839800   -1.152600    3.016200
H      -5.496900   -0.344000    4.482800
N      -5.812300    2.017300    3.611600
H      -5.520800    2.825600    3.060100
H      -5.359600    1.958200    4.512000
C      -1.268300   -2.465200    3.315100
O      -1.133800   -2.404100    2.065700
N      -0.835100   -3.558000    4.018300
H      -0.654400   -4.417400    3.480800
H      -1.202700   -3.702600    4.948000
N      -1.793500   -1.438400    4.014300
H      -2.156600   -0.618300    3.513800
H      -1.894200   -1.486700    5.014800
C       3.283300   -4.544100    2.972400
O       4.346800   -4.333400    2.334900
N       2.826400   -5.815200    3.206300
H       3.353300   -6.532500    2.732000
H       1.813900   -5.967500    3.244200
N       2.559300   -3.541300    3.527200
H       2.742600   -2.579900    3.231700
H       1.638800   -3.732100    3.901300
C      -3.332900    5.042200   -1.041800
O      -2.833900    5.376600   -2.120000
N      -3.541300    3.740600   -0.675200
H      -3.004200    3.038100   -1.171000
H      -3.780900    3.544000    0.291200
N      -3.740600    5.976600   -0.099900
H      -3.964600    6.878900   -0.494300
H      -4.321100    5.643500    0.667700
C       0.824300    2.628500   -1.405500
O       0.820600    2.831300   -2.651400
N       1.184900    1.431800   -0.886900
H       1.507500    0.698200   -1.505300
H       1.315500    1.308800    0.108200
N       0.430900    3.582200   -0.530100
H       0.376100    4.529600   -0.891000
H       0.568000    3.441700    0.466100
C       6.305000   -0.325000   -1.558900
O       5.924700   -0.032900   -2.721200
N       6.308900   -1.609000   -1.106700
H       5.802800   -2.290300   -1.651100
H       6.378300   -1.769900   -0.105900
N       6.787400    0.610300   -0.695700
H       6.547700    1.575000   -0.884200
H       6.841700    0.351700    0.287500
C      -6.305000    0.325000   -1.558900
O      -5.924700    0.032900   -2.721200
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N	-6.787400	-0.610300	-0.695700
H	-6.547700	-1.575000	-0.884200
H	-6.841700	-0.351700	0.287500
N	-6.308900	1.609000	-1.106700
H	-5.802800	2.290300	-1.651100
H	-6.378300	1.769900	-0.105900
C	-0.824300	-2.628500	-1.405500
O	-0.820600	-2.831300	-2.651400
N	-0.430900	-3.582200	-0.530100
H	-0.376100	-4.529600	-0.891000
H	-0.568000	-3.441700	0.466100
N	-1.184900	-1.431800	-0.886900
H	-1.507500	-0.698200	-1.505300
H	-1.315500	-1.308800	0.108200
C	3.332900	-5.042200	-1.041800
O	2.833900	-5.376600	-2.120000
N	3.740600	-5.976600	-0.099900
H	3.964600	-6.878900	-0.494300
H	4.321100	-5.643500	0.667700
N	3.541300	-3.740600	-0.675200
H	3.004200	-3.038100	-1.171000
H	3.780900	-3.544000	0.291200
C	0.325000	6.305000	1.558900
O	0.032900	5.924700	2.721200
N	1.609000	6.308900	1.106700
H	2.290300	5.802800	1.651100
H	1.769900	6.378300	0.105900
N	-0.610300	6.787400	0.695700
H	-1.575000	6.547700	0.884200
H	-0.351700	6.841700	-0.287500
C	5.042200	3.332900	1.041800
O	5.376600	2.833900	2.120000
N	5.976600	3.740600	0.099900
H	6.878900	3.964600	0.494300
H	5.643500	4.321100	-0.667700
N	3.740600	3.541300	0.675200
H	3.038100	3.004200	1.171000
H	3.544000	3.780900	-0.291200
C	-2.628500	0.824300	1.405500
O	-2.831300	0.820600	2.651400
N	-1.431800	1.184900	0.886900
H	-0.698200	1.507500	1.505300
H	-1.308800	1.315500	-0.108200
N	-3.582200	0.430900	0.530100
H	-4.529600	0.376100	0.891000
H	-3.441700	0.568000	-0.466100
C	2.628500	-0.824300	1.405500
O	2.831300	-0.820600	2.651400
N	3.582200	-0.430900	0.530100
H	4.529600	-0.376100	0.891000
H	3.441700	-0.568000	-0.466100
N	1.431800	-1.184900	0.886900
H	0.698200	-1.507500	1.505300
H	1.308800	-1.315500	-0.108200
C	-5.042200	-3.332900	1.041800
O	-5.376600	-2.833900	2.120000
N	-3.740600	-3.541300	0.675200
H	-3.038100	-3.004200	1.171000
H	-3.544000	-3.780900	-0.291200
N	-5.976600	-3.740600	0.099900
H	-6.878900	-3.964600	0.494300
H	-5.643500	-4.321100	-0.667700
C	-0.325000	-6.305000	1.558900

O	-0.032900	-5.924700	2.721200
N	0.610300	-6.787400	0.695700
H	1.575000	-6.547700	0.884200
H	0.351700	-6.841700	-0.287500
N	-1.609000	-6.308900	1.106700
H	-2.290300	-5.802800	1.651100
H	-1.769900	-6.378300	0.105900
C	0.862600	5.993900	-2.910600
O	0.888300	6.252600	-1.684700
N	2.017300	5.812300	-3.611600
H	2.825600	5.520800	-3.060100
H	1.958200	5.359600	-4.512000
N	-0.318000	5.964900	-3.589700
H	-1.152600	5.839800	-3.016200
H	-0.344000	5.496900	-4.482800
C	4.544100	3.283300	-2.972400
O	4.333400	4.346800	-2.334900
N	5.815200	2.826400	-3.206300
H	6.532500	3.353300	-2.732000
H	5.967500	1.813900	-3.244200
N	3.541300	2.559300	-3.527200
H	2.579900	2.742600	-3.231700
H	3.732100	1.638800	-3.901300
C	-2.465200	1.268300	-3.315100
O	-2.404100	1.133800	-2.065700
N	-1.438400	1.793500	-4.014300
H	-0.618300	2.156600	-3.513800
H	-1.486700	1.894200	-5.014800
N	-3.558000	0.835100	-4.018300
H	-4.417400	0.654400	-3.480800
H	-3.702600	1.202700	-4.948000
C	2.465200	-1.268300	-3.315100
O	2.404100	-1.133800	-2.065700
N	3.558000	-0.835100	-4.018300
H	4.417400	-0.654400	-3.480800
H	3.702600	-1.202700	-4.948000
N	1.438400	-1.793500	-4.014300
H	0.618300	-2.156600	-3.513800
H	1.486700	-1.894200	-5.014800
C	-4.544100	-3.283300	-2.972400
O	-4.333400	-4.346800	-2.334900
N	-3.541300	-2.559300	-3.527200
H	-2.579900	-2.742600	-3.231700
H	-3.732100	-1.638800	-3.901300
N	-5.815200	-2.826400	-3.206300
H	-6.532500	-3.353300	-2.732000
H	-5.967500	-1.813900	-3.244200
C	-0.862600	-5.993900	-2.910600
O	-0.888300	-6.252600	-1.684700
N	0.318000	-5.964900	-3.589700
H	1.152600	-5.839800	-3.016200
H	0.344000	-5.496900	-4.482800
N	-2.017300	-5.812300	-3.611600
H	-2.825600	-5.520800	-3.060100
H	-1.958200	-5.359600	-4.512000

n=4 urea cluster optimized with AM1

C	0.715100	0.818100	0.029800
O	1.347300	1.256400	-0.979400
N	-0.404500	1.503400	0.499300
H	-0.462600	2.456300	0.210500

H	-0.703500	1.318900	1.431800
N	1.077900	-0.409000	0.581200
H	1.939500	-0.779000	0.259300
H	0.824600	-0.603100	1.522400
C	0.874800	4.828300	-0.126100
O	0.246600	4.389900	0.885500
N	0.508100	6.054200	-0.677700
H	-0.353400	6.422500	-0.353200
H	0.756500	6.246800	-1.620600
N	1.993800	4.144100	-0.598800
H	2.054200	3.191500	-0.309200
H	2.288700	4.327600	-1.532900
C	0.741200	3.729200	-4.028300
O	1.037600	4.726000	-3.309800
N	-0.071500	3.922400	-5.149700
H	-0.181100	4.868400	-5.430400
H	-0.073000	3.245000	-5.871700
N	1.236800	2.464600	-3.715200
H	1.589600	2.365400	-2.785600
H	0.764400	1.666900	-4.068400
C	0.868600	1.922300	3.913700
O	0.547400	0.922000	3.211000
N	0.362300	3.185700	3.611400
H	-0.019900	3.279200	2.693000
H	0.851100	3.984400	3.939800
N	1.719500	1.734500	5.007300
H	1.836100	0.790000	5.290000
H	1.746400	2.416100	5.724900

n=7 urea cluster optimized with AM1

C	0.264400	-0.248200	0.786800
O	0.539400	0.511800	-0.185900
N	0.097800	0.274600	2.065300
H	0.447600	1.203800	2.198400
H	0.193900	-0.331200	2.844300
N	0.112200	-1.618200	0.547300
H	0.018100	-1.870000	-0.408000
H	-0.379600	-2.175100	1.201400
C	0.375100	6.163100	-0.114200
O	1.603800	5.892900	-0.291700
N	0.006400	7.467400	0.202200
H	0.755100	8.061800	0.495100
H	-0.854700	7.628100	0.673500
N	-0.572300	5.146100	-0.246400
H	-0.263400	4.374000	-0.803600
H	-1.518600	5.409300	-0.393500
C	0.486900	10.562400	-0.348300
O	1.544900	10.076600	0.159500
N	-0.677000	10.543600	0.402600
H	-0.611400	10.213100	1.339300
H	-1.474000	11.058100	0.132100
N	0.524100	11.135800	-1.623300
H	1.302700	10.831100	-2.177700
H	-0.330700	11.178600	-2.129100
C	1.103500	3.386900	-3.206300
O	0.178800	4.202700	-2.922900
N	1.854100	3.576200	-4.370400
H	1.759100	4.474500	-4.787000
H	2.751900	3.161400	-4.434700
N	1.363800	2.323000	-2.350500
H	0.654700	2.115800	-1.681200

H	1.907000	1.554700	-2.658400
C	1.881200	8.014900	-2.784200
O	1.405300	9.019300	-3.387900
N	2.795600	8.198700	-1.746600
H	2.806900	9.116300	-1.356400
H	2.926500	7.453300	-1.100400
N	1.580000	6.722700	-3.239400
H	0.795800	6.679900	-3.850800
H	1.622800	5.980000	-2.573500
C	2.070100	3.490100	1.973900
O	1.692300	2.685500	2.877200
N	2.558100	4.750100	2.335100
H	2.330700	5.036200	3.257100
H	2.595400	5.461400	1.641800
N	2.082000	3.088600	0.649700
H	1.697400	2.197300	0.439500
H	2.182700	3.752500	-0.080300
C	0.925400	8.617400	3.335700
O	-0.207600	8.689100	2.780200
N	1.891500	9.587500	3.075900
H	1.735600	10.117500	2.240900
H	2.840300	9.379700	3.277500
N	1.187300	7.554100	4.210000
H	0.378100	7.062100	4.513700
H	1.907100	7.657200	4.884300

n=12 urea cluster optimized with AM1

C	0.204300	4.729600	0.502000
O	-0.832800	5.442800	0.624900
N	1.394500	5.123400	1.094200
H	1.337400	5.832100	1.792100
H	2.160200	4.488500	1.155000
N	0.135900	3.539100	-0.236400
H	-0.617400	3.503500	-0.882600
H	0.991700	3.124300	-0.532100
C	6.528200	3.031300	1.548600
O	6.118700	1.941600	2.074100
N	7.798500	3.475200	1.839400
H	8.292300	3.015700	2.570100
H	8.134700	4.355700	1.531800
N	5.716400	3.681800	0.613100
H	4.757300	3.388300	0.638600
H	5.833200	4.665700	0.523200
C	10.504800	2.739300	4.071600
O	9.323500	3.034300	4.435400
N	11.140900	3.561600	3.158200
H	10.678200	4.407000	2.907200
H	12.104400	3.470600	2.964500
N	11.138300	1.620300	4.616400
H	10.508900	0.943700	5.004300
H	11.900000	1.228100	4.113800
C	0.244100	8.077600	3.299400
O	1.330800	7.415800	3.245700
N	-0.011400	8.884400	4.409700
H	0.798100	9.142500	4.939500
H	-0.687900	9.605400	4.316700
N	-0.667400	7.969100	2.262700
H	-0.530400	7.220500	1.615400
H	-1.596100	8.288900	2.384200
C	4.953800	8.026900	1.213200
O	5.333600	8.866700	2.091600

N	5.882500	7.577500	0.275400
H	6.696100	8.147700	0.169100
H	5.552700	7.134300	-0.548300
N	3.635900	7.584400	1.188800
H	3.107800	7.758400	2.018800
H	3.452700	6.700300	0.767900
C	11.521100	8.234100	1.066400
O	11.824000	9.454100	0.925200
N	10.722500	7.596800	0.115300
H	10.204000	8.217700	-0.468700
H	10.246600	6.766600	0.389100
N	12.080700	7.503700	2.118300
H	12.555200	8.045900	2.799700
H	11.604300	6.692700	2.436900
C	2.699600	1.262800	0.995800
O	2.808600	2.450900	0.573200
N	3.817500	0.427100	1.006600
H	4.692500	0.906000	0.926600
H	3.816100	-0.361500	1.607800
N	1.458200	0.799700	1.422800
H	0.680000	1.383700	1.226900
H	1.289700	-0.171100	1.507000
C	8.127400	-0.136600	3.675000
O	9.283400	-0.541400	3.988700
N	7.474800	0.805400	4.478700
H	8.090200	1.318400	5.075600
H	6.762700	1.353100	4.047900
N	7.463800	-0.719400	2.592200
H	8.027400	-1.306500	2.024900
H	6.757900	-0.193100	2.131700
C	3.515100	4.385900	3.485400
O	3.938700	4.996200	2.459500
N	3.673300	3.005800	3.575100
H	4.272800	2.593400	2.892300
H	3.633900	2.565000	4.460600
N	2.900600	5.108100	4.509400
H	2.579700	6.015500	4.246100
H	2.331700	4.623200	5.160900
C	8.511400	6.497200	2.985100
O	9.460800	5.988700	2.303600
N	7.961100	5.758300	4.017100
H	8.436800	4.922300	4.279900
H	7.341800	6.172800	4.666200
N	8.069700	7.779100	2.684500
H	8.375100	8.135900	1.804400
H	7.171800	8.082500	2.988500
C	3.443600	10.113100	4.501000
O	2.340800	10.581400	4.904600
N	4.457100	10.983700	4.102000
H	4.186900	11.931800	4.002200
H	5.177100	10.645400	3.509000
N	3.679800	8.736300	4.562200
H	2.853700	8.180900	4.622600
H	4.405100	8.363600	3.991300
C	8.528000	10.463300	0.583000
O	8.376600	9.322500	0.046000
N	9.636300	11.244500	0.251500
H	10.400600	10.718400	-0.130000
H	9.910600	11.951800	0.893300
N	7.561500	10.907900	1.473400
H	6.735300	10.357100	1.551700
H	7.524200	11.854500	1.751800

n=24 urea cluster optimized with AM1

C	1.523200	2.266700	1.245100
O	0.921000	2.196300	2.360900
N	1.494600	3.462400	0.530100
H	1.210300	4.265000	1.049500
H	2.178600	3.622800	-0.168200
N	2.093600	1.120800	0.705300
H	2.190600	0.346600	1.328200
H	2.774000	1.202800	-0.009400
C	5.773500	2.408200	1.680900
O	5.209200	2.838000	2.737200
N	6.723700	3.199200	1.036000
H	7.057200	3.975300	1.567800
H	7.421600	2.725900	0.508300
N	5.332700	1.213700	1.103700
H	4.750500	0.660900	1.700700
H	6.008400	0.695300	0.587000
C	11.399900	3.146500	1.650700
O	12.017700	2.682400	2.657700
N	11.787900	4.381300	1.121300
H	12.412000	4.897400	1.697300
H	11.095900	4.918500	0.651200
N	10.429700	2.376000	1.012400
H	10.120100	1.574500	1.520000
H	9.715500	2.857400	0.516900
C	0.307400	9.145700	1.782900
O	-0.241100	8.616600	2.797400
N	0.173100	10.521600	1.570600
H	-0.190000	11.027200	2.344800
H	0.878000	10.980800	1.041100
N	0.945800	8.347700	0.844900
H	1.079200	7.392000	1.099100
H	1.625200	8.757800	0.251000
C	5.534800	8.413700	1.750700
O	6.080900	7.858700	2.756100
N	6.008100	9.649200	1.300900
H	6.612200	10.124500	1.939400
H	5.362400	10.233000	0.816500
N	4.561200	7.729500	1.034600
H	4.227600	6.879800	1.438700
H	3.906400	8.253700	0.503800
C	9.403200	8.521700	1.124400
O	9.978800	8.455800	2.254000
N	9.087900	9.765300	0.586500
H	9.106400	10.528900	1.230600
H	8.406800	9.820700	-0.131200
N	9.211100	7.351100	0.396000
H	9.326900	6.502000	0.904600
H	8.558300	7.340900	-0.347700
C	-0.210500	2.690900	5.556800
O	-0.533000	2.631500	6.779900
N	1.081100	3.097400	5.203900
H	1.528000	3.697900	5.864500
H	1.260800	3.296300	4.244200
N	-1.128900	2.318700	4.586100
H	-1.928900	1.828900	4.902100
H	-0.845500	2.200100	3.641300
C	5.310200	2.908200	6.214000
O	5.337500	2.988300	7.480900
N	6.445500	3.254500	5.479700
H	7.098000	3.836700	5.961300

H	6.337000	3.433800	4.504500
N	4.153100	2.466100	5.582300
H	3.514400	1.961600	6.159700
H	4.186800	2.217000	4.618900
C	11.796900	2.510400	6.067500
O	11.561100	2.657700	7.307600
N	12.946700	3.055400	5.522600
H	13.474700	3.661500	6.098700
H	13.096400	3.064300	4.541400
N	10.878800	1.840200	5.267200
H	10.235900	1.243600	5.740000
H	11.135800	1.589100	4.338700
C	0.065800	8.912400	6.202600
O	0.341900	8.880500	7.441800
N	0.558900	9.936800	5.416100
H	1.232000	10.545500	5.825700
H	0.467800	9.906300	4.429500
N	-0.704900	7.889300	5.653400
H	-1.232700	7.357300	6.302900
H	-1.075600	7.988700	4.736500
C	5.811700	7.895500	6.226000
O	5.652300	8.023000	7.482000
N	6.978800	8.359400	5.644100
H	7.564700	8.931700	6.208400
H	7.077100	8.404200	4.656900
N	4.804000	7.323300	5.455200
H	4.128400	6.785100	5.954700
H	5.023700	7.025100	4.530300
C	11.076700	8.444300	5.495900
O	11.339300	8.650900	6.718000
N	11.910900	8.973700	4.518500
H	12.549100	9.668000	4.821500
H	11.619700	8.993900	3.568500
N	9.940600	7.714200	5.144800
H	9.585200	7.105600	5.850400
H	9.855200	7.400200	4.203600
C	3.242000	-0.330900	3.968600
O	3.454100	-0.572500	2.741900
N	4.258800	-0.595500	4.895000
H	4.956400	-1.224300	4.568900
H	4.016200	-0.667900	5.857500
N	2.028400	0.200200	4.370300
H	1.477200	0.633100	3.660400
H	1.914900	0.525800	5.302800
C	8.169500	0.335000	3.135900
O	8.111300	0.770800	1.944300
N	9.334500	-0.280200	3.577300
H	9.958300	-0.600700	2.878200
H	9.365900	-0.707600	4.473300
N	7.069600	0.459000	3.978300
H	6.378900	1.119500	3.700500
H	7.203800	0.349200	4.959400
C	2.325400	5.714100	3.137000
O	2.359800	5.939800	1.883100
N	3.419600	5.102000	3.740300
H	4.011200	4.574200	3.134800
H	3.335800	4.777700	4.677700
N	1.211700	6.091400	3.867300
H	0.578600	6.721100	3.422500
H	1.246400	6.097600	4.861600
C	8.915800	4.997100	3.293500
O	9.034000	4.768200	2.045700
N	9.955900	4.657200	4.152200

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H      10.623100    4.014000    3.786800
H       9.772800    4.592200    5.130200
N       7.749900    5.582900    3.769400
H       7.197900    6.069600    3.096300
H       7.721200    5.924100    4.704000
C       3.039300   10.552400    2.885200
O       3.130300   10.320800    1.637600
N       3.487100    9.613300    3.786600
H       3.790400    8.736100    3.442600
H       3.403500    9.745600    4.766900
N       2.421400   11.729000    3.327600
H       2.425400   12.465200    2.659900
H       2.557700   12.003900    4.277800
C       8.130700   11.556300    3.802000
O       7.909300   11.663800    2.556900
N       9.017800   10.597700    4.266300
H       9.288300    9.893600    3.614700
H       9.055700   10.377800    5.235200
N       7.468500   12.409800    4.679800
H       7.083500   13.229700    4.279300
H       7.726400   12.433600    5.638000
C       1.958200    0.323300    8.310400
O       2.745500    0.317200    7.318300
N       1.805100   -0.849300    9.049000
H       2.476200   -1.558900    8.877200
H       1.404600   -0.816900    9.952900
N       1.289900    1.494100    8.673800
H       1.250300    2.183400    7.946300
H       0.433600    1.400800    9.171600
C       8.224900    0.665600    7.561700
O       8.642200    0.099400    6.503600
N       9.130500    1.264000    8.419200
H      10.062300    1.387700    8.086700
H       8.815800    1.863000    9.140000
N       6.868700    0.573700    7.902000
H       6.285900    0.265200    7.156200
H       6.473100    1.309700    8.447000
C       2.475900    5.495900    7.830300
O       2.502200    5.503900    6.559400
N       2.860900    4.347200    8.512900
H       3.399400    3.688600    7.988300
H       3.080700    4.409500    9.477100
N       2.057200    6.637200    8.507500
H       1.567300    7.309400    7.954400
H       1.769600    6.560800    9.452600
C       8.658800    5.417700    7.925600
O       8.512100    5.366700    6.665100
N       9.453900    4.459000    8.558400
H      10.045700    3.934200    7.945700
H       9.848800    4.681700    9.440700
N       8.020500    6.415300    8.646600
H       7.317000    6.933900    8.163700
H       7.918100    6.326300    9.626600
C       3.857900   10.647000    7.117300
O       3.169800   11.282200    6.254000
N       5.213200   10.950200    7.272200
H       5.608800   11.492500    6.538500
H       5.816500   10.248500    7.647500
N       3.240800    9.737100    7.952300
H       2.263000    9.593000    7.829800
H       3.774000    9.033100    8.405700
C       8.709700   10.948900    8.247300
O       8.100700   10.850700    7.138200
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N	10.096900	10.825900	8.292500
H	10.502500	10.388800	7.488300
H	10.521900	10.581000	9.155500
N	7.973600	11.219200	9.394600
H	7.027100	11.486500	9.262200
H	8.422500	11.510100	10.225700

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C	-0.400000	3.660800	2.283500
O	-0.761600	2.909000	3.246300
N	-0.959300	4.926700	2.158700
H	-1.484900	5.251700	2.934100
H	-0.492300	5.627400	1.627900
N	0.468800	3.179100	1.318400
H	0.846900	2.269300	1.466800
H	0.998700	3.819300	0.777700
C	5.698000	2.779800	1.399200
O	5.343400	3.283200	2.512700
N	6.833000	3.274300	0.735000
H	7.363300	3.919900	1.287400
H	7.391200	2.590500	0.273000
N	4.935800	1.771600	0.847700
H	4.049100	1.576700	1.259400
H	5.118800	1.430300	-0.060600
C	11.173000	3.431600	1.592500
O	11.209100	3.139200	2.829300
N	12.168000	4.234300	1.043500
H	12.746800	4.710400	1.706700
H	11.969500	4.734800	0.209600
N	10.135700	2.922700	0.819700
H	9.608800	2.183700	1.234400
H	10.211300	2.926400	-0.167000
C	16.544700	2.382700	1.681400
O	17.194500	3.072100	2.531800
N	15.473800	2.942900	1.005100
H	15.160200	3.829100	1.334500
H	14.798400	2.343900	0.589100
N	16.985900	1.097300	1.365100
H	17.672200	0.723700	1.975700
H	16.329800	0.454300	0.981700
C	-0.357500	8.616000	1.532300
O	-0.899800	7.794300	2.340400
N	-0.928000	9.875200	1.353400
H	-1.619200	10.124000	2.019400
H	-0.355000	10.609800	1.001500
N	0.731700	8.220300	0.777000
H	1.123600	7.330300	0.990100
H	1.320100	8.907800	0.366900
C	5.468300	7.854200	1.361100
O	5.145600	8.440300	2.445700
N	6.694400	8.147700	0.753200
H	7.324000	8.668100	1.329800
H	7.132200	7.410000	0.247900
N	4.556200	7.019700	0.748800
H	3.708100	6.819700	1.227000
H	4.822100	6.433900	-0.000900
C	11.434800	7.885400	1.706900
O	11.679300	7.766000	2.950400
N	12.164600	8.792000	0.959900
H	12.785800	9.390100	1.460500
H	11.802200	9.122300	0.100300

N	10.535200	6.999500	1.084900
H	9.962700	6.505200	1.741700
H	10.001000	7.394400	0.340200
C	16.895500	7.308900	2.719700
O	17.322400	8.059700	3.657500
N	15.982800	7.806000	1.804000
H	15.609000	8.710500	1.992700
H	15.410700	7.170500	1.300400
N	17.433900	6.034300	2.568500
H	17.988200	5.713900	3.325800
H	16.911400	5.333000	2.089300
C	0.208900	3.201600	6.563200
O	0.588700	3.349100	7.767300
N	1.086600	3.521800	5.528300
H	1.826700	4.142300	5.770600
H	0.728300	3.600300	4.602300
N	-1.054200	2.707000	6.291400
H	-1.544000	2.292500	7.044800
H	-1.325000	2.486500	5.360700
C	5.191000	2.894200	5.930000
O	5.128100	2.688900	7.185100
N	6.384600	3.350100	5.368900
H	6.979800	3.855700	5.991200
H	6.361900	3.677900	4.426100
N	4.071600	2.645400	5.148400
H	3.388100	2.037900	5.549600
H	4.160100	2.620900	4.155700
C	10.596200	2.606400	6.143900
O	10.353500	2.438300	7.383800
N	11.858200	3.042300	5.752600
H	12.376500	3.530900	6.452000
H	11.984900	3.354600	4.814000
N	9.602700	2.339900	5.210500
H	8.840200	1.789000	5.529800
H	9.846000	2.245300	4.247100
C	17.732200	2.874100	5.612900
O	17.271800	3.374100	6.684700
N	18.779500	3.516700	4.952800
H	18.987200	4.428900	5.282300
H	18.908000	3.348400	3.981100
N	17.255700	1.651100	5.163700
H	16.475200	1.269000	5.652400
H	17.363400	1.413100	4.207400
C	-1.080700	8.060800	5.739100
O	-0.909000	7.925900	6.988800
N	-0.225700	8.885900	5.016000
H	0.285500	9.562200	5.540500
H	-0.459400	9.123300	4.080500
N	-2.100200	7.365000	5.104600
H	-2.543300	6.653500	5.632000
H	-2.133100	7.311500	4.113400
C	5.687800	8.786400	5.819900
O	5.935000	8.865900	7.066500
N	6.629000	9.238600	4.907600
H	7.320500	9.866600	5.257300
H	6.376300	9.323800	3.947700
N	4.472400	8.256400	5.401400
H	3.991200	7.690800	6.067100
H	4.351000	8.017800	4.441700
C	11.515300	7.897100	6.374700
O	11.331300	8.101700	7.617100
N	12.626300	8.467400	5.751000
H	13.057000	9.213900	6.252300

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H      12.652100    8.524600    4.756400
N      10.679500    7.034300    5.693700
H       9.879600    6.694400    6.176600
H      10.693000    6.984200    4.701100
C      16.443900    8.163900    6.978900
O      16.073400    8.238600    8.193700
N      17.516800    8.935000    6.542400
H      18.124800    9.266700    7.252200
H      17.913500    8.762700    5.644700
N      15.771200    7.316900    6.111400
H      14.841900    7.075000    6.361300
H      15.987300    7.332800    5.139000
C       2.331700    0.510300    3.145500
O       2.257300    0.820200    1.915900
N       3.533300   -0.019000    3.631000
H       4.116000   -0.426100    2.937000
H       3.536800   -0.455700    4.526500
N       1.258200    0.730700    3.982700
H       0.501400    1.270900    3.624800
H       1.351900    0.626500    4.965900
C       7.802700    0.446600    3.245300
O       8.108000    1.011800    2.152400
N       8.753000   -0.342900    3.898200
H       9.496500   -0.670800    3.329000
H       8.458600   -0.930800    4.645200
N       6.539400    0.621300    3.788100
H       5.996700    1.365500    3.412400
H       6.356500    0.347700    4.726800
C      14.179200    0.288800    2.939800
O      14.168900    0.352100    1.675300
N      15.271600   -0.327400    3.572900
H      15.708300   -1.035100    3.029000
H      15.203600   -0.517200    4.549500
N      13.141400    0.835400    3.678800
H      12.550100    1.479900    3.201500
H      13.257100    0.961200    4.659600
C       2.272300    5.822700    3.188900
O       2.043200    5.704700    1.942500
N       3.525100    5.498200    3.691200
H       4.104000    4.940000    3.100300
H       3.643100    5.388100    4.673300
N       1.250000    6.274300    4.022300
H       0.518400    6.771400    3.558100
H       1.484200    6.587400    4.940000
C       7.912200    5.738200    3.307200
O       7.932100    5.870500    2.043900
N       8.971000    5.094400    3.937000
H       9.545500    4.521300    3.359400
H       8.891800    4.838800    4.894500
N       6.837300    6.234400    4.040000
H       6.238500    6.861100    3.548200
H       6.950000    6.390600    5.017100
C      14.425200    5.180800    3.889800
O      14.550700    5.319000    2.630000
N      15.460300    4.616300    4.619100
H      16.123900    4.089500    4.095500
H      15.344700    4.394600    5.584300
N      13.259800    5.614300    4.498600
H      12.670300    6.196700    3.946600
H      13.191100    5.666900    5.488200
C       1.892600   10.950700    2.820000
O       1.792700   10.884500    1.559200
N       3.020200   10.474100    3.461800
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H       3.636100    9.904700    2.924700
H       3.017400   10.364300    4.450500
N       0.817800   11.490300    3.551100
H       0.288300   12.162600    3.045300
H       0.973500   11.708800    4.511900
C       9.226000   10.370600    2.527200
O       9.275300    9.584000    1.534100
N      10.367000   10.584100    3.303100
H      11.054500    9.864400    3.245500
H      10.251000   10.999200    4.201900
N       8.042600   11.031600    2.817500
H       7.342200   11.041900    2.117800
H       7.991600   11.680000    3.565000
C      14.277900   10.575100    3.763600
O      14.350100   10.307300    2.528400
N      15.186500   10.019500    4.647600
H      15.990700    9.583400    4.250000
H      15.217900   10.318300    5.593600
N      13.203100   11.343800    4.228600
H      12.736000   11.867200    3.524500
H      13.273000   11.767600    5.125000
C       3.434300    0.431900    7.575200
O       2.853900    0.128500    6.488100
N       4.632500   -0.192800    7.914700
H       5.103700   -0.657100    7.169200
H       5.219600    0.246000    8.582900
N       2.804400    1.297500    8.467900
H       1.988800    1.756100    8.122400
H       3.370600    1.816400    9.094300
C       8.100300    0.113300    7.251100
O       7.253800   -0.495100    6.527100
N       9.406000   -0.365700    7.301000
H       9.539700   -1.311700    7.040800
H      10.062000    0.048200    7.919300
N       7.720500    1.232200    7.986000
H       6.862300    1.659800    7.705400
H       8.433100    1.852900    8.302600
C      14.112000    1.238800    7.332600
O      14.587000    0.627900    6.325000
N      14.925300    2.071100    8.086800
H      15.822200    2.273000    7.696100
H      14.505700    2.800200    8.614800
N      12.802200    0.952600    7.739300
H      12.254600    0.502400    7.040700
H      12.308700    1.643900    8.260700
C       2.363100    5.602600    7.716900
O       2.799400    6.019700    6.595800
N       3.093300    4.649800    8.426700
H       3.814200    4.196100    7.905200
H       2.582300    4.065000    9.048500
N       1.237700    6.202200    8.279600
H       0.713700    6.782300    7.657500
H       0.692300    5.653300    8.905300
C       8.154100    5.715900    8.006100
O       8.069000    5.594600    6.744000
N       8.767900    4.710400    8.745500
H       9.303800    4.051600    8.221400
H       9.078900    4.902500    9.666100
N       7.637200    6.852600    8.616000
H       7.026500    7.407000    8.053000
H       7.457600    6.844700    9.590000
C      14.444000    5.537100    8.191600
O      13.912400    4.760000    7.332600
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N	15.753600	5.306200	8.597200
H	16.273400	4.671700	8.030000
H	16.261300	6.061900	8.997600
N	13.678100	6.529200	8.790400
H	12.778300	6.696100	8.395900
H	14.143300	7.310300	9.191500
C	2.311500	10.161500	7.331300
O	1.857900	10.694200	6.270600
N	3.633700	10.418700	7.712900
H	4.191500	10.815400	6.989500
H	4.110700	9.734900	8.257400
N	1.469800	9.424900	8.140300
H	0.549600	9.233500	7.811200
H	1.817200	8.892700	8.896600
C	9.499400	10.602700	6.847500
O	8.911000	11.112800	5.842000
N	10.827400	10.952400	7.110400
H	11.311300	11.394900	6.364400
H	11.380800	10.348400	7.679100
N	8.809000	9.783000	7.718800
H	7.859500	9.577600	7.500700
H	9.303200	9.168200	8.320700
C	14.016700	11.424700	8.332200
O	13.730800	11.096300	7.140000
N	15.233100	11.033500	8.887000
H	15.695100	10.287700	8.407500
H	15.328700	11.029300	9.874200
N	13.119200	12.200100	9.051200
H	12.348600	12.579800	8.556600
H	13.374200	12.616400	9.909900

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C	2.429300	2.228000	1.448200
O	1.720800	2.220200	2.502500
N	2.403200	3.346600	0.617800
H	2.019200	4.171000	1.030400
H	3.158300	3.493400	-0.006700
N	3.114700	1.076100	1.083000
H	3.185000	0.363600	1.777100
H	3.851000	1.129900	0.423600
C	6.313500	2.401400	2.130600
O	5.413800	3.003100	2.800800
N	7.329400	3.132800	1.533000
H	7.359300	4.103200	1.747800
H	8.197500	2.694300	1.326900
N	6.185200	1.035200	1.887900
H	5.502400	0.575700	2.451000
H	7.010000	0.506500	1.701300
C	10.961000	2.349800	1.644300
O	10.146200	2.958400	2.415100
N	12.018800	3.046000	1.086700
H	12.149000	3.991400	1.367200
H	12.798000	2.552200	0.724600
N	10.720300	1.025800	1.304400
H	9.998200	0.566400	1.817100
H	11.479600	0.467600	0.988200
C	16.695500	2.937700	0.795500
O	16.718200	3.445600	1.958300
N	17.284200	3.629000	-0.252600
H	17.809700	4.437900	-0.021700
H	17.448700	3.196700	-1.125200

N	16.106400	1.692400	0.595900
H	15.493000	1.384400	1.321800
H	15.859800	1.414400	-0.322900
C	0.555600	9.234700	1.916300
O	-0.041200	8.525100	2.790700
N	0.060700	10.498800	1.598800
H	-0.614100	10.866300	2.228600
H	0.679100	11.173800	1.205900
N	1.639000	8.713900	1.240700
H	1.911900	7.777500	1.432900
H	2.250300	9.300800	0.729600
C	5.957600	8.329000	1.516300
O	5.519200	8.699000	2.654800
N	6.967200	9.054100	0.911800
H	7.389100	9.784300	1.440500
H	7.489500	8.658700	0.171700
N	5.335500	7.273800	0.847600
H	4.646500	6.788200	1.384900
H	5.908400	6.700400	0.272800
C	11.058200	8.590100	1.216700
O	11.073400	8.591200	2.486500
N	12.050100	9.277800	0.521000
H	12.579200	9.927700	1.067200
H	11.878300	9.541400	-0.419000
N	10.059400	7.891100	0.547700
H	9.509400	7.272100	1.106300
H	10.195900	7.633600	-0.398400
C	16.068000	7.575000	1.737200
O	16.746600	8.205900	2.608500
N	15.050600	8.217200	1.063900
H	14.878200	9.173400	1.277300
H	14.366600	7.701800	0.566900
N	16.416400	6.256600	1.409200
H	16.995000	5.807200	2.085600
H	15.691000	5.671300	1.049800
C	0.513100	14.246000	1.391900
O	-0.103700	13.367300	2.077500
N	-0.058100	15.505100	1.225300
H	-0.846000	15.698000	1.794200
H	0.527700	16.269800	0.976800
N	1.693900	13.917500	0.748800
H	2.075800	13.022000	0.957600
H	2.321000	14.638400	0.475400
C	5.825600	14.090100	1.422000
O	5.744000	14.101400	2.690800
N	6.806800	14.845400	0.801800
H	7.324400	15.475700	1.376400
H	6.757700	15.037200	-0.166400
N	4.913000	13.335900	0.686300
H	4.415600	12.643700	1.209400
H	5.140900	13.088600	-0.246600
C	11.161800	14.607100	1.765100
O	11.650300	14.124000	2.836100
N	11.701900	15.785600	1.232700
H	12.292900	16.280700	1.871900
H	11.066900	16.368200	0.732200
N	10.200600	13.888500	1.066200
H	9.845600	13.074900	1.521700
H	9.558800	14.390300	0.500600
C	15.468200	14.446400	1.427000
O	16.083500	14.451400	2.537300
N	14.942200	15.632000	0.933700
H	14.882800	16.390400	1.580700

H	14.261200	15.605600	0.215700
N	15.445100	13.274000	0.664200
H	15.681100	12.448100	1.174000
H	14.701500	13.155700	0.017600
C	0.381200	2.539300	5.622900
O	0.032100	2.470800	6.839900
N	1.503500	3.289700	5.263600
H	1.759300	4.007500	5.906600
H	1.645100	3.494800	4.298300
N	-0.332200	1.831500	4.669800
H	-0.984000	1.167000	5.003900
H	-0.003100	1.752900	3.736200
C	5.527100	3.175600	6.268700
O	5.595900	3.218700	7.540700
N	6.576700	3.671900	5.503500
H	7.199200	4.289700	5.975400
H	6.431200	3.827500	4.530600
N	4.425800	2.594500	5.675300
H	3.779000	2.127500	6.268200
H	4.351500	2.497800	4.690100
C	10.552600	2.518600	5.820300
O	10.615600	2.481600	7.091600
N	11.398500	3.373000	5.127400
H	11.909100	4.029800	5.676300
H	11.208300	3.600500	4.179200
N	9.735700	1.619300	5.153200
H	9.086000	1.113000	5.714500
H	9.524300	1.736600	4.186500
C	17.249000	3.162000	5.346700
O	17.289400	3.254000	6.610200
N	18.267300	3.724300	4.583800
H	18.857400	4.363500	5.060300
H	18.132800	3.860900	3.609300
N	16.172500	2.517400	4.741500
H	15.667000	1.885300	5.325100
H	16.233300	2.285300	3.775700
C	0.275000	8.916300	6.205800
O	0.424100	9.041900	7.463000
N	1.376000	9.077500	5.368700
H	2.134300	9.600800	5.745000
H	1.226600	9.156600	4.386900
N	-0.970200	8.601800	5.687800
H	-1.649200	8.275700	6.330000
H	-1.074500	8.372000	4.725300
C	5.576700	8.595600	6.102800
O	5.637200	8.504200	7.368100
N	6.669300	9.097900	5.401700
H	7.321900	9.634400	5.931400
H	6.556400	9.346200	4.443100
N	4.417500	8.196200	5.441200
H	3.830700	7.565700	5.947000
H	4.445000	8.074900	4.452000
C	11.246300	8.529700	5.928300
O	11.295500	8.543900	7.196700
N	12.387800	8.854500	5.193000
H	13.068700	9.388600	5.692100
H	12.277500	9.085100	4.229100
N	10.058300	8.184100	5.292600
H	9.405800	7.667100	5.841500
H	10.067900	8.000100	4.314400
C	16.433000	7.746100	6.041600
O	16.281900	7.582900	7.292900
N	17.693000	8.006200	5.524400

H	18.385300	8.287800	6.174800
H	17.797700	8.283900	4.574900
N	15.321100	7.676600	5.205700
H	14.527800	7.202000	5.575600
H	15.461500	7.606200	4.222900
C	-0.644300	13.594700	5.478400
O	-0.639900	13.478000	6.741100
N	0.311400	14.402400	4.864700
H	0.735800	15.090300	5.448600
H	0.189700	14.644300	3.908800
N	-1.577900	12.900700	4.722000
H	-2.084300	12.190800	5.192200
H	-1.474500	12.831800	3.736100
C	6.139700	14.235800	6.100100
O	6.269500	14.346300	7.363200
N	7.185400	14.609400	5.269400
H	7.891800	15.180300	5.679900
H	7.015500	14.734200	4.294900
N	4.937100	13.760100	5.582200
H	4.398900	13.191600	6.201600
H	4.902100	13.508500	4.617900
C	11.413700	13.962100	6.275500
O	11.324800	13.909500	7.544700
N	12.625500	14.309200	5.692000
H	13.270400	14.786100	6.286500
H	12.649700	14.553200	4.726200
N	10.291300	13.668600	5.502800
H	9.597600	13.112300	5.958400
H	10.425100	13.492000	4.529900
C	16.942800	13.697600	5.777800
O	17.192200	13.653500	7.018500
N	17.950200	14.056000	4.890100
H	18.752200	14.477700	5.289400
H	17.733000	14.270000	3.944400
N	15.654500	13.413100	5.318900
H	15.110600	12.831000	5.917800
H	15.519800	13.287500	4.340000
C	3.572400	-0.639500	4.491900
O	4.149000	-0.729700	3.364900
N	4.020000	-1.456000	5.533600
H	4.462200	-2.299000	5.254600
H	3.518300	-1.463100	6.390700
N	2.527800	0.249500	4.672900
H	2.378100	0.917100	3.946300
H	2.232800	0.494700	5.590400
C	8.339900	-0.967800	4.093500
O	8.527400	-0.260800	3.054900
N	9.442200	-1.443600	4.809500
H	10.304700	-1.010500	4.568300
H	9.313000	-1.632900	5.778800
N	7.053100	-1.360700	4.440100
H	6.309300	-0.991000	3.891300
H	6.861200	-1.554000	5.395700
C	13.716400	0.383300	3.151100
O	13.608200	0.658000	1.913900
N	14.914100	-0.137300	3.626600
H	15.497500	-0.578000	2.958100
H	14.983900	-0.431800	4.574400
N	12.639500	0.599000	4.003600
H	11.944300	1.218300	3.657400
H	12.798200	0.620500	4.989300
C	2.787600	5.873200	3.251800
O	2.817000	5.953800	1.983900

N	3.923400	5.427100	3.931200
H	4.557500	4.889500	3.377700
H	3.824500	5.144500	4.881300
N	1.636600	6.241400	3.933600
H	0.971000	6.775500	3.414200
H	1.680200	6.398200	4.914600
C	8.066600	6.065300	3.102100
O	7.872000	6.200800	1.852400
N	9.298400	5.596000	3.552600
H	9.816500	5.059100	2.888700
H	9.384800	5.318900	4.505000
N	7.044900	6.378100	3.991100
H	6.306200	6.935500	3.618400
H	7.267900	6.517200	4.952500
C	13.500300	5.558800	2.994500
O	13.540300	5.614000	1.725800
N	14.586200	5.015700	3.681400
H	15.176000	4.424500	3.135900
H	14.463300	4.749300	4.635500
N	12.382700	6.039300	3.671500
H	11.830800	6.701500	3.166600
H	12.446700	6.183100	4.656400
C	2.977000	11.425600	3.199800
O	2.908900	11.381100	1.930100
N	4.166200	11.096000	3.838900
H	4.810400	10.563900	3.290100
H	4.145700	10.899800	4.815500
N	1.845500	11.805200	3.921900
H	1.160700	12.306800	3.395600
H	1.959600	12.081600	4.873400
C	8.558000	11.409100	3.238700
O	8.566200	11.451500	1.970600
N	9.700400	10.995700	3.919500
H	10.344000	10.454000	3.382600
H	9.621900	10.761200	4.884800
N	7.401800	11.780600	3.926100
H	6.761800	12.343100	3.406400
H	7.471900	11.979000	4.899600
C	14.136400	11.068600	3.179100
O	14.124900	11.015100	1.906600
N	15.227300	10.560100	3.864600
H	15.856900	9.988100	3.344000
H	15.181900	10.426900	4.848200
N	13.048500	11.616100	3.852600
H	12.458400	12.209900	3.308000
H	13.152700	11.854700	4.814000
C	2.563000	16.599900	3.029500
O	2.610800	16.572500	1.764100
N	3.619000	16.116200	3.782700
H	4.281200	15.545700	3.304800
H	3.497000	15.963900	4.758600
N	1.407500	17.108500	3.647500
H	0.918100	17.777100	3.098700
H	1.448300	17.305000	4.624500
C	8.951500	16.756700	3.361900
O	9.026300	16.435900	2.133600
N	10.026100	16.535600	4.203500
H	10.748800	15.939300	3.870900
H	9.924500	16.634600	5.188800
N	7.769800	17.318000	3.844500
H	7.172800	17.716200	3.160500
H	7.756800	17.719900	4.754700
C	13.878800	17.065700	4.220500

O	13.665300	17.349100	3.001600
N	15.057200	16.442300	4.588300
H	15.574600	15.999300	3.861100
H	15.173100	16.100600	5.514900
N	12.894700	17.371700	5.167500
H	12.250200	18.071500	4.880300
H	13.146400	17.376300	6.131600
C	2.696500	0.634900	8.759100
O	3.143100	0.478400	7.583000
N	3.071700	-0.283600	9.742700
H	3.864200	-0.840600	9.518100
H	2.963500	-0.042400	10.697400
N	1.874700	1.716700	9.056700
H	1.505200	2.199600	8.258600
H	1.260200	1.645800	9.832000
C	7.299400	0.575000	7.750300
O	7.930900	-0.237100	7.006000
N	7.971900	1.626600	8.356800
H	8.915200	1.763900	8.065600
H	7.453900	2.434300	8.619400
N	5.950900	0.330700	8.048400
H	5.513000	-0.322400	7.436200
H	5.382200	1.126300	8.256400
C	14.186100	1.222100	7.578000
O	14.348500	0.695600	6.432000
N	15.282100	1.747100	8.244700
H	16.115600	1.868200	7.710400
H	15.150600	2.354400	9.015000
N	12.935000	1.149700	8.192700
H	12.177300	0.937600	7.579000
H	12.716300	1.811900	8.898900
C	2.639000	5.703300	7.940900
O	2.776800	5.804700	6.683200
N	3.069700	4.550900	8.583100
H	3.687600	3.961500	8.065200
H	3.179300	4.547400	9.566400
N	2.051900	6.751600	8.649400
H	1.581300	7.432500	8.089800
H	1.652500	6.566600	9.536900
C	8.538900	5.822500	7.774300
O	8.579100	5.812100	6.503100
N	9.053800	4.736800	8.475200
H	9.627900	4.112900	7.947100
H	9.283300	4.842800	9.432700
N	7.986600	6.916600	8.430400
H	7.449800	7.541400	7.862400
H	7.680300	6.813000	9.366600
C	14.070800	5.689900	7.475600
O	13.444400	5.357900	6.418800
N	15.167800	4.925500	7.892900
H	15.521500	4.306200	7.191800
H	15.878000	5.406500	8.401000
N	13.581700	6.721900	8.265200
H	12.848400	7.269600	7.864900
H	14.221500	7.200600	8.853400
C	2.531700	11.079500	7.680500
O	3.109600	11.550500	6.648000
N	3.126000	10.042700	8.383400
H	3.920500	9.613500	7.958400
H	2.553200	9.463700	8.949400
N	1.374700	11.703100	8.162200
H	0.942200	12.321000	7.505600
H	0.732000	11.125500	8.659700

C	8.414000	11.099700	7.915400
O	8.529200	11.327700	6.671300
N	8.879000	9.902300	8.431100
H	9.474000	9.356000	7.844300
H	8.968800	9.777400	9.407100
N	7.825400	12.064900	8.735800
H	7.350100	12.794900	8.246600
H	7.409700	11.771900	9.586600
C	14.022600	10.915400	7.882300
O	14.106600	11.035900	6.622800
N	14.631600	9.833100	8.505600
H	15.257300	9.296500	7.942700
H	14.822800	9.869500	9.475800
N	13.330500	11.878100	8.622900
H	12.757800	12.490100	8.075200
H	12.941300	11.603400	9.493200
C	2.504400	15.603100	7.478900
O	2.160900	16.239500	6.435300
N	3.835200	15.689200	7.918800
H	4.458000	16.039300	7.222900
H	4.208600	14.917000	8.425800
N	1.550900	14.932300	8.218500
H	0.648000	14.817900	7.811100
H	1.812400	14.310700	8.941900
C	8.089100	16.493100	7.817700
O	8.472700	17.041600	6.738200
N	8.873600	15.521900	8.415200
H	9.670400	15.207400	7.906300
H	8.466200	14.886000	9.054800
N	6.926100	16.959400	8.447800
H	6.382500	17.576100	7.888800
H	6.402600	16.302600	8.979400
C	14.619400	15.466600	8.515700
O	14.340000	16.161200	7.492600
N	15.953600	15.351000	8.936500
H	16.606800	15.578700	8.213700
H	16.196400	14.515500	9.420300
N	13.581100	14.936300	9.266700
H	12.675800	14.953100	8.849900
H	13.761800	14.243800	9.947300

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C	1.495300	2.567500	1.436600
O	0.978700	2.415100	2.588000
N	1.361800	3.794900	0.783800
H	1.108200	4.554800	1.380900
H	2.028000	4.030200	0.086200
N	2.072600	1.478500	0.804300
H	2.196800	0.651800	1.347900
H	2.676100	1.609600	0.032000
C	5.790800	2.460900	1.899600
O	5.236300	2.987300	2.918500
N	6.859400	3.103700	1.291700
H	7.203600	3.921900	1.744200
H	7.515900	2.561000	0.782500
N	5.232900	1.310600	1.334100
H	4.559800	0.852400	1.915000
H	5.858500	0.694600	0.863300
C	11.082200	2.555000	1.686300
O	10.605300	3.060000	2.754900
N	12.108500	3.207800	1.013400

H	12.493900	4.004500	1.471500
H	12.729500	2.667200	0.460100
N	10.500600	1.415500	1.149800
H	9.766100	1.000500	1.679500
H	11.049800	0.818300	0.581100
C	16.543400	2.903900	0.939000
O	16.515500	3.210200	2.169500
N	17.590800	3.372500	0.144300
H	18.126900	4.110100	0.540900
H	17.479400	3.395300	-0.840100
N	15.537700	2.111800	0.405000
H	14.933400	1.659700	1.059200
H	15.667200	1.668200	-0.469900
C	0.318300	9.185300	1.849800
O	-0.226600	8.472700	2.753400
N	-0.235300	10.422200	1.514400
H	-0.895900	10.782200	2.164700
H	0.357500	11.108300	1.101500
N	1.391800	8.680400	1.140100
H	1.733700	7.782500	1.399000
H	1.996700	9.293800	0.650300
C	5.988500	8.196700	1.563300
O	5.505000	8.645200	2.654600
N	7.051700	8.849700	0.981600
H	7.398800	9.674300	1.413500
H	7.536200	8.465500	0.213000
N	5.391400	7.100500	0.934100
H	4.648300	6.678700	1.452600
H	5.995700	6.465900	0.463400
C	11.113700	8.517400	1.420100
O	10.999100	8.661900	2.677100
N	12.200800	9.089400	0.768300
H	12.717900	9.765200	1.293100
H	12.162500	9.227600	-0.211600
N	10.149100	7.791500	0.725000
H	9.532200	7.243400	1.290600
H	10.386000	7.404600	-0.156400
C	16.222900	7.378300	1.839200
O	16.919600	8.006200	2.695600
N	15.276000	8.049500	1.086500
H	15.114500	9.005000	1.320000
H	14.522100	7.538300	0.690300
N	16.503100	6.023900	1.581700
H	17.028600	5.583600	2.307200
H	15.732800	5.469000	1.266100
C	0.130400	14.220000	1.554700
O	-0.456100	13.302800	2.217000
N	-0.469900	15.472300	1.449900
H	-1.235500	15.630300	2.059100
H	0.094100	16.256600	1.210500
N	1.305000	13.939900	0.882400
H	1.701000	13.037700	1.024300
H	1.904700	14.679200	0.597700
C	5.550200	14.108700	1.385600
O	5.446600	14.222500	2.648800
N	6.556400	14.784700	0.730000
H	7.172400	15.353700	1.265300
H	6.652400	14.759700	-0.250700
N	4.605300	13.356100	0.686600
H	4.063000	12.732700	1.248700
H	4.838400	13.021600	-0.217300
C	11.151800	14.330700	1.652800
O	11.683000	13.889600	2.723400

N	11.684600	15.462200	1.040600
H	12.374800	15.949600	1.574000
H	11.067200	16.028300	0.506400
N	10.131200	13.605700	1.044000
H	9.775200	12.837300	1.572500
H	9.458900	14.109500	0.514200
C	16.296300	13.936100	1.780800
O	16.705500	14.213000	2.951200
N	15.787400	14.946500	0.983000
H	15.573500	15.809600	1.437500
H	15.267400	14.723800	0.171700
N	16.485900	12.642500	1.277000
H	16.719300	11.971000	1.976500
H	15.827300	12.307300	0.609900
C	0.644500	2.557500	6.000800
O	0.604300	2.501300	7.270900
N	1.634600	3.308800	5.371400
H	2.023800	4.038800	5.929800
H	1.532000	3.505200	4.398200
N	-0.271200	1.826000	5.266500
H	-0.829800	1.173200	5.754000
H	-0.231100	1.787500	4.275100
C	5.440100	2.909300	6.367200
O	5.598800	2.852500	7.631800
N	6.093700	3.898800	5.656800
H	6.806800	4.403700	6.133800
H	6.110900	3.883700	4.663200
N	4.636100	1.974100	5.733400
H	4.047000	1.424700	6.321600
H	4.320100	2.150100	4.805300
C	10.907100	2.764700	6.230900
O	11.024900	2.667800	7.497000
N	11.510200	3.816800	5.574700
H	12.089200	4.430300	6.100200
H	11.469100	3.907300	4.587800
N	10.224600	1.777000	5.529500
H	9.649800	1.175100	6.078900
H	9.927100	1.960800	4.596500
C	16.871100	3.118100	5.604700
O	16.890500	3.293000	6.861700
N	17.867600	3.699900	4.827300
H	18.404600	4.406000	5.269400
H	17.767200	3.744900	3.840700
N	15.858400	2.367300	5.026300
H	15.348700	1.764600	5.634200
H	15.917600	2.113600	4.067200
C	-0.381000	8.486100	6.181900
O	-0.377700	8.339200	7.445300
N	0.751300	8.968900	5.539900
H	1.390400	9.493900	6.096500
H	0.692200	9.207500	4.574700
N	-1.519700	8.143600	5.463500
H	-2.175100	7.571100	5.936700
H	-1.482600	8.081800	4.470600
C	5.526400	8.596900	6.117700
O	5.553500	8.529600	7.390600
N	6.628600	9.104300	5.436800
H	7.252800	9.666900	5.975900
H	6.527500	9.341400	4.473400
N	4.403800	8.154200	5.437700
H	3.783900	7.560100	5.944300
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C	11.074700	8.615600	6.128300

O	11.131000	8.546300	7.399000
N	12.153400	9.129900	5.423200
H	12.808400	9.668400	5.948500
H	12.041000	9.362900	4.461700
N	9.929500	8.178100	5.473200
H	9.329200	7.575600	5.995100
H	9.958700	8.041300	4.487200
C	17.091000	8.074200	6.158800
O	17.101000	8.248600	7.417200
N	18.239100	8.357800	5.423700
H	18.909900	8.927100	5.880900
H	18.185300	8.425000	4.432300
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H	15.270800	7.153800	6.108600
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C	-0.715300	13.644700	5.686700
O	-0.722800	13.519800	6.948800
N	0.387500	14.220000	5.060200
H	0.969300	14.786100	5.641600
H	0.302200	14.497200	4.109500
N	-1.801600	13.191600	4.945000
H	-2.413600	12.570000	5.416100
H	-1.718100	13.089400	3.958200
C	5.533700	14.100500	6.099700
O	5.542000	14.081000	7.373500
N	6.586000	14.685800	5.416200
H	7.195200	15.271000	5.945600
H	6.500900	14.867600	4.441600
N	4.458800	13.537900	5.418600
H	3.913800	12.876600	5.928100
H	4.523700	13.402600	4.434300
C	11.392400	13.858600	6.163000
O	11.268400	13.846400	7.430700
N	12.588700	14.284600	5.596800
H	13.167700	14.845100	6.186100
H	12.614900	14.489700	4.621700
N	10.325900	13.444700	5.375200
H	9.620000	12.915300	5.842500
H	10.489400	13.231300	4.415200
C	16.863200	14.095100	6.362700
O	16.842600	14.240100	7.626000
N	17.989700	14.493300	5.657000
H	18.626900	15.077000	6.139800
H	17.972500	14.540700	4.664100
N	15.755000	13.569500	5.708100
H	15.136200	13.024100	6.269100
H	15.846900	13.295300	4.754600
C	0.493900	2.703200	10.694000
O	0.498200	2.686200	11.962200
N	1.308100	3.585700	10.007100
H	1.716500	4.321500	10.537300
H	1.218200	3.697500	9.023200
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H	-0.953500	1.287400	10.547800
H	-0.408900	1.834800	9.035800
C	5.600100	2.986300	11.028200
O	5.583200	3.020400	12.300800
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H	6.798000	4.621900	10.830000
H	6.380400	3.902500	9.346100
N	5.033500	1.891000	10.375500
H	4.346600	1.398500	10.904900
H	4.857300	1.958500	9.395400

C	10.838700	2.608400	10.927200
O	10.727500	2.611100	12.196400
N	11.380600	3.716100	10.294300
H	11.913600	4.332000	10.869900
H	11.632100	3.660200	9.333000
N	10.421000	1.489400	10.212100
H	9.789300	0.885400	10.696400
H	10.294000	1.570000	9.226700
C	17.296600	2.951500	10.220400
O	17.307600	3.036500	11.486400
N	18.367300	3.459600	9.491600
H	18.963900	4.078700	9.985700
H	18.268900	3.602400	8.512300
N	16.205800	2.368100	9.582200
H	15.661600	1.745900	10.139900
H	16.273700	2.155500	8.612000
C	0.301300	8.738000	10.781400
O	0.548400	8.918700	12.017300
N	1.020500	9.450200	9.825200
H	1.470600	10.270300	10.164700
H	0.684600	9.481700	8.886500
N	-0.628000	7.788500	10.407100
H	-1.036700	7.237700	11.117700
H	-0.844900	7.613200	9.455400
C	5.692000	8.746400	10.836400
O	5.686700	8.890800	12.102500
N	6.132100	9.788600	10.033600
H	6.662400	10.504400	10.477500
H	6.315000	9.622700	9.068700
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H	4.707300	6.963900	10.867500
H	5.083800	7.503100	9.300300
C	11.468700	8.514400	10.818500
O	11.532400	8.612800	12.083100
N	12.578100	8.861300	10.041500
H	13.242300	9.442300	10.508800
H	12.427700	9.064200	9.076200
N	10.305800	8.042200	10.232300
H	9.663400	7.567600	10.826000
H	10.278500	7.839700	9.260100
C	16.670600	7.770200	10.816800
O	16.476000	7.674100	12.069100
N	17.948900	8.021600	10.340400
H	18.611300	8.338500	11.004700
H	18.091200	8.252300	9.384300
N	15.594800	7.643400	9.940800
H	14.797600	7.173000	10.310000
H	15.780100	7.511600	8.969700
C	-1.001000	13.836800	10.302100
O	-0.920600	13.605300	11.549000
N	0.030000	14.496000	9.665300
H	0.765600	14.861700	10.223800
H	0.016900	14.664300	8.689100
N	-2.147400	13.457200	9.605100
H	-2.734800	12.816700	10.082300
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C	5.946600	14.093700	10.807200
O	6.088700	14.090000	12.070900
N	6.404400	15.172700	10.070900
H	7.031200	15.797300	10.531700
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H	4.777100	12.433100	10.784300

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O	11.460200	13.932100	12.126200
N	11.829300	15.005200	10.127800
H	12.462100	15.601300	10.617100
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C	16.933800	14.040600	11.052100
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N	17.414500	15.187000	10.393700
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H	3.952800	-2.526700	4.036500
H	3.347200	-1.838600	5.461900
N	2.387800	0.321400	4.311000
H	2.023500	1.025800	3.711800
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O	7.835300	0.385800	2.262300
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N	3.858400	5.490200	3.932100
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H	0.902400	6.848900	3.504600
H	1.640200	6.448300	4.983200
C	8.117400	5.971600	3.202700
O	7.945700	5.988100	1.942100
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H	6.325800	6.846700	3.622300
H	7.248100	6.498900	5.004600
C	13.605700	5.694000	3.234700
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N	14.666700	5.063700	3.893100
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H	14.569700	4.867700	4.867200
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H	12.002100	6.930900	3.417800
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C	14.395300	10.946600	3.237900
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O	8.972500	16.198200	1.895200
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O	3.162300	-0.416500	7.080100
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H	14.729700	2.281300	13.722000
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O	2.884800	5.928100	11.430700
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H	1.111700	7.060200	12.740400
H	1.529800	6.428500	14.260700
C	8.284500	5.814700	12.642300
O	8.408400	5.917500	11.382100
N	8.853400	4.725700	13.294000
H	9.527800	4.208500	12.767600
H	9.001100	4.768900	14.272500
N	7.580500	6.792700	13.341700
H	7.034500	7.413900	12.778500
H	7.200300	6.564700	14.228100
C	14.345800	5.741400	12.348400
O	13.740800	5.371400	11.290900
N	15.427500	4.990600	12.815200

H	15.782500	4.323500	12.161300
H	16.124300	5.475600	13.334400
N	13.842200	6.801500	13.091400
H	13.113000	7.330700	12.661200
H	14.474500	7.308000	13.664100
C	2.302900	11.230900	12.237800
O	2.775000	11.782100	11.191900
N	3.051200	10.261500	12.900400
H	3.874100	9.953800	12.427200
H	2.556300	9.567200	13.409400
N	1.106300	11.699100	12.779800
H	0.591000	12.318600	12.188000
H	0.555400	11.049400	13.294000
C	8.097500	10.804200	12.479900
O	8.471300	11.337800	11.385100
N	8.804600	9.734300	12.980300
H	9.656800	9.475600	12.538600
H	8.555700	9.301100	13.831100
N	7.005700	11.337000	13.176700
H	6.551100	12.091200	12.700400
H	6.392700	10.684100	13.611700
C	14.180200	10.975500	12.619800
O	14.307000	11.087000	11.359800
N	14.849800	9.956800	13.277400
H	15.505500	9.426600	12.746000
H	14.956500	9.974500	14.259500
N	13.393500	11.894000	13.313500
H	12.762000	12.421800	12.745300
H	13.052100	11.643400	14.210500
C	2.476400	15.342400	12.424300
O	2.318500	15.796700	11.247600
N	3.721200	15.462600	13.041000
H	4.478200	15.677200	12.427200
H	3.951000	14.843100	13.781100
N	1.379300	14.848000	13.112000
H	0.540900	14.713800	12.588200
H	1.506100	14.285200	13.915200
C	9.433500	16.287100	12.089600
O	8.749900	16.830500	11.163400
N	10.697800	16.791100	12.403600
H	11.088400	17.403000	11.723800
H	11.356300	16.178300	12.832800
N	8.872800	15.270100	12.838900
H	7.955400	14.968100	12.597200
H	9.452800	14.655600	13.355700
C	14.471000	16.225400	12.512300
O	13.613400	16.846100	11.804100
N	15.740800	16.772900	12.678300
H	15.960500	17.531900	12.080600
H	16.487100	16.177900	12.959500
N	14.106800	15.068900	13.177900
H	13.201400	14.707900	12.974300
H	14.807100	14.432900	13.482300

n=93 urea cluster optimized with AM1

C	0.444700	3.989600	2.325900
O	-0.090800	3.375900	3.305600
N	-0.010600	5.263800	1.976200
H	-0.565500	5.717700	2.665500
H	0.613300	5.867600	1.486800
N	1.400100	3.351800	1.562300

H	1.659900	2.424300	1.813300
H	2.000800	3.871800	0.971000
C	6.045300	2.412000	1.708500
O	5.567600	2.930700	2.771300
N	7.192400	2.950300	1.139100
H	7.630300	3.686900	1.647100
H	7.782600	2.358500	0.604600
N	5.349800	1.389300	1.080400
H	4.540600	1.052900	1.557400
H	5.854800	0.740100	0.527100
C	11.144800	2.443300	1.694000
O	10.725200	2.886400	2.814000
N	12.196300	3.078000	1.058400
H	12.644100	3.823300	1.543600
H	12.723500	2.591500	0.376400
N	10.465800	1.396800	1.071300
H	9.747900	0.970300	1.618100
H	10.993400	0.785200	0.492800
C	16.453000	2.626300	1.310100
O	16.460700	2.637500	2.580800
N	17.494200	3.234700	0.615300
H	18.059500	3.860800	1.151500
H	17.362500	3.476000	-0.337000
N	15.408200	1.998800	0.643100
H	14.806900	1.429700	1.200000
H	15.515300	1.741900	-0.306600
C	21.764900	1.972100	1.507100
O	22.453500	2.789900	2.196300
N	20.668300	2.422800	0.793200
H	20.405400	3.372200	0.939300
H	19.961900	1.778900	0.523000
N	22.185900	0.644400	1.402700
H	22.873500	0.373900	2.065200
H	21.507100	-0.043700	1.162700
C	0.617300	8.964400	1.742900
O	0.045000	8.174800	2.565700
N	0.047600	10.202800	1.467600
H	-0.680400	10.494300	2.075300
H	0.614100	10.930500	1.091900
N	1.742900	8.538600	1.063000
H	2.122600	7.653600	1.315900
H	2.343000	9.200800	0.631600
C	6.191800	8.079000	1.527600
O	5.732000	8.509600	2.637400
N	7.203500	8.778400	0.905400
H	7.587900	9.565700	1.376300
H	7.706000	8.384900	0.151700
N	5.597000	6.974400	0.913400
H	4.894900	6.521700	1.462600
H	6.194800	6.361300	0.406500
C	11.112000	8.340800	1.321300
O	11.028200	8.426200	2.586400
N	12.088100	9.063800	0.655500
H	12.590800	9.741300	1.189000
H	12.030700	9.201400	-0.321700
N	10.207600	7.536500	0.626800
H	9.673300	6.911800	1.197300
H	10.473500	7.185800	-0.262000
C	16.491900	8.703700	1.473900
O	17.136100	8.242200	2.474800
N	16.943200	9.860800	0.844300
H	17.661700	10.354900	1.332500
H	16.265000	10.429800	0.389900

N	15.431400	7.978200	0.955400
H	15.143200	7.172300	1.465000
H	14.736800	8.450500	0.429500
C	21.416600	7.916200	1.782500
O	22.137300	8.791900	2.361500
N	20.036600	8.051100	1.795100
H	19.669800	8.966500	1.939700
H	19.470000	7.423400	1.271500
N	22.026200	6.824500	1.174700
H	22.980800	6.682900	1.403000
H	21.485800	6.015400	0.962100
C	0.428700	14.043000	1.365600
O	-0.184500	13.122100	1.998300
N	-0.161600	15.298400	1.251700
H	-0.959600	15.452000	1.818100
H	0.409600	16.083500	1.035700
N	1.625500	13.765200	0.732400
H	2.014800	12.861900	0.886700
H	2.239400	14.506000	0.484100
C	5.777900	14.047900	1.367900
O	5.728700	14.099900	2.637800
N	6.718100	14.809700	0.699500
H	7.247000	15.460700	1.237300
H	6.674900	14.932700	-0.279300
N	4.863000	13.252400	0.678400
H	4.395000	12.565200	1.233600
H	5.076600	12.977100	-0.250300
C	11.312100	14.509300	1.894300
O	12.077800	13.965000	2.758700
N	11.625900	15.769000	1.406700
H	12.413100	16.224600	1.812400
H	10.910300	16.330200	1.010500
N	10.231900	13.806000	1.392400
H	10.044700	12.911500	1.786300
H	9.471800	14.295900	0.985100
C	16.045800	14.465500	1.826000
O	16.704900	13.878500	2.745400
N	16.653600	15.469300	1.093400
H	17.573100	15.735200	1.371200
H	16.093300	16.138300	0.625400
N	14.764000	14.020800	1.502800
H	14.369100	13.362500	2.137800
H	14.121800	14.686100	1.137100
C	21.852000	13.007300	2.079600
O	22.384000	13.692800	3.012000
N	20.869900	13.574700	1.289900
H	20.563900	14.493500	1.523200
H	20.253400	12.992400	0.776800
N	22.342700	11.728700	1.795700
H	22.935100	11.347200	2.497000
H	21.717700	11.069000	1.383900
C	-0.107700	3.174600	6.727700
O	-0.051700	2.954500	7.981500
N	0.989600	3.700000	6.070100
H	1.691400	4.136100	6.624500
H	0.912300	3.977600	5.117200
N	-1.278800	2.878600	6.039800
H	-1.910900	2.273600	6.504100
H	-1.280400	2.870400	5.043900
C	5.720100	2.955200	6.192900
O	5.815000	2.940300	7.465400
N	6.806100	3.386800	5.438000
H	7.456300	3.968200	5.923100

H	6.663900	3.592200	4.471500
N	4.550100	2.526600	5.594500
H	3.920200	2.002800	6.161000
H	4.511700	2.394000	4.608100
C	11.045000	2.720900	6.292200
O	11.141500	2.703700	7.563600
N	11.614000	3.761100	5.587900
H	12.203200	4.390900	6.083700
H	11.631500	3.764600	4.595000
N	10.411600	1.669400	5.634900
H	9.807300	1.108600	6.196000
H	10.145700	1.789800	4.681700
C	16.594600	2.784100	6.013700
O	16.693900	2.769600	7.283800
N	17.592600	3.387300	5.262200
H	18.198900	4.012300	5.747600
H	17.443900	3.556400	4.292700
N	15.488400	2.201400	5.411700
H	14.974900	1.556300	5.972800
H	15.494300	2.035600	4.430200
C	22.854400	2.854200	5.598800
O	22.909600	3.123800	6.837500
N	23.953500	3.125500	4.791400
H	24.632300	3.735400	5.177800
H	23.858900	3.110300	3.801200
N	21.692100	2.307100	5.065000
H	21.082800	1.855000	5.712700
H	21.716500	1.941500	4.140500
C	-0.161800	8.195500	6.007700
O	-0.099000	7.997300	7.261600
N	0.808400	8.962000	5.382500
H	1.376300	9.544300	5.956800
H	0.696100	9.213500	4.427300
N	-1.204100	7.633600	5.280400
H	-1.715100	6.917400	5.736700
H	-1.165900	7.614900	4.286500
C	5.793900	8.577900	6.081300
O	5.811400	8.579800	7.356700
N	6.872000	9.096900	5.380200
H	7.493700	9.685600	5.892100
H	6.781200	9.267300	4.402300
N	4.697000	8.042500	5.424000
H	4.111100	7.441200	5.959500
H	4.726900	7.900100	4.439200
C	11.051500	8.461400	6.045200
O	11.088000	8.445700	7.318700
N	12.167400	8.882100	5.338400
H	12.837600	9.415600	5.847500
H	12.090800	9.058000	4.361500
N	9.892600	8.065300	5.386800
H	9.266200	7.500200	5.918400
H	9.935900	7.884600	4.407600
C	16.926100	8.211000	5.948600
O	16.806500	8.290100	7.215400
N	18.066600	8.718100	5.340500
H	18.602400	9.358500	5.885100
H	18.088100	8.832100	4.350900
N	15.917700	7.617900	5.204300
H	15.262600	7.060200	5.708900
H	16.083000	7.387600	4.249500
C	22.343900	8.435200	5.873400
O	22.379900	8.554500	7.137800
N	23.419600	8.882800	5.119500

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H      24.070700    9.464700    5.587500
H      23.346600    8.963100    4.131000
N      21.221500    7.885100    5.263600
H      20.630800    7.329900    5.845600
H      21.274300    7.623600    4.305800
C      -0.631400   13.339000    5.425900
O      -0.648500   13.120300    6.675800
N       0.422600   14.055500    4.869800
H       0.953900   14.617800    5.499600
H       0.343200   14.376400    3.933000
N      -1.659200   12.846900    4.629600
H      -2.234300   12.155100    5.046000
H      -1.553500   12.822800    3.640300
C       5.649400   13.981600    6.056800
O       5.565200   13.991700    7.328700
N       6.737900   14.575500    5.445500
H       7.311600   15.157900    6.014000
H       6.751800   14.714800    4.461400
N       4.634000   13.386300    5.317400
H       4.061700   12.734600    5.810400
H       4.777800   13.214100    4.347000
C      11.700300   14.134200    6.221000
O      11.588500   14.153400    7.491300
N      12.456800   15.117200    5.580300
H      13.096500   15.604600    6.173700
H      12.777500   14.931900    4.653100
N      11.027600   13.167100    5.507000
H      10.373100   12.597500    5.994600
H      11.037700   13.154200    4.513800
C      16.831800   13.817500    6.157700
O      16.808600   13.817900    7.434100
N      17.901000   14.393900    5.493900
H      18.484500   15.004200    6.023700
H      17.866000   14.518900    4.506700
N      15.782500   13.231700    5.472000
H      15.198300   12.617100    5.992000
H      15.829500   13.109600    4.485300
C      22.437400   13.688500    6.446900
O      22.418800   13.857600    7.707700
N      23.632900   13.849400    5.757400
H      24.348900   14.334000    6.241200
H      23.628000   13.905800    4.762900
N      21.263100   13.364700    5.780300
H      20.553300   12.922300    6.322400
H      21.310800   13.120500    4.815400
C       0.416500    3.413400   11.322900
O       0.806900    3.484600   12.530500
N       0.625500    4.487100   10.465400
H       1.347500    5.115600   10.740200
H       0.507900    4.353600    9.482800
N      -0.222900    2.256800   10.884100
H      -0.644600    1.702100   11.588800
H      -0.636500    2.240200    9.978500
C       5.842900    2.830100   10.845900
O       5.805500    2.812300   12.118600
N       6.643500    3.743100   10.201000
H       7.216600    4.338700   10.753100
H       6.736300    3.755200    9.212700
N       5.118000    1.863700   10.137500
H       4.367600    1.462200   10.658400
H       4.933700    2.025600    9.169500
C      10.892700    2.473300   10.986300
O      10.671400    2.430000   12.241400
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N	11.528900	3.576000	10.443900
H	12.046900	4.145400	11.078800
H	11.848300	3.544000	9.501500
N	10.494500	1.396900	10.193000
H	9.793500	0.813400	10.599400
H	10.436400	1.530500	9.205800
C	16.477800	2.428100	10.674000
O	16.343100	2.356100	11.938500
N	17.106000	3.542700	10.134400
H	17.665900	4.079400	10.759500
H	17.350100	3.563900	9.171900
N	15.998900	1.404700	9.870700
H	15.368000	0.764400	10.303700
H	15.906800	1.551700	8.890700
C	23.282400	3.038300	10.203200
O	23.247400	3.301500	11.445500
N	24.388500	3.427500	9.450300
H	24.975300	4.100500	9.881200
H	24.315000	3.455000	8.458800
N	22.226100	2.362200	9.620300
H	21.584100	1.907500	10.228200
H	22.262500	2.085300	8.668000
C	0.328400	8.444800	10.625600
O	0.560900	8.591200	11.867300
N	0.956800	9.286000	9.709800
H	1.316600	10.131700	10.090600
H	0.619700	9.324800	8.772500
N	-0.508200	7.429000	10.202900
H	-0.782300	6.758400	10.876900
H	-0.617600	7.217200	9.239400
C	6.045600	8.868900	10.769000
O	6.092300	9.078300	12.024000
N	7.121600	9.237400	9.968900
H	7.766300	9.876500	10.377300
H	6.994200	9.303600	8.981900
N	4.918900	8.268200	10.219800
H	4.355600	7.741800	10.852200
H	4.947400	7.961400	9.272700
C	11.306300	8.551100	10.734900
O	11.370200	8.628500	11.999600
N	12.442500	8.825000	9.976100
H	13.139300	9.368900	10.439300
H	12.339800	8.977200	8.996400
N	10.098900	8.199000	10.131000
H	9.463700	7.699000	10.716400
H	10.105200	7.936500	9.169500
C	16.536500	7.992400	10.637200
O	16.466200	7.799600	11.894000
N	17.725600	8.448900	10.082300
H	18.347600	8.910700	10.710500
H	17.733600	8.751000	9.133300
N	15.419500	7.748900	9.842500
H	14.718900	7.172200	10.255700
H	15.544000	7.653600	8.857000
C	22.012500	8.068800	10.516300
O	21.844700	7.891900	11.764900
N	22.954500	8.977600	10.078200
H	23.460800	9.482800	10.759400
H	23.111800	9.148900	9.114400
N	21.192300	7.397800	9.612200
H	20.713300	6.609500	9.985900
H	21.463200	7.345800	8.654200
C	-1.127500	13.276900	9.967900

O	-1.029900	12.949500	11.191400
N	-0.217900	14.168000	9.424700
H	0.546800	14.441200	9.998500
H	-0.154900	14.295400	8.443400
N	-2.197500	12.802500	9.215700
H	-2.720900	12.072000	9.633400
H	-2.147600	12.827100	8.223700
C	5.797000	14.184400	10.708900
O	5.785900	14.332900	11.974600
N	6.524800	15.072100	9.930400
H	7.218200	15.602800	10.407500
H	6.659600	14.894200	8.960900
N	5.089900	13.135100	10.148000
H	4.426200	12.679400	10.733900
H	4.955400	13.082900	9.165200
C	11.788100	14.433500	10.892500
O	11.980500	14.480400	12.153500
N	12.342500	15.427600	10.084300
H	13.110200	15.915700	10.489200
H	12.405000	15.266100	9.100800
N	11.020700	13.420100	10.359300
H	10.472700	12.875300	10.987400
H	10.774100	13.420500	9.396300
C	17.074900	14.034200	10.810600
O	17.154500	14.181200	12.074800
N	17.945500	14.740600	9.988900
H	18.771800	15.079800	10.428200
H	18.023000	14.496800	9.025500
N	16.099900	13.212500	10.283100
H	15.443700	12.804200	10.905800
H	15.938300	13.155600	9.305400
C	21.627400	13.655500	11.053500
O	21.372700	13.507900	12.289000
N	22.742000	14.374000	10.667500
H	23.221600	14.881500	11.367500
H	22.943100	14.545600	9.711500
N	20.745800	13.128700	10.104000
H	20.179300	12.383600	10.448000
H	21.067400	13.032800	9.163400
C	2.653700	0.534000	3.669200
O	2.656000	0.675400	2.409700
N	3.720800	-0.136400	4.274200
H	4.265000	-0.702100	3.667600
H	3.634800	-0.437600	5.217300
N	1.620200	1.056200	4.427900
H	1.005000	1.693400	3.969900
H	1.704300	1.108300	5.416000
C	7.904400	-0.003900	3.356600
O	7.836100	0.190000	2.104600
N	9.039100	-0.618300	3.883000
H	9.583100	-1.138600	3.237800
H	9.043000	-0.919500	4.830100
N	6.856000	0.392100	4.180100
H	6.235200	1.066800	3.789600
H	7.008200	0.445100	5.162800
C	13.324800	0.043000	3.036400
O	13.143600	0.293100	1.803100
N	13.876000	-1.173600	3.419900
H	14.335800	-1.685600	2.707000
H	14.186600	-1.300400	4.356500
N	12.977700	0.996000	3.986300
H	12.340800	1.696800	3.682900
H	12.940500	0.737300	4.947900

C	19.482100	0.030700	3.218300
O	19.404600	-0.045900	1.956100
N	20.610200	-0.519200	3.855400
H	21.020100	-1.275600	3.357100
H	20.575600	-0.634200	4.845600
N	18.494400	0.667200	3.945500
H	17.861600	1.240100	3.432700
H	18.639000	0.872800	4.908600
C	3.003500	5.844100	3.374100
O	2.926700	5.896100	2.106700
N	4.143800	5.322300	3.975900
H	4.705700	4.740700	3.389100
H	4.102800	5.073900	4.939600
N	1.938100	6.323000	4.133500
H	1.328500	6.954100	3.658500
H	2.064900	6.471100	5.109900
C	8.235400	5.795500	3.256900
O	8.087000	5.808500	1.994000
N	9.449400	5.398500	3.804700
H	10.044800	4.869200	3.204000
H	9.494700	5.189200	4.777000
N	7.177900	6.190000	4.070000
H	6.462200	6.717300	3.622100
H	7.343300	6.379400	5.033000
C	13.779100	5.568500	3.184600
O	13.778000	5.579200	1.915300
N	14.854200	4.990900	3.860200
H	15.395900	4.349400	3.321800
H	14.753000	4.780500	4.829000
N	12.709400	6.127600	3.875700
H	12.121600	6.735400	3.346800
H	12.817600	6.340900	4.842800
C	19.653300	5.321700	2.951700
O	19.604600	5.137900	1.691100
N	20.818300	4.990800	3.638900
H	21.421900	4.354000	3.159800
H	20.771300	4.891900	4.631200
N	18.548800	5.858700	3.601000
H	17.921700	6.371300	3.016000
H	18.661600	6.197500	4.531700
C	2.915400	11.150500	3.026800
O	2.898200	11.188900	1.753700
N	4.075100	10.775000	3.691000
H	4.744800	10.278700	3.139900
H	4.011800	10.519800	4.652600
N	1.759100	11.495400	3.722100
H	1.101700	12.040400	3.206300
H	1.822600	11.684800	4.699000
C	8.546200	11.358600	3.241300
O	8.517200	11.384900	1.973100
N	9.680400	10.868600	3.887700
H	10.258800	10.271500	3.335000
H	9.616200	10.643500	4.856500
N	7.450900	11.830400	3.961900
H	6.828300	12.417900	3.450500
H	7.566500	12.035100	4.930100
C	14.254500	10.806700	3.158000
O	14.346700	10.624900	1.905100
N	15.320900	10.463700	3.982900
H	16.020400	9.885600	3.574200
H	15.168700	10.359800	4.961600
N	13.080400	11.338400	3.690300
H	12.527100	11.872800	3.053800

H	13.089900	11.655900	4.634400
C	19.422000	11.110100	3.380200
O	19.472300	11.062200	2.110500
N	20.536700	10.700800	4.110400
H	21.157100	10.090800	3.621400
H	20.443600	10.543400	5.089300
N	18.265500	11.556300	4.007100
H	17.651200	12.096700	3.434300
H	18.304700	11.791200	4.974300
C	2.414800	16.409300	3.095200
O	2.473000	16.415700	1.829900
N	3.468300	15.920900	3.845200
H	4.153700	15.388000	3.356900
H	3.347100	15.747900	4.818100
N	1.243600	16.882300	3.715400
H	0.749300	17.555200	3.176000
H	1.278400	17.065300	4.695400
C	8.721900	16.482600	3.470500
O	8.868500	16.356000	2.213600
N	9.551800	15.775600	4.332800
H	10.382100	15.409100	3.931700
H	9.566700	15.991600	5.304400
N	7.707200	17.279900	3.963000
H	7.077900	17.677800	3.313400
H	7.559100	17.400500	4.935600
C	14.399400	16.969900	3.683000
O	14.328000	16.813500	2.424400
N	15.263800	16.181300	4.426900
H	15.969400	15.694700	3.923300
H	15.427900	16.381900	5.386200
N	13.593600	17.918200	4.298800
H	12.869300	18.306300	3.748300
H	13.506800	17.946200	5.287200
C	19.488900	16.400600	3.339000
O	19.470800	16.218400	2.084800
N	20.533600	15.913700	4.094400
H	21.190800	15.316300	3.643300
H	20.507800	15.945400	5.086100
N	18.408200	17.068200	3.943500
H	17.903700	17.656800	3.321400
H	18.539500	17.426400	4.864200
C	2.880700	0.235100	8.363100
O	2.911000	0.371200	7.102900
N	3.554000	-0.832400	8.943600
H	4.185400	-1.324500	8.360800
H	3.691400	-0.870800	9.925100
N	2.202500	1.163000	9.147200
H	1.534000	1.728500	8.667700
H	2.010100	0.938800	10.097000
C	8.085600	-0.316200	8.012400
O	8.277600	-0.276700	6.759000
N	8.219900	-1.529200	8.682400
H	8.703200	-2.239000	8.186000
H	8.293600	-1.539100	9.674800
N	7.754000	0.849800	8.694900
H	7.341000	1.574300	8.145400
H	7.454900	0.778300	9.640900
C	13.900300	-0.424300	7.632300
O	14.092300	-0.358900	6.377400
N	14.309800	-1.556100	8.324700
H	14.946200	-2.148300	7.849500
H	14.334500	-1.552100	9.319200
N	13.300100	0.640800	8.292700

H	12.764200	1.266400	7.732100
H	13.015300	0.528300	9.239800
C	19.957100	0.543500	7.882800
O	19.903900	0.340300	6.628400
N	20.727700	-0.296800	8.667800
H	21.113900	-1.094800	8.231200
H	20.694100	-0.255000	9.659000
N	19.334500	1.661300	8.428500
H	18.623000	2.071200	7.860800
H	19.203400	1.702100	9.415600
C	3.248800	5.904500	8.062500
O	3.149100	5.730100	6.805500
N	4.366400	5.430500	8.728400
H	4.942000	4.790200	8.225600
H	4.380500	5.394700	9.721800
N	2.224500	6.561500	8.736600
H	1.593500	7.078200	8.161300
H	2.390700	6.908800	9.654800
C	8.532300	5.746200	7.948600
O	8.499800	5.650300	6.678200
N	9.633300	5.272300	8.638400
H	10.252100	4.668800	8.141600
H	9.614100	5.209000	9.630300
N	7.453200	6.316800	8.613800
H	6.832300	6.861000	8.055100
H	7.552000	6.580700	9.567800
C	13.796800	5.559700	7.860400
O	13.858300	5.654300	6.591200
N	14.852300	4.981000	8.547100
H	15.491500	4.440500	8.006500
H	14.750700	4.750100	9.510000
N	12.673900	6.034100	8.523200
H	12.095300	6.667300	8.014400
H	12.684800	6.120800	9.514600
C	19.561900	5.344400	7.624300
O	19.622200	5.517100	6.362200
N	20.551400	4.610100	8.261000
H	21.136700	4.055000	7.673200
H	20.394000	4.279500	9.187400
N	18.511000	5.905200	8.333600
H	17.981600	6.607700	7.866000
H	18.541700	5.936200	9.327600
C	2.812300	11.238600	7.706500
O	2.849900	11.075400	6.443000
N	3.815000	10.696300	8.490100
H	4.412200	10.030200	8.050800
H	3.706900	10.647500	9.477900
N	1.758200	11.950500	8.268800
H	1.209300	12.488100	7.632200
H	1.855000	12.303900	9.194900
C	8.709600	11.457300	7.937500
O	8.681300	11.378200	6.667100
N	9.810300	10.966800	8.628900
H	10.376300	10.309100	8.135300
H	9.761000	10.867400	9.618600
N	7.643300	12.042100	8.602900
H	7.002500	12.564800	8.048400
H	7.717300	12.267600	9.568600
C	13.997400	11.074300	7.849000
O	13.947700	11.053300	6.575500
N	15.127300	10.591700	8.491000
H	15.729700	10.008200	7.951300
H	15.115400	10.450000	9.475300

N	12.918000	11.580900	8.558000
H	12.280700	12.150400	8.044100
H	13.007700	11.760900	9.531800
C	19.293000	10.945000	8.049700
O	19.374700	11.146900	6.795000
N	20.341400	10.314800	8.708100
H	20.982800	9.817900	8.128400
H	20.208700	9.981100	9.636200
N	18.163400	11.371900	8.725300
H	17.557900	11.988100	8.228200
H	18.135300	11.377500	9.718200
C	2.066300	15.963200	7.778300
O	2.009900	16.128700	6.518900
N	2.787700	14.889300	8.304000
H	3.516100	14.545300	7.712500
H	2.993100	14.898600	9.280500
N	1.370000	16.827000	8.603000
H	0.719600	17.436100	8.174400
H	1.311900	16.673800	9.583000
C	8.570900	16.847600	8.134400
O	8.354700	16.792300	6.882600
N	9.392700	15.901300	8.734700
H	10.015100	15.414100	8.127000
H	9.697200	16.048200	9.671500
N	7.962100	17.844300	8.883100
H	7.213900	18.325700	8.448200
H	7.985000	17.813100	9.876600
C	14.658400	17.129300	8.333600
O	14.321300	17.103100	7.109800
N	15.215800	15.998500	8.922700
H	15.631100	15.344600	8.292600
H	15.640100	16.088900	9.819900
N	14.435200	18.283200	9.071800
H	13.846600	18.964000	8.659500
H	14.531900	18.277800	10.061000
C	19.755300	16.964900	7.963500
O	19.415200	16.792400	6.750800
N	20.455600	15.972200	8.625100
H	20.874300	15.258300	8.074000
H	20.790900	16.122000	9.547500
N	19.422000	18.153100	8.605100
H	18.733800	18.705500	8.155000
H	19.487200	18.213400	9.596900
C	2.993400	0.058300	13.073300
O	3.251700	0.085800	11.831900
N	3.416200	-1.034100	13.831600
H	4.094100	-1.615500	13.394600
H	3.484200	-0.945900	14.816200
N	2.296700	1.107200	13.653800
H	1.872400	1.762500	13.031700
H	1.887100	1.001800	14.547900
C	7.489300	0.278200	12.278700
O	8.229900	-0.341300	11.452800
N	8.051500	1.197500	13.151800
H	9.002700	1.441000	12.971700
H	7.470100	1.914700	13.522100
N	6.130400	-0.064600	12.381100
H	5.784500	-0.572400	11.596200
H	5.513700	0.661200	12.686800
C	13.037000	0.218800	11.904000
O	13.766300	-0.402200	11.069200
N	13.451100	1.447300	12.384500
H	14.418500	1.672000	12.308900

H	12.902100	1.936700	13.049100
N	11.832400	-0.351100	12.328800
H	11.493500	-1.079800	11.744000
H	11.133500	0.254600	12.701800
C	19.947400	1.451300	12.481400
O	20.058000	0.995300	11.299900
N	21.053600	2.008800	13.102000
H	21.857500	2.174300	12.535000
H	20.944100	2.573300	13.906600
N	18.748000	1.271000	13.170900
H	17.966400	1.028900	12.598100
H	18.539400	1.877400	13.927200
C	2.862400	5.562100	12.627900
O	3.281400	6.035300	11.521700
N	3.542200	4.511400	13.226900
H	4.283800	4.106600	12.699000
H	3.046100	3.909100	13.838500
N	1.796400	6.178800	13.279300
H	1.328500	6.888600	12.756300
H	1.224300	5.616300	13.864700
C	8.454800	5.832600	12.662300
O	8.510800	5.887900	11.393800
N	9.056200	4.772800	13.325900
H	9.675100	4.204900	12.784700
H	9.252100	4.846700	14.293400
N	7.784300	6.838000	13.355300
H	7.210400	7.437600	12.799200
H	7.470900	6.661800	14.278300
C	14.310700	5.860400	12.341600
O	13.721100	5.424600	11.299000
N	15.373200	5.144700	12.879000
H	15.669200	4.342600	12.366900
H	16.068700	5.635500	13.387700
N	13.808900	6.979000	12.993100
H	13.091100	7.484500	12.519400
H	14.420600	7.504000	13.569200
C	19.992400	5.668000	12.114400
O	19.496000	5.094200	11.091600
N	21.185200	5.186900	12.657900
H	21.682500	4.550600	12.067500
H	21.759000	5.845000	13.137000
N	19.274800	6.673400	12.753200
H	18.440900	6.973800	12.295900
H	19.784000	7.369600	13.245700
C	2.281100	10.924600	12.182600
O	2.697700	11.555900	11.158200
N	3.099800	9.980800	12.789000
H	3.950400	9.764100	12.316500
H	2.671000	9.241300	13.294800
N	1.059000	11.291800	12.758300
H	0.486100	11.856800	12.163200
H	0.563000	10.571200	13.237000
C	8.220000	11.137100	12.423500
O	8.747900	11.679500	11.397800
N	8.851000	10.064100	13.025000
H	9.647800	9.681800	12.564100
H	8.341300	9.471500	13.631800
N	7.075600	11.700000	12.993700
H	6.663200	12.437600	12.462000
H	6.432000	11.076100	13.425800
C	14.158200	11.092200	12.550200
O	14.129400	11.132900	11.281300
N	14.867000	10.082000	13.184000

H	15.463300	9.527700	12.605900
H	15.127500	10.182300	14.133600
N	13.490800	12.077300	13.278400
H	12.843200	12.629200	12.753200
H	13.232200	11.881900	14.215400
C	19.675500	11.072000	12.604400
O	19.212400	10.700400	11.477700
N	20.702400	10.349400	13.179200
H	21.106000	9.614000	12.643800
H	21.218000	10.720900	13.935900
N	19.065500	12.126300	13.296600
H	18.398300	12.631100	12.748100
H	19.673700	12.709700	13.829400
C	1.993800	14.961100	12.372800
O	1.996700	15.372800	11.170700
N	3.158000	15.077500	13.131500
H	3.988600	15.253200	12.607600
H	3.266900	14.501800	13.930400
N	0.808100	14.521500	12.945100
H	0.050200	14.351900	12.317800
H	0.836900	13.963400	13.762600
C	8.444200	16.189400	12.737100
O	8.670000	16.609500	11.561500
N	9.491500	15.659200	13.477000
H	10.320800	15.435400	12.972700
H	9.304500	15.139200	14.297200
N	7.178600	16.384500	13.312000
H	6.460900	16.517900	12.628200
H	6.911800	15.743900	14.026300
C	14.144000	16.461600	12.637800
O	14.879600	16.986300	11.742800
N	14.569100	15.320200	13.303500
H	15.375900	14.869700	12.926300
H	13.883800	14.735100	13.719500
N	12.966000	17.109300	13.016000
H	12.686400	17.852000	12.419600
H	12.233100	16.559500	13.400800
C	18.973800	16.590600	12.276200
O	19.743200	17.004700	11.354900
N	19.447100	15.662300	13.205900
H	20.323500	15.245600	12.974000
H	18.779000	15.057900	13.626200
N	17.704300	17.146800	12.416900
H	17.386100	17.685700	11.645100
H	16.997800	16.612900	12.870600

n=120 urea cluster optimized with AM1

O	0.646400	0.157100	-0.014200
N	1.288800	-0.810800	0.029200
H	2.318900	-0.669500	0.040500
C	6.567500	0.441800	0.560200
O	5.788200	1.263500	-0.025000
N	7.882600	0.311900	0.124700
H	8.179600	0.959500	-0.570700
H	8.572200	0.021100	0.777400
N	6.068800	-0.375500	1.561400
H	5.119000	-0.224900	1.820900
H	6.689800	-0.735600	2.245200
C	11.244000	1.317300	0.695500
O	10.339600	2.102900	0.259000
N	12.397800	1.107100	-0.053600

H	12.553800	1.739400	-0.807600
H	13.212600	0.803900	0.429000
N	11.014800	0.597100	1.858200
H	10.175900	0.807900	2.352800
H	11.792600	0.272300	2.383300
C	16.778200	2.434700	0.109400
O	17.067600	3.522400	0.711100
N	17.431400	2.107400	-1.069900
H	18.054900	2.791400	-1.439600
H	16.980300	1.508500	-1.720300
N	15.906700	1.533200	0.705500
H	15.424500	1.855700	1.517100
H	15.417300	0.896500	0.122600
C	20.238600	3.542900	2.087500
O	21.017300	4.499000	1.777700
N	19.888400	2.604700	1.123100
H	20.110900	2.853200	0.182700
H	19.057200	2.077400	1.251000
N	19.853000	3.381000	3.416700
H	20.054100	4.153500	4.007200
H	19.017900	2.882900	3.631100
C	0.906800	-1.244100	-5.689300
O	0.668500	-0.002100	-5.579000
N	1.632800	-1.711100	-6.783200
H	2.130800	-1.010100	-7.290300
H	2.086300	-2.590400	-6.702400
N	0.312000	-2.132700	-4.790200
H	-0.035600	-1.706100	-3.962500
H	0.732300	-3.024300	-4.666400
C	6.190800	0.260000	-4.937500
O	5.427500	1.115000	-5.494100
N	7.367000	-0.120500	-5.572600
H	7.619500	0.409000	-6.379600
H	8.116400	-0.447700	-5.009600
N	5.777200	-0.376600	-3.766400
H	4.948900	-0.003500	-3.350600
H	6.486400	-0.651500	-3.123400
C	11.683300	1.292600	-5.102500
O	11.528300	2.543000	-4.939700
N	12.794900	0.830400	-5.807800
H	13.280400	1.527800	-6.337200
H	12.756900	-0.072600	-6.215300
N	10.756000	0.420200	-4.557700
H	10.088500	0.805700	-3.923400
H	10.954900	-0.545300	-4.484800
C	16.826200	2.623200	-5.136300
O	17.040500	3.773800	-4.632300
N	17.571300	2.200600	-6.226500
H	18.190100	2.872600	-6.626900
H	17.181800	1.527000	-6.840400
N	15.928100	1.762000	-4.509500
H	15.402900	2.155900	-3.759500
H	15.462700	1.083200	-5.063000
C	23.127900	3.804400	-4.067200
O	22.794800	4.898300	-4.621000
N	23.951900	2.926000	-4.756000
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O	0.577900	-0.094200	-11.453500

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H       0.735400   -1.246400   -9.321000
H       2.067400   -2.177500   -9.671000
C       6.728200    0.258400  -10.964100
O       6.317700    1.451100  -11.118100
N       7.956300   -0.102800  -11.497500
H       8.396400    0.551100  -12.109600
H       8.207600   -1.054500  -11.580500
N       5.928700   -0.660000  -10.290300
H       5.148900   -0.274600   -9.796100
H       6.350700   -1.459100   -9.884100
C      11.806300    1.609700  -10.773800
O      12.089800    2.736800  -10.252000
N      12.485800    1.176300  -11.912500
H      13.116700    1.844600  -12.305200
H      11.972600    0.635800  -12.571800
N      10.903300    0.778700  -10.132900
H      10.402400    1.153900   -9.358800
H      10.493300    0.022800  -10.620000
C      17.351200    2.986000  -10.358800
O      17.170400    4.222700  -10.120400
N      18.178200    2.615700  -11.399300
H      18.747400    3.321800  -11.812300
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N      16.734000    2.032100   -9.545200
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H      21.590000    3.719800  -10.493100
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H      22.171000    3.664100   -6.949100
C       2.160500   -0.298700  -17.812500
O       1.261400    0.384000  -17.230800
N       2.047900   -0.553200  -19.182100
H       1.383600    0.014500  -19.653100
H       2.879500   -0.768900  -19.685400
N       3.186400   -0.864100  -17.073900
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H       4.032300   -1.111700  -17.529000
C       6.978300    0.259100  -16.320500
O       6.840400    1.510600  -16.144800
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H       8.555300    0.478100  -17.578700
H       7.997300   -1.111500  -17.475900
N       6.058700   -0.605800  -15.755600
H       5.402000   -0.222000  -15.111200
H       6.214700   -1.580600  -15.740600
C      12.217300    2.040500  -16.476100
O      12.308000    3.190500  -15.940200
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H	16.466000	2.101200	-15.524700
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N	21.538700	4.038500	-16.613300
H	21.242200	4.452800	-17.470300
H	21.191000	3.140100	-16.390300
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H	22.550100	5.105500	-13.689900
H	21.893700	3.601500	-14.008600
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O	-0.300600	4.467600	0.690500
N	0.090800	3.010300	-1.047400
H	0.741700	3.672300	-1.412400
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N	-1.232300	2.375500	0.878900
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H	6.576600	4.817300	-1.111000
H	6.238700	3.193300	-0.740500
N	4.361300	3.718000	1.037800
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H	4.610100	2.754800	1.096400
C	10.178100	5.596300	0.468200
O	10.067800	6.864200	0.509200
N	10.959600	5.019400	-0.518200
H	11.586800	5.630100	-0.995600
H	11.188300	4.053000	-0.471900
N	9.521600	4.819300	1.414500
H	8.827100	5.280600	1.961200
H	9.398900	3.846700	1.242800
C	16.011000	6.875500	0.770600
O	15.635700	8.092300	0.760200
N	17.268400	6.548300	0.292200
H	17.758600	7.252700	-0.213300
H	17.523400	5.598800	0.145900
N	15.151400	5.900100	1.254500
H	14.376400	6.213400	1.798000
H	15.487900	4.977600	1.412300
C	21.127600	7.885800	1.467200
O	21.090800	9.099100	1.092600
N	22.332300	7.199900	1.423600
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H	22.362200	6.216900	1.564400
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H	19.230200	7.856500	2.203100
H	20.023100	6.362300	2.314100
C	-0.246200	3.290700	-5.561100
O	-0.500900	4.512400	-5.313000
N	0.994300	2.936200	-6.077700
H	1.489400	3.659800	-6.554300
H	1.127000	2.008000	-6.414800
N	-1.210000	2.331800	-5.284600
H	-1.957400	2.617500	-4.701100
H	-0.975200	1.365700	-5.305900

C	4.919500	4.542800	-5.537300
O	4.803300	5.803300	-5.403000
N	6.068600	4.021900	-6.115800
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H	6.082100	3.069900	-6.406400
N	3.893700	3.712900	-5.107100
H	3.234200	4.118500	-4.478800
H	4.050100	2.732700	-5.030400
C	10.773000	5.910600	-4.971400
O	10.450600	7.140700	-5.036500
N	12.078600	5.524200	-5.253600
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H	10.098200	4.058700	-4.361100
C	16.120400	7.096800	-4.593600
O	15.792700	8.326600	-4.569600
N	17.394100	6.749200	-5.016500
H	17.897100	7.443300	-5.524600
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N	15.193100	6.133900	-4.212700
H	14.414800	6.466600	-3.682000
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C	22.078700	8.270300	-4.128600
O	21.749000	9.491800	-4.231400
N	23.353300	7.880000	-4.527200
H	23.849700	8.532100	-5.084400
H	23.558300	6.916100	-4.655400
N	21.166200	7.341900	-3.639700
H	20.413500	7.715100	-3.100000
H	21.491600	6.433100	-3.396400
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H	-1.088200	1.260300	-11.276800
C	5.520000	4.761700	-10.775600
O	5.227600	5.994400	-10.639900
N	6.745500	4.412500	-11.323800
H	7.243300	5.138500	-11.791900
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N	4.604100	3.799300	-10.374300
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H	4.897800	2.852800	-10.282000
C	11.152200	6.077500	-10.194500
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C	16.399400	7.603300	-10.023000
O	16.120500	8.846500	-9.989600
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H	15.683800	5.728000	-9.537000
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O	22.003500	9.978600	-9.699700
N	23.616100	8.350600	-9.832000
H	24.092500	8.929200	-10.480200
H	23.834500	7.380000	-9.834400
N	21.452700	7.918800	-8.842400
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H	21.763500	7.026000	-8.533200
C	0.407300	3.685400	-16.847400
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H	2.147200	4.093200	-17.826200
H	1.749100	2.444500	-17.810200
N	-0.541100	2.714400	-16.566100
H	-1.288700	2.984900	-15.976300
H	-0.317500	1.748800	-16.632400
C	6.034500	4.854200	-16.015000
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H	10.839300	4.605700	-15.223800
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H	15.540900	7.255800	-13.990500
H	16.660900	6.112300	-14.572500
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N	22.699800	9.037600	-16.414100
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H	20.938600	7.656900	-15.056200
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N	-0.408100	7.292000	-0.415900
H	0.061300	7.944600	-1.003300
H	-0.061800	6.360500	-0.371100
N	-1.616100	6.983700	1.663800
H	-2.430300	7.326600	2.119400
H	-1.589700	5.996500	1.522400
C	4.017600	9.130400	0.505800
O	3.671800	10.354000	0.585900
N	4.609000	8.656300	-0.655000
H	4.984900	9.350400	-1.267000
H	5.071900	7.774200	-0.632800
N	3.791000	8.296000	1.598800

H	3.105500	8.624600	2.245100
H	3.830900	7.308800	1.463900
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N	9.867600	9.704600	-0.531400
H	10.291800	10.411600	-1.095900
H	10.352500	8.836000	-0.470900
N	8.937200	9.333600	1.678800
H	8.215300	9.643700	2.293400
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C	14.571800	11.343400	1.005100
O	14.140800	12.537400	1.077700
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H	15.825900	10.098500	-0.075900
N	14.273200	10.451600	2.025800
H	13.528800	10.720700	2.635600
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H	-2.083500	7.793800	-3.950700
H	-1.465500	6.274500	-4.451600
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O	3.764800	10.371400	-5.244400
N	4.731200	8.627300	-6.387000
H	5.202100	9.302300	-6.951100
H	5.161100	7.731200	-6.319500
N	3.712900	8.319500	-4.205200
H	3.005000	8.682700	-3.604600
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H	10.368900	10.738100	-6.461800
H	10.488000	9.128300	-5.939900
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H	13.962700	10.930500	-2.472800
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C	20.690300	12.749900	-4.012300
O	20.169200	13.908400	-4.047400
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H	21.981100	13.122600	-5.542100
H	22.085100	11.525700	-4.949700

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O	-1.163200	9.055200	-11.308700
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N	-1.895200	7.013200	-10.564300
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H	-1.771700	6.032400	-10.486300
C	4.720400	9.388100	-10.853700
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C	9.839900	10.564800	-10.084800
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H	8.755900	10.029600	-8.454000
H	9.543600	8.722800	-9.198400
C	14.933600	12.045800	-9.526500
O	14.509700	13.225500	-9.315200
N	15.542400	11.743900	-10.747300
H	15.929300	12.531400	-11.226000
H	16.074400	10.902700	-10.809200
N	14.785500	11.080100	-8.539700
H	14.104300	11.273400	-7.838100
H	14.923400	10.121000	-8.773700
C	21.144600	13.235400	-9.311600
O	20.639500	14.396700	-9.226700
N	21.632600	12.800900	-10.537200
H	21.801300	13.500000	-11.218900
H	22.148700	11.953800	-10.599100
N	21.207600	12.423100	-8.179900
H	20.547700	12.644500	-7.470300
H	21.409900	11.453200	-8.296100
C	-0.195700	8.317000	-16.521600
O	-0.266000	9.580400	-16.446200
N	0.475200	7.722700	-17.569600
H	1.001700	8.314000	-18.173900
H	0.650500	6.745900	-17.576500
N	-0.777100	7.543000	-15.503300
H	-1.493300	8.011400	-14.998400
H	-0.932100	6.575100	-15.680100
C	4.957200	9.412900	-16.094800
O	4.719200	10.661600	-16.136900
N	5.640700	8.826400	-17.157600
H	6.163800	9.458200	-17.725000
H	6.008900	7.906900	-17.054100
N	4.539500	8.667200	-15.000200
H	3.831300	9.088500	-14.435400
H	4.526800	7.673700	-15.070700
C	10.250800	11.019400	-15.925000
O	10.001800	12.269400	-15.890800
N	10.943700	10.501700	-17.021300
H	11.494100	11.170200	-17.520800

H	11.338800	9.588600	-16.939800
N	9.818100	10.208400	-14.891100
H	9.116000	10.592200	-14.294100
H	9.831200	9.218900	-15.006100
C	15.486900	12.451900	-14.975700
O	15.128400	13.670900	-14.919300
N	16.204200	12.014600	-16.089800
H	16.712300	12.730500	-16.563500
H	16.650600	11.122200	-16.050100
N	15.159300	11.589200	-13.935100
H	14.412900	11.896600	-13.347300
H	15.215300	10.605700	-14.094600
C	20.437700	13.868300	-14.614300
O	19.848100	14.972800	-14.395100
N	21.095000	13.688800	-15.828400
H	21.352800	14.517700	-16.306400
H	21.661600	12.882400	-15.967000
N	20.429300	12.869000	-13.647700
H	19.727300	12.955900	-12.946100
H	20.669700	11.938200	-13.918200
C	2.798600	1.504600	2.486100
O	3.118000	0.407600	1.939500
N	3.505700	1.947300	3.593200
H	4.071400	1.281200	4.057600
H	3.218700	2.757400	4.089100
N	1.729800	2.240900	1.964700
H	1.519100	2.003700	1.020500
H	1.654800	3.208400	2.199100
C	7.817300	2.247100	3.351300
O	8.196600	1.070700	3.056600
N	8.061400	2.807100	4.776900
H	8.700800	2.295800	5.334700
H	7.979700	3.784400	4.941400
N	7.137400	2.995700	2.410400
H	6.968200	2.585800	1.525700
H	6.862600	3.932700	2.582500
C	13.471000	3.171800	2.786700
O	13.558300	1.932400	2.509900
N	14.464300	3.790900	3.518500
H	15.187700	3.224200	3.900900
H	14.344300	4.712700	3.866600
N	12.417700	3.904200	2.245000
H	11.651900	3.371200	1.908400
H	12.226000	4.823400	2.575000
C	17.290800	5.014200	4.486100
O	17.202500	3.772100	4.721700
N	17.058800	5.932600	5.506100
H	17.095100	5.566600	6.426400
H	17.320400	6.884100	5.376800
N	17.625100	5.442800	3.205800
H	17.513500	4.770200	2.480100
H	17.528200	6.404900	2.971400
C	2.746900	1.030800	-2.300000
O	2.992900	-0.214200	-2.312400
N	3.004300	1.773700	-1.139900
H	3.652700	1.330800	-0.515600
H	3.120700	2.758800	-1.245200
N	2.161800	1.611900	-3.407300
H	1.869100	1.016100	-4.146400
H	1.899000	2.567300	-3.420600
C	8.038800	2.381700	-2.858600
O	8.203700	1.131900	-3.026000
N	9.024400	3.120200	-2.219600

H	9.680800	2.599800	-1.679700
H	8.833700	4.053300	-1.931100
N	6.873500	2.991300	-3.317600
H	6.337300	2.460700	-3.965800
H	6.859500	3.980900	-3.436000
C	14.150800	3.603300	-1.962700
O	14.496800	2.389600	-1.798100
N	14.980600	4.622600	-1.509900
H	15.704700	4.347500	-0.886300
H	14.604000	5.537200	-1.382800
N	12.950600	3.894500	-2.597900
H	12.564000	3.177800	-3.171100
H	12.750500	4.836600	-2.852400
C	19.609700	4.945800	-1.687000
O	19.947700	3.719400	-1.724900
N	20.438400	5.913700	-0.857400
H	20.922400	5.485100	-0.093700
H	20.070900	6.825700	-0.686200
N	18.507900	5.362200	-2.414000
H	18.160800	4.722100	-3.094600
H	18.342200	6.332000	-2.559900
C	2.954400	1.132000	-8.653500
O	3.240300	-0.094200	-8.846300
N	3.843700	1.935200	-7.948800
H	4.498200	1.452100	-7.371100
H	3.540900	2.830600	-7.635300
N	1.759000	1.641400	-9.146000
H	1.318800	1.102800	-9.860200
H	1.636500	2.629600	-9.196800
C	8.616600	2.476900	-7.934600
O	8.828700	1.224200	-7.933400
N	9.459800	3.315900	-7.215900
H	10.032700	2.877700	-6.528700
H	9.175300	4.253300	-7.034300
N	7.543600	2.989200	-8.659500
H	7.180400	2.392100	-9.369700
H	7.504700	3.969700	-8.833700
C	14.466500	3.882400	-7.367000
O	14.817700	2.666600	-7.214500
N	15.359500	4.895800	-7.035900
H	16.129000	4.625200	-6.465200
H	15.017300	5.824000	-6.916000
N	13.202900	4.177600	-7.858300
H	12.750100	3.449400	-8.367200
H	12.993300	5.115000	-8.121900
C	19.622200	5.155200	-7.141600
O	19.908900	3.927300	-7.290400
N	20.491000	5.973400	-6.418000
H	21.062700	5.499700	-5.751800
H	20.184200	6.885400	-6.157700
N	18.455100	5.663400	-7.704300
H	18.029500	5.089800	-8.401300
H	18.374400	6.649300	-7.828100
C	3.298800	1.293800	-13.989500
O	3.591400	0.064200	-14.160800
N	4.046600	2.048200	-13.102700
H	4.655000	1.556900	-12.488100
H	3.751400	2.960400	-12.839300
N	2.232700	1.844700	-14.686700
H	1.876900	1.299800	-15.443000
H	2.145600	2.834700	-14.750700
C	9.490400	2.881800	-13.280800
O	9.855000	1.662900	-13.201900

N	10.095200	3.829800	-12.483400
H	10.872800	3.557100	-11.931900
H	9.826600	4.784900	-12.506800
N	8.518000	3.248100	-14.204200
H	8.005600	2.505300	-14.624100
H	8.074400	4.135100	-14.131200
C	14.414500	4.110200	-12.950900
O	14.787400	2.904400	-13.071200
N	15.294000	5.044400	-12.416800
H	16.053300	4.680700	-11.885100
H	14.957200	5.946600	-12.167400
N	13.124400	4.477500	-13.342900
H	12.688800	3.835900	-13.971700
H	12.939400	5.442400	-13.510300
C	20.241300	5.610100	-12.240900
O	20.525500	4.370400	-12.173400
N	21.100100	6.539800	-11.668100
H	21.755000	6.175500	-11.008200
H	20.782200	7.473600	-11.530600
N	19.078900	6.000000	-12.890800
H	18.662600	5.320700	-13.490900
H	18.934700	6.956700	-13.120700
C	4.654800	1.507100	-19.470900
O	4.860000	0.263700	-19.338900
N	5.474300	2.425100	-18.822500
H	5.985000	2.064400	-18.045300
H	5.171200	3.372800	-18.750400
N	3.595200	1.932200	-20.278700
H	3.345200	1.309000	-21.008600
H	3.495600	2.904900	-20.468600
C	9.440600	3.072700	-18.638500
O	9.803600	1.874900	-18.424300
N	10.034700	4.104300	-17.914600
H	10.903800	3.876500	-17.487100
H	9.910500	5.046000	-18.212400
N	8.451300	3.335800	-19.573800
H	7.916400	2.558600	-19.877600
H	8.036800	4.237400	-19.626500
C	15.272700	4.654200	-18.098900
O	15.602000	3.465800	-17.792100
N	15.903700	5.726600	-17.474700
H	16.796200	5.523200	-17.082500
H	15.786900	6.642600	-17.849700
N	14.270500	4.864600	-19.037300
H	13.692800	4.086900	-19.245600
H	13.896000	5.774500	-19.175000
C	19.557100	6.415900	-18.696100
O	19.830600	5.183100	-18.823100
N	20.469400	7.264100	-18.099500
H	21.222800	6.842800	-17.604100
H	20.243100	8.211900	-17.911500
N	18.313100	6.879900	-19.136500
H	17.879200	6.309200	-19.823500
H	18.170900	7.861500	-19.222200
C	2.136400	5.936000	3.488000
O	2.574600	4.748100	3.405400
N	2.422700	6.695500	4.614100
H	3.135800	6.343800	5.206000
H	2.262800	7.677500	4.611900
N	1.389700	6.465100	2.437400
H	0.982400	5.795000	1.820700
H	0.874900	7.300600	2.592800
C	7.203700	6.826400	3.707700

O	7.584200	5.614200	3.698600
N	7.363800	7.586700	4.861100
H	8.004400	7.226700	5.526900
H	7.256900	8.576200	4.817900
N	6.640500	7.377100	2.563700
H	6.270500	6.738500	1.893800
H	6.214700	8.274600	2.620500
C	12.631000	7.692500	3.533500
O	13.112400	6.517800	3.456200
N	12.731100	8.385700	4.731400
H	13.386500	8.030700	5.384500
H	12.517400	9.356900	4.767600
N	12.032500	8.266700	2.417600
H	11.710200	7.636600	1.715600
H	11.515400	9.110600	2.532400
C	17.692400	9.579000	3.688500
O	17.951800	8.350900	3.895600
N	17.699000	10.464200	4.756600
H	18.144900	10.151700	5.583300
H	17.647400	11.444600	4.595200
N	17.437400	10.016400	2.392200
H	17.106000	9.316800	1.762000
H	17.083100	10.938500	2.261000
C	2.094800	5.688500	-2.519500
O	2.381300	4.446400	-2.510500
N	2.478600	6.482700	-1.446800
H	3.190400	6.109300	-0.856300
H	2.435400	7.473500	-1.536000
N	1.398000	6.215600	-3.593700
H	0.964500	5.565700	-4.212500
H	1.027700	7.137100	-3.548700
C	7.335900	6.999800	-2.503400
O	7.664900	5.772100	-2.605200
N	7.644800	7.683700	-1.337300
H	8.348600	7.277400	-0.759600
H	7.536100	8.672800	-1.299600
N	6.683300	7.616600	-3.560400
H	6.269900	7.010500	-4.236900
H	6.256300	8.506000	-3.417500
C	12.770000	8.097300	-1.936300
O	13.072000	6.862100	-2.023500
N	13.031500	8.786500	-0.761200
H	13.684500	8.367500	-0.134700
H	12.945700	9.778400	-0.741900
N	12.191600	8.732600	-3.027400
H	11.808400	8.138700	-3.731800
H	11.764900	9.624300	-2.901500
C	18.357600	9.432300	-1.669500
O	18.793500	8.239100	-1.783000
N	18.611900	10.131100	-0.498100
H	19.320000	9.747200	0.091200
H	18.467200	11.115400	-0.467000
N	17.630500	9.994400	-2.704600
H	17.238700	9.364100	-3.368500
H	17.177600	10.871200	-2.568800
C	2.041800	5.738000	-8.478600
O	2.278000	4.490000	-8.368900
N	2.792600	6.628900	-7.739800
H	3.388600	6.259900	-7.033700
H	2.583200	7.599800	-7.735400
N	1.008400	6.175900	-9.305200
H	0.677500	5.503000	-9.965200
H	1.010600	7.126800	-9.606800

C	7.641700	7.068500	-7.748000
O	7.941800	5.831700	-7.808500
N	7.854500	7.767900	-6.567600
H	8.499900	7.358800	-5.925700
H	7.792000	8.761800	-6.574900
N	7.106000	7.690600	-8.867400
H	6.714600	7.087100	-9.558600
H	6.698700	8.594600	-8.771300
C	13.045600	8.394000	-7.302700
O	13.448400	7.192600	-7.440200
N	13.208600	9.034600	-6.085700
H	13.860800	8.626500	-5.451100
H	13.052500	10.015500	-6.018700
N	12.458600	9.041700	-8.386400
H	12.099000	8.443800	-9.100800
H	11.962500	9.890700	-8.220200
C	18.704300	9.740400	-6.843700
O	19.071400	8.528700	-6.983000
N	19.461800	10.601300	-6.045200
H	20.073200	10.136000	-5.404500
H	19.017500	11.425200	-5.697000
N	17.579200	10.181800	-7.510800
H	17.226400	9.609400	-8.245400
H	17.327800	11.142300	-7.496000
C	2.598300	5.916000	-13.714200
O	2.749900	4.649600	-13.733300
N	2.945200	6.621500	-12.575300
H	3.538900	6.160800	-11.923100
H	2.949500	7.617400	-12.587700
N	2.104100	6.562300	-14.840000
H	1.636500	5.981900	-15.503400
H	1.790800	7.505500	-14.759700
C	8.084300	7.373900	-13.300800
O	8.334200	6.123700	-13.281700
N	8.374800	8.145500	-12.187500
H	9.001100	7.746700	-11.520900
H	8.351300	9.139100	-12.262700
N	7.525500	7.930300	-14.444800
H	7.075100	7.286700	-15.059600
H	7.154900	8.854600	-14.407200
C	13.334700	8.702000	-12.892800
O	13.640700	7.468800	-12.968800
N	13.619100	9.406200	-11.732200
H	14.278100	8.997200	-11.106200
H	13.522700	10.396000	-11.718500
N	12.728900	9.326600	-13.978300
H	12.315500	8.719500	-14.653300
H	12.289200	10.209700	-13.841100
C	18.930100	10.133200	-12.157500
O	19.355300	8.958800	-12.407400
N	19.325200	10.766800	-10.995900
H	20.097400	10.370800	-10.506200
H	19.107200	11.724700	-10.841400
N	18.093500	10.768300	-13.076300
H	17.633400	10.166400	-13.727000
H	17.583200	11.569900	-12.775500
C	3.440500	6.006400	-19.288200
O	3.570500	4.741200	-19.311400
N	3.407400	6.671100	-18.070700
H	3.849900	6.212500	-17.303400
H	3.418700	7.667400	-18.067100
N	3.319700	6.697900	-20.491300
H	3.050700	6.148500	-21.271500

H	3.010800	7.646000	-20.480500
C	8.179100	7.580100	-18.999100
O	8.349900	6.322700	-18.955500
N	8.672400	8.378800	-17.974100
H	9.368700	7.973400	-17.387200
H	8.696700	9.364600	-18.097600
N	7.488600	8.137400	-20.067300
H	6.969200	7.505400	-20.627000
H	7.185000	9.083500	-20.030200
C	13.994700	9.149600	-18.488200
O	14.154800	7.892300	-18.550000
N	14.081300	9.803600	-17.263100
H	14.609600	9.338900	-16.554200
H	14.117000	10.798400	-17.259600
N	13.716000	9.854300	-19.656700
H	13.410300	9.305800	-20.424300
H	13.378300	10.788500	-19.600900
C	18.600600	11.005200	-18.350600
O	18.790300	9.752100	-18.399500
N	19.085600	11.735100	-17.273600
H	19.796700	11.298600	-16.727500
H	19.079100	12.728100	-17.315400
N	17.893100	11.626400	-19.374900
H	17.382700	11.025600	-19.975400
H	17.560600	12.554500	-19.257300
C	0.688800	9.869600	2.878900
O	1.705900	9.432700	3.510500
N	0.859800	10.629700	1.737400
H	1.790100	10.722900	1.395600
H	0.108600	10.742800	1.097100
N	-0.581600	9.638800	3.396000
H	-0.631500	9.015300	4.163500
H	-1.372300	9.706800	2.797200
C	5.740300	10.841100	2.965000
O	6.707900	10.258600	3.559100
N	6.002600	11.658300	1.880300
H	6.936800	11.673800	1.535600
H	5.270300	11.906300	1.257900
N	4.451000	10.719700	3.468300
H	4.315200	10.037500	4.174700
H	3.669300	10.906300	2.881100
C	10.799100	11.724300	3.076400
O	11.671100	10.978500	3.627800
N	11.186700	12.595800	2.077400
H	12.141800	12.586100	1.798500
H	10.514400	12.987100	1.464000
N	9.484900	11.721400	3.550000
H	9.250100	10.957400	4.141200
H	8.760600	12.010500	2.930300
C	17.107200	14.001000	2.480600
O	17.556600	12.947500	3.032000
N	17.989800	14.867200	1.861500
H	18.934200	14.565200	1.760500
H	17.664500	15.578300	1.257600
N	15.750800	14.321600	2.612400
H	15.178000	13.546300	2.876800
H	15.343100	14.891700	1.907200
C	0.980900	10.261300	-2.461300
O	1.215500	9.011000	-2.453800
N	1.536600	11.068300	-1.468600
H	2.298000	10.659300	-0.966200
H	1.607800	12.043900	-1.632400
N	0.150600	10.784200	-3.434100

H	-0.326700	10.142200	-4.027600
H	-0.180000	11.713000	-3.381700
C	6.751200	11.501000	-2.703900
O	6.549700	10.321500	-2.260900
N	7.659000	12.337300	-2.054100
H	8.179200	11.902700	-1.320100
H	8.167700	12.982700	-2.614300
N	5.982600	11.965700	-3.752900
H	5.357300	11.324400	-4.186500
H	6.269200	12.758800	-4.268700
C	12.187000	12.643700	-2.294300
O	11.950900	11.486900	-1.810400
N	13.034700	13.512400	-1.614800
H	13.513800	13.116300	-0.833700
H	13.545900	14.173500	-2.152500
N	11.504600	13.064500	-3.428400
H	10.920000	12.388300	-3.866900
H	11.933300	13.736400	-4.019900
C	17.782200	13.747300	-2.223600
O	17.411800	12.738800	-1.538200
N	18.655000	14.676800	-1.652700
H	19.099400	14.367400	-0.813600
H	19.236400	15.193000	-2.275200
N	17.227900	13.975200	-3.473900
H	16.602500	13.282000	-3.817600
H	17.760400	14.461900	-4.157100
C	0.762400	9.902000	-8.118300
O	1.506700	9.176800	-8.858800
N	1.295100	10.522300	-6.998700
H	2.233800	10.290500	-6.760000
H	0.690500	10.779800	-6.254500
N	-0.551100	10.125700	-8.494000
H	-0.868600	9.685900	-9.328400
H	-1.216700	10.413600	-7.819000
C	6.587800	11.692500	-7.669900
O	6.842800	10.448300	-7.631100
N	7.195100	12.547000	-6.751600
H	7.953800	12.147900	-6.236100
H	7.286900	13.506300	-6.984000
N	5.698500	12.177000	-8.619400
H	5.178600	11.493800	-9.129800
H	5.271500	13.060000	-8.488400
C	12.310700	12.948000	-7.414000
O	12.136500	11.746900	-7.024900
N	13.162100	13.789200	-6.696400
H	13.690600	13.341500	-5.976400
H	13.640400	14.496700	-7.204000
N	11.565000	13.434900	-8.471900
H	10.983100	12.788600	-8.956700
H	11.872200	14.237200	-8.961600
C	18.144000	13.774000	-7.177400
O	17.578900	13.031800	-6.312000
N	19.038800	14.748800	-6.765200
H	19.356900	14.687200	-5.822100
H	19.652700	15.162500	-7.430900
N	17.869100	13.565300	-8.527300
H	16.963500	13.213100	-8.737300
H	18.278100	14.159000	-9.214100
C	1.154700	10.059800	-12.858800
O	1.961200	9.280600	-13.465000
N	1.431600	10.469300	-11.555400
H	2.204200	10.015100	-11.120000
H	0.660300	10.657900	-10.956200

N	0.065700	10.571400	-13.543800
H	-0.071700	10.245800	-14.475400
H	-0.726800	10.877800	-13.034300
C	6.518600	11.624700	-12.813400
O	7.256500	10.719500	-13.327400
N	6.981800	12.337500	-11.717300
H	7.815200	11.998800	-11.288100
H	6.321000	12.776900	-11.123700
N	5.322000	11.974500	-13.434900
H	5.048000	11.380400	-14.189300
H	4.581100	12.294100	-12.852800
C	12.094000	13.273600	-12.597100
O	12.431400	12.050800	-12.671400
N	12.585700	14.051700	-11.557500
H	13.325600	13.653800	-11.016900
H	12.564500	15.038600	-11.629500
N	11.252100	13.809500	-13.570300
H	10.772800	13.137000	-14.135000
H	10.741700	14.632900	-13.357900
C	18.036800	14.548300	-12.096700
O	17.859300	13.418700	-11.531800
N	19.035400	15.395900	-11.633900
H	19.655300	15.010400	-10.953800
H	19.416300	16.063900	-12.261800
N	17.160600	14.960800	-13.089500
H	16.478300	14.299900	-13.387800
H	17.465500	15.627300	-13.757100
C	2.975900	10.347500	-18.635300
O	2.545000	9.300100	-19.218000
N	4.195900	10.902200	-19.031200
H	4.764900	10.310200	-19.591900
H	4.700200	11.449700	-18.368200
N	2.183800	10.981600	-17.696700
H	1.319400	10.547700	-17.456300
H	2.598700	11.592400	-17.035400
C	7.760000	11.789300	-18.159900
O	7.154400	10.892100	-18.833000
N	8.944000	12.329100	-18.655600
H	9.348100	11.846300	-19.420900
H	9.564400	12.796100	-18.033700
N	7.202000	12.263700	-16.991800
H	6.352600	11.849100	-16.679200
H	7.742000	12.795200	-16.352000
C	13.370300	13.406100	-17.521300
O	12.979800	12.458200	-18.272800
N	14.591400	14.048000	-17.791100
H	15.201400	13.516700	-18.375600
H	15.056300	14.459400	-17.006700
N	12.545900	13.868300	-16.514700
H	11.682300	13.392400	-16.377000
H	12.927700	14.380400	-15.755600
C	17.439000	15.491600	-17.685700
O	17.481100	14.235300	-17.862100
N	18.078100	16.052700	-16.594200
H	18.674500	15.459600	-16.058500
H	18.226300	17.028200	-16.537300
N	16.753300	16.283900	-18.606500
H	16.149000	15.792300	-19.224000
H	16.472500	17.198800	-18.350900
N	3.277700	-2.289700	-4.275100
H	3.194600	-1.292000	-4.343400
H	4.214200	-2.540200	-4.521000
H	3.136100	-2.528800	-3.312800

n=160 urea cluster optimized with AM1

C	-7.004300	-11.106200	-7.568800
O	-5.803300	-11.457200	-7.795800
N	-7.553300	-11.326200	-6.302800
H	-6.881300	-11.501200	-5.585800
H	-8.312300	-10.753200	-6.012800
N	-7.776300	-10.625200	-8.609800
H	-7.319300	-10.452200	-9.477800
H	-8.627300	-10.154200	-8.434800
C	-7.271300	-6.867200	-7.905800
O	-6.171300	-7.339200	-7.469800
N	-7.963300	-5.924200	-7.153800
H	-7.481300	-5.566200	-6.357800
H	-8.549300	-5.282200	-7.636800
N	-7.833300	-7.398200	-9.065800
H	-7.230300	-7.996200	-9.591800
H	-8.419300	-6.801200	-9.603800
C	-8.135300	-1.181200	-7.817800
O	-6.967300	-1.435200	-7.378800
N	-8.858300	-0.122200	-7.272800
H	-8.336300	0.496800	-6.686800
H	-9.548300	0.305800	-7.843800
N	-8.719300	-2.043200	-8.735800
H	-8.136300	-2.771200	-9.089800
H	-9.417300	-1.689200	-9.344800
C	-8.712300	4.074800	-8.077800
O	-7.444300	4.130800	-8.126800
N	-9.425300	5.150800	-7.560800
H	-8.892300	5.808800	-7.030800
H	-10.363300	5.014800	-7.271800
N	-9.357300	2.936800	-8.551800
H	-8.794300	2.307800	-9.086800
H	-10.317300	2.982800	-8.786800
C	-8.974300	9.263800	-9.401800
O	-8.305300	10.076800	-8.684800
N	-9.620300	8.190800	-8.809800
H	-9.410300	8.030800	-7.849800
H	-9.862300	7.402800	-9.366800
N	-9.122300	9.520800	-10.760800
H	-8.548300	10.238800	-11.130800
H	-9.379300	8.775800	-11.368800
C	-6.452300	-11.601200	-0.588800
O	-5.534300	-12.156200	-1.275800
N	-6.651300	-11.986200	0.738200
H	-5.914300	-12.523200	1.134200
H	-7.069300	-11.331200	1.363200
N	-7.306300	-10.701200	-1.198800
H	-7.129300	-10.474200	-2.151800
H	-7.817300	-10.054200	-0.647800
C	-7.374300	-6.282200	-2.311800
O	-6.253300	-6.650200	-1.827800
N	-8.032300	-5.184200	-1.761800
H	-7.530300	-4.682200	-1.063800
H	-8.626300	-4.650200	-2.350800
N	-7.976300	-7.043200	-3.300800
H	-7.453300	-7.820200	-3.641800
H	-8.601300	-6.603200	-3.931800
C	-7.898300	-0.847200	-2.891800
O	-6.765300	-1.032200	-2.343800
N	-8.656300	0.276800	-2.544800
H	-8.181300	0.907800	-1.931800

H	-9.183300	0.707800	-3.271800
N	-8.412300	-1.810200	-3.735800
H	-7.836300	-2.589200	-3.960800
H	-9.182300	-1.612200	-4.322800
C	-8.235300	4.755800	-2.328800
O	-7.160300	5.123800	-2.907800
N	-8.825300	5.588800	-1.408800
H	-8.394300	6.463800	-1.214800
H	-9.588300	5.293800	-0.854800
N	-8.840300	3.547800	-2.704800
H	-8.281300	2.998800	-3.326800
H	-9.277300	3.026800	-1.975800
C	-8.390300	10.308800	-4.442800
O	-7.511300	11.005800	-3.838800
N	-9.088300	9.339800	-3.739800
H	-8.777300	9.149800	-2.812800
H	-9.539300	8.607800	-4.235800
N	-8.714300	10.598800	-5.765800
H	-8.089300	11.208800	-6.237800
H	-9.122300	9.886800	-6.331800
C	-6.628300	-10.873200	4.497200
O	-6.034300	-11.609200	3.645200
N	-6.980300	-11.402200	5.732200
H	-6.579300	-12.281200	5.957200
H	-7.200300	-10.792200	6.487200
N	-6.890300	-9.548200	4.185200
H	-6.901300	-9.306200	3.218200
H	-7.421300	-8.987200	4.810200
C	-7.256300	-5.733200	3.115200
O	-6.155300	-6.133200	3.621200
N	-7.918300	-4.656200	3.683200
H	-7.431300	-4.155200	4.394200
H	-8.558300	-4.141200	3.129200
N	-7.837300	-6.456200	2.076200
H	-7.272300	-7.186200	1.696200
H	-8.399300	-5.960200	1.424200
C	-7.881300	-0.370200	2.883200
O	-6.617300	-0.262200	2.812200
N	-8.620300	0.651800	3.473200
H	-8.093300	1.322800	3.995200
H	-9.532300	0.454800	3.809200
N	-8.492300	-1.499200	2.357200
H	-7.921300	-2.091200	1.790200
H	-9.464300	-1.498200	2.175200
C	-8.039300	5.048800	2.491200
O	-7.024300	5.565800	1.920200
N	-8.680300	5.741800	3.508200
H	-8.243300	6.587800	3.808200
H	-9.180300	5.226800	4.193200
N	-8.565300	3.852800	2.008200
H	-8.012300	3.384800	1.322200
H	-9.045300	3.265800	2.651200
C	-8.072300	10.847800	1.111200
O	-7.231300	11.477800	1.829200
N	-8.746300	9.766800	1.642200
H	-8.525300	9.491800	2.572200
H	-9.221300	9.129800	1.051200
N	-8.356300	11.306800	-0.175800
H	-7.717300	11.979800	-0.529800
H	-8.721300	10.661800	-0.841800
C	-6.456300	-10.246200	10.567200
O	-5.660300	-10.949200	9.866200
N	-6.510300	-10.452200	11.947200

H	-5.750300	-10.971200	12.319200
H	-6.859300	-9.712200	12.516200
N	-7.325300	-9.364200	9.948200
H	-7.211300	-9.246200	8.966200
H	-7.697300	-8.602200	10.467200
C	-7.398300	-5.237200	9.020200
O	-6.135300	-5.109200	8.966200
N	-8.164300	-4.184200	9.504200
H	-7.666300	-3.445200	9.952200
H	-9.092300	-4.348200	9.805200
N	-7.982300	-6.431200	8.605200
H	-7.396300	-7.026200	8.056200
H	-8.946300	-6.439200	8.374200
C	-7.733300	0.054800	8.524200
O	-6.682300	0.462800	7.931200
N	-8.345300	0.871800	9.469200
H	-7.849300	1.699800	9.717200
H	-8.883300	0.443800	10.184200
N	-8.324300	-1.140200	8.135200
H	-7.796300	-1.703200	7.501200
H	-8.876300	-1.627200	8.800200
C	-7.784300	5.713800	8.150200
O	-6.782300	6.293800	7.616200
N	-8.380300	6.273800	9.280200
H	-7.850300	6.996800	9.719200
H	-8.842300	5.650800	9.904200
N	-8.350300	4.607800	7.528200
H	-7.869300	4.254800	6.732200
H	-8.827300	3.942800	8.091200
C	-8.238300	10.137800	7.669200
O	-7.163300	10.774800	7.902200
N	-8.865300	9.465800	8.699200
H	-8.398300	9.421800	9.578200
H	-9.595300	8.822800	8.525200
N	-8.822300	10.219800	6.399200
H	-8.207300	10.565800	5.693200
H	-9.386300	9.458800	6.096200
C	-2.361300	-11.507200	-7.859800
O	-1.091300	-11.521200	-7.914800
N	-3.022300	-10.404200	-7.312800
H	-2.476300	-9.876200	-6.663800
H	-3.986300	-10.512200	-7.076800
N	-3.066300	-12.562200	-8.403800
H	-2.560300	-13.244200	-8.906800
H	-4.058300	-12.590200	-8.399800
C	-2.737300	-6.832200	-7.839800
O	-1.491300	-6.598200	-7.975800
N	-3.414300	-6.259200	-6.777800
H	-2.959300	-5.512200	-6.302800
H	-4.405300	-6.314200	-6.724800
N	-3.388300	-7.637200	-8.763800
H	-2.797300	-8.175200	-9.361800
H	-4.277300	-8.022200	-8.534800
C	-3.554300	-1.149200	-7.722800
O	-2.301300	-0.993200	-7.894800
N	-4.177300	-0.522200	-6.656800
H	-3.671300	0.215800	-6.217800
H	-5.170300	-0.500200	-6.599800
N	-4.268300	-1.935200	-8.618800
H	-3.718300	-2.533200	-9.199800
H	-5.182300	-2.247200	-8.376800
C	-4.003300	4.354800	-8.393800
O	-2.745300	4.487800	-8.544800

N	-4.618300	4.882800	-7.267800
H	-4.103300	5.574800	-6.765800
H	-5.611300	4.955800	-7.246800
N	-4.733300	3.681800	-9.366800
H	-4.208300	3.083800	-9.967800
H	-5.666300	3.400800	-9.162800
C	-4.867300	10.334800	-9.202800
O	-3.612300	10.405800	-9.027800
N	-5.649300	11.464800	-8.984800
H	-5.211300	12.199800	-8.482800
H	-6.637300	11.378800	-8.900800
N	-5.441300	9.130800	-9.593800
H	-4.830300	8.470800	-10.026800
H	-6.392300	9.120800	-9.880800
C	-2.129300	-11.890200	-1.435800
O	-0.890300	-11.758200	-1.691800
N	-2.884300	-10.774200	-1.095800
H	-2.382300	-10.001200	-0.715800
H	-3.815300	-10.910200	-0.768800
N	-2.707300	-13.152200	-1.519800
H	-2.194300	-13.827200	-2.032800
H	-3.699300	-13.243200	-1.509800
C	-2.787300	-6.378200	-2.024800
O	-1.526300	-6.225200	-2.136800
N	-3.559300	-5.310200	-1.593800
H	-3.075300	-4.552200	-1.163800
H	-4.508300	-5.460200	-1.334800
N	-3.361300	-7.604200	-2.331800
H	-2.808300	-8.220200	-2.889800
H	-4.351300	-7.669200	-2.421800
C	-3.335300	-0.777200	-2.425800
O	-2.089300	-0.576200	-2.611800
N	-4.068300	0.160800	-1.722800
H	-3.560300	0.869800	-1.242800
H	-5.004300	-0.024200	-1.449800
N	-3.922300	-1.938200	-2.909800
H	-3.385300	-2.455200	-3.572800
H	-4.914300	-1.984200	-2.987800
C	-3.702300	5.179800	-3.082800
O	-2.428300	5.186800	-3.126800
N	-4.350300	5.841800	-2.051800
H	-3.814300	6.529800	-1.565800
H	-5.335300	5.982800	-2.101800
N	-4.409300	4.507800	-4.069800
H	-3.894300	3.853800	-4.618800
H	-5.384300	4.345800	-3.959800
C	-4.085300	11.204800	-3.956800
O	-2.827300	11.216800	-3.782800
N	-4.811300	12.371800	-3.745800
H	-4.348300	13.084800	-3.237800
H	-5.804300	12.338800	-3.695800
N	-4.721300	10.029800	-4.339800
H	-4.152300	9.338800	-4.776800
H	-5.678300	10.068800	-4.609800
C	-2.520300	-11.329200	4.032200
O	-1.265300	-11.224200	3.874200
N	-3.251300	-10.236200	4.487200
H	-2.728300	-9.525200	4.954200
H	-4.185300	-10.378200	4.795200
N	-3.146300	-12.530200	3.725200
H	-2.613300	-13.176200	3.195200
H	-4.137300	-12.580200	3.655200
C	-2.677300	-5.731200	3.426200

O	-1.423300	-5.551200	3.281200
N	-3.466300	-4.676200	3.859200
H	-2.987300	-3.917200	4.292200
H	-4.408300	-4.844200	4.135200
N	-3.227300	-6.976200	3.152200
H	-2.678300	-7.579200	2.577200
H	-4.218300	-7.064200	3.084200
C	-3.199300	-0.004200	2.741200
O	-1.929300	0.096800	2.707200
N	-3.897300	0.555800	3.799200
H	-3.409300	1.229800	4.348200
H	-4.887300	0.641800	3.744200
N	-3.852300	-0.675200	1.715200
H	-3.286300	-1.292200	1.172200
H	-4.808300	-0.929200	1.833200
C	-3.555300	5.705800	2.102200
O	-2.282300	5.749800	2.148200
N	-4.290300	6.837800	2.434200
H	-3.815300	7.512800	2.997200
H	-5.273300	6.749800	2.571200
N	-4.179300	4.527800	1.721200
H	-3.603300	3.852800	1.266200
H	-5.146300	4.535800	1.485200
C	-3.819300	11.651800	1.685200
O	-2.553300	11.647800	1.797200
N	-4.530300	12.783800	2.060200
H	-4.045300	13.432800	2.630200
H	-5.522300	12.746800	2.144200
N	-4.469300	10.521800	1.203200
H	-3.913300	9.888800	0.670200
H	-5.433300	10.587800	0.965200
C	-2.226300	-10.769200	9.866200
O	-0.982300	-10.706200	9.620200
N	-2.951300	-9.596200	10.043200
H	-2.420300	-8.797200	10.317200
H	-3.881300	-9.655200	10.394200
N	-2.843300	-12.014200	9.935200
H	-2.335300	-12.769200	9.543200
H	-3.837300	-12.076200	9.923200
C	-2.717300	-4.892200	8.801200
O	-1.443300	-4.845200	8.776200
N	-3.401300	-4.166200	9.765200
H	-2.889300	-3.448200	10.229200
H	-4.386300	-4.046200	9.689200
N	-3.385300	-5.666200	7.868200
H	-2.838300	-6.335200	7.370200
H	-4.356300	-5.852200	7.978200
C	-3.233300	0.636800	8.019200
O	-1.961300	0.647800	8.107200
N	-3.985300	1.291800	8.984200
H	-3.491300	1.952800	9.543200
H	-4.951300	1.466800	8.816200
N	-3.834300	-0.035200	6.967200
H	-3.259300	-0.678200	6.467200
H	-4.814300	-0.207200	6.982200
C	-3.305300	6.349800	7.842200
O	-2.033300	6.339800	7.923200
N	-4.043300	7.043800	8.788200
H	-3.535300	7.664800	9.379200
H	-5.005300	7.236800	8.626200
N	-3.921300	5.658800	6.812200
H	-3.369300	4.987800	6.327200
H	-4.908300	5.542800	6.806200

C	-3.800300	11.363800	7.649200
O	-2.530300	11.402800	7.722200
N	-4.551300	12.211800	8.452200
H	-4.076300	12.633800	9.211200
H	-5.537300	12.106800	8.514200
N	-4.412300	10.476800	6.783200
H	-3.842300	10.063800	6.080200
H	-5.393300	10.527800	6.627200
C	2.347700	-11.426200	-8.019800
O	3.613700	-11.359200	-8.139800
N	1.669700	-10.457200	-7.296800
H	2.213700	-9.911200	-6.664800
H	0.707700	-10.591200	-7.075800
N	1.667700	-12.466200	-8.638800
H	2.165700	-12.961200	-9.336800
H	0.674700	-12.460200	-8.685800
C	1.865700	-6.103200	-7.835800
O	3.132700	-6.006200	-7.730800
N	1.060700	-5.651200	-6.800800
H	1.489700	-5.020200	-6.157800
H	0.081700	-5.549200	-6.954800
N	1.328700	-6.659200	-8.987800
H	1.957700	-7.174200	-9.562800
H	0.367700	-6.916200	-9.015800
C	1.101700	-0.762200	-8.005800
O	2.371700	-0.672200	-8.046800
N	0.414700	-0.201200	-6.936800
H	0.921700	0.469800	-6.398800
H	-0.570300	-0.071200	-7.006800
N	0.437700	-1.422200	-9.030800
H	0.999700	-2.018200	-9.599800
H	-0.517300	-1.678200	-8.912800
C	0.673700	4.551800	-8.802800
O	1.938700	4.611800	-8.937800
N	0.065700	5.227800	-7.752800
H	0.604700	5.944800	-7.317800
H	-0.922300	5.348800	-7.756800
N	-0.067300	3.802800	-9.703800
H	0.439700	3.148800	-10.259800
H	-1.023300	3.600800	-9.513800
C	-0.251300	10.765800	-9.454800
O	1.014700	10.858800	-9.402800
N	-1.022300	11.903800	-9.243800
H	-0.554300	12.666800	-8.816800
H	-1.999300	11.815800	-9.081800
N	-0.839300	9.536800	-9.710800
H	-0.254300	8.847800	-10.132800
H	-1.814300	9.490800	-9.900800
C	2.498700	-11.553200	-1.612800
O	3.745700	-11.406200	-1.821800
N	1.749700	-10.488200	-1.140800
H	2.256700	-9.754200	-0.696800
H	0.807700	-10.636200	-0.855800
N	1.913700	-12.790200	-1.872800
H	2.439700	-13.397200	-2.452800
H	0.922700	-12.863200	-1.914800
C	1.887700	-5.882200	-2.226800
O	3.160700	-5.854200	-2.175800
N	1.158700	-5.172200	-1.291800
H	1.644700	-4.483200	-0.764800
H	0.171700	-5.089200	-1.378800
N	1.258700	-6.609200	-3.230800
H	1.827700	-7.280200	-3.698800

H	0.289700	-6.821200	-3.141800
C	1.303700	-0.237200	-2.694800
O	2.571700	-0.115200	-2.721800
N	0.594700	0.298800	-1.627800
H	1.077700	0.984800	-1.087800
H	-0.395300	0.383800	-1.690800
N	0.664700	-0.906200	-3.728800
H	1.240700	-1.481200	-4.302800
H	-0.289300	-1.173200	-3.627800
C	0.989700	5.411800	-3.300800
O	2.247700	5.565800	-3.435800
N	0.350700	5.951800	-2.194800
H	0.849700	6.661800	-1.704800
H	-0.644300	5.994800	-2.173800
N	0.289700	4.704800	-4.268800
H	0.833700	4.122800	-4.867800
H	-0.648300	4.424800	-4.091800
C	0.600700	11.283800	-3.979800
O	1.871700	11.275800	-3.949800
N	-0.076300	12.383800	-3.468800
H	0.453700	12.995800	-2.897800
H	-1.059300	12.345800	-3.326800
N	-0.090300	10.196800	-4.497800
H	0.427700	9.584800	-5.090800
H	-1.066300	10.281800	-4.677800
C	2.151700	-11.051200	3.837200
O	3.404700	-10.918200	3.674200
N	1.436700	-10.084200	4.530200
H	1.969700	-9.461200	5.098200
H	0.499700	-10.273200	4.806200
N	1.518700	-12.163200	3.297200
H	2.031700	-12.667200	2.616200
H	0.526700	-12.206200	3.258200
C	2.028700	-5.369200	3.254200
O	3.296700	-5.257200	3.174200
N	1.292700	-4.316200	3.766200
H	1.795700	-3.601200	4.240200
H	0.327700	-4.431200	3.974200
N	1.412700	-6.545200	2.845200
H	1.968700	-7.150200	2.281200
H	0.430700	-6.546200	2.680200
C	1.466700	0.320800	2.561200
O	2.736700	0.415800	2.506200
N	0.792700	0.864800	3.645200
H	1.297700	1.528800	4.190200
H	-0.197300	0.967800	3.608200
N	0.788700	-0.319200	1.533200
H	1.337700	-0.916200	0.953200
H	-0.167300	-0.567200	1.662200
C	1.143700	6.051800	2.077200
O	2.416700	6.128800	2.085200
N	0.387700	7.089800	2.611200
H	0.881700	7.701800	3.226200
H	-0.572300	6.923800	2.823200
N	0.543700	4.940800	1.516200
H	1.117700	4.347800	0.959200
H	-0.439300	4.913800	1.374200
C	0.831700	11.774800	1.509200
O	2.097700	11.751800	1.618200
N	0.145700	12.928800	1.878200
H	0.649700	13.559800	2.453200
H	-0.842300	12.898800	1.991200
N	0.158700	10.658800	1.037200

H	0.701700	10.004800	0.515200
H	-0.810300	10.727800	0.820200
C	2.432700	-10.498200	9.609200
O	3.683700	-10.416200	9.401200
N	1.685700	-9.340200	9.768200
H	2.194700	-8.525200	10.034200
H	0.737700	-9.402200	10.061200
N	1.835700	-11.754200	9.660200
H	2.369700	-12.499200	9.285200
H	0.845700	-11.832200	9.621200
C	1.945700	-4.494200	8.694200
O	3.214700	-4.375200	8.696200
N	1.202700	-3.795200	9.634200
H	1.670700	-3.052200	10.105200
H	0.214700	-3.726200	9.538200
N	1.341700	-5.317200	7.757200
H	1.930700	-5.965200	7.281200
H	0.376700	-5.546200	7.839200
C	1.454700	0.926800	7.993200
O	2.725700	1.015800	7.966200
N	0.756700	1.526800	9.031200
H	1.254700	2.211800	9.557200
H	-0.231300	1.632800	8.965200
N	0.797700	0.236800	6.982200
H	1.364700	-0.381200	6.442200
H	-0.154300	-0.026200	7.116200
C	1.360700	6.301800	7.736200
O	2.625700	6.378800	7.592200
N	0.774700	6.880800	8.854200
H	1.333700	7.535800	9.354200
H	-0.212300	6.998800	8.892200
N	0.608700	5.640800	6.781200
H	1.107700	5.032800	6.169200
H	-0.346300	5.427800	6.964200
C	0.872700	11.682800	7.590200
O	2.143700	11.694800	7.660200
N	0.148700	12.606800	8.334200
H	0.635700	13.038800	9.080200
H	-0.838300	12.510800	8.422200
N	0.234700	10.745800	6.792200
H	0.796700	10.308800	6.094200
H	-0.738300	10.840800	6.604200
C	7.036700	-11.147200	-7.916800
O	8.297700	-11.019200	-7.905800
N	6.268700	-10.604200	-6.906800
H	6.715700	-9.959200	-6.294800
H	5.277700	-10.569200	-6.990800
N	6.440700	-11.820200	-8.999800
H	7.035700	-12.493200	-9.424800
H	5.486700	-12.098200	-8.902800
C	6.534700	-5.857200	-7.833800
O	7.804700	-5.794200	-7.921800
N	5.901700	-5.423200	-6.678800
H	6.443700	-4.829200	-6.084800
H	4.919700	-5.256200	-6.702800
N	5.815700	-6.366200	-8.911800
H	6.342700	-6.934200	-9.540800
H	4.861700	-6.623200	-8.775800
C	5.797700	-0.594200	-8.239800
O	7.064700	-0.567200	-8.343800
N	5.183700	-0.009200	-7.138800
H	5.738700	0.653800	-6.640800
H	4.202700	0.160800	-7.170800

N	5.052700	-1.216200	-9.238800
H	5.555700	-1.870200	-9.799800
H	4.091700	-1.421200	-9.069800
C	5.347700	4.619800	-9.180800
O	6.616700	4.597800	-9.251800
N	4.740700	5.255800	-8.100800
H	5.302700	5.938800	-7.636800
H	3.763700	5.450800	-8.147800
N	4.598700	4.008800	-10.181800
H	5.089700	3.337800	-10.736800
H	3.633700	3.825800	-10.013800
C	4.409700	11.164800	-9.551800
O	5.676700	11.241800	-9.562800
N	3.697700	11.871800	-8.585800
H	4.189700	12.614800	-8.151800
H	2.710700	11.959800	-8.665800
N	3.760700	10.365800	-10.477800
H	4.324700	9.715800	-10.978800
H	2.788700	10.187800	-10.394800
C	7.075700	-10.717200	-1.470800
O	8.289700	-10.346200	-1.414800
N	6.217700	-10.446200	-0.408800
H	6.510700	-9.715200	0.201200
H	5.233700	-10.527200	-0.553800
N	6.629700	-11.404200	-2.590800
H	7.327700	-11.784200	-3.182800
H	5.727700	-11.821200	-2.599800
C	6.539700	-5.545200	-2.325800
O	7.807700	-5.486200	-2.337800
N	5.842700	-4.979200	-1.259800
H	6.347700	-4.302200	-0.729800
H	4.861700	-4.830200	-1.349800
N	5.871700	-6.175200	-3.372800
H	6.433700	-6.776200	-3.936800
H	4.921700	-6.447200	-3.242800
C	5.972700	0.051800	-3.018800
O	7.234700	0.126800	-3.169800
N	5.381700	0.606800	-1.890800
H	5.928700	1.271800	-1.387800
H	4.392700	0.719800	-1.860800
N	5.209700	-0.590200	-3.984800
H	5.704700	-1.174200	-4.621800
H	4.262700	-0.828200	-3.791800
C	5.648700	5.496800	-3.800800
O	6.910700	5.475800	-3.976800
N	5.127700	6.031800	-2.629800
H	5.728700	6.651800	-2.130800
H	4.148700	6.208800	-2.571800
N	4.819700	4.981800	-4.790800
H	5.253700	4.377800	-5.452800
H	3.863700	4.795800	-4.576800
C	5.233700	10.715800	-4.460800
O	6.466700	10.484800	-4.674800
N	4.866700	11.773800	-3.648800
H	5.580700	12.216800	-3.127800
H	3.916700	11.938800	-3.415800
N	4.272700	9.867800	-5.007800
H	4.595700	9.327800	-5.779800
H	3.323700	10.173800	-5.046800
C	6.805700	-10.861200	3.863200
O	8.054700	-10.629200	3.864200
N	6.076700	-10.754200	5.041200
H	6.501700	-10.218200	5.762200

H	5.081700	-10.722200	4.998200
N	6.190700	-11.224200	2.667200
H	6.788700	-11.601200	1.972200
H	5.245700	-11.536200	2.675200
C	6.653700	-4.512200	3.335200
O	7.884700	-4.207200	3.408200
N	5.799700	-4.154200	4.371200
H	6.147700	-3.471200	5.007200
H	4.815700	-4.171200	4.221200
N	6.178700	-5.194200	2.213200
H	6.877700	-5.693200	1.701200
H	5.288700	-5.639200	2.274200
C	6.131700	0.644800	2.208200
O	7.396700	0.717800	2.112200
N	5.493700	1.226800	3.298200
H	6.019700	1.906800	3.800200
H	4.504700	1.341800	3.282200
N	5.406700	-0.012200	1.219200
H	5.935700	-0.624200	0.637200
H	4.461700	-0.271200	1.403200
C	5.829700	6.462800	1.882200
O	7.097700	6.526800	1.925200
N	5.069700	7.553800	2.305200
H	5.561700	8.210800	2.871200
H	4.110700	7.408800	2.533200
N	5.223700	5.321800	1.385200
H	5.796700	4.681800	0.885200
H	4.241700	5.290800	1.234200
C	5.495700	11.478800	1.390200
O	6.753700	11.434800	1.216200
N	4.948700	12.528800	2.112200
H	5.551700	13.282800	2.325200
H	3.966700	12.674800	2.138200
N	4.698700	10.428800	0.953200
H	5.133700	9.778800	0.339200
H	3.714700	10.553800	0.869200
C	7.071700	-9.894200	9.159200
O	8.322700	-9.712200	9.050200
N	6.334700	-9.136200	10.050200
H	6.784700	-8.336200	10.436200
H	5.342700	-9.168200	10.043200
N	6.455700	-10.848200	8.343200
H	7.068700	-11.530200	7.962200
H	5.534700	-11.151200	8.566200
C	6.597700	-3.810200	8.739200
O	7.840700	-3.539200	8.729200
N	5.812700	-3.345200	9.789200
H	6.211700	-2.611200	10.337200
H	4.821700	-3.345200	9.691200
N	6.050700	-4.558200	7.701200
H	6.697700	-5.114200	7.183200
H	5.134700	-4.934200	7.811200
C	6.134700	1.480800	8.030200
O	7.390700	1.692800	8.067200
N	5.342700	1.950800	9.075200
H	5.755700	2.669800	9.631200
H	4.354700	1.988800	8.954200
N	5.583700	0.789800	6.962200
H	6.222700	0.249800	6.418200
H	4.649700	0.449800	7.038200
C	6.007700	6.655800	7.592200
O	7.272700	6.826800	7.592200
N	5.263700	7.158800	8.656200

H	5.720700	7.860800	9.197200
H	4.276700	7.257800	8.548200
N	5.407700	5.961800	6.559200
H	6.000700	5.406800	5.983200
H	4.451700	5.689800	6.633200
C	5.560700	11.976800	7.447200
O	6.823700	12.085800	7.407200
N	4.854700	12.700800	8.420200
H	5.330700	13.504800	8.755200
H	3.865700	12.782800	8.326200
N	4.914700	11.059800	6.642200
H	5.454700	10.628800	5.926200
H	3.924700	11.076800	6.546200
C	-5.147300	-9.337200	-11.002800
O	-6.417300	-9.316200	-10.970800
N	-4.480300	-8.388200	-11.768800
H	-5.023300	-7.923200	-12.452800
H	-3.500300	-8.460200	-11.914800
N	-4.455300	-10.284200	-10.269800
H	-4.972300	-10.783200	-9.580800
H	-3.466300	-10.243200	-10.187800
C	-6.042300	-4.343200	-10.040800
O	-7.254300	-4.566200	-9.730800
N	-5.750300	-3.431200	-11.036800
H	-6.498300	-2.898200	-11.402800
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N	-5.022300	-4.980200	-9.331800
H	-5.304300	-5.813200	-8.864800
H	-4.102300	-4.987200	-9.718800
C	-6.838300	0.714800	-10.351800
O	-8.065300	0.582800	-10.045800
N	-6.479300	0.863800	-11.683800
H	-7.208300	1.103800	-12.309800
H	-5.550300	1.125800	-11.923800
N	-5.876300	0.722800	-9.344800
H	-6.157300	0.292800	-8.490800
H	-4.916300	0.621800	-9.598800
C	-7.360300	6.790800	-11.230800
O	-8.621300	6.665800	-11.168800
N	-6.822300	7.730800	-12.127800
H	-7.414300	7.931800	-12.899800
H	-5.849300	7.671800	-12.337800
N	-6.547300	6.104800	-10.357800
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H	-5.559300	6.102800	-10.458800
C	-5.440300	-9.573200	-4.235800
O	-6.696300	-9.718200	-4.091800
N	-4.959300	-8.444200	-4.896800
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N	-4.582300	-10.528200	-3.718800
H	-4.970300	-11.167200	-3.057800
H	-3.604300	-10.355200	-3.685800
C	-5.912300	-4.293200	-4.726800
O	-7.158300	-4.483200	-4.537800
N	-5.490300	-3.119200	-5.333800
H	-6.185300	-2.602200	-5.823800
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N	-5.006300	-5.265200	-4.328800
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C	-6.494300	1.764800	-5.107800
O	-7.753300	1.642800	-4.973800

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C      -7.164300    7.620800   -6.048800
O      -8.439300    7.618800   -6.063800
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O      -6.514300   -9.068200    1.177200
N      -4.703300   -7.794200    0.547200
H      -5.321300   -7.274200   -0.038800
H      -3.739300   -7.798200    0.296200
N      -4.443300   -9.957200    1.621200
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H      -3.475300   -9.774200    1.769200
C      -5.864300   -3.690200    0.647200
O      -7.102300   -3.845200    0.901200
N      -5.458300   -2.606200   -0.117800
H      -6.163300   -2.146200   -0.648800
H      -4.522300   -2.563200   -0.451800
N      -4.939300   -4.616200    1.118200
H      -5.263300   -5.229200    1.832200
H      -3.977300   -4.356200    1.161200
C      -6.247300    2.353800   -0.330800
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N      -5.521300    2.986800   -1.326800
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H      -4.558300    3.199800   -1.194800
N      -5.621300    1.824800    0.789200
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H      -4.631300    1.721800    0.797200
C      -6.710300    8.581800   -0.870800
O      -7.978300    8.507800   -0.978800
N      -6.035300    9.643800   -1.476800
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H      -6.583300    7.034800    0.453200
H      -5.071300    7.744800    0.080200
C      -5.478300   -8.615200    6.778200
O      -6.731300   -8.706200    7.003200
N      -5.007300   -7.582200    5.988200
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H      -4.062300   -7.589200    5.675200
N      -4.621300   -9.575200    7.313200
H      -4.999300  -10.093200    8.080200
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C      -5.750300   -2.659200    5.895200
O      -7.010300   -2.799200    5.929200
N      -5.150300   -2.206200    4.725200
H      -5.751300   -1.731200    4.087200
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N      -4.996300   -2.952200    7.032200
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H	-4.820300	2.273800	5.954200
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C	-5.096300	-7.558200	11.989200
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C	-5.990300	-1.531200	11.016200
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H	-4.180300	-1.244200	10.063200
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H	-6.107300	-1.878200	13.012200
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N	-5.581300	2.772800	11.386200
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O	-7.274300	8.481800	11.064200
N	-5.506300	9.671800	10.211200
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H	-4.217300	8.035800	11.823200
C	-0.476300	-8.970200	-10.883800
O	-1.732300	-9.150200	-10.934800
N	0.092700	-7.965200	-11.662800
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H	1.077700	-7.942200	-11.798800
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H	1.253700	-9.534200	-9.894800
C	-1.480300	-3.640200	-10.829800
O	-2.747300	-3.651200	-10.719800
N	-0.902300	-2.965200	-11.895800
H	-1.489300	-2.344200	-12.394800
H	0.078700	-2.807200	-11.918800
N	-0.695300	-4.274200	-9.874800
H	-1.154300	-4.963200	-9.318800
H	0.270700	-4.423200	-10.068800

C	-2.285300	1.332800	-11.235800
O	-3.547300	1.402800	-11.085800
N	-1.732300	1.657800	-12.471800
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N	-1.483300	0.943800	-10.174800
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H	-0.517300	0.760800	-10.331800
C	-2.701300	7.098800	-11.589800
O	-3.967300	7.139800	-11.463800
N	-2.065300	8.146800	-12.244800
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H	-1.095300	8.093800	-12.455800
N	-1.984300	6.024800	-11.094800
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H	-0.990300	6.073800	-11.043800
C	-0.791300	-9.015200	-4.658800
O	-2.055300	-9.176200	-4.673800
N	-0.178300	-8.387200	-5.730800
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H	0.780700	-8.127200	-5.678800
N	-0.060300	-9.463200	-3.567800
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C	-1.301300	-3.566200	-5.056800
O	-2.562300	-3.744200	-5.095800
N	-0.660300	-3.037200	-6.169800
H	-1.243300	-2.550200	-6.815800
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N	-0.600300	-3.898200	-3.904800
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H	0.390700	-3.986200	-3.945800
C	-1.802300	2.126800	-5.452800
O	-3.075300	2.059800	-5.399800
N	-1.197300	2.583800	-6.614800
H	-1.784300	3.089800	-7.241800
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N	-1.053300	1.742800	-4.351800
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H	-0.069300	1.617800	-4.443800
C	-2.495300	7.762800	-6.174800
O	-3.759300	7.633800	-6.062800
N	-1.979300	8.877800	-6.827800
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H	0.358700	-2.307200	-0.847800
N	-0.543300	-3.198200	1.457200
H	-1.024300	-3.715200	2.162200

H	0.447700	-3.285200	1.427200
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H	0.169700	2.161800	0.754200
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H	0.770700	-7.240200	5.441200
N	-0.095300	-9.042200	7.150200
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H	0.880700	-8.891200	7.280200
C	-1.074300	-2.366200	5.680200
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C	-1.639300	3.171800	5.109200
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O	-3.077300	8.755800	4.591200
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N	0.179700	-6.644200	10.705200
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H	-0.124300	-8.229200	13.544200
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O	2.929700	-8.516200	-10.899800
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H	5.851700	-8.056200	-12.068800
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O	1.949700	-3.338200	-10.970800
N	3.858700	-2.998200	-12.203800
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O	1.131700	1.579800	-11.506800
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N	3.119700	1.158800	-10.425800
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N	2.416700	8.368800	-12.602800
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C	3.899700	-8.738200	-4.833800
O	2.634700	-8.890200	-4.830800
N	4.509700	-8.148200	-5.936800
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H	5.460700	-7.862200	-5.864800
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C	3.379700	-3.205200	-5.144800
O	2.111700	-3.278200	-5.049800
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H	3.340700	-2.218200	-6.923800
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N	4.171700	-3.593200	-4.069800
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H	5.147700	-3.730200	-4.214800
C	2.890700	2.354800	-5.745800
O	1.621700	2.316800	-5.625800
N	3.447700	2.705800	-6.963800
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H	4.425700	2.882800	-7.028800
N	3.688700	2.057800	-4.646800
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H	4.660700	1.887800	-4.789800
C	2.139700	8.031800	-6.733800
O	0.883700	8.036800	-6.517800
N	2.687700	8.982800	-7.577800
H	2.050700	9.516800	-8.126800
H	3.624700	8.891800	-7.898800
N	2.923700	7.070800	-6.115800
H	2.510700	6.580800	-5.352800
H	3.914700	7.138800	-6.142800
C	4.070700	-8.206200	1.007200
O	2.828700	-8.443200	0.846200
N	4.792700	-7.629200	-0.035800
H	4.243700	-7.173200	-0.734800
H	5.682700	-7.230200	0.166200
N	4.675700	-8.542200	2.202200
H	4.170700	-9.159200	2.800200
H	5.666700	-8.513200	2.292200
C	3.466700	-2.641200	0.146200
O	2.196700	-2.716200	0.222200
N	4.052700	-2.229200	-1.044800
H	3.455700	-1.754200	-1.685800
H	5.016700	-1.984200	-1.057800
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H	3.791700	-3.522200	1.953200
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C	3.068700	2.960800	-0.512800
O	1.796700	2.902800	-0.448800
N	3.675700	3.357800	-1.696800
H	3.097700	3.857800	-2.337800
H	4.643700	3.587800	-1.690800
N	3.814700	2.624800	0.609200
H	3.341700	2.087800	1.304200
H	4.795700	2.478800	0.515200
C	2.705700	8.594800	-1.068800
O	1.436700	8.618800	-0.957800
N	3.343700	9.544800	-1.858800
H	2.760700	10.014800	-2.517800
H	4.289700	9.386800	-2.129800
N	3.424700	7.623800	-0.388800
H	2.945700	7.158800	0.350200
H	4.414700	7.696800	-0.318800
C	3.840700	-7.694200	6.426200
O	2.578700	-7.871200	6.404200
N	4.377700	-6.585200	5.790200
H	3.811700	-6.161200	5.089200
H	5.364700	-6.503200	5.694200
N	4.647700	-8.616200	7.083200
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H	5.589700	-8.369200	7.293200
C	3.598700	-1.888200	5.641200
O	2.338700	-2.076200	5.605200
N	4.247700	-1.418200	4.509200
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N       3.657700    3.827800    3.666200
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H       3.362700    2.628800    6.691200
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C       2.896700    9.143800    4.580200
O       1.624700    9.076800    4.627200
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H       4.469700   10.160800    3.698200
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H       4.630700    8.262800    5.299200
C       4.216700   -7.042200   11.580200
O       2.966700   -7.279200   11.584200
N       4.770700   -6.288200   10.555200
H       4.133700   -5.727200   10.033200
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N       4.006700    3.584800   12.042200
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O       2.050700    9.113800   10.606200
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C       8.363700   -8.810200  -10.160800
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N       8.587700  -10.092200  -10.657800
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H       8.928700  -10.793200  -10.039800
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H	6.491700	-0.784200	-11.850800
H	7.679700	-0.794200	-10.667800
C	6.343700	7.696800	-11.162800
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N	7.058700	8.737800	-10.608800
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N	6.940700	6.450800	-11.390800
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C	8.601700	-8.292200	-4.873800
O	7.340700	-8.451200	-4.913800
N	9.228700	-7.540200	-5.868800
H	8.619700	-6.953200	-6.399800
H	10.131700	-7.172200	-5.688800
N	9.326700	-8.893200	-3.862800
H	8.843700	-9.524200	-3.260800
H	10.312700	-8.938200	-3.895800
C	7.882700	-2.343200	-4.940800
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N	8.375700	-1.203200	-5.583800
H	7.787700	-0.856200	-6.314800
H	8.793700	-0.505200	-5.010800
N	8.584700	-2.938200	-3.915800
H	8.208700	-3.757200	-3.497800
H	9.337700	-2.478200	-3.473800
C	7.403700	3.177800	-5.673800
O	6.339700	2.565800	-6.016800
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C	6.674700	8.522800	-6.808800
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H	6.942700	7.093800	-5.387800
H	7.973700	8.416800	-5.223800
C	8.429700	-8.238200	0.734200
O	7.484700	-7.718200	1.416200
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H	8.327700	-6.830200	-0.737800
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N	9.079700	-9.364200	1.221200
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O	6.915700	-2.381200	-0.055800

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H	9.119700	4.829800	-1.318800
N	8.414700	3.184800	0.624200
H	7.988700	2.510800	1.224200
H	9.396700	3.282800	0.667200
C	7.180700	9.263800	-0.976800
O	6.152700	8.576800	-1.278800
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O	7.248700	-7.115200	6.534200
N	7.467700	-7.796200	4.354200
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H	8.793700	-8.968200	7.122200
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H	8.404700	-3.257200	6.706200
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C	7.782700	3.779800	4.663200
O	6.513700	3.760800	4.747200
N	8.378700	4.281800	3.516200
H	7.786700	4.790800	2.892200
H	9.335700	4.529800	3.526200
N	8.541700	3.306800	5.733200
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H	9.294700	8.609800	5.398200
C	8.709700	-6.312200	10.810200
O	7.614700	-6.666200	11.350200
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H	9.661700	-4.630200	10.105200
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