

C–H Bond Addition across a Transient Uranium–Nitrido Moiety and Formation of a Parent Uranium Imido Complex

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Experimental Procedures

General Methods. All reactions and manipulations were performed under an inert atmosphere (N_2) using standard Schlenk techniques or in a Vacuum Atmospheres, Inc. Nexus II drybox equipped with a molecular sieves 13X / Q5 Cu-0226S catalyst purifier system. Glassware was oven-dried overnight at 150 °C prior to use. 1H and $^{31}P\{^1H\}$ NMR spectra were obtained on a Bruker DMX-300 or Bruker DMX-360 Fourier transform NMR spectrometer operating at 300 MHz (1H) or 360 MHz (1H) and 146 MHz (^{31}P) respectively. Unless specified, NMR spectra were recorded at 300 K; variable-temperature 1H NMR were performed on a Bruker UNI-400 operating at 400 MHz (1H). Chemical shifts were recorded in units of parts per million downfield from residual protio solvent peaks. Following abbreviations are used: b, broad; d, doublet; m, multiplet; s, singlet. Elemental analyses were performed on a Costech ECS 4010 analyzer at the Earth & Environmental Science department of the University of Pennsylvania. The infrared spectra were obtained from 400–4000 cm⁻¹ using a Perkin Elmer 1600 series infrared spectrometer.

Materials. Tetrahydrofuran (THF), Et₂O, CH₂Cl₂, hexanes, pentane, and toluene were purchased from Fisher Scientific. These solvents were sparged for 20 min with dry argon and dried using a commercial two-column solvent purification system comprising columns packed with Q5 reactant and neutral alumina respectively (for hexanes and pentane), or two columns of neutral alumina (for THF, Et₂O and CH₂Cl₂). All solvents were stored over 3 Å molecular sieves. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc. and stored over potassium mirror overnight prior to use. Starting materials: HPN^[1], UI₃(THF)₄^[2] and UCl₄^[3] were prepared according to the reported procedures. NaN₃ was dried under vacuum at room temperature overnight. Subsequently it was stirred in THF, toluene, and pentane in series for 24 hours each.

Electrochemistry. Voltammetry experiments (CV, DPV) were performed using a CH Instruments 620D Electrochemical Analyzer/Workstation and the data were processed using CHI software v9.24. All experiments were performed in an N_2 atmosphere drybox using electrochemical cells that consisted of a 4 mL vial, glassy carbon working electrode, a platinum wire counter electrode, and a silver wire plated with AgCl as a quasi-reference electrode. The quasi-reference electrode was prepared by dipping a length of silver wire in concentrated hydrochloric acid. The working electrode surfaces were polished prior to each set of experiments. Potentials were reported versus ferrocene, which was added as an internal standard for calibration at the end of each run. Solutions employed during these studies were ~3 mM in analyte and 100 mM in [⁷Pr₄N][BAr^F] in 2 mL of THF. All data were collected in a positive-feedback IR compensation mode.

X-Ray Crystallography. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-Kα radiation ($\lambda=0.71073 \text{ \AA}$) at a temperature of 143(1) K. In all cases, rotation frames were integrated using SAINT,^[4] producing a listing of unaveraged F² and σ(F²) values which were then passed to the SHELXTL^[5] program package for further processing and structure solution. The intensity data were corrected for Lorentz and polarization effects and for absorption using TWINABS^[6] or SADABS.^[7] The structures were solved by direct methods (SHELXS-97).^[8] Refinement was by full-matrix least squares based on F² using SHELXL-97.^[8] All reflections were used during refinements. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model.

Potassium N-(2-(Diisopropylphosphino)-4-methylphenyl)-2,4,6-trimethylaniline (KPN). Potassium benzyl (3.58 g, 27.5 mmol, 1.5 equiv) was added in a solid portion to *N*-(2-(Diisopropylphosphino)-4-methylphenyl)-2,4,6-trimethylaniline (6.00 g, 18.3 mmol, 1 equiv) in a solution of diethyl ether and hexanes in a 1:1 mixture. The reaction mixture was stirred at room temperature for 1 h and filtered through a medium-porosity frit. Volatiles were removed under reduced pressure from the filtrate to give an oily residue. This residue was dissolved in hexanes and volatiles were subsequently removed to yield KPN as a yellow solid. Yield: 95% (6.26 g, 17.1 mmol). 1H NMR (360 MHz, C₆D₆): δ 6.97 (s, 2H, Ar-H), 6.90 (m, 1H, Ar-H), 6.75 (dd, $J = 8.43, 2.12 \text{ Hz}$, 1H, Ar-H), 5.93 (dd, $J = 8.37, 5.82 \text{ Hz}$, 1H, Ar-H), 2.33 (s, 3H, Ar-CH₃), 2.27 (s, 3H, Ar-CH₃), 2.14 (s, 6H, Ar-CH₃), 2.07 (m, 2H, PCH(CH₃)₂), 1.10 (m, 12H, PCH(CH₃)₂). $^{31}P\{^1H\}$ (146 MHz, C₆D₆): δ -5.68 (s). IR (KBr) : 2953 (s), 2727 (m), 2548 (w), 2406 (w), 2256 (w), 2140 (w), 2052 (w), 1893 (w), 1757 (w), 1590 (s), 1463 (s), 1344 (s), 1273 (m), 1209 (m), 1146 (m), 1030 (m), 927 (w), 865 (m), 813 (m), 733 (w), 687 (w), 653 (w), 607 (w), 541 (w), 498 (m). Anal. found (calcd) for C₂₂H₃₁KNP: C, 69.97 (69.62); H, 8.16 (8.23); N, 3.51 (3.69).

(PN)₂U^{III}I (1). A solution of KPN (8.50 g, 22.05 mmol, 2 equiv) in THF (30 mL) was added dropwise to a suspension of UI₃(THF)₄ (10.00 g, 11.02 mmol, 1 equiv) in THF (40 mL). The reaction mixture was stirred for 3 h, filtered over Celite, and volatiles were removed under reduced pressure. The residue was extracted with

hexanes, filtered over Celite and crystallized at -21°C to yield $(\text{PN})_2\text{UI}$ as a black crystalline solid. Yield: 48% (5.39 g, 5.30 mmol). ^1H NMR (300 MHz, C_6D_6 , 300 K): δ 54.13 (s, 2H), 31.81 (s, 2H), 21.94 (s, 2H), 14.03 (s, 6H), -4.26 (s, 4H), -4.65 (s, 6H), -33.29 (s, 12H). The peaks associated with the isopropyl groups were not observed at 300 K because of large broadening but were resolved at 200 K. ^1H NMR (400 MHz, Tol-d_8 , 200 K): δ 92.50 (s, 2H) 51.03 (s, 2H), 34.62 (s, 2H), 31.89 (bs, 6H), 23.83 (s, 6H), 10.75 (s, 2H), 1.10 (bs, 6H, overlapped with Tol-d_8 and residual hexanes), -9.74 (s, 6H), -12.61 (s, 2H), -14.71 (s, 2H), -16.56 (s, 6H), -60.65 (s, 6H), -65.00 (s, 6H), -87.71 (s, 2H). IR (KBr) : 2956 (w), 2919 (w), 2867 (w), 1597 (m), 1558(w), 1540 (w), 1467(s), 1391 (m), 1305 (m), 1274 (s), 1249 (s), 1215 (m), 1188 (m), 1153 (w), 1134 (w), 1027 (m), 926 (m), 891 (s), 856 (s), 813 (s), 729 (w), 709 (m), 691 (m), 654 (w), 617 (w), 584 (w), 563 (m), 543 (m), 490 (m), 465 (w), 435 (m). Anal. found (calcd) for $\text{C}_{44}\text{H}_{62}\text{IN}_2\text{P}_2\text{U}$: C, 50.12 (50.53); H, 5.35 (5.98); N, 2.37 (2.68). No ^{31}P signal was observed for this compound.

(PN)₂U^{IV}Cl₂ (2). A solution of KPN (4.00 g, 10.94 mmol, 2.2 equiv) in THF (20 mL) was added dropwise to a solution of uranium tetrachloride (1.88 g, 4.98 mmol, 1 equiv) in THF (30 mL). The reaction mixture stirred at room temperature for 2 h, filtered through a medium-porosity frit, and volatiles were removed under reduced pressure. Pentane was added to the residue and volatiles were removed under reduced pressure. A subsequent portion of pentane was added and solid was collected on a medium-porosity frit. This solid was recrystallized from fluorobenzene at -21°C to yield $(\text{PN})_2\text{UCl}_2$ as an orange solid. Yield: 62% (2.96 g, 3.08 mmol). ^1H NMR (300 MHz, C_6D_6): δ 36.02 (s, 2H), 28.77 (s, 2H), 28.57 (s, 2H), 15.50 (s, 6H), 10.76 (s, 4H), -0.84 (s, 12H), -6.18 (s, 6H), -7.66 (s, 12H), -9.33 (s, 4H), -12.55 (s, 12H). IR (KBr) : 2963 (s), 2919 (s), 2868 (s), 2733 (w), 1946 (w), 1884 (w), 18750 (w), 1714 (w), 1597 (m), 1490 (s), 1466 (s), 1389 (m), 1274 (m), 1240 (s), 1213 (m), 1187 (m), 1060 (m), 1025 (m), 928 (w), 890 (m), 857 (m), 830 (m), 810 (m), 754 (m), 714 (m), 685 (m), 651 (w), 609 (w), 543 (w), 517 (w), 493 (w), 436 (w). Anal. found (calcd) for $\text{C}_{44}\text{H}_{62}\text{Cl}_2\text{N}_2\text{P}_2\text{U}$: C, 53.71 (53.39); H, 6.01 (6.31); N, 2.53 (2.83). No ^{31}P signal was observed for this compound.

(PN)₂U^{IV}(N₃)₂ (3). To a solution of **2** (1.50 g, 1.56 mmol, 1 equiv) in THF (5 mL) was added sodium azide (0.22 g, 3.44 mmol, 2.2 equiv) as a solid portion. The reaction mixture was stirred for 1 h at room temperature and volatiles were removed under reduced pressure. The residue was extracted with pentane, filtered, and volatiles were removed. The compound was then crystallized from fluorobenzene at -21°C to yield $(\text{PN})_2\text{U}(\text{N}_3)_2$ as X-ray quality red/orange crystals. Yield: 94% (1.43 g, 1.47 mmol). ^1H NMR (300 MHz, C_6D_6): δ 16.03 (s, 2H), 15.87 (s, 2H), 11.06 (m, 4H), 4.73 (s, 12H), 0.25 (s, 12H), -4.77 (s, 4H), -7.53 (s, 6H), -9.16 (s, 4H), -12.14 (s, 12H), -16.91 (s, 2H), -28.69 (s, 2H). IR (KBr) : 2966 (m), 2920 (m), 2869 (m), 2724 (w), 2665 (w), 2538 (w), 2363 (w), 2077 (s, azide), 1761 (w), 1597 (m), 1542 (w), 1464 (s), 1360 (s), 1251 (s), 1154 (m), 1100 (w), 1061 (w), 1027 (m), 929 (w), 888 (m), 863 (m), 818 (m), 752 (m), 711 (w), 684 (w), 649 (w), 602 (w), 543 (w), 493 (w), 433 (w). Anal. found (calcd) for $\text{C}_{44}\text{H}_{62}\text{N}_8\text{P}_2\text{U}\cdot\text{C}_{12}\text{H}_{10}\text{F}_2$: C, 56.06 (56.28); H, 5.69 (6.07); N, 9.39 (9.38). No ^{31}P signal was observed for this compound.

[K(THF)₃][(PN)U^{IV}(=NH)[ⁱP₂P(C₆H₃Me)N(C₆H₂Me₂CH₂)] (4). To a solution of $(\text{PN})_2\text{U}(\text{N}_3)_2$ (100 mg, 0.10 mmol, 1 equiv) in THF was added potassium graphite (55 mg, 0.41 mmol, 4 equiv) as a solid portion. The reaction mixture, which immediately turned green and subsequently to red over the course of seconds, was then filtered and volatiles were removed under reduced pressure. The residue was dissolved in minimal THF and layered with pentane. The layered solution was crystallized at -21°C to yield **4** as red crystals. Yield: 15%, (18 mg, 0.02 mmol). ^1H (300 MHz, C_6D_6): δ 52.64 (3H), 41.26 (1H), 40.38 (3H), 22.09 (1H), 18.79 (1H), 18.44 (1H), 13.79 (3H), 12.69 (1H), 9.11 (3H), 2.20 (12H, THF), 1.14 (12H, THF), -1.75 (3H), -3.83 (1H), -4.74 (1H), -5.61 (3H), -7.41 (1H), -7.56 (1H), -9.26 (1H), -2.76 (3H), -9.74 (3H), -12.34 (1H), -14.40 (3H), -16.93 (3H), -19.53 (1H), -29.47 (3H), -32.00 (3H), -32.93 (1H), -39.03 (1H). Twelve protons are obscured by THF and benzene solvent peaks. IR (KBr) : 3355 (w, N-H), 2950 (s), 2919 (s), 2864 (s), 1600 (m), 1496 (s), 1464 (s), 1391 (m), 1270 (s), 1213 (w), 1192 (w), 1153 (w), 1032 (w), 881 (m), 856 (m), 812 (m), 748 (w), 730 (w), 699 (w), 660 (w), 611 (w), 545 (w), 497 (m). EA was not obtainable for this compound, as it was unstable toward desolvation and associated decomposition upon drying, as indicated by ^1H NMR spectroscopy. No ^{31}P signal was observed for this compound.

Electronic Absorption Spectra

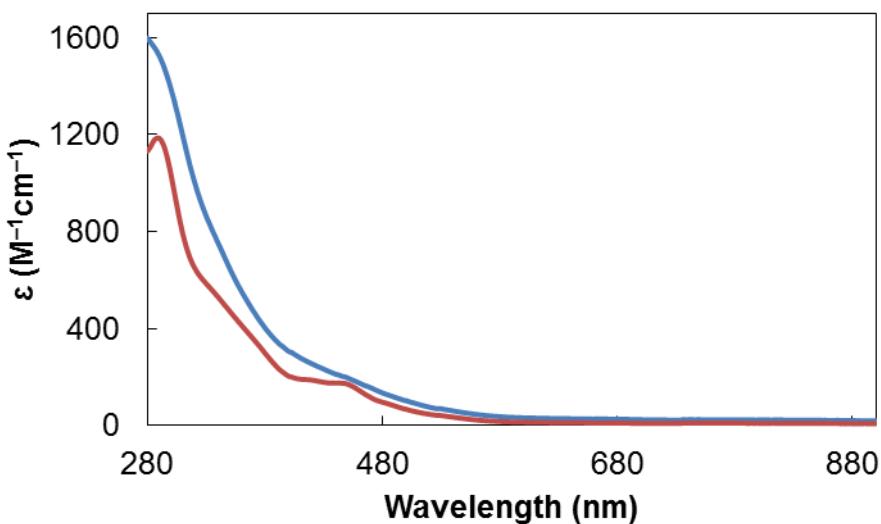


Figure S1. Electronic absorption spectrum of $\text{Cl}_2\text{U}(\text{PN})_2$ (red trace) and $(\text{N}_3)_2\text{U}(\text{PN})_2$ (blue trace).

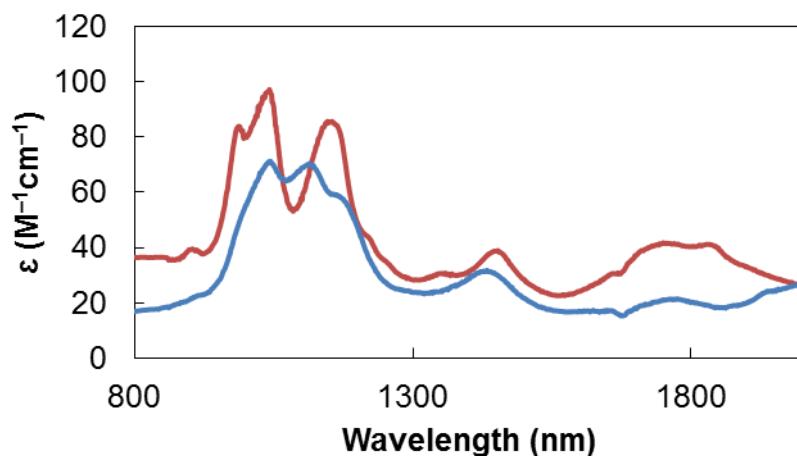


Figure S2. Near-IR spectrum of $\text{Cl}_2\text{U}(\text{PN})_2$ (red trace) and $(\text{N}_3)_2\text{U}(\text{PN})_2$ (blue trace).

Electrochemical Data

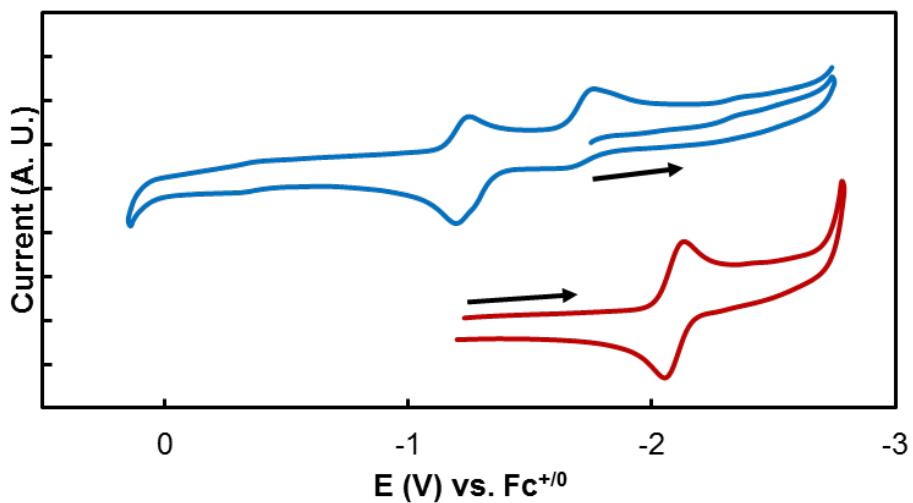


Figure S3. Cyclic voltammograms of $(PN)_2U^{III}I$ (**1**) (top) and $(PN)_2U^{IV}Cl_2$ (**2**) (bottom) at a scan rate of 250 mV/s in THF with 0.1 M $[^nPr_4N][BAr^F]$ supporting electrolyte. Arrows indicate the open circuit potential and scan direction.

Electrochemical analysis allowed us to compare the redox properties of these new compounds with the previously reported low and mid-valent uranium PNP complexes, $(PNP)_2U^{III}I$ and $(PNP)_2U^{IV}Cl_2$ (Figure S3). The measurements were performed in THF with $[^nPr_4N][BAr^F]$ supporting electrolyte and referenced to $Fc^{+/-}$. With an open circuit potential at -1.75 V, we observed a reversible anodic wave for **1** at $E_{1/2} = -1.22$ V in the cyclic voltammogram, which we assigned as the $U^{III/IV}$ couple. This was slightly shifted compared to $(PNP)_2U^{III}I$, which had a $U^{III/IV}$ couple at -1.47 V.^[9] This 250 mV shift can be attributed to the additional phosphine arms that are coordinated in the case of $(PNP)_2U^{III}I$. Compound **1** also featured an irreversible reduction wave with an E_{pc} of -1.76 V. Upon oxidation of **1**, we propose the stability of the *cisoid*-(N,N) geometry increased. Thus the return reduction wave of the $U(III/IV)$ couple observed at $E_{1/2} = -1.22$ V shows a smaller current, and the second reduction wave at -1.76 V (observed only in the second sweep) corresponds to the *cis*-(N,N)- $U^{IV}I(PNP)_2^+$ complex generated on the electrochemical timescale. To summarize, the *transoid*-(N,N) compound had E_{pc} of -1.25 V and the *cisoid*-(N,N) compound had an E_{pc} of -1.76 V. These assignments were supported by the identification of the *transoid* configuration of amide nitrogen atoms in both uranium(IV) complexes that were isolated (**2** and **3**) for this system. We expect that the relative orientations of the PN^- are governed by primarily steric interactions at the metal cation. A similar effect was observed by Kiplinger and coworkers for $U^{III}I(PNP)_2$, in which upon oxidation the PNP^- coordination mode changed from κ^3 -(P,N,P) to κ^2 -(P,N), resulting in a second metal-based feature at -1.9 V. Complex **2** and the analogous PNP complex, $(PNP)_2U^{IV}Cl_2$, had more similar electrochemical behavior due to the two dangling phosphine arms in $(PNP)_2U^{IV}Cl_2$. The $U^{III/IV}$ couple for **2** was at -2.09 V, while the PNP complex was at -2.19 V. Both compounds also exhibited ligand oxidation processes between -0.1 and 0.67 V (Figure S10).^[9]

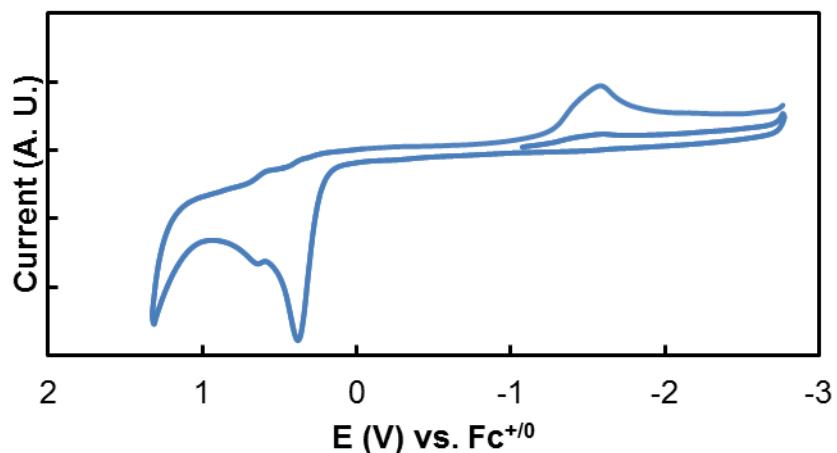


Figure S4. CV of HPN in THF with $[n\text{Pr}_4\text{N}][\text{BAr}^{\text{F}}]$ supporting electrolyte.

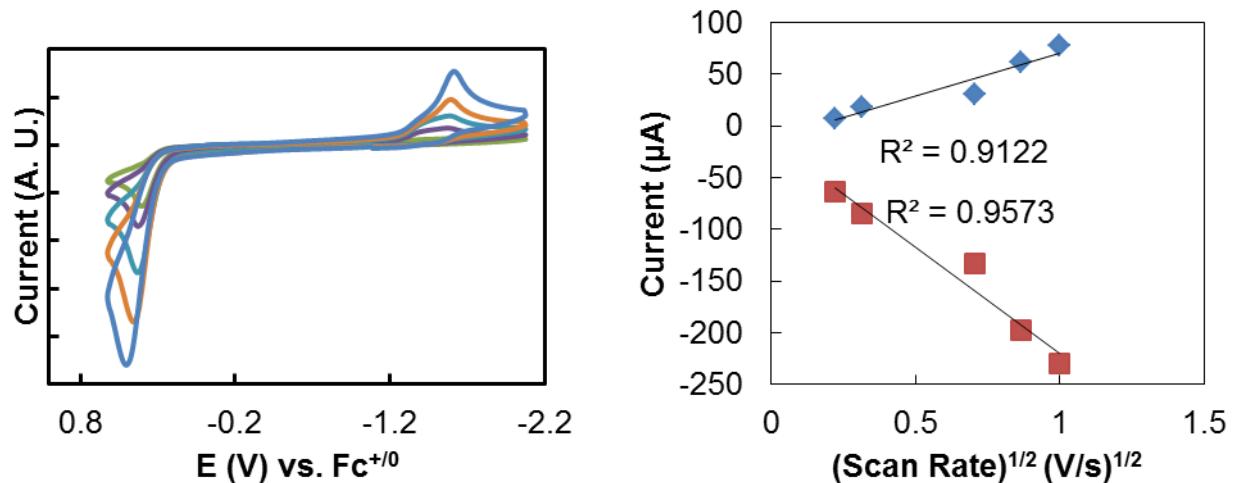


Figure S5. Scan rate dependence of HPN^{0+} couple with Randles-Sevcik plot.

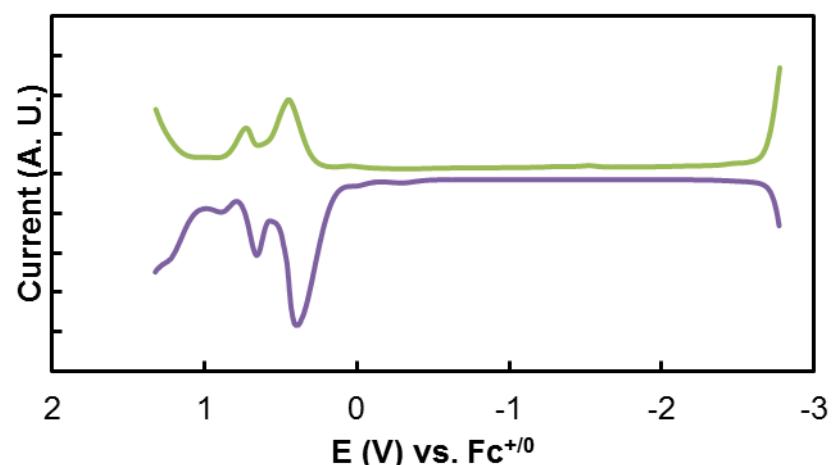


Figure S6. DPV of HPN in THF with $[n\text{Pr}_4\text{N}][\text{BAr}^{\text{F}}]$ supporting electrolyte

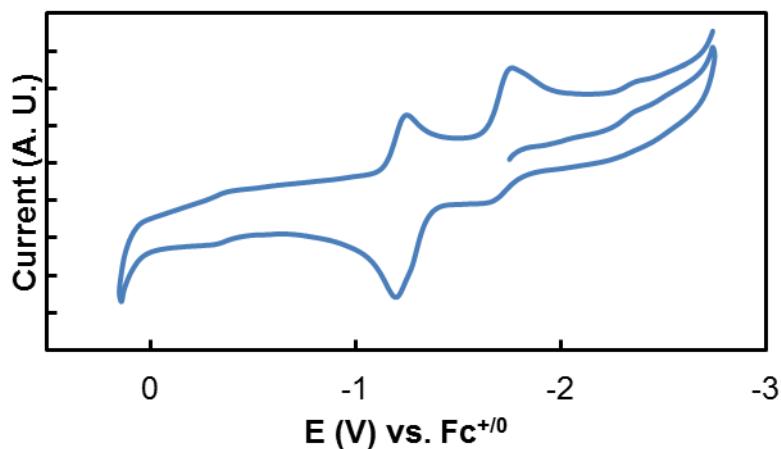


Figure S7. CV of $(\text{PN})_2\text{U}^{\text{III}}\text{I}$ in THF with $[n\text{Pr}_4\text{N}][\text{BArF}]$ supporting electrolyte.

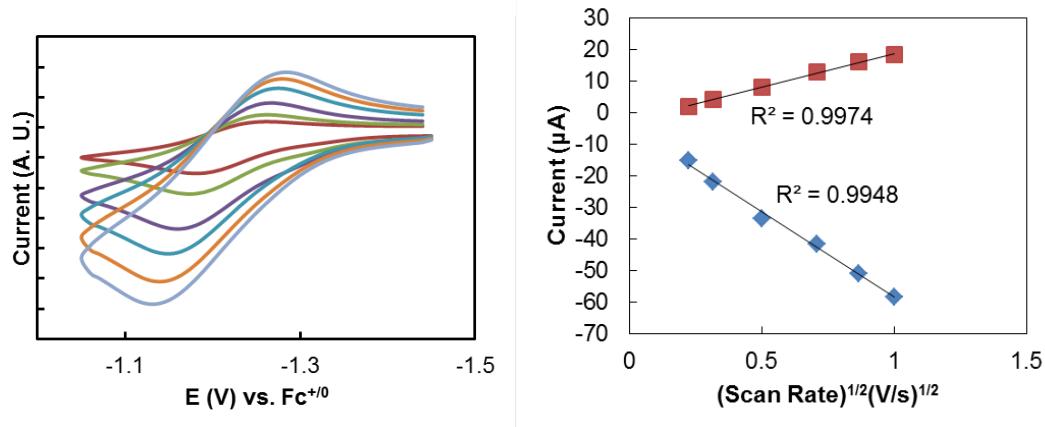


Figure S8. Scan rate dependence of $\text{U}^{\text{III/IV}}$ couple with Randles-Sevcik plot.

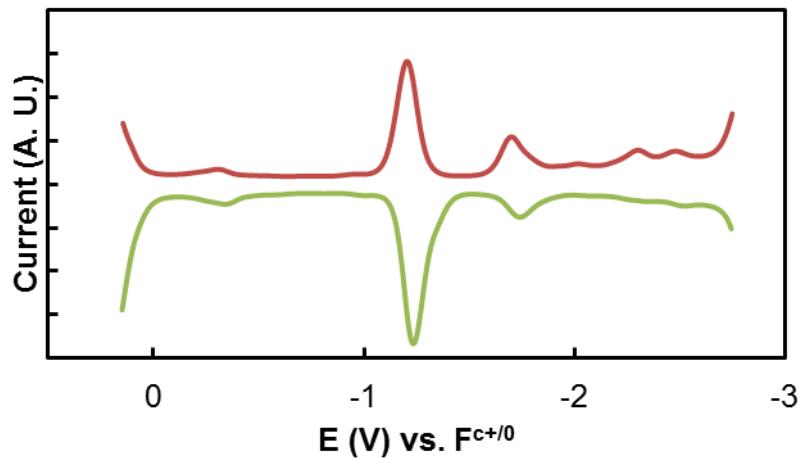


Figure S9. DPV of $(\text{PN})_2\text{U}^{\text{III}}\text{I}$ in THF with $[n\text{Pr}_4\text{N}][\text{BArF}]$ supporting electrolyte.

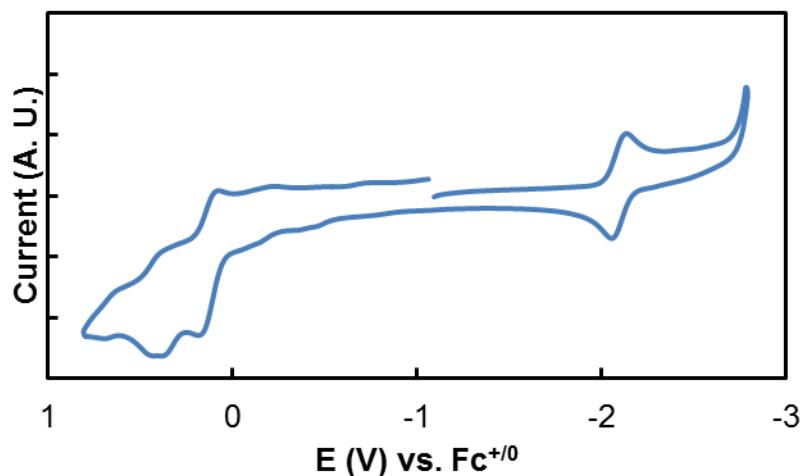


Figure S10. CV of $(\text{PN})_2\text{U}^{\text{IV}}\text{Cl}_2$ in THF with $[n\text{Pr}_4\text{N}][\text{BArF}]$ supporting electrolyte.

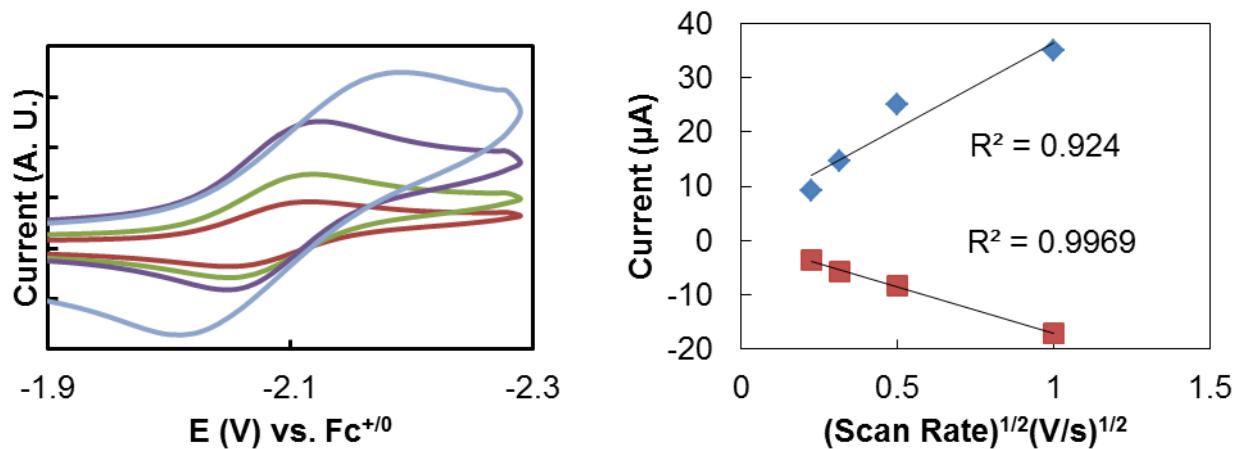


Figure S11. Scan rate dependence of $\text{U}^{\text{III/IV}}$ couple with Randles-Sevcik plot.

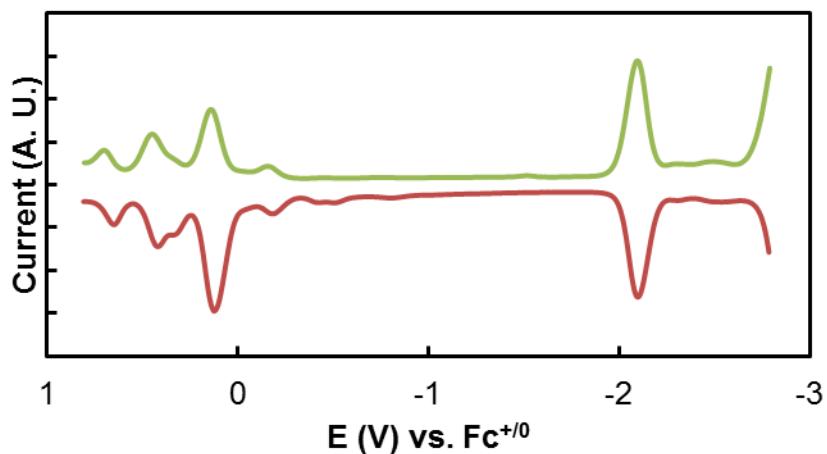


Figure S12. DPV of $(\text{PN})_2\text{U}^{\text{IV}}\text{Cl}_2$ in THF with $[n\text{Pr}_4\text{N}][\text{BArF}]$ supporting electrolyte.

X-Ray Crystallography Discussion

X-ray crystal structures of **1** and **2** allowed for comparison of these compounds with $(\text{PNP})_2\text{U}^{\text{III}}\text{I}$ and $(\text{PNP})_2\text{U}^{\text{IV}}\text{Cl}_2$ reported by Kiplinger and coworkers (Figure 1).^[9] The structure of compound **1** revealed a C_2 symmetric complex with amide ligands positioned *trans* to one another. The geometry of **1** was distorted from an idealized trigonal bipyramidal geometry, with a τ_5 value of 0.72. Upon comparison with the asymmetrical PNP complex, $(\text{PNP})_2\text{U}^{\text{III}}\text{I}$, all uranium–ligand bond lengths for **1** were found to be shorter than those in $(\text{PNP})_2\text{U}^{\text{III}}\text{I}$. For example, the U–N bond lengths in **1** were 2.337(4) Å, while in $(\text{PNP})_2\text{U}^{\text{III}}\text{I}$ the average U–N bond length was 2.408(5) Å. While **2** was also C_2 symmetric, the amide ligands in this compound were positioned *cis* to one another in contrast with **1**. The previously reported structure of $(\text{PNP})_2\text{U}^{\text{IV}}\text{Cl}_2$ was significantly different from **2**, with *cis*-chlorides and a Cl–U–Cl bond angle of 101.37(4)°. In contrast, compound **2** had *trans* chloride ligands, with a Cl(1)–U(1)–Cl(1) bond angle of 166.58(3)°. The amide bond lengths in $(\text{PNP})_2\text{U}^{\text{IV}}\text{Cl}_2$ and **2** were similar with distances of 2.285(3) and 2.276(4) Å respectively. However, the U–P bonds were significantly longer in **2** at 3.1495(6) Å, while the coordinated phosphines in $(\text{PNP})_2\text{U}^{\text{IV}}\text{Cl}_2$ had an average bond length of 3.000(1) Å.^[9]

The crystal structure of **3** revealed *cis* amide and phosphine ligands and *trans* azide ligands, similar to the coordination environment found in **2** (Figure 2). The axial geometry was more linear in **3** with a N(3)–U(1)–N(6) bond angle of 170.6(8)° compared to the 166.58(3)° Cl(1)–U(1)–Cl(1) bond angle found in **2**. The average U–N_{amide} bond lengths in **3** were slightly longer than those in **2** with bond lengths of 2.283(3) and 2.2763(17) Å respectively. The average U–N_{azide} bond lengths in **3** were shorter than those reported for $\{[\text{Na}(\text{THF})_4][\text{U}^{\text{IV}}(\text{N}(\text{SiMe}_3)_2)_3(\text{N}_3)_2]\}_x$ with bond lengths of 2.24(4) and 2.337(6) Å respectively.^[10] Surprisingly, the U–N_{azide} bonds in **3** were of similar lengths to those in the uranium(V) azide, $\text{U}^{\text{V}}[\text{N}(\text{SiMe}_3)_2]_3(\text{N}_3)_2$, which has U–N_{azide} bond lengths of 2.226(3) Å.^[10]

NMR Data

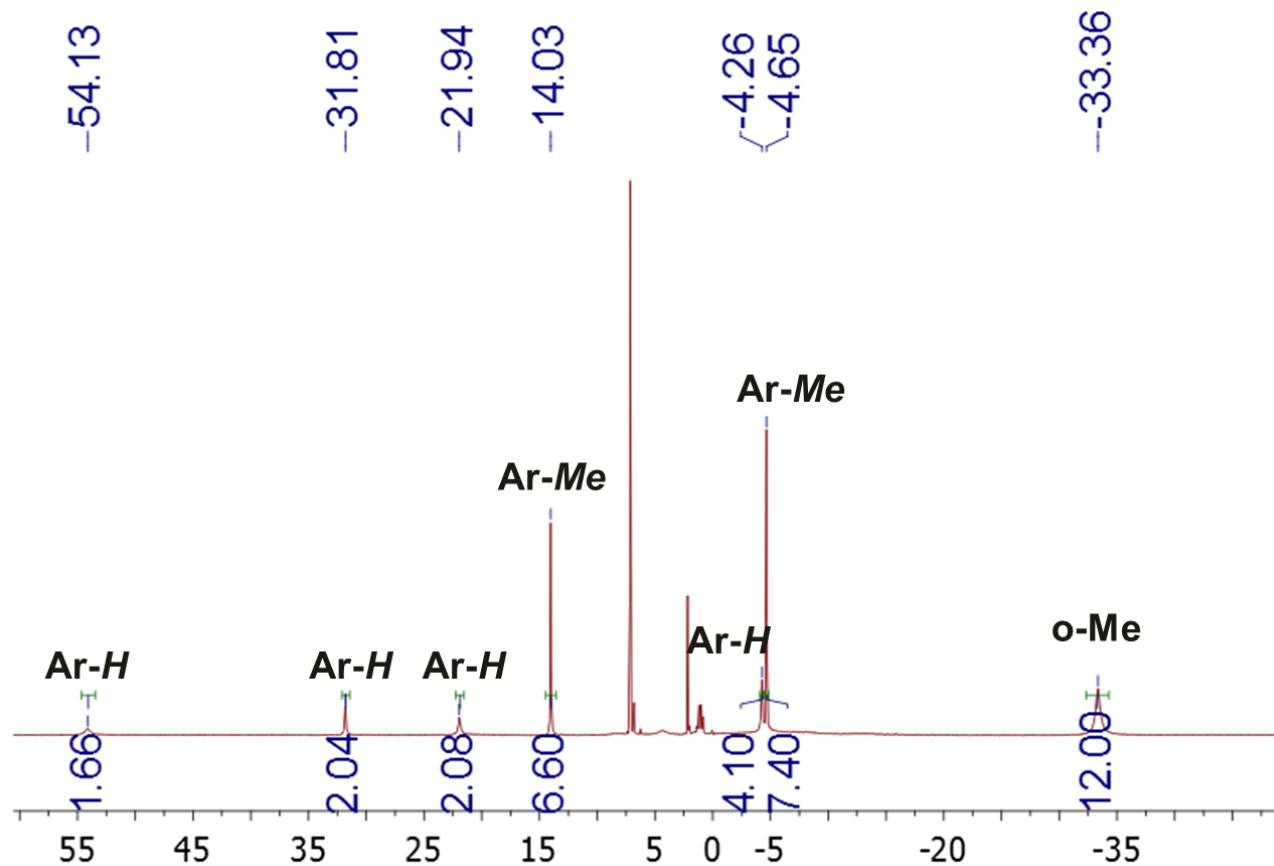


Figure S13. 1H NMR of **1** in C_6D_6 at 300 K.

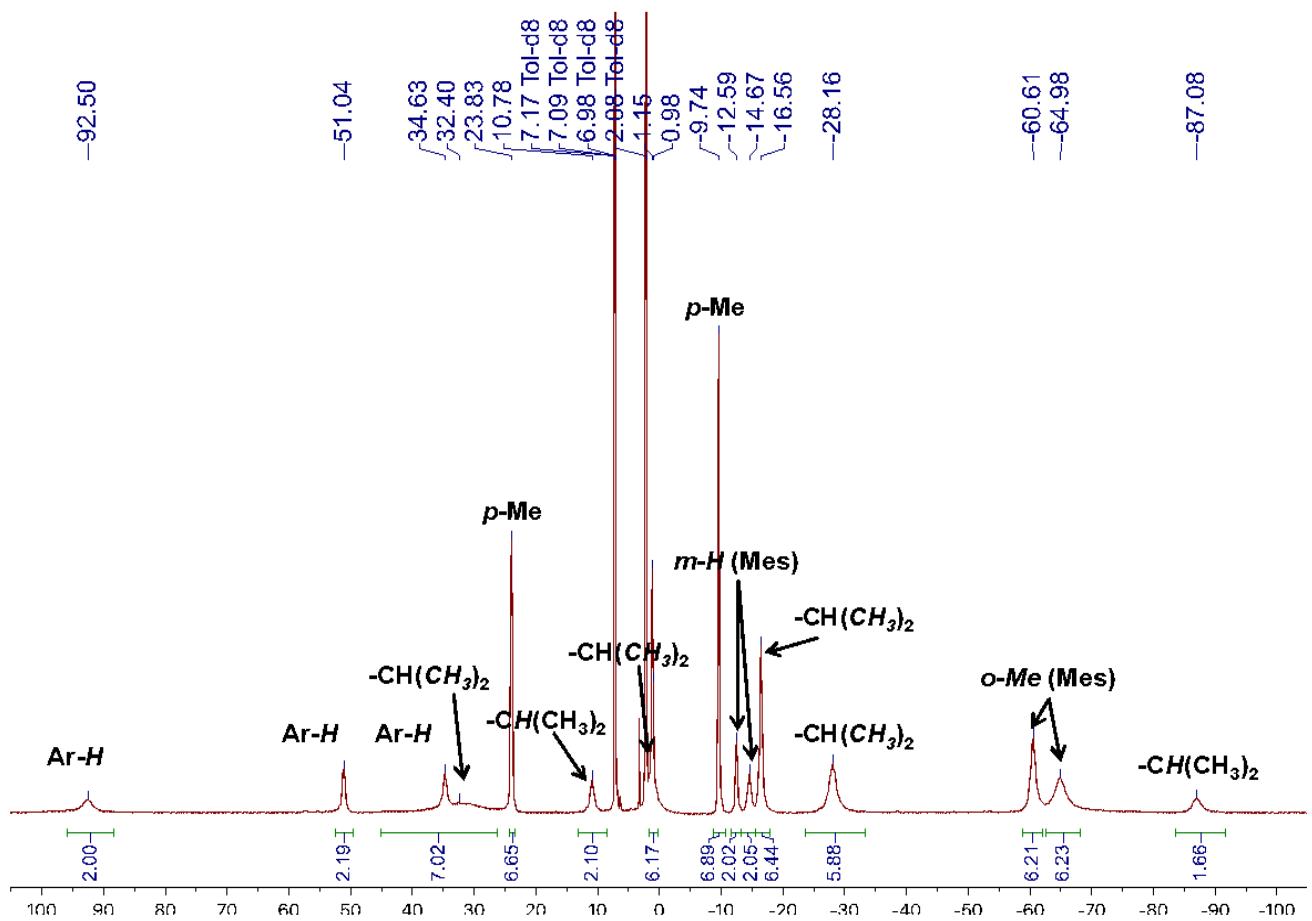


Figure S14. ^1H NMR of **1** in Tol-d_8 at 200 K.

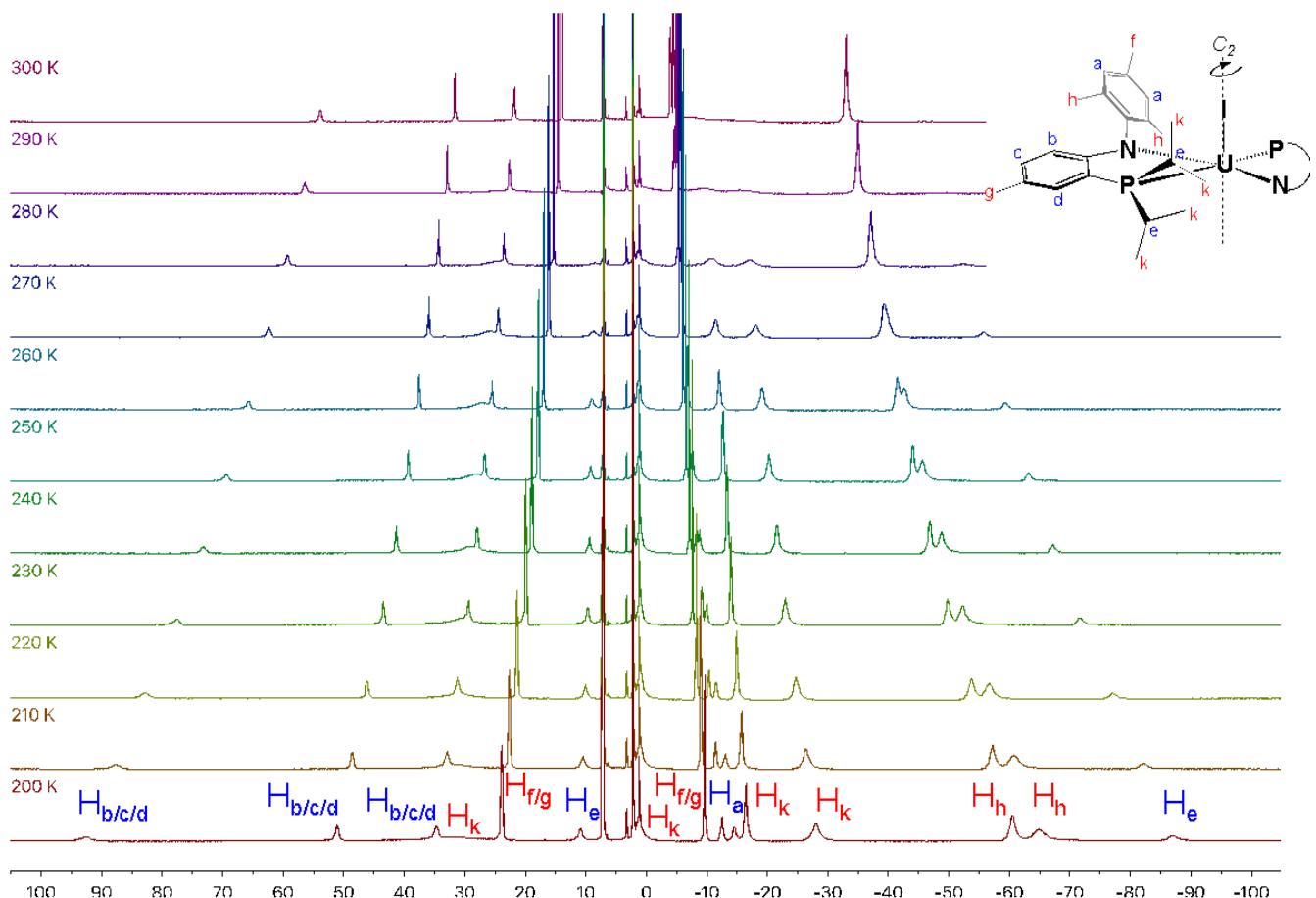


Figure S15. VT^{-1}H NMR of **1** in $\text{Tol}-d_8$.

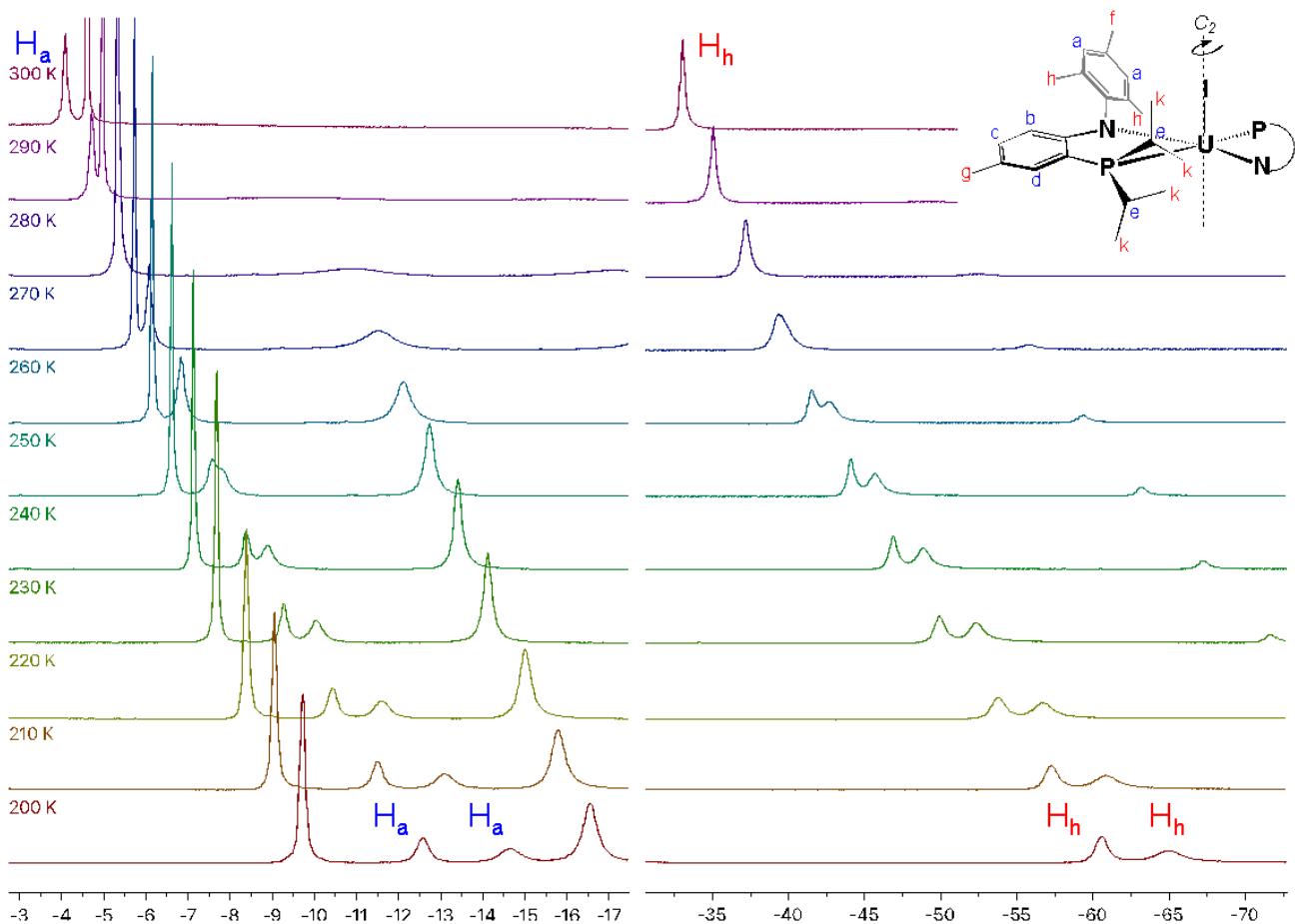
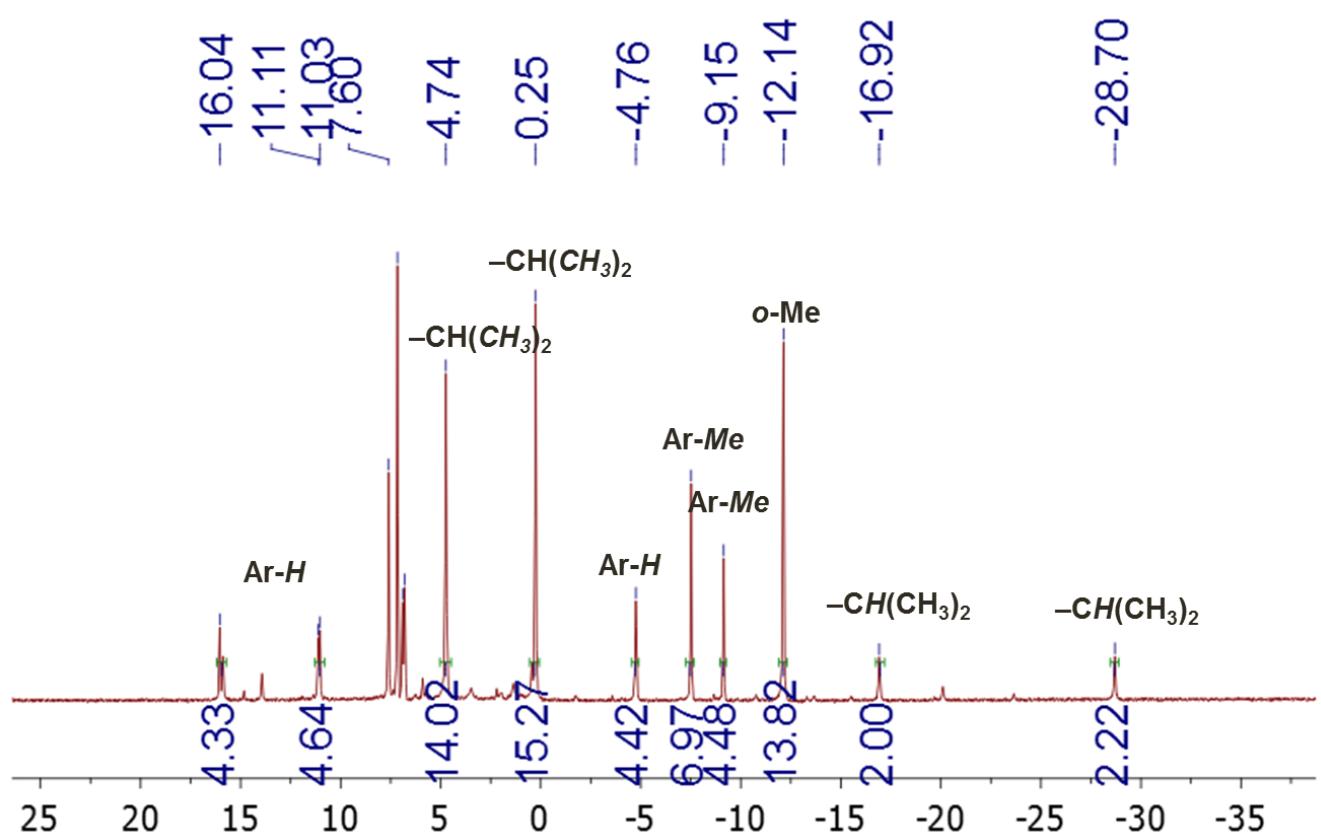
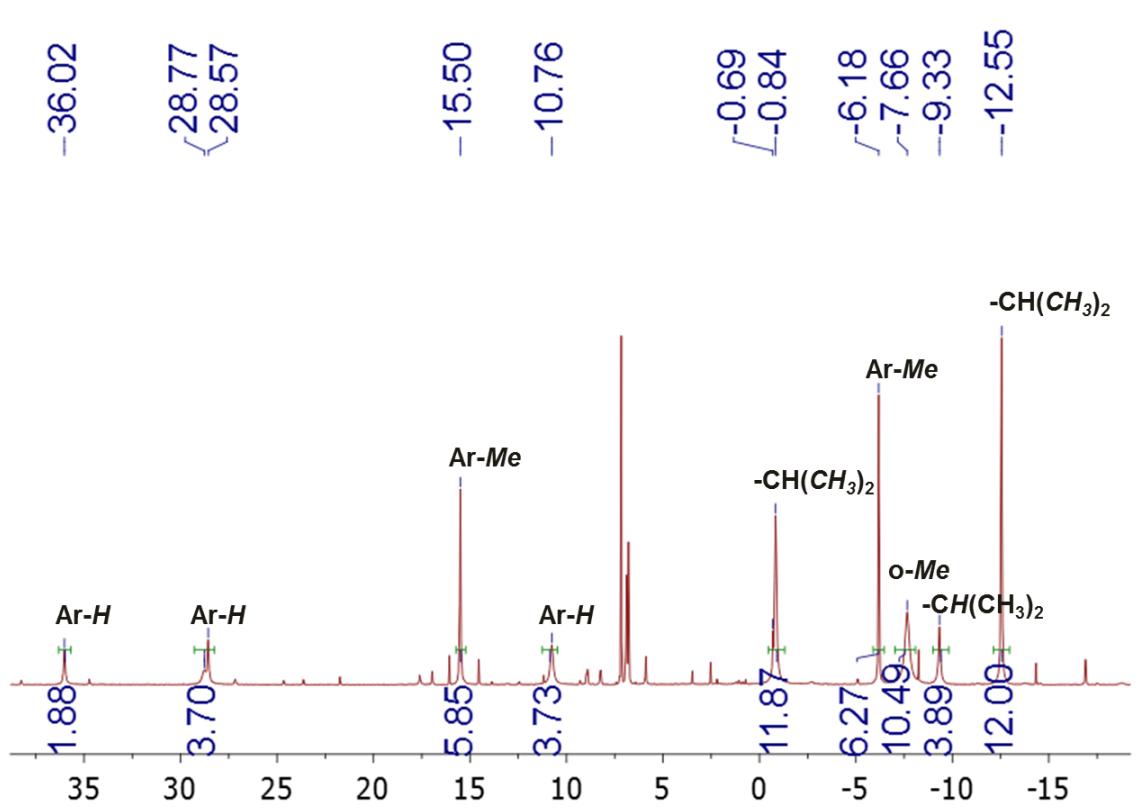


Figure S16. Zoom on the decoalescence of H_a (left) and H_h (right) of **1** in Tol-d₈.

Comments on solution behavior of **1**: At room temperature (300 K), complex **1** was characterized by an average C_{2v} symmetry (free rotation of the mesityl moieties) and the absence of signals for the *iso*-propyl groups. At 200 K, a pure C_2 symmetry, consistent with X-ray diffraction study, was observed. Notably, *iso*-propyl groups were totally desymmetrized resulting in 4 sets of CH₃ resonances (H_k, **Figure S15**) and 2 sets of CH resonances (H_e, **Figure S15**). Moreover, limitation of the mesityl free rotation and decoalescence of the resulting signals was observed between 260–270 K (**Figure S16**).



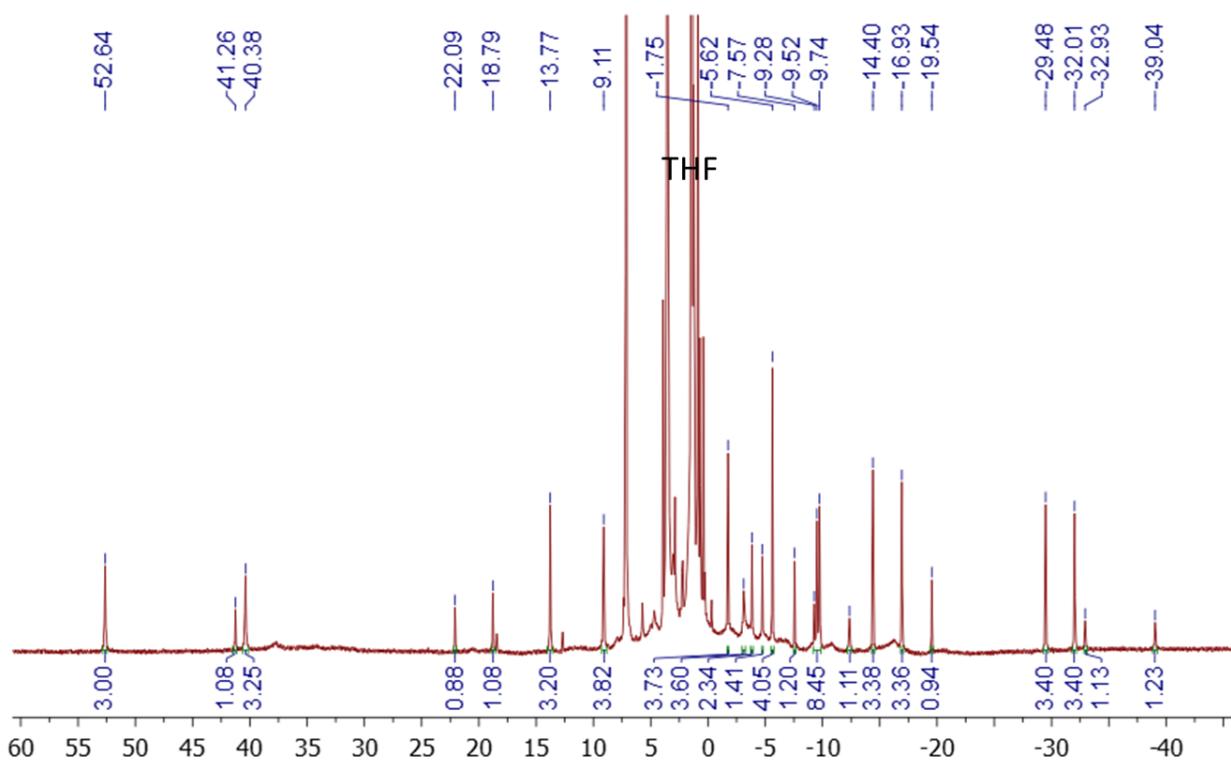


Figure S19. ^1H NMR of **4** in $C_6\text{D}_6$.

Computational Details

All calculations were performed by the ADF 2017.105 modeling suite.^[11,12] The geometry optimizations were carried out with the PBE^[13,14] exchange-correlation functional and the all-electron triple-zeta basis set with polarization functions (TZP). The spin-free relativistic zeroth-order regular approximation (SF-ZORA) Hamiltonian is used to include relativistic effects. The zero-point energy (ZPE) and entropy corrections were obtained from the vibrational calculations at the same level of theory and were used to obtain the Gibbs free energy. Solvation free energies were evaluated by a conductor-like screening model (COSMO)^[15] approach with the tetrahydrofuran (dielectric constant, $\epsilon = 7.43$)^[16] using the optimized gas phase structures.

The free energy in solution phase G(sol) has been calculated as follows:

$$G(\text{sol}) = G(\text{gas}) + G(\text{solv}) \quad (1)$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas}) \quad (2)$$

$$H(\text{gas}) = E(\text{SCF}) + ZPE \quad (3)$$

$$\Delta E(\text{SCF}) = \sum E(\text{SCF}) \text{ for products} - \sum E(\text{SCF}) \text{ for reactants} \quad (4)$$

$$\Delta G(\text{sol}) = \sum G(\text{sol}) \text{ for products} - \sum G(\text{sol}) \text{ for reactants} \quad (5)$$

$\Delta G(\text{gas})$ is the free energy in gas phase; $\Delta G(\text{solv})$ is the free energy of solvation as computed using the continuum solvation model; $\Delta H(\text{gas})$ is the enthalpy in gas phase; T is the temperature (298.15K); $\Delta E(\text{SCF})$ is the self-consistent field energy. Note that by entropy here we refer specifically to the vibrational / rotational / translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model.

Computational Results

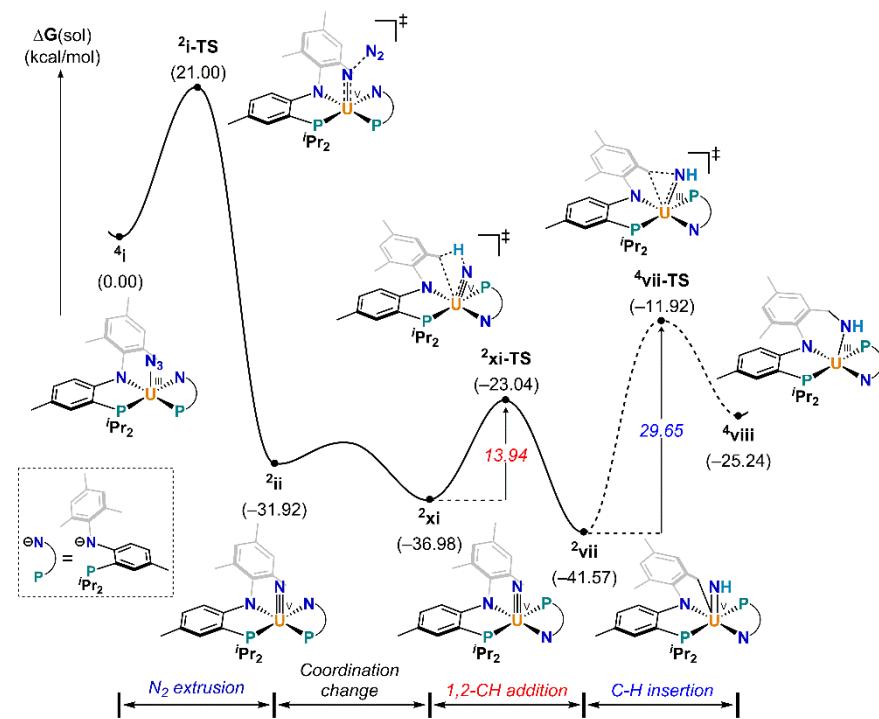


Figure S20. Computed energy profile of starting from U(III) azide complex without considering one electron reduction via potassium graphite.

Figure S20 details the proposed mechanism for the computed energy profile of starting from U(III) azide complex without considering one electron reduction via potassium graphite in the reaction coordinate. Extruding N_2 and oxidative process at the uranium(III) azide intermediate, 4_i gives the U(V)-nitrido complex, 2_{ii} , $(\text{PN})_2\text{U}^{\text{V}}(\equiv\text{N})$, that is located at relative free energy is 31.9 kcal/mol lower than 4_i . The transition state of the N_2 extrusion, 2_i-TS is located at 21.0 kcal/mol, which is feasible under very mild conditions. In that transition state, a quartet to doublet spin-crossover takes place. The intersystem crossing in uranium is quite common due to the strong spin-orbit interaction on the uranium since uranium is a very heavy metal. After the oxidative process, rearranging one of the PN^- ligand at the *cisoid*-(N,N) intermediate, 2_{ii} to the *transoid*-(N,N) intermediate, 2_{xi} occurs. The coordination change is thermodynamically downhill process by 5.1 kcal/mol. At the *transoid*-(N,N) intermediate, 2_{xi} , a 1,2-CH addition is performed at one of the proximal methyl groups to form the cyclometallated imido intermediate, 2_{vii} . The transition state, 2_{xi}-TS is associated with the activation barrier of 13.9 kcal/mol. The C-H insertion, involving the transformation $2_{vii} \rightarrow 4_{vii}$ via 4_{vii}-TS is quite uphill energetically by 16.3 kcal/mol and is kinetically prohibitive with a calculated barrier of 29.7 kcal/mol.

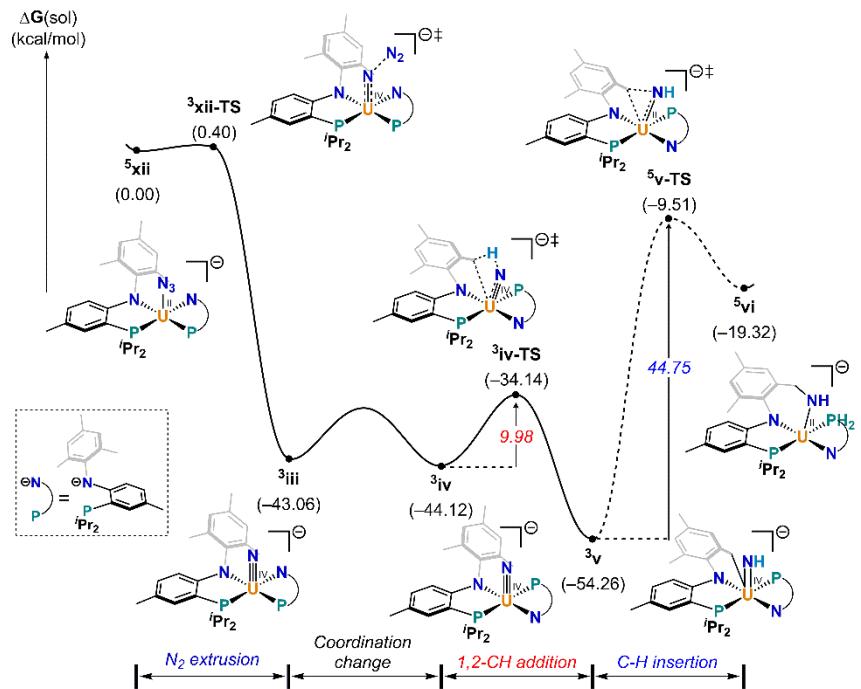


Figure S21. Computed energy profile of starting from U(II) azide complex.

Figure S21 illustrates the proposed mechanism for the computed energy profile of starting from U(II) azide complex without considering one electron reduction via potassium graphite in the reaction coordinate. Extruding N_2 and oxidative process from the uranium(III) azide intermediate, ^5xii gives the U(V)-nitrido complex, ^3iii , $(\text{PN})_2\text{U}^{\text{V}}(\equiv\text{N})$, that is located at relative free energy of -43.1 kcal/mol. The transition state of the N_2 extrusion, $^3\text{xii-TS}$ is located at 0.4 kcal/mol, which is barrier-less process. In that transition state, a quintet to triplet spin-crossover takes place. After the oxidative process, rearranging one of the PN^- ligand from the *cisoid*-(N,N) intermediate, ^3iii to the *transoid*-(N,N) intermediate, ^2ix takes place. The coordination change is thermoneutral process by 1.1 kcal/mol downhill. At the *transoid*-(N,N) intermediate, ^3iv , a C–H activation occurs at one of the proximal methyl groups of the PN^- ligand to form the uranium(IV) imido intermediate, ^3v . In 1,2-CH addition step, $^3\text{iv-TS}$ is associated with the step barrier of 10.0 kcal/mol, which is relatively faster than the proton-transfer at the uranium(V) nitride intermediate. Our DFT calculations suggest that the C–H insertion step with spin-crossover, involving the transformation $^3\text{v} \rightarrow ^5\text{vi}$ via $^5\text{vii-TS}$ is extremely uphill energetically by 34.9 kcal/mol and is kinetically harsh to overcome a calculated barrier of 44.8 kcal/mol.

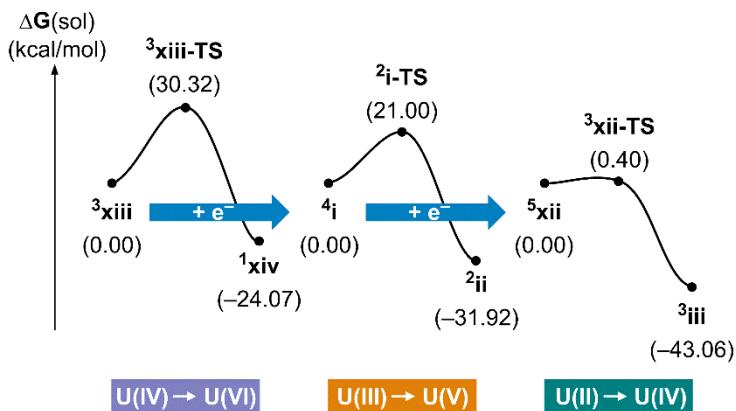


Figure S22. Comparison of the N_2 extrusion step adopting different oxidation state at the uranium center.

Figure S22 summarizes the calculated changes of the energy profiles for the N_2 extrusion with the spin-crossover between spin state surfaces when different oxidation states are considered for the uranium center. If the intermediate, ${}^3\text{xiii}$ is reduced to become ${}^4\text{i}$ containing a U(III)-center, the oxidative process and N_2 extrusion become much easier with a barrier of only 21.0 kcal/mol and exergonic by 31.9 kcal/mol. If one electron is obtained to afford the U(II) analogue, ${}^5\text{xii}$, the oxidative process is predicted to be barrier-less process, which is only 0.4 kcal/mol. But, the uranium(II) azide complex could be achieved by giving only over-reduction condition. Thus, the oxidative process is only predicted to be feasible for the U(III) oxidation state.

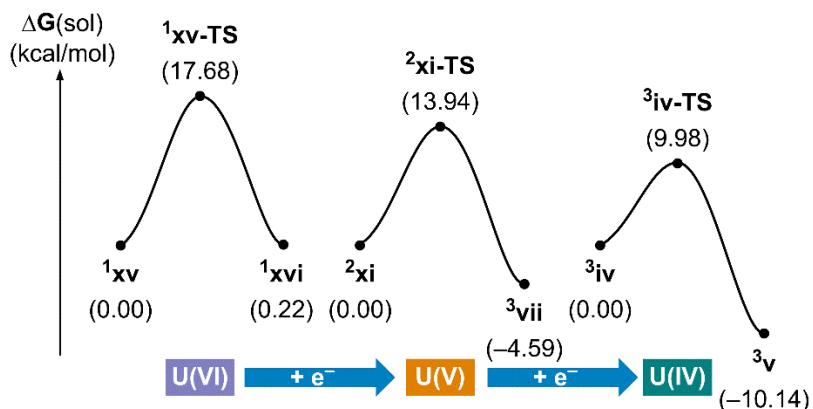


Figure S23. Comparison of the 1,2-CH insertion step adopting different oxidation state at the uranium center.

Figure S23 summarizes the calculated changes of the energy profiles for the 1,2-CH insertion step when different oxidation states are considered for the uranium center. The 1,2-CH insertion step becomes much easier as the uranium center is reduced. It means that the 1,2-CH insertion takes place readily as the uranium center is reduced since the interaction between the uranium cation and the nitrido ligand becomes less covalent. Therefore, the nitrido ligand of the $\text{U(IV)}\equiv\text{N}$ is much more basic and is a better nucleophile.

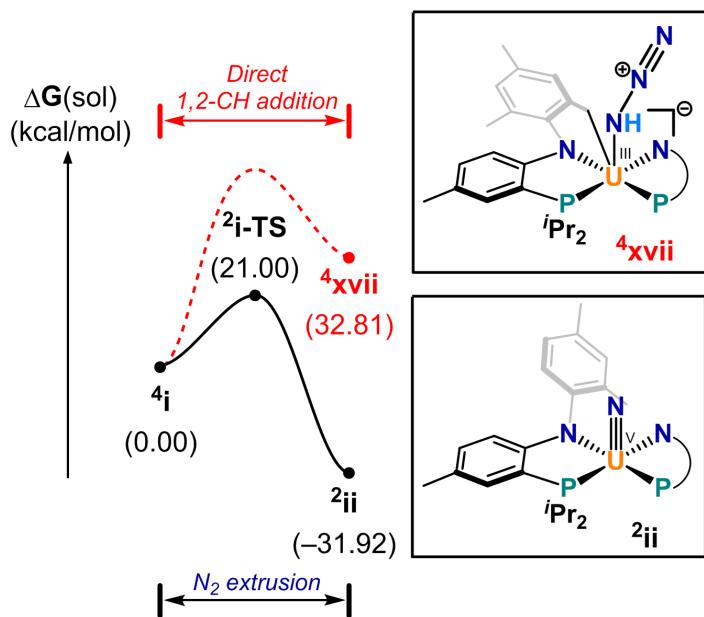


Figure S24. Comparison of N_2 extrusion and direct 1,2-CH addition by azide ligand.

We calculated a product complex that is generated by 1,2-CH addition without N_2 extrusion and isomerization of one of the PN^- ligands. Then, we observed that the product complex, $^4\text{xvii}$ has much higher energy, as shown in Figure S24. This means that the structure is unstable because the basicity of the azide ligand and the electrophilicity of the U(III) center are not matched well enough to directly give rise to 1,2-CH addition without N_2 extrusion. The N_2 extrusion from the intermediate ^4i oxidizes the uranium center so that the methyl carbanion from the PN^- ligand can readily coordinate to the uranium center. Unless the electrophilicity of the uranium is increased as the uranium is oxidized, the 1,2-CH addition does not occur. So, the direct 1,2-CH addition is unlikely to occur prior to N_2 extrusion, according to our calculations.

XYZ Coordinates

=====			
4i			
=====			
114			
UC44P2N5H62			
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P	8.482224000	3.142816000	3.382601000
P	11.455296000	1.943642000	6.167751000
N	7.458806000	5.178321000	5.266694000
N	11.339978000	4.822050000	7.090689000
N	8.247799000	2.790159000	7.848838000
N	7.600664000	2.374667000	8.785041000
N	6.983399000	1.964454000	9.675183000
C	6.698806000	5.144083000	4.108634000
C	5.589712000	6.001182000	3.885796000
H	5.305253000	6.708372000	4.667260000
C	4.876406000	5.967963000	2.693854000
H	4.033667000	6.653823000	2.564222000
C	5.215625000	5.088583000	1.651337000
C	6.302628000	4.235348000	1.871776000
H	6.584005000	3.551140000	1.067684000
C	7.036198000	4.232651000	3.068954000
C	4.440994000	5.066218000	0.357588000
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H	10.786609000	4.896859000	2.434251000
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H	6.173703000	1.461409000	1.898239000
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H	4.476372000	4.482151000	6.439083000
=====			
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=====			
114			
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N	7.604978000	1.882892000	8.334081000

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H	6.211372000	1.616039000	1.724800000	H	10.369865000	10.973661000	7.117165000
C	6.982154000	5.962465000	6.504888000	C	9.830544000	5.853848000	9.192218000
C	7.427647000	7.307874000	6.599235000	H	9.620796000	6.374196000	10.136205000
C	7.020642000	8.088149000	7.686860000	H	10.408182000	4.947921000	9.421164000
H	7.362026000	9.125989000	7.745585000	H	8.841239000	5.545102000	8.802552000
C	6.182299000	7.585035000	8.689095000	=====	=====	=====	=====
C	5.712783000	6.273240000	8.554252000	=====	=====	=====	=====
H	5.016777000	5.876298000	9.299500000	³ iii	=====	=====	=====
C	6.071670000	5.454942000	7.474670000	=====	=====	=====	=====
C	8.276739000	7.911113000	5.510891000	112	=====	=====	=====
H	8.384208000	8.992937000	5.663071000	UC44P2N3H62	=====	=====	=====
H	7.830319000	7.739609000	4.521005000	U	9.400616000	3.971053000	6.059576000
H	9.288790000	7.479700000	5.490113000	P	8.263912000	2.961998000	3.506199000
C	5.794057000	8.431065000	9.875201000	P	11.577160000	1.947588000	6.209219000
H	4.789727000	8.174021000	10.240234000	N	7.389054000	5.209034000	5.310408000
H	5.807070000	9.501519000	9.626406000	N	11.443788000	4.740578000	7.256826000
H	6.492563000	8.281086000	10.714956000	N	8.602976000	2.839232000	7.243471000
C	5.436264000	4.099137000	7.316697000	C	6.611668000	5.124138000	4.186793000
H	4.708952000	3.922527000	8.120207000	C	5.496554000	5.983325000	3.944439000
H	6.188163000	3.295691000	7.332642000	H	5.230051000	6.716143000	4.708667000
H	4.910015000	4.030112000	6.352314000	C	4.760056000	5.921127000	2.767952000
C	12.393279000	4.132236000	7.579299000	H	3.921883000	6.613814000	2.633160000
C	13.312363000	4.788093000	8.439247000	C	5.066932000	5.001834000	1.749692000
H	13.226798000	5.866467000	8.579031000	C	6.133045000	4.126202000	1.994120000
C	14.299961000	4.088317000	9.122541000	H	6.376466000	3.396197000	1.217336000
H	14.975358000	4.641282000	9.782220000	C	6.891874000	4.144598000	3.175567000
C	14.439876000	2.696628000	9.000057000	C	4.286525000	4.960664000	0.459003000
C	13.555465000	2.048237000	8.131321000	H	3.202391000	4.862457000	0.636452000
H	13.644102000	0.964567000	8.020798000	H	4.597573000	4.108591000	-0.163592000
C	12.558611000	2.724732000	7.410598000	H	4.429961000	5.875583000	-0.141853000
C	15.491995000	1.940211000	9.770452000	C	9.128081000	2.915071000	1.820235000
H	15.458744000	0.866274000	9.540978000	H	8.344138000	2.746357000	1.063393000
H	15.354933000	2.053246000	10.857465000	C	9.780601000	4.271183000	1.534576000
H	16.505117000	2.302200000	9.534704000	H	10.563395000	4.495254000	2.276661000
C	12.621589000	1.453335000	4.776135000	H	9.043320000	5.084910000	1.569199000
H	11.932955000	1.061286000	4.008566000	H	10.250835000	4.269617000	0.536854000
C	13.247504000	2.751532000	4.255305000	C	10.146664000	1.776704000	1.723010000
H	13.966048000	3.152511000	4.984402000	H	10.621954000	1.772501000	0.727865000
H	12.493013000	3.529466000	4.072061000	H	9.688850000	0.789693000	1.879349000
H	13.786263000	2.566609000	3.313374000	H	10.943428000	1.901165000	2.469986000
C	13.700997000	0.399821000	5.037799000	C	7.414177000	1.254765000	3.570035000
H	14.286327000	0.240330000	4.118017000	H	8.266773000	0.578961000	3.762019000
H	13.283800000	-0.572761000	5.331545000	C	6.491637000	1.211152000	4.793521000
H	14.402105000	0.729926000	5.817573000	H	5.625748000	1.875028000	4.644823000
C	11.105398000	0.188578000	6.988871000	H	7.015151000	1.535254000	5.707245000
H	12.073472000	-0.332853000	7.070186000	H	6.110837000	0.187391000	4.945221000
C	10.491746000	0.311859000	8.387328000	C	6.681587000	0.774016000	2.314152000
H	9.541717000	0.863983000	8.343863000	H	6.333910000	-0.263075000	2.460398000
H	11.164600000	0.828668000	9.084920000	H	7.313885000	0.783486000	1.413781000
H	10.295556000	-0.695617000	8.787236000	H	5.793396000	1.391266000	2.117010000
C	10.188966000	-0.609118000	6.050747000	C	7.042366000	6.177847000	6.287804000
H	10.007415000	-1.611569000	6.468051000	C	7.524383000	7.508114000	6.172395000
H	10.621709000	-0.741366000	5.047647000	C	7.211625000	8.442772000	7.164853000
H	9.217353000	-0.103623000	5.950975000	H	7.586805000	9.466261000	7.060675000
C	11.298056000	6.231172000	7.147052000	C	6.439818000	8.104482000	8.282903000
C	11.993958000	7.107670000	6.274594000	C	5.957573000	6.794057000	8.373846000

H	5.334017000	6.512127000	9.229096000		^{3iv}
C	6.228046000	5.825796000	7.397109000		=====
C	8.334267000	7.916237000	4.968968000		112
H	8.630985000	8.971677000	5.039525000		UC44P2N3H62
H	7.763409000	7.769185000	4.039284000	U	0.441596000 -0.013873000 0.052452000
H	9.249546000	7.312354000	4.873293000	P	1.412766000 -2.754876000 0.740686000
C	6.167029000	9.112741000	9.371742000	P	-0.631959000 2.545447000 -1.226729000
H	5.234052000	8.883147000	9.907127000	N	1.966097000 -1.068502000 -1.690536000
H	6.086836000	10.132467000	8.965889000	N	-0.096880000 1.814658000 1.530089000
H	6.979388000	9.123018000	10.118353000	N	-1.204693000 -0.716729000 -0.285669000
C	5.642329000	4.444835000	7.502555000	H	-2.465818000 0.360767000 1.915210000
H	5.005430000	4.361605000	8.394896000	C	2.420880000 -2.356217000 -1.831068000
H	6.443761000	3.685937000	7.551524000	C	3.113466000 -2.814761000 -2.996145000
H	5.034250000	4.210225000	6.614854000	H	3.309474000 -2.102168000 -3.799688000
C	12.490615000	4.046544000	7.806660000	C	3.523695000 -4.133000000 -3.141000000
C	13.420263000	4.625449000	8.723502000	H	4.040105000 -4.424544000 -4.062488000
H	13.307446000	5.680010000	8.983819000	C	3.285853000 -5.100885000 -2.148536000
C	14.439912000	3.881232000	9.301568000	C	2.640077000 -4.658483000 -0.987561000
H	15.116087000	4.374213000	10.008819000	H	2.434078000 -5.392470000 -0.203095000
C	14.619500000	2.515535000	9.013870000	C	2.226741000 -3.331442000 -0.795777000
C	13.737044000	1.947971000	8.086337000	C	3.687548000 -6.542659000 -2.336855000
H	13.8555404000	0.886698000	7.848938000	H	3.549205000 -7.116246000 -1.408486000
C	12.704960000	2.669559000	7.469378000	H	4.745526000 -6.638890000 -2.632445000
C	15.699128000	1.702007000	9.683404000	H	3.090358000 -7.039848000 -3.121003000
H	15.761458000	0.694013000	9.247400000	C	2.705313000 -3.021537000 2.102615000
H	15.515245000	1.580481000	10.764962000	H	2.223466000 -2.554068000 2.978655000
H	16.691712000	2.171112000	9.578999000	C	3.950869000 -2.196985000 1.757536000
C	12.729661000	1.617287000	4.734868000	H	4.664470000 -2.206234000 2.597696000
H	12.062760000	1.117377000	4.011725000	H	3.693864000 -1.150280000 1.539910000
C	13.156547000	2.965762000	4.144238000	H	4.457974000 -2.608836000 0.872063000
H	13.784863000	3.519726000	4.857826000	C	3.086650000 -4.460021000 2.461843000
H	12.287102000	3.597035000	3.904823000	H	3.614759000 -4.952187000 1.632385000
H	13.737055000	2.820922000	3.218358000	H	2.214561000 -5.073774000 2.729124000
C	13.945012000	0.716087000	4.965022000	H	3.767676000 -4.459787000 3.330078000
H	14.477282000	0.554944000	4.012084000	C	0.109054000 -4.066761000 1.093167000
H	13.666812000	-0.273107000	5.356782000	H	0.630311000 -5.033993000 1.200847000
H	14.653422000	1.177744000	5.667455000	C	-0.879420000 -4.156459000 -0.075258000
C	11.218801000	0.215254000	6.860370000	H	-1.664824000 -4.894221000 0.159913000
H	12.183053000	-0.315734000	6.944873000	H	-0.378274000 -4.470919000 -1.001334000
C	10.560183000	0.290761000	8.242603000	H	-1.350062000 -3.175634000 -0.253447000
H	9.651109000	0.912298000	8.194571000	C	-0.616372000 -3.732058000 2.402121000
H	11.236621000	0.734070000	8.986084000	H	-1.117574000 -2.755783000 2.320606000
H	10.290701000	-0.723920000	8.580953000	H	0.064239000 -3.693875000 3.265648000
C	10.320892000	-0.535811000	5.869778000	H	-1.386121000 -4.492686000 2.612526000
H	10.125469000	-1.557246000	6.235635000	C	2.089004000 -0.221503000 -2.819137000
H	10.769720000	-0.620343000	4.868474000	C	3.151714000 0.716059000 -2.901516000
H	9.354421000	-0.019189000	5.774723000	C	3.245512000 1.560643000 -4.013641000
C	11.217022000	6.068407000	7.691436000	H	4.074321000 2.275112000 -4.063856000
C	11.637825000	7.155465000	6.881440000	C	2.319158000 1.510698000 -5.064315000
C	11.382780000	8.466934000	7.297908000	C	1.284801000 0.570314000 -4.977376000
H	11.721832000	9.296535000	6.668163000	H	0.555012000 0.502536000 -5.791553000
C	10.716003000	8.745246000	8.497461000	C	1.151824000 -0.298106000 -3.886213000
C	10.300975000	7.663232000	9.282634000	C	4.185110000 0.775030000 -1.808194000
H	9.771344000	7.857028000	10.221330000	H	4.984552000 1.485560000 -2.061459000
C	10.532684000	6.333838000	8.909791000	H	4.630352000 -0.214537000 -1.627678000
C	12.384523000	6.892316000	5.598365000	H	3.731460000 1.090972000 -0.853141000
H	12.721084000	7.834232000	5.142843000	C	2.415529000 2.459485000 -6.234181000
H	11.757719000	6.365535000	4.859013000	H	3.461939000 2.714807000 -6.459123000
H	13.259104000	6.248192000	5.7711335000	H	1.886583000 3.406581000 -6.031683000
C	10.416008000	10.164538000	8.910452000	H	1.968059000 2.025015000 -7.140250000
H	11.142690000	10.870126000	8.481492000	C	0.055590000 -1.329743000 -3.855079000
H	10.434015000	10.277210000	10.004700000	H	-0.657464000 -1.165975000 -4.675242000
H	9.414041000	10.475299000	8.569108000	H	-0.486245000 -1.315297000 -2.894762000
C	10.093567000	5.202227000	9.802915000	H	0.473400000 -2.344127000 -3.959620000
H	9.437766000	5.573591000	10.602424000	C	-0.733672000 3.019796000 1.501141000
H	10.964120000	4.711433000	10.268109000	C	-1.059383000 3.783067000 2.658250000
H	9.559313000	4.418207000	9.242055000	H	-0.791715000 3.384183000 3.639769000
				C	-1.703076000 5.010963000 2.554521000
				H	-1.937897000 5.563733000 3.470822000

C	-2.067826000	5.556736000	1.310329000	C	3.880798000	-6.649373000	-1.849701000
C	-1.738717000	4.812686000	0.167456000	H	3.345187000	-7.271418000	-1.117381000
H	-2.031447000	5.211538000	-0.807942000	H	4.960966000	-6.781006000	-1.662981000
C	-1.075981000	3.580564000	0.230313000	H	3.676297000	-7.062916000	-2.850504000
C	-2.793074000	6.876439000	1.211890000	C	2.360179000	-2.803949000	2.346552000
H	-3.785129000	6.839692000	1.693538000	H	1.779241000	-2.248298000	3.101598000
H	-2.949018000	7.162712000	0.161424000	C	3.645668000	-2.017105000	2.063523000
H	-2.231814000	7.692521000	1.697214000	H	4.231510000	-1.902401000	2.989449000
C	0.478767000	3.641917000	-2.305716000	H	3.431560000	-1.013239000	1.672838000
H	0.806560000	2.936812000	-3.089197000	H	4.266964000	-2.540789000	1.321970000
C	1.716417000	4.042139000	-1.494927000	C	2.686748000	-4.196433000	2.892630000
H	2.462876000	4.523474000	-2.147444000	H	3.270098000	-4.782090000	2.166574000
H	2.185068000	3.163785000	-1.026583000	H	1.786556000	-4.769688000	3.155829000
H	1.448271000	4.748852000	-0.694880000	H	3.298212000	-4.103832000	3.806345000
C	-0.145984000	4.865004000	-2.984119000	C	-0.024031000	-4.079303000	1.087330000
H	-0.427895000	5.631874000	-2.248045000	H	0.513680000	-5.010870000	1.334608000
H	-1.035474000	4.613253000	-3.578806000	C	-0.847528000	-4.296675000	-0.188305000
H	0.587851000	5.324785000	-3.668103000	H	-1.608638000	-5.074584000	-0.010428000
C	-2.261501000	2.497992000	-2.178232000	H	-0.216741000	-4.620441000	-1.027767000
H	-2.556105000	3.546276000	-2.361137000	H	-1.360631000	-3.363980000	-0.473524000
C	-3.341403000	1.815406000	-1.330721000	C	-0.934840000	-3.691265000	2.258971000
H	-4.280152000	1.751036000	-1.906446000	H	-1.482054000	-2.767069000	2.021643000
H	-3.542519000	2.377801000	-0.408299000	H	-0.379975000	-3.529306000	3.194630000
H	-3.020683000	0.798745000	-1.050333000	H	-1.676809000	-4.486590000	2.438016000
C	-2.089227000	1.780687000	-3.520646000	C	2.309979000	-0.256058000	-2.516016000
H	-1.808200000	0.730978000	-3.357065000	C	3.430617000	0.565179000	-2.796258000
H	-1.320533000	2.241946000	-4.157289000	C	3.367810000	1.473452000	-3.858260000
H	-3.041214000	1.790702000	-4.076990000	H	4.241871000	2.095107000	-4.078544000
C	0.128079000	1.061138000	2.686571000	C	2.205666000	1.609005000	-4.643151000
C	-0.927324000	0.418919000	3.409144000	C	1.098027000	0.814642000	-4.344798000
C	-0.607928000	-0.396839000	4.496150000	H	0.199421000	0.896411000	-4.964204000
H	-1.424707000	-0.880029000	5.042854000	C	1.108047000	-0.132762000	-3.293023000
C	0.722358000	-0.647815000	4.887262000	C	4.675843000	0.433409000	-1.959756000
C	1.745843000	-0.052241000	4.148763000	H	5.420357000	1.191511000	-2.240374000
H	2.787445000	-0.227415000	4.438604000	H	5.133578000	-0.562724000	-2.071240000
C	1.482982000	0.795501000	3.057136000	H	4.443107000	0.543678000	-0.889004000
C	-2.357863000	0.610146000	2.983277000	C	2.159804000	2.611046000	-5.771545000
H	-2.683681000	1.654968000	3.108521000	H	3.067671000	2.560124000	-6.393273000
H	-3.025562000	-0.036186000	3.569851000	H	2.087840000	3.645104000	-5.392641000
C	1.020865000	-1.570305000	6.042235000	H	1.291701000	2.437448000	-6.423510000
H	2.081018000	-1.520669000	6.329321000	C	-0.042389000	-1.016020000	-2.993114000
H	0.793735000	-2.620765000	5.790559000	H	-0.833397000	-0.916425000	-3.750112000
H	0.416678000	-1.317614000	6.928116000	H	-0.924568000	-0.949088000	-1.868378000
C	2.605020000	1.550535000	2.389206000	H	0.254636000	-2.072883000	-2.914717000
H	3.582749000	1.151699000	2.693359000	C	-0.572243000	2.783286000	1.519891000
H	2.567961000	2.621124000	2.651560000	C	-0.787779000	3.469278000	2.754086000
H	2.552225000	1.534878000	1.281544000	H	-0.422936000	3.012477000	3.676331000
C				C	-1.455621000	4.686347000	2.814159000
H				H	-1.596827000	5.161965000	3.791065000
C				C	-1.962509000	5.312135000	1.662115000
C				C	-1.740177000	4.657329000	0.444029000

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UC44P2N3H62			
U	0.297708000	-0.073750000	-0.426213000
P	1.257527000	-2.732136000	0.809483000
P	-0.752045000	2.592603000	-1.262891000
N	2.264406000	-1.141254000	-1.417433000
N	0.060141000	1.5669855000	1.439134000
N	-1.452418000	-0.794969000	-0.589992000
H	-2.035178000	-0.184101000	1.890179000
C	2.672987000	-2.441830000	-1.545425000
C	3.413249000	-2.934883000	-2.658351000
H	3.662095000	-2.242524000	-3.465783000
C	3.788975000	-4.270123000	-2.744694000
H	4.347396000	-4.604792000	-3.625854000
C	3.459278000	-5.204442000	-1.746121000
C	2.716328000	-4.730464000	-0.655316000
H	2.408468000	-5.448894000	0.110814000
C	2.319675000	-3.392748000	-0.534062000

C	-3.493474000	1.974998000	-1.305342000	C	-0.430514000	-4.393176000	0.568140000
H	-4.462048000	2.011588000	-1.832081000	H	-1.086293000	-3.541426000	0.337647000
H	-3.627176000	2.420985000	-0.310006000	H	-0.384226000	-4.497936000	1.662264000
H	-3.199086000	0.921794000	-1.167072000	H	-0.896549000	-5.306514000	0.162663000
C	-2.360902000	2.204082000	-3.552816000	C	3.800455000	0.999898000	-0.641055000
H	-2.087404000	1.139150000	-3.558399000	C	4.438735000	1.798347000	0.345339000
H	-1.626358000	2.747016000	-4.165285000	C	5.055056000	2.997495000	-0.029523000
H	-3.345162000	2.301384000	-4.040259000	H	5.553822000	3.595680000	0.740562000
C	0.422469000	0.940808000	2.654924000	C	5.059052000	3.447656000	-1.356256000
C	-0.528401000	0.195465000	3.404514000	C	4.419759000	2.655703000	-2.316324000
C	-0.121765000	-0.429266000	4.591235000	H	4.417527000	2.981626000	-3.362328000
H	-0.861740000	-1.001312000	5.161353000	C	3.794717000	1.443440000	-1.991140000
C	1.190388000	-0.338466000	5.073009000	C	4.489939000	1.329114000	1.775138000
C	2.111958000	0.408902000	4.328054000	H	5.044266000	2.042707000	2.400597000
H	3.141314000	0.504957000	4.689628000	H	4.973708000	0.343836000	1.849903000
C	1.754745000	1.044257000	3.132823000	H	3.481802000	1.208841000	2.199849000
C	-1.961249000	0.117583000	2.948247000	C	5.699970000	4.761377000	-1.729581000
H	-2.446038000	1.104449000	3.023437000	H	6.576895000	4.973590000	-1.100008000
H	-2.528179000	-0.593051000	3.566085000	H	4.996975000	5.602127000	-1.600811000
C	1.607518000	-1.052594000	6.335531000	H	6.024044000	4.765132000	-2.780583000
H	2.406761000	-0.507744000	6.859478000	C	3.185556000	0.587841000	-3.071538000
H	1.991833000	-2.063980000	6.118198000	H	3.106041000	1.148093000	-4.014142000
H	0.761366000	-1.168466000	7.028500000	H	2.188418000	0.211388000	-2.788613000
C	2.757069000	1.874468000	2.373645000	H	3.806760000	-0.304712000	-3.252794000
H	3.737555000	1.857301000	2.869710000	C	-0.969719000	2.864584000	1.445747000
H	2.420363000	2.918892000	2.289910000	C	-1.748801000	3.336191000	2.540237000
H	2.884438000	1.516364000	1.339164000	H	-1.614359000	2.866756000	3.516745000
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3v							
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112				H	-2.402507000	4.883513000	-0.948561000
UC44P2N3H62				C	-1.232143000	3.457709000	0.168892000
U	0.720869000	0.117261000	0.015784000	C	-3.957200000	6.045681000	0.971396000
P	1.766951000	-2.642332000	0.657588000	H	-4.875527000	5.838570000	1.543674000
P	-0.292376000	2.719795000	-1.220886000	H	-4.243359000	6.173454000	-0.083300000
N	3.192052000	-0.228236000	-0.275578000	H	-3.571340000	7.018363000	1.324456000
N	-0.042906000	1.854733000	1.540035000	C	0.867695000	4.119981000	-1.765279000
N	0.014511000	-0.667659000	-1.661041000	H	1.536728000	3.632865000	-2.495417000
H	-0.392711000	-1.032781000	-2.529184000	C	1.714308000	4.545421000	-0.560544000
C	3.958625000	-1.360233000	-0.444932000	H	2.472606000	5.281458000	-0.871454000
C	5.296564000	-1.338408000	-0.943417000	H	2.240417000	3.694478000	-0.108849000
H	5.751706000	-0.376555000	-1.187010000	H	1.082824000	5.007317000	0.212837000
C	6.028431000	-2.505122000	-1.135310000	C	0.213768000	5.337842000	-2.423639000
H	7.048164000	-2.427152000	-1.528613000	H	-0.450141000	5.859479000	-1.718554000
C	5.498160000	-3.773292000	-0.846206000	H	-0.368848000	5.078243000	-3.318976000
C	4.199341000	-3.803378000	-0.319012000	H	0.992799000	6.055403000	-2.732740000
H	3.764863000	-4.778022000	-0.076643000	C	-1.542006000	2.612731000	-2.622006000
C	3.437175000	-2.649158000	-0.099989000	H	-1.962776000	3.619056000	-2.789702000
C	6.276540000	-5.038439000	-1.110409000	C	-2.676185000	1.658569000	-2.228998000
H	5.849055000	-5.890092000	-0.560261000	H	-3.398018000	1.567745000	-3.057972000
H	7.330392000	-4.939003000	-0.804514000	H	-3.215495000	2.017989000	-1.341637000
H	6.277333000	-5.310172000	-2.180834000	H	-2.271069000	0.659483000	-2.005257000
C	2.103075000	-3.149164000	2.457565000	C	-0.836576000	2.140159000	-3.899771000
H	1.110694000	-3.052279000	2.929237000	H	-0.350509000	1.168446000	-3.723762000
C	3.024262000	-2.108600000	3.103265000	H	-0.067714000	2.849525000	-4.240405000
H	3.156010000	-2.332904000	4.174136000	H	-1.567315000	2.019155000	-4.716320000
H	2.609523000	-1.094976000	3.023811000	C	0.081236000	1.120716000	2.746262000
H	4.016411000	-2.116813000	2.627379000	C	-0.494377000	-0.197804000	2.755526000
C	2.632584000	-4.565197000	2.698620000	C	-0.326118000	-0.969389000	3.936766000
H	3.626220000	-4.701148000	2.246572000	H	-0.792524000	-1.959403000	3.977994000
H	1.963808000	-5.343862000	2.304472000	C	0.364220000	-0.496329000	5.049536000
H	2.738165000	-4.740923000	3.782704000	C	0.933400000	0.790740000	5.000586000
C	0.953032000	-4.185131000	-0.060055000	H	1.493395000	1.167572000	5.862757000
H	1.592129000	-5.047828000	0.194855000	C	0.802867000	1.601651000	3.866915000
C	0.853534000	-4.081011000	-1.585092000	C	-1.124202000	-0.706169000	1.551006000
H	0.328114000	-4.962941000	-1.988536000	H	-1.787330000	0.015241000	1.037791000
H	1.847003000	-4.026964000	-2.050721000	H	-1.599522000	-1.687130000	1.648380000
H	0.300429000	-3.172891000	-1.866890000	C	0.524675000	-1.352011000	6.283501000

H	0.277416000	-0.791683000	7.199125000	C	2.803608000	0.061761000	-3.464011000
H	1.563422000	-1.706633000	6.393643000	H	2.644032000	0.383471000	-4.502728000
H	-0.125669000	-2.237420000	6.240904000	H	1.832642000	-0.212453000	-3.016503000
C	1.417624000	2.976829000	3.833864000	H	3.405551000	-0.860687000	-3.470924000
H	2.129239000	3.108125000	4.661238000	C	-1.141420000	2.853565000	1.486231000
H	0.649896000	3.764232000	3.911788000	C	-2.089262000	3.244428000	2.468990000
H	1.938806000	3.152625000	2.881008000	H	-2.107183000	2.708569000	3.421002000
				C	-2.993236000	4.276405000	2.224054000
				H	-3.712466000	4.546177000	3.005088000
⁵v-TS				C	-3.016118000	4.971560000	1.003492000
				C	-2.096527000	4.569651000	0.019885000
112				H	-2.129303000	5.068994000	-0.953573000
UC44P2N3H62				C	-1.176994000	3.535180000	0.229758000
U	0.859776000	0.197180000	0.321986000	C	-3.975886000	6.110993000	0.762280000
P	1.960778000	-2.498334000	0.883098000	H	-4.948811000	5.929232000	1.245101000
P	0.014300000	2.882821000	-1.008551000	H	-4.158639000	6.258258000	-0.312966000
N	3.146439000	-0.170890000	-0.591757000	H	-3.592689000	7.067656000	1.159717000
N	-0.215353000	1.859813000	1.657372000	C	1.277756000	4.292249000	-1.177580000
N	-0.930368000	-0.747447000	-0.401219000	H	2.083729000	3.842598000	-1.780793000
H	-1.590838000	-1.331751000	-0.918664000	C	1.845494000	4.609129000	0.211502000
C	3.957613000	-1.288556000	-0.642653000	H	2.698557000	5.300725000	0.122038000
C	5.220495000	-1.302569000	-1.304439000	H	2.195456000	3.704694000	0.726883000
H	5.576832000	-0.383898000	-1.773932000	H	1.080871000	5.080943000	0.846451000
C	6.002420000	-2.452815000	-1.383798000	C	0.797727000	5.574945000	-1.862625000
H	6.959934000	-2.403184000	-1.913964000	H	-0.011603000	6.053107000	-1.290539000
C	5.589007000	-3.667689000	-0.815098000	H	0.441361000	5.403460000	-2.888217000
C	4.3611199000	-3.659770000	-0.139018000	H	1.629401000	6.298209000	-1.920685000
H	4.016614000	-4.597162000	0.306042000	C	-0.954304000	2.976064000	-2.625442000
C	3.555478000	-2.514829000	-0.019470000	H	-1.294914000	4.017315000	-2.756013000
C	6.435738000	-4.913614000	-0.904567000	C	-2.181753000	2.060455000	-2.555118000
H	5.879772000	-5.795346000	-0.552832000	H	-2.712338000	2.064028000	-3.522131000
H	7.351088000	-4.837411000	-0.291863000	H	-2.882897000	2.387906000	-1.775375000
H	6.759574000	-5.115554000	-1.938889000	H	-1.882572000	1.027199000	-2.320221000
C	2.410666000	-2.968186000	2.674356000	C	-0.051948000	2.598423000	-3.805467000
H	1.430885000	-2.902686000	3.178089000	H	0.301739000	1.561598000	-3.705750000
C	3.302107000	-1.862671000	3.251472000	H	0.834386000	3.244003000	-3.884164000
H	3.479254000	-2.032238000	4.326251000	H	-0.612187000	2.673109000	-4.752213000
H	2.836655000	-0.871807000	3.139878000	C	-0.300565000	0.898055000	2.679914000
H	4.277634000	-1.841211000	2.741385000	C	-0.947204000	-0.352357000	2.334493000
C	3.013401000	-4.350022000	2.942970000	C	-0.935095000	-1.400750000	3.301149000
H	4.022659000	-4.434958000	2.514989000	H	-1.443438000	-2.339516000	3.060754000
H	2.398491000	-5.168250000	2.540239000	C	-0.350519000	-1.244951000	4.550691000
H	3.104131000	-4.513461000	4.030896000	C	0.292203000	-0.015610000	4.858214000
C	1.120615000	-4.073182000	0.248818000	H	0.774437000	0.108051000	5.833103000
H	1.809696000	-4.915325000	0.433007000	C	0.344724000	1.036588000	3.938214000
C	0.886492000	-3.955858000	-1.260943000	C	-1.781441000	-0.452521000	1.102950000
H	0.390124000	-4.8644483000	-1.642148000	H	-2.366108000	0.454446000	0.911221000
H	1.831869000	-3.823959000	-1.804752000	H	-2.432589000	-1.332632000	1.158515000
H	0.244510000	-3.088944000	-1.480779000	C	-0.366464000	-2.358652000	5.567032000
C	-0.194604000	-4.334127000	0.988895000	H	-0.799437000	-2.024512000	6.525063000
H	-0.881792000	-3.486945000	0.845437000	H	0.652535000	-2.721226000	5.789220000
H	-0.047452000	-4.472761000	2.069711000	H	-0.956087000	-3.215752000	5.211062000
H	-0.682365000	-5.241867000	0.595117000	C	1.049435000	2.325249000	4.266457000
C	3.637820000	0.981903000	-1.257262000	H	1.576432000	2.251229000	5.228107000
C	4.336202000	1.982706000	-0.527901000	H	0.344532000	3.171039000	4.318871000
C	4.836368000	3.104912000	-1.199416000	H	1.777610000	2.583727000	3.481036000
H	5.376499000	3.864297000	-0.623557000				
C	4.677432000	3.278555000	-2.580695000				
C	3.996679000	2.277891000	-3.290828000				
H	3.869228000	2.383413000	-4.373816000				
C	3.481136000	1.138701000	-2.661669000				
C	4.574835000	1.802142000	0.946758000				
H	5.083998000	2.677567000	1.374124000				
H	5.186196000	0.907494000	1.141591000				
H	3.629320000	1.641087000	1.496402000				
C	5.192471000	4.515011000	-3.275256000				
H	6.126822000	4.874010000	-2.817643000				
H	4.465885000	5.344240000	-3.220309000				
H	5.387014000	4.323874000	-4.341043000				

C	2.803608000	0.061761000	-3.464011000
H	2.644032000	0.383471000	-4.502728000
H	1.832642000	-0.212453000	-3.016503000
H	3.405551000	-0.860687000	-3.470924000
C	-1.141420000	2.853565000	1.486231000
C	-2.089262000	3.244428000	2.468990000
H	-2.107183000	2.708569000	3.421002000
C	-2.993236000	4.276405000	2.224054000
H	-3.712466000	4.546177000	3.005088000
C	-3.016118000	4.971560000	1.003492000
C	-2.096527000	4.569651000	0.019885000
H	-2.129303000	5.068994000	-0.953573000
C	-1.176994000	3.535180000	0.229758000
C	-3.975886000	6.110993000	0.762280000
H	-4.948811000	5.929232000	1.245101000
H	-4.158639000	6.258258000	-0.312966000
H	-3.592689000	7.067656000	1.159717000
C	1.277756000	4.292249000	-1.177580000
H	2.083729000	3.842598000	-1.780793000
C	1.845494000	4.609129000	0.211502000
H	2.698557000	5.300725000	0.122038000
H	2.195456000	3.704694000	0.726883000
H	1.080871000	5.080943000	0.846451000
C	0.797727000	5.574945000	-1.862625000
H	-0.011603000	6.053107000	-1.290539000
H	0.441361000	5.403460000	-2.888217000
C	1.629401000	6.298209000	-1.920685000
C	-0.954304000	2.976064000	-2.625442000
H	-1.294914000	4.017315000	-2.756013000
C	-2.181753000	2.060455000	-2.555118000
H	-2.712338000	2.064028000	-3.522131000
H	-2.882897000	2.387906000	-1.775375000
H	-1.882572000	1.027199000	-2.320221000
C	-0.051948000	2.598423000	-3.805467000
H	0.301739000	1.561598000	-3.705750000
H	0.834386000	3.244003000	-3.884164000
H	-0.612187000	2.673109000	-4.752213000
C	-0.300565000	0.898055000	2.679914000
C	-0.947204000	-0.352357000	2.334493000
C	-0.935095000	-1.400750000	3.301149000
H	-1.443438000	-2.339516000	3.060754000
C	-0.350519000	-1.244951000	4.550691000
C	0.292203000	-0.015610000	4.858214000
C	0.774437000	0.108051000	5.833103000
C	0.344724000	1.036588000	3.938214000
C	-1.781441000	-0.452521000	1.102950000
H	-2.366108000	0.454446000	0.911221000
H	-2.432589000	-1.332632000	1.158515000
C	-0.366464000	-2.358652000	5.567032000
H	-0.799437000	-2.024512000	6.525063000
H	0.652535000	-2.721226000	5.789220000
H	-0.956087000	-3.215752000	5.211062000
C	1.049435000	2.325249000	4.266457000
H	1.576432000	2.251229000	5.228107000
H	0.344532000	3.171039000	4.318871000
H	1.777610000	2.583727000	3.481036000

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UC44P2N3H62			
U	0.906469000	0.173283000	-0.002569000
P	2.141737000	-2.292269000	1.01858

C	4.121087000	-1.260045000	-0.627783000	H	2.859055000	5.011234000	0.525771000	
C	5.385819000	-1.312170000	-1.277377000	H	2.330955000	3.345997000	0.868589000	
H	5.682310000	-0.475456000	-1.913640000	H	1.263973000	4.708009000	1.269582000	
C	6.237621000	-2.407065000	-1.141651000	C	0.928312000	5.669533000	-1.321598000	
H	7.195795000	-2.401033000	-1.672719000	H	0.178563000	6.096542000	-0.639031000	
C	5.889474000	-3.519420000	-0.356164000	H	0.512699000	5.677411000	-2.339243000	
C	4.651662000	-3.471480000	0.298704000	H	1.799529000	6.346774000	-1.316897000	
H	4.358561000	-4.333363000	0.904959000	C	-0.960196000	3.278582000	-2.443163000	
C	3.774089000	-2.377324000	0.200900000	H	-1.293497000	4.329779000	-2.408506000	
C	6.810579000	-4.707045000	-0.219618000	C	-2.193216000	2.369113000	-2.480622000	
H	6.343505000	-5.501167000	0.381496000	H	-2.758952000	2.529725000	-3.413442000	
H	7.761496000	-4.437995000	0.271809000	H	-2.862734000	2.560676000	-1.631024000	
H	7.069649000	-5.141950000	-1.199694000	H	-1.893434000	1.309257000	-2.437776000	
C	2.480856000	-2.461703000	2.890308000	C	-0.085487000	3.069743000	-3.683050000	
H	1.474082000	-2.316185000	3.320403000	H	0.284531000	2.033370000	-3.721144000	
C	3.350911000	-1.282232000	3.334239000	H	0.790825000	3.733169000	-3.698963000	
H	3.428050000	-1.249813000	4.433513000	H	-0.670475000	3.255989000	-4.599129000	
H	2.925939000	-0.325160000	2.995252000	C	-0.539226000	0.486531000	2.645518000	
H	4.366386000	-1.365743000	2.917487000	C	-1.371529000	-0.642468000	2.400582000	
C	3.055249000	-3.781649000	3.415025000	C	-1.580887000	-1.574361000	3.420083000	
H	4.086568000	-3.933884000	3.064584000	H	-2.220683000	-2.439654000	3.217438000	
H	2.458281000	-4.655385000	3.117036000	C	-0.988769000	-1.439902000	4.688399000	
H	3.084821000	-3.766065000	4.518595000	C	-0.169059000	-0.324981000	4.911637000	
C	1.398236000	-3.992165000	0.610714000	H	0.308397000	-0.202028000	5.890238000	
H	2.126504000	-4.758450000	0.927493000	C	0.063755000	0.640046000	3.925887000	
C	1.206990000	-4.103570000	-0.905252000	C	-2.042359000	-0.821355000	1.045120000	
H	0.806456000	-5.096817000	-1.170636000	H	-2.755462000	0.017941000	0.899697000	
H	2.153491000	-3.956492000	-1.443557000	H	-2.653684000	-1.741855000	1.102847000	
H	0.491280000	-3.344568000	-1.259332000	C	-1.252612000	-2.449440000	5.777362000	
C	0.074576000	-4.216573000	1.346235000	H	-2.270585000	-2.343044000	6.191893000	
H	-0.644123000	-3.428043000	1.077496000	H	-0.544539000	-2.332296000	6.610367000	
H	0.192423000	-4.202379000	2.439152000	H	-1.166355000	-3.481878000	5.403810000	
H	-0.360141000	-5.191029000	1.065576000	C	0.958206000	1.818410000	4.190469000	
C	3.671844000	0.914732000	-1.505282000	H	1.373329000	1.778206000	5.207368000	
C	4.475288000	1.910817000	-0.878876000	H	0.420529000	2.771274000	4.067220000	
C	4.875492000	3.035065000	-1.607078000	H	1.793926000	1.844251000	3.469551000	
H	5.489035000	3.792841000	-1.107277000	<hr/> <hr/> <hr/> <hr/> <hr/>				
C	4.515663000	3.220504000	-2.951654000	<hr/> <hr/> <hr/> <hr/> <hr/>				
C	3.740012000	2.227157000	-3.561084000	<hr/> <hr/> <hr/> <hr/> <hr/>				
H	3.459932000	2.340134000	-4.614019000	<hr/> <hr/> <hr/> <hr/> <hr/>				
C	3.320583000	1.080401000	-2.872850000	112				
C	4.908824000	1.732483000	0.550575000	UC44P2N3H62				
H	5.408904000	2.635481000	0.927471000	U	0.793447000	0.173632000	0.072132000	
H	5.599322000	0.880056000	0.650335000	P	1.780888000	-2.621800000	0.775320000	
H	4.048449000	1.501395000	1.200337000	P	-0.253491000	2.699725000	-1.252493000	
C	4.944562000	4.455453000	-3.705305000	N	3.114145000	-0.205626000	-0.301507000	
H	6.028165000	4.631838000	-3.610655000	N	0.036908000	1.856463000	1.489973000	
H	4.438396000	5.359360000	-3.326721000	N	0.128664000	-0.696846000	-1.537708000	
H	4.709201000	4.369271000	-4.775803000	H	-0.215864000	-1.166939000	-2.382340000	
C	2.532461000	0.009929000	-3.575766000	C	3.886651000	-1.349503000	-0.494101000	
H	2.399951000	0.250701000	-4.640429000	C	5.187836000	-1.317712000	-1.061301000	
H	1.526436000	-0.108280000	-3.121211000	H	5.624229000	-0.355952000	-1.334970000	
H	3.024311000	-0.970165000	-3.487651000	C	5.911529000	-2.483113000	-1.288537000	
C	-1.163261000	2.545626000	1.586839000	H	6.906109000	-2.405662000	-1.738224000	
C	-2.090125000	2.867377000	2.619356000	C	5.398435000	-3.749485000	-0.965201000	
H	-2.168966000	2.201345000	3.480707000	C	4.134408000	-3.783462000	-0.363847000	
C	-2.901201000	3.995713000	2.543087000	H	3.722054000	-4.757486000	-0.088085000	
H	-3.597345000	4.200619000	3.363898000	C	3.385095000	-2.626418000	-0.108862000	
C	-2.861515000	4.867970000	1.442821000	C	6.170699000	-5.011130000	-1.256668000	
C	-1.968589000	4.542801000	0.410155000	H	5.717329000	-5.880213000	-0.759731000	
H	-1.950676000	5.184341000	-0.476172000	H	7.214180000	-4.934413000	-0.914829000	
C	-1.129845000	3.421682000	0.457071000	H	6.200891000	-5.227431000	-2.337158000	
C	-3.729088000	6.100915000	1.379493000	C	2.257382000	-3.050552000	2.557389000	
H	-4.754044000	5.895859000	1.727658000	H	1.291913000	-3.008343000	3.088178000	
H	-3.797189000	6.486223000	0.351109000	C	3.149982000	-1.942579000	3.125054000	
H	-3.334255000	6.918816000	2.007855000	H	3.372686000	-2.145226000	4.184198000	
C	1.359540000	4.272446000	-0.866247000	H	2.666023000	-0.958396000	3.070514000	
H	2.120589000	3.887159000	-1.565563000	H	4.105914000	-1.892293000	2.583537000	
C	1.989105000	4.334671000	0.531003000	C	2.890600000	-4.426411000	2.779640000	

H	3.862759000	-4.505442000	2.272468000	H	-1.006802000	-2.044940000	3.669686000
H	2.252460000	-5.253093000	2.437984000	C	0.191658000	-0.713977000	4.858727000
H	3.069322000	-4.575528000	3.856675000	C	0.841690000	0.540813000	4.900679000
C	0.921353000	-4.187424000	0.184706000	H	1.382813000	0.830923000	5.806185000
H	1.633119000	-5.011347000	0.359419000	C	0.814150000	1.418941000	3.819913000
C	0.613795000	-4.124163000	-1.313773000	C	-1.213892000	-0.606038000	1.333674000
H	0.181991000	-5.081799000	-1.644717000	H	-1.805542000	0.185687000	0.841653000
H	1.516730000	-3.930638000	-1.908309000	H	-1.723296000	-1.571295000	1.320650000
H	-0.110511000	-3.325685000	-1.524071000	C	0.243817000	-1.626169000	6.058279000
C	-0.347920000	-4.463060000	0.999798000	H	-0.151078000	-1.126105000	6.955971000
H	-1.081931000	-3.656543000	0.863887000	H	1.279893000	-1.922473000	6.287213000
H	-0.146439000	-4.565475000	2.075370000	H	-0.342259000	-2.540229000	5.894020000
H	-0.813367000	-5.400756000	0.658431000	C	1.493079000	2.760569000	3.895205000
C	3.716925000	1.031185000	-0.687002000	H	2.239255000	2.778765000	4.700465000
C	4.380386000	1.822711000	0.288789000	H	0.764949000	3.564191000	4.090149000
C	5.010672000	3.008101000	-0.102291000	H	1.982431000	3.013658000	2.944292000
H	5.531285000	3.601220000	0.655790000				
C	5.010277000	3.446129000	-1.433129000				
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H	4.354149000	2.969446000	-3.429892000				
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C	4.468232000	1.359099000	1.718454000				
H	5.018567000	2.086432000	2.329663000				
H	4.981206000	0.388405000	1.785893000				
H	3.475456000	1.215691000	2.169246000				
C	5.680197000	4.738740000	-1.823278000				
H	6.600049000	4.904103000	-1.244418000				
H	5.019755000	5.601142000	-1.633961000				
H	5.938510000	4.750789000	-2.891069000				
C	3.105101000	0.600659000	-3.124455000				
H	2.957777000	1.181830000	-4.044802000				
H	2.145019000	0.161194000	-2.816279000				
H	3.770614000	-0.245249000	-3.361590000				
C	-0.907118000	2.873478000	1.407459000				
C	-1.659445000	3.334765000	2.513565000				
H	-1.505922000	2.873480000	3.490445000				
C	-2.608804000	4.340429000	2.362315000				
H	-3.174847000	4.667245000	3.239660000				
C	-2.873195000	4.932088000	1.115760000				
C	-2.150139000	4.453596000	0.014604000				
H	-2.375317000	4.865459000	-0.972776000				
C	-1.182972000	3.447616000	0.136605000				
C	-3.893968000	6.032249000	0.971623000				
H	-4.815003000	5.803199000	1.528245000				
H	-4.166271000	6.189537000	-0.081342000				
H	-3.511886000	6.990513000	1.360217000				
C	0.886070000	4.084847000	-1.844450000				
H	1.569333000	3.577276000	-2.545878000				
C	1.711339000	4.585585000	-0.653606000				
H	2.462363000	5.311582000	-0.999434000				
H	2.243740000	3.769505000	-0.147999000				
H	1.067201000	5.086418000	0.083492000				
C	0.205372000	5.252130000	-2.565158000				
H	-0.473643000	5.795493000	-1.892415000				
H	-0.361493000	4.937927000	-3.452019000				
H	0.971589000	5.968842000	-2.901539000				
C	-1.521721000	2.500822000	-2.619139000				
H	-1.958076000	3.496617000	-2.804487000				
C	-2.637615000	1.548617000	-2.173440000				
H	-3.376784000	1.435625000	-2.981942000				
H	-3.161901000	1.924205000	-1.284131000				
H	-2.228717000	0.554052000	-1.940548000				
C	-0.838498000	2.006239000	-3.899930000				
H	-0.350346000	1.036189000	-3.725771000				
H	-0.077558000	2.708626000	-4.269102000				
H	-1.585815000	1.874026000	-4.697572000				
C	0.099154000	1.041069000	2.649237000				
C	-0.581134000	-0.224401000	2.576357000				
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C	3.225997000	1.060602000	-2.712439000	112			
C	4.733485000	1.755778000	0.744249000	UC44P2N3H62			
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H	5.364055000	0.864417000	0.885238000	P	2.576943000	-1.878997000	1.514525000
H	3.858089000	1.618224000	1.398229000	P	0.668361000	3.329382000	-0.169705000
C	5.012366000	4.337436000	-3.586603000	N	3.143569000	-0.339665000	-0.950554000
H	6.000793000	4.661295000	-3.231029000	N	-0.588099000	1.216630000	1.477172000
H	4.330840000	5.197714000	-3.479770000	N	-0.696239000	-0.695416000	-0.894829000
H	5.089642000	4.113304000	-4.659541000	H	-0.770321000	-1.137084000	-1.814412000
C	2.450096000	-0.016149000	-3.426499000	C	4.142194000	-1.262696000	-0.696682000
H	2.283174000	0.255329000	-4.477325000	C	5.257005000	-1.462476000	-1.553812000
H	1.470255000	-0.209224000	-2.959456000	H	5.339909000	-0.859927000	-2.460478000
H	2.994082000	-0.972683000	-3.397302000	C	6.230032000	-2.414518000	-1.272359000
C	-1.087448000	2.834554000	1.548786000	H	7.068722000	-2.531989000	-1.965636000
C	-1.999653000	3.201752000	2.568256000	C	6.158008000	-3.235973000	-0.134379000
H	-2.052532000	2.598325000	3.476930000	C	5.053683000	-3.055198000	0.706427000
C	-2.841634000	4.299133000	2.412410000	H	4.964041000	-3.704597000	1.580984000
H	-3.537171000	4.550071000	3.219023000	C	4.060319000	-2.093777000	0.460783000
C	-2.833635000	5.081936000	1.245958000	C	7.226089000	-4.256645000	0.169150000
C	-1.951295000	4.699647000	0.224593000	H	6.900821000	-4.952131000	0.955754000
H	-1.964650000	5.268411000	-0.709281000	H	8.158152000	-3.780183000	0.515784000
C	-1.090024000	3.603061000	0.351187000	H	7.481439000	-4.852196000	-0.720678000
C	-3.732502000	6.284211000	1.100706000	C	3.198959000	-1.295353000	3.200653000
H	-4.732050000	6.093901000	1.519079000	H	2.272425000	-1.246358000	3.799420000
H	-3.856712000	6.565697000	0.045358000	C	3.747008000	0.129406000	3.051201000
H	-3.323545000	7.162351000	1.627841000	H	4.046793000	0.533514000	4.030899000
C	1.377931000	4.331273000	-1.035707000	H	2.997562000	0.818666000	2.627529000
H	2.143180000	3.893310000	-1.696991000	H	4.628032000	0.146005000	2.392435000
C	1.994464000	4.506341000	0.358369000	C	4.203793000	-2.197633000	3.920993000
H	2.874582000	5.164996000	0.299623000	H	5.159183000	-2.236856000	3.379266000
H	2.320249000	3.550728000	0.791143000	H	3.835024000	-3.225719000	4.044029000
H	1.271359000	4.960187000	1.051477000	H	4.409705000	-1.798114000	4.927187000
C	0.942517000	5.684953000	-1.603607000	C	2.025761000	-3.654239000	1.809638000
H	0.182766000	6.160695000	-0.966612000	H	2.924694000	-4.222034000	2.102522000
H	0.543316000	5.611862000	-2.624574000	C	1.492695000	-4.229843000	0.491947000
H	1.809717000	6.364402000	-1.638182000	H	1.200765000	-5.282695000	0.630421000
C	-0.944745000	3.200063000	-2.532009000	H	2.250015000	-4.188013000	-0.303265000
H	-1.264993000	4.254395000	-2.576254000	H	0.606831000	-3.670936000	0.152069000
C	-2.190798000	2.307777000	-2.489810000	C	0.985184000	-3.752472000	2.926476000
H	-2.758885000	2.412021000	-3.427591000	H	0.100054000	-3.141119000	2.701324000
H	-2.854477000	2.578201000	-1.657316000	H	1.380511000	-3.430366000	3.900045000
H	-1.908329000	1.250561000	-2.371422000	H	0.6526666000	-4.797275000	3.034044000
C	-0.083308000	2.893522000	-3.761726000	C	3.250828000	0.455524000	-2.122437000
H	0.244057000	1.843918000	-3.758454000	C	4.068180000	1.624339000	-2.125575000
H	0.814613000	3.524419000	-3.817777000	C	4.165035000	2.392808000	-3.286937000
H	-0.669008000	3.057466000	-4.679831000	H	4.810683000	3.276849000	-3.281448000
C	-0.380686000	0.760129000	2.603317000	C	3.461488000	2.066762000	-4.457218000
C	-1.052648000	-0.446531000	2.179288000	C	2.655751000	0.926547000	-4.438497000
C	-1.132112000	-1.534332000	3.094314000	H	2.111679000	0.643945000	-5.345303000
H	-1.661250000	-2.439619000	2.787755000	C	2.549111000	0.102233000	-3.305533000
C	-0.634709000	-1.437821000	4.386323000	C	4.866875000	1.988513000	-0.902698000
C	0.022955000	-0.245272000	4.774563000	H	5.352802000	2.965664000	-1.026347000
H	0.435194000	-0.173201000	5.785754000	H	5.647616000	1.237862000	-0.703409000
C	0.172130000	0.839758000	3.911109000	H	4.233943000	2.017191000	-0.002714000
C	-1.719765000	-0.474183000	0.883355000	C	3.554841000	2.940501000	-5.681956000
H	-2.205260000	0.453049000	0.578289000	H	4.586386000	3.280990000	-5.853655000
H	-2.321869000	-1.366549000	0.7076666000	H	2.929713000	3.842094000	-5.573721000
C	-0.784358000	-2.569389000	5.372099000	H	3.214797000	2.408646000	-6.580948000
H	-1.338639000	-2.245892000	6.266884000	C	1.790194000	-1.197432000	-3.415491000
H	0.195948000	-2.933545000	5.719549000	H	0.864587000	-1.071308000	-3.995525000
H	-1.323622000	-3.417959000	4.930252000	H	1.546774000	-1.620720000	-2.432111000
C	0.890333000	2.088987000	4.343052000	H	2.402428000	-1.950373000	-3.938062000
H	1.408396000	1.936666000	5.298850000	C	-1.196285000	2.446671000	1.689621000
H	0.194161000	2.934496000	4.458538000	C	-2.352264000	2.618825000	2.494943000
H	1.623373000	2.401554000	3.583649000	H	-2.796281000	1.745245000	2.975189000
				C	-2.942800000	3.866161000	2.663578000
				H	-3.833878000	3.946293000	3.293770000
⁴ viii				C	-2.438230000	5.016892000	2.035897000
				C	-1.321367000	4.846595000	1.209259000

H	-0.946292000	5.718249000	0.667747000	H	7.081944000	-4.973593000	-1.142314000
C	-0.691418000	3.605459000	1.029805000	H	6.055096000	-5.184889000	-2.567488000
C	-3.072549000	6.369372000	2.240932000	C	2.241067000	-3.093750000	2.506116000
H	-4.170475000	6.311722000	2.193875000	H	1.286534000	-3.050417000	3.056239000
H	-2.740271000	7.086220000	1.476702000	C	3.164779000	-2.015292000	3.078976000
H	-2.813825000	6.794529000	3.224923000	H	3.404913000	-2.250007000	4.126745000
C	2.085478000	4.476262000	0.326934000	H	2.698980000	-1.020905000	3.060474000
H	2.869836000	4.211573000	-0.403429000	H	4.111976000	-1.969746000	2.522644000
C	2.581230000	4.087227000	1.724990000	C	2.854115000	-4.486624000	2.677659000
H	3.484206000	4.661779000	1.983689000	H	3.812363000	-4.571715000	2.146343000
H	2.830885000	3.017683000	1.788073000	H	2.192863000	-5.294670000	2.337852000
H	1.813501000	4.297743000	2.484307000	H	3.056734000	-4.660562000	3.745742000
C	1.832833000	5.985068000	0.242007000	C	0.811678000	-4.164316000	0.150843000
H	1.124738000	6.314299000	1.014888000	H	1.534930000	-4.986705000	0.278228000
H	1.448545000	6.299556000	-0.737955000	C	0.436731000	-4.084687000	-1.331451000
H	2.777359000	6.525572000	0.414524000	H	0.073962000	-5.066591000	-1.670084000
C	-0.051960000	4.099483000	-1.730158000	H	1.290182000	-3.802607000	-1.962517000
H	-0.387879000	5.115091000	-1.461366000	H	-0.371723000	-3.358239000	-1.488504000
C	-1.275372000	3.283621000	-2.166839000	C	-0.414023000	-4.468258000	1.020656000
H	-1.723115000	3.729871000	-3.068487000	H	-1.172992000	-3.679032000	0.927954000
H	-2.044073000	3.253294000	-1.382867000	H	-0.164498000	-4.585768000	2.083840000
H	-0.994850000	2.246031000	-2.409575000	H	-0.876554000	-5.408592000	0.685735000
C	0.986457000	4.187692000	-2.849714000	C	3.641800000	1.035064000	-0.601196000
H	1.364556000	3.191697000	-3.121179000	C	4.290747000	1.797490000	0.411735000
H	1.850551000	4.809735000	-2.577153000	C	4.922711000	2.990984000	0.058065000
H	0.528624000	4.628791000	-3.749461000	H	5.435461000	3.563578000	0.835859000
C	-1.149312000	0.068123000	2.098943000	C	4.949277000	3.457736000	-1.264837000
C	-1.840695000	-0.887191000	1.305234000	C	4.305271000	2.694448000	-2.244792000
C	-2.414092000	-2.005652000	1.922213000	H	4.331845000	3.032115000	-3.284859000
H	-2.958203000	-2.725316000	1.302904000	C	3.651044000	1.491737000	-1.948644000
C	-2.332166000	-2.217463000	3.304146000	C	4.378143000	1.291919000	1.826437000
C	-1.612527000	-1.288135000	4.066347000	H	4.919426000	2.006076000	2.459217000
H	-1.515838000	-1.445260000	5.145456000	H	4.905007000	0.327412000	1.865214000
C	-1.005335000	-0.163801000	3.495957000	H	3.388890000	1.125642000	2.277649000
C	-1.996591000	-0.693206000	-0.197191000	C	5.645316000	4.746071000	-1.611144000
H	-2.548722000	0.250535000	-0.377602000	H	6.609013000	4.830708000	-1.089538000
H	-2.636324000	-1.509368000	-0.571366000	H	5.039167000	5.614055000	-1.305386000
C	-2.950609000	-3.434878000	3.942937000	H	5.826784000	4.829786000	-2.690342000
H	-3.225947000	-3.243086000	4.989371000	C	3.067485000	0.668564000	-3.066871000
H	-2.247832000	-4.284639000	3.939366000	H	2.859969000	1.294019000	-3.944675000
H	-3.852589000	-3.756129000	3.403291000	H	2.144850000	0.152020000	-2.768102000
C	-0.244317000	0.805417000	4.359889000	H	3.777633000	-0.114607000	-3.377400000
H	0.004991000	0.353929000	5.329528000	C	-0.904022000	2.865258000	1.353680000
H	-0.829018000	1.719819000	4.549442000	C	-1.652399000	3.326940000	2.456580000
H	0.682544000	1.134472000	3.867100000	H	-1.474275000	2.900864000	3.444724000
				C	-2.631507000	4.300471000	2.287098000
=====				H	-3.197869000	4.636864000	3.159325000
1ix				C	-2.923546000	4.846643000	1.025553000
=====				C	-2.196284000	4.362377000	-0.071582000
112				H	-2.441022000	4.742980000	-1.065945000
UC44P2N3H62				C	-1.197154000	3.391645000	0.071491000
U	0.869762000	0.218211000	0.123916000	C	-3.979085000	5.907636000	0.862524000
P	1.733397000	-2.636853000	0.742953000	H	-4.887513000	5.658669000	1.429514000
P	-0.239040000	2.660434000	-1.305188000	H	-4.259021000	6.039751000	-0.190888000
N	3.070899000	-0.235778000	-0.269776000	H	-3.622217000	6.880344000	1.236547000
N	0.073060000	1.8666691000	1.456924000	C	0.868539000	4.061247000	-1.907759000
N	0.182377000	-0.725661000	-1.394504000	H	1.584816000	3.557762000	-2.577858000
H	-0.175674000	-1.264891000	-2.192124000	C	1.642381000	4.631248000	-0.713192000
C	3.833993000	-1.382161000	-0.534233000	H	2.379531000	5.365481000	-1.068964000
C	5.116347000	-1.331491000	-1.124757000	H	2.183900000	3.853692000	-0.158078000
H	5.558986000	-0.364269000	-1.366601000	H	0.964541000	5.144866000	-0.016886000
C	5.816490000	-2.498926000	-1.410475000	C	0.154630000	5.173297000	-2.682598000
H	6.803670000	-2.421994000	-1.873598000	H	-0.563905000	5.709843000	-2.047082000
C	5.285106000	-3.768023000	-1.127813000	H	-0.370620000	4.808979000	-3.575074000
C	4.029925000	-3.813331000	-0.504996000	H	0.899827000	5.910048000	-3.019930000
H	3.612004000	-4.791774000	-0.258202000	C	-1.486999000	2.367145000	-2.668719000
C	3.310187000	-2.654055000	-0.188602000	H	-1.937052000	3.350140000	-2.885867000
C	6.035923000	-5.025256000	-1.477875000	C	-2.594012000	1.414363000	-2.203737000
H	5.574997000	-5.910648000	-1.020563000	H	-3.322673000	1.271981000	-3.015613000

H	-3.134618000	1.806813000	-1.331940000	H	0.113897000	-4.516474000	2.288741000
H	-2.182403000	0.428418000	-1.942540000	H	-0.405828000	-5.490018000	0.900359000
C	-0.784390000	1.853201000	-3.931368000	C	3.488414000	0.921419000	-1.250517000
H	-0.291073000	0.889175000	-3.740698000	C	4.217251000	1.919905000	-0.551482000
H	-0.027711000	2.555126000	-4.308820000	C	4.726449000	3.009704000	-1.264078000
H	-1.523781000	1.701222000	-4.731458000	H	5.311410000	3.762887000	-0.728817000
C	0.157440000	1.077529000	2.633393000	C	4.533321000	3.148788000	-2.646104000
C	-0.510398000	-0.192478000	2.577280000	C	3.798778000	2.159065000	-3.313562000
C	-0.412004000	-1.041917000	3.708897000	H	3.653618000	2.242208000	-4.394379000
H	-0.923085000	-2.007771000	3.682923000	C	3.277890000	1.041847000	-2.649885000
C	0.247990000	-0.641764000	4.863891000	C	4.520566000	1.765801000	0.917566000
C	0.887429000	0.621222000	4.886728000	H	5.100236000	2.620794000	1.287273000
H	1.416021000	0.928432000	5.793436000	H	5.095772000	0.847771000	1.108421000
C	0.865432000	1.487976000	3.798367000	H	3.609166000	1.696162000	1.535808000
C	-1.124573000	-0.580131000	1.324775000	C	5.087289000	4.336515000	-3.387943000
H	-1.742072000	0.190609000	0.832292000	H	6.027702000	4.685235000	-2.940162000
H	-1.584912000	-1.567889000	1.280986000	H	4.381188000	5.182552000	-3.361529000
C	0.288281000	-1.520876000	6.085535000	H	5.272744000	4.099648000	-4.443971000
H	-0.190998000	-1.023163000	6.942048000	C	2.599879000	-0.055308000	-3.427554000
H	1.325546000	-1.737105000	6.383821000	H	2.389548000	0.266381000	-4.455089000
H	-0.227927000	-2.474347000	5.916365000	H	1.659221000	-0.381149000	-2.958614000
C	1.525156000	2.838480000	3.863560000	H	3.244398000	-0.947076000	-3.476176000
H	2.310209000	2.855429000	4.630030000	C	-1.064858000	2.818207000	1.513758000
H	0.794382000	3.622232000	4.118295000	C	-1.966672000	3.172312000	2.539354000
H	1.960387000	3.121499000	2.895329000	H	-2.007243000	2.577732000	3.453603000
				C	-2.828091000	4.253711000	2.378300000
				H	-3.521187000	4.502428000	3.186143000
³ix-TS				C	-2.844363000	5.018176000	1.199690000
				C	-1.965739000	4.641061000	0.172597000
112				H	-1.998759000	5.197032000	-0.767330000
UC44P2N3H62				C	-1.080879000	3.565323000	0.310498000
U	0.974049000	0.256135000	0.223598000	C	-3.771328000	6.195182000	1.047038000
P	2.023265000	-2.549683000	0.970489000	H	-4.772207000	5.971539000	1.442791000
P	0.067475000	2.963646000	-0.984292000	H	-3.878156000	6.490145000	-0.005327000
N	3.067296000	-0.258516000	-0.555781000	H	-3.393969000	7.070472000	1.599613000
N	-0.206314000	1.722007000	1.578719000	C	1.343773000	4.343999000	-1.129496000
N	-0.352487000	-0.704036000	-0.918189000	H	2.135276000	3.892754000	-1.748990000
H	-1.054294000	-1.203934000	-1.474618000	C	1.926580000	4.639639000	0.258720000
C	3.964179000	-1.338059000	-0.581378000	H	2.788503000	5.316525000	0.164201000
C	5.213738000	-1.282615000	-1.241351000	H	2.273592000	3.730672000	0.769705000
H	5.518209000	-0.361262000	-1.739584000	H	1.181039000	5.127135000	0.902637000
C	6.056260000	-2.388364000	-1.276079000	C	0.861993000	5.634285000	-1.799650000
H	7.012186000	-2.306506000	-1.800345000	H	0.073864000	6.125912000	-1.211935000
C	5.705731000	-3.605162000	-0.667783000	H	0.489755000	5.475078000	-2.820205000
C	4.475706000	-3.652768000	-0.000709000	H	1.702667000	6.342561000	-1.865442000
H	4.183749000	-4.592626000	0.472381000	C	-0.943362000	3.040710000	-2.562089000
C	3.614889000	-2.546951000	0.068890000	H	-1.274645000	4.088077000	-2.657218000
C	6.618365000	-4.801910000	-0.730486000	C	-2.181411000	2.143296000	-2.462707000
H	6.188644000	-5.663441000	-0.202562000	H	-2.767136000	2.217560000	-3.391150000
H	7.596714000	-4.582325000	-0.276413000	H	-2.833760000	2.433799000	-1.628336000
H	6.808441000	-5.105575000	-1.771169000	H	-1.891670000	1.091248000	-2.326755000
C	2.499869000	-2.790466000	2.779127000	C	-0.084618000	2.680707000	-3.779313000
H	1.524752000	-2.776023000	3.292385000	H	0.247043000	1.633745000	-3.729769000
C	3.299360000	-1.566155000	3.244381000	H	0.807388000	3.315223000	-3.872478000
H	3.516971000	-1.641842000	4.320361000	H	-0.677288000	2.798586000	-4.698763000
H	2.745894000	-0.626737000	3.091062000	C	-0.297283000	0.768707000	2.601036000
H	4.259081000	-1.494029000	2.712278000	C	-0.896863000	-0.484607000	2.215531000
C	3.224118000	-4.090503000	3.138000000	C	-0.926087000	-1.548409000	3.160068000
H	4.230471000	-4.125256000	2.699222000	H	-1.383877000	-2.496646000	2.873055000
H	2.673721000	-4.986983000	2.821186000	C	-0.473277000	-1.366456000	4.458398000
H	3.343122000	-4.151011000	4.231005000	C	0.106382000	-0.122198000	4.809569000
C	1.248408000	-4.174889000	0.432518000	H	0.494457000	0.005799000	5.824259000
H	1.998731000	-4.947957000	0.668074000	C	0.219274000	0.940823000	3.915857000
C	1.013225000	-4.174390000	-1.082103000	C	-1.535700000	-0.583344000	0.923734000
H	0.594122000	-5.143059000	-1.392906000	H	-2.055294000	0.299815000	0.555079000
H	1.944998000	-4.013473000	-1.639904000	H	-2.017168000	-1.533199000	0.693249000
H	0.303061000	-3.385573000	-1.369027000	C	-0.588500000	-2.456230000	5.491433000
C	-0.035705000	-4.498265000	1.200181000	H	-1.242679000	-2.141959000	6.318675000
H	-0.826077000	-3.769655000	0.968690000	H	0.391535000	-2.691452000	5.933888000

H	-1.004734000	-3.377517000	5.064619000	H	1.778226000	-0.916987000	-2.678985000
C	0.862820000	2.236763000	4.324339000	H	3.015454000	-1.008816000	-3.924305000
H	1.482599000	2.103718000	5.219692000	C	-1.052105000	2.627015000	1.559378000
H	0.106987000	3.005395000	4.548358000	C	-1.986945000	2.888117000	2.584579000
H	1.484329000	2.644753000	3.514222000	H	-2.066516000	2.200782000	3.428132000
<hr/>				C	-2.819282000	4.001439000	2.526344000
<hr/>				H	-3.531357000	4.170688000	3.338442000
³ x				C	-2.775746000	4.903503000	1.450219000
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112				H	-1.847530000	5.293305000	-0.443410000
UC44P2N3H62				C	-1.008941000	3.516886000	0.458018000
U	1.138366000	0.353859000	0.164295000	C	-3.674154000	6.112007000	1.406111000
P	2.171209000	-2.373380000	1.129039000	H	-4.715329000	5.846885000	1.640537000
P	0.140055000	3.069346000	-0.891459000	H	-3.659660000	6.587988000	0.416553000
N	3.182021000	-0.290495000	-0.630084000	H	-3.360251000	6.867964000	2.143097000
N	-0.193270000	1.516517000	1.574294000	C	1.411621000	4.457719000	-0.947784000
N	-0.725301000	-0.637680000	-0.381390000	H	2.155566000	4.086238000	-1.672046000
H	-0.997388000	-1.104207000	-1.252447000	C	2.089947000	4.563773000	0.424408000
C	4.079801000	-1.366392000	-0.583244000	H	2.926374000	5.276932000	0.376772000
C	5.278143000	-1.403271000	-1.328263000	H	2.498464000	3.601092000	0.765815000
H	5.534427000	-0.564136000	-1.977258000	H	1.383379000	4.920233000	1.187377000
C	6.129022000	-2.502025000	-1.253353000	C	0.906620000	5.826951000	-1.412889000
H	7.047535000	-2.499723000	-1.846407000	H	0.193637000	6.258131000	-0.696592000
C	5.832083000	-3.615000000	-0.449570000	H	0.431318000	5.795005000	-2.402366000
C	4.638086000	-3.576346000	0.282573000	H	1.756620000	6.523579000	-1.481654000
H	4.379799000	-4.444020000	0.893625000	C	-0.898347000	3.270400000	-2.442585000
C	3.770317000	-2.475094000	0.241844000	H	-1.275923000	4.306100000	-2.419072000
C	6.765838000	-4.795000000	-0.374819000	C	-2.097092000	2.316151000	-2.413468000
H	6.293750000	-5.650522000	0.126244000	H	-2.710294000	2.463350000	-3.315032000
H	7.680432000	-4.544399000	0.185458000	H	-2.735731000	2.488736000	-1.537170000
H	7.081456000	-5.120160000	-1.376804000	H	-1.768769000	1.266030000	-2.394878000
C	2.576658000	-2.447756000	2.964544000	C	-0.058049000	3.081814000	-3.708954000
H	1.584742000	-2.341785000	3.437290000	H	0.335181000	2.056826000	-3.773192000
C	3.412576000	-1.213904000	3.330153000	H	0.794328000	3.772645000	-3.759988000
H	3.581438000	-1.177643000	4.416703000	H	-0.683250000	3.254423000	-4.597773000
H	2.911104000	-0.274403000	3.048818000	C	-0.494749000	0.455264000	2.481602000
H	4.394588000	-1.239368000	2.836057000	C	-1.316798000	-0.613229000	2.033875000
C	3.237078000	-3.731708000	3.473919000	C	-1.678634000	-1.614779000	2.942687000
H	4.256491000	-3.841313000	3.079250000	H	-2.337517000	-2.420462000	2.608805000
H	2.665769000	-4.634530000	3.218669000	C	-1.239653000	-1.601390000	4.271337000
H	3.315723000	-3.692990000	4.571411000	C	-0.387238000	-0.561849000	4.678816000
C	1.3865555000	-4.024841000	0.698187000	H	-0.028450000	-0.542614000	5.712173000
H	2.143179000	-4.782882000	0.961590000	C	-0.001186000	0.466192000	3.815530000
C	1.132054000	-4.099527000	-0.812139000	C	-1.832434000	-0.658343000	0.600010000
H	0.742028000	-5.093867000	-1.075943000	H	-2.518444000	0.193400000	0.431522000
H	2.048695000	-3.931810000	-1.393345000	H	-2.429735000	-1.576759000	0.485974000
H	0.381393000	-3.354632000	-1.117149000	C	-1.656098000	-2.675534000	5.241000000
C	0.109819000	-4.302251000	1.493030000	H	-2.097317000	-2.238439000	6.148685000
H	-0.672877000	-3.574805000	1.239741000	H	-0.791731000	-3.276109000	5.564928000
H	0.268121000	-4.266491000	2.579522000	H	-2.393084000	-3.356309000	4.796700000
H	-0.269250000	-5.304803000	1.243735000	C	0.851760000	1.602900000	4.310743000
C	3.505615000	0.814124000	-1.472434000	H	1.369009000	1.332460000	5.239672000
C	4.310626000	1.876449000	-0.967940000	H	0.237026000	2.494049000	4.513412000
C	4.658217000	2.924205000	-1.820837000	H	1.596239000	1.912075000	3.563342000
H	5.293181000	3.727890000	-1.436931000	<hr/>			
C	4.234648000	2.967067000	-3.160626000	² xi			
C	3.433975000	1.923559000	-3.632998000	<hr/>			
H	3.103089000	1.937676000	-4.675142000	112			
C	3.066325000	0.839042000	-2.822048000	UC44P2N3H62			
C	4.850393000	1.827468000	0.438213000	U	-0.008725000	-0.199433000	-0.263717000
H	5.341258000	2.771925000	0.703314000	P	0.789541000	-2.958973000	0.672659000
H	5.585395000	1.014837000	0.544940000	P	-1.135955000	2.369926000	-1.353705000
H	4.068014000	1.627233000	1.187346000	N	1.951474000	-1.044415000	-1.321626000
C	4.652904000	4.100534000	-4.059719000	N	0.244168000	1.649080000	1.200425000
H	5.740590000	4.083181000	-4.228625000	N	-1.590678000	-0.943239000	-0.696839000
H	4.416778000	5.077206000	-3.611482000	H	-1.157264000	-0.841969000	2.149051000
H	4.160336000	4.043219000	-5.038595000	C	2.422180000	-2.342708000	-1.497881000
C	2.314340000	-0.317908000	-3.429211000	C	3.361509000	-2.685261000	-2.506472000
H	1.602134000	0.023485000	-4.192208000				

H	3.756843000	-1.897799000	-3.150431000	H	1.011674000	4.505675000	-1.104658000
C	3.772831000	-3.998576000	-2.703500000	C	-0.979813000	4.723174000	-3.071263000
H	4.492398000	-4.210439000	-3.500275000	H	-1.168094000	5.428700000	-2.249436000
C	3.281828000	-5.055530000	-1.919699000	H	-1.939250000	4.478114000	-3.546982000
C	2.372822000	-4.721379000	-0.909306000	H	-0.367675000	5.251391000	-3.819916000
H	1.972367000	-5.527345000	-0.288898000	C	-2.904710000	2.317565000	-1.976587000
C	1.949001000	-3.405029000	-0.672780000	H	-3.216256000	3.361685000	-2.148379000
C	3.702124000	-6.482166000	-2.169054000	C	-3.834536000	1.683817000	-0.935905000
H	3.375783000	-7.142697000	-1.353661000	H	-4.863285000	1.660804000	-1.328878000
H	4.795654000	-6.571710000	-2.257303000	H	-3.842327000	2.253174000	0.003574000
H	3.270230000	-6.874170000	-3.104398000	H	-3.521572000	0.651209000	-0.720157000
C	1.762445000	-3.291149000	2.262090000	C	-2.959298000	1.550829000	-3.304435000
H	1.110380000	-2.869526000	3.046563000	H	-2.657533000	0.503878000	-3.151511000
C	3.056332000	-2.470482000	2.230712000	H	-2.313511000	1.993121000	-4.077294000
H	3.585191000	-2.565115000	3.191512000	H	-3.989559000	1.548983000	-3.692730000
H	2.861988000	-1.402767000	2.060500000	C	0.995391000	1.212745000	2.326355000
H	3.727076000	-2.829847000	1.436889000	C	0.424000000	0.268309000	3.216674000
C	2.051307000	-4.756332000	2.599751000	C	1.172325000	-0.176897000	4.314913000
H	2.712429000	-5.216555000	1.851686000	H	0.717070000	-0.888599000	5.010439000
H	1.139577000	-5.363973000	2.679967000	C	2.471706000	0.279464000	4.558324000
H	2.569592000	-4.812608000	3.570575000	C	3.018106000	1.216336000	3.669305000
C	-0.523133000	-4.300624000	0.635938000	H	4.029141000	1.594769000	3.849171000
H	-0.005257000	-5.256218000	0.823891000	C	2.309463000	1.696615000	2.563586000
C	-1.208369000	-4.368434000	-0.733199000	C	-1.003672000	-0.189611000	3.031628000
H	-1.978964000	-5.155463000	-0.718447000	H	-1.685076000	0.664526000	2.913410000
H	-0.493914000	-4.607094000	-1.532658000	H	-1.332946000	-0.782773000	3.895424000
H	-1.6906668000	-3.408917000	-0.972016000	C	3.272094000	-0.234461000	5.727655000
C	-1.544051000	-4.059174000	1.755142000	H	3.885206000	0.560539000	6.175425000
H	-2.087240000	-3.118340000	1.581057000	H	3.960467000	-1.036041000	5.413155000
H	-1.080073000	-4.016861000	2.751674000	H	2.620286000	-0.648008000	6.509305000
H	-2.285050000	-4.873432000	1.767561000	C	2.904970000	2.752315000	1.671988000
C	2.502506000	-0.036343000	-2.163411000	H	3.974306000	2.885272000	1.881354000
C	3.711548000	0.619401000	-1.811180000	H	2.401736000	3.720065000	1.825576000
C	4.226828000	1.599573000	-2.665572000	H	2.778521000	2.504383000	0.609201000
H	5.163311000	2.095397000	-2.391849000	=====	=====	=====	=====
C	3.594049000	1.948917000	-3.866655000	² xi-TS	=====	=====	=====
C	2.409531000	1.284518000	-4.202090000	=====	=====	=====	=====
H	1.912747000	1.523717000	-5.147497000	112	=====	=====	=====
C	1.849984000	0.299589000	-3.376735000	UC44P2N3H62	=====	=====	=====
C	4.464961000	0.213082000	-0.573182000	U	0.260565000	-0.116922000	-0.399283000
H	5.294566000	0.904194000	-0.374819000	P	1.127653000	-2.775542000	0.787261000
H	4.881278000	-0.800214000	-0.687856000	P	-0.794418000	2.584240000	-1.308340000
H	3.812907000	0.179795000	0.310317000	N	2.238281000	-1.049163000	-1.278687000
C	4.165929000	3.021443000	-4.758273000	N	0.099864000	1.527881000	1.321827000
H	5.264530000	2.984414000	-4.776407000	N	-1.502032000	-0.740208000	-0.578346000
H	3.881590000	4.025614000	-4.403074000	H	-1.990103000	-0.194605000	1.904561000
H	3.801521000	2.921791000	-5.789898000	C	2.698375000	-2.353178000	-1.434849000
C	0.623607000	-0.458645000	-3.824056000	C	3.536330000	-2.758527000	-2.501705000
H	0.262309000	-0.076291000	-4.788029000	C	3.839791000	-2.022484000	-3.248507000
H	-0.222666000	-0.397791000	-3.116702000	C	3.952482000	-4.080468000	-2.625428000
H	0.845604000	-1.530462000	-3.937363000	H	4.593561000	-4.354443000	-3.468627000
C	-0.449453000	2.852023000	1.300912000	C	3.561634000	-5.071421000	-1.709590000
C	-0.478700000	3.618428000	2.494591000	H	2.715821000	-4.676311000	-0.664495000
H	0.088455000	3.271122000	3.360116000	C	2.364072000	-5.438938000	0.035808000
C	-1.228736000	4.785389000	2.590076000	C	2.280008000	-3.353419000	-0.513244000
H	-1.225179000	5.336974000	3.535096000	C	4.031697000	-6.497166000	-1.849169000
C	-1.997527000	5.263248000	1.516214000	H	3.439684000	-7.176291000	-1.219961000
C	-1.961701000	4.517664000	0.332007000	H	5.087060000	-6.605651000	-1.549724000
H	-2.561324000	4.862909000	-0.514276000	H	3.954324000	-6.847215000	-2.889444000
C	-1.203836000	3.345212000	0.195843000	C	2.156266000	-2.864107000	2.370325000
C	-2.832983000	6.512403000	1.641123000	H	1.570298000	-2.272284000	3.092492000
H	-3.658910000	6.376814000	2.357858000	C	3.494729000	-2.151146000	2.136914000
H	-3.275793000	6.793143000	0.675507000	H	4.023021000	-2.027159000	3.094301000
H	-2.234614000	7.365385000	1.996786000	H	3.362621000	-1.154306000	1.695749000
C	-0.225750000	3.484188000	-2.581374000	H	4.136029000	-2.736567000	1.462695000
H	-0.048256000	2.814565000	-3.440477000	C	2.384387000	-4.266716000	2.941380000
C	1.135585000	3.865800000	-1.990343000	H	2.962594000	-4.893890000	2.247053000
H	1.724272000	4.424060000	-2.734135000	H	1.448009000	-4.787370000	3.183010000

H	2.968420000	-4.191283000	3.872847000	C	2.268653000	0.474233000	4.173680000
C	-0.162093000	-4.125035000	0.949530000	H	3.302786000	0.606203000	4.506262000
H	0.369830000	-5.054355000	1.213658000	C	1.872132000	1.050392000	2.961952000
C	-0.899881000	-4.329785000	-0.378599000	C	-1.849187000	0.093719000	2.957245000
H	-1.646064000	-5.131880000	-0.266393000	H	-2.340397000	1.072647000	3.077376000
H	-0.214287000	-4.615063000	-1.188233000	H	-2.372255000	-0.629926000	3.596240000
H	-1.429267000	-3.410065000	-0.670220000	C	1.836534000	-0.882771000	6.266730000
C	-1.143191000	-3.764604000	2.073020000	H	2.635600000	-0.295323000	6.740446000
H	-1.695500000	-2.848172000	1.818609000	H	2.237005000	-1.895147000	6.091324000
H	-0.643404000	-3.607633000	3.039667000	H	1.009006000	-0.979391000	6.983096000
H	-1.877592000	-4.574673000	2.201671000	C	2.847437000	1.864383000	2.151117000
C	2.292324000	-0.165047000	-2.386025000	H	3.810887000	1.949572000	2.670772000
C	3.407476000	0.672537000	-2.649058000	H	2.458616000	2.875195000	1.960477000
C	3.359907000	1.529226000	-3.749721000	H	3.037381000	1.413341000	1.163557000
H	4.227050000	2.160511000	-3.965877000				
C	2.232291000	1.600033000	-4.591721000				
C	1.128862000	0.799543000	-4.302341000				
H	0.251915000	0.837604000	-4.954183000				
C	1.125298000	-0.099826000	-3.212697000				
C	4.628439000	0.603840000	-1.7711677000				
H	5.343028000	1.396136000	-2.029699000				
H	5.138316000	-0.367119000	-1.870887000				
H	4.361326000	0.700250000	-0.708976000				
C	2.228624000	2.533399000	-5.776394000				
H	3.086822000	2.340081000	-6.437741000				
H	2.302523000	3.585062000	-5.456279000				
H	1.311379000	2.424969000	-6.370218000				
C	-0.025990000	-0.984658000	-2.910759000				
H	-0.797091000	-0.938265000	-3.690808000				
H	-1.012172000	-0.878764000	-1.833794000				
H	0.284746000	-2.030820000	-2.764890000				
C	-0.530581000	2.759887000	1.448161000				
C	-0.666854000	3.434619000	2.691278000				
H	-0.245017000	2.980855000	3.589571000				
C	-1.332525000	4.650637000	2.789841000				
H	-1.414482000	5.127944000	3.771142000				
C	-1.907746000	5.274739000	1.670158000				
C	-1.754097000	4.627195000	0.438993000				
H	-2.195312000	5.092650000	-0.445997000				
C	-1.073210000	3.408399000	0.302518000				
C	-2.662418000	6.574278000	1.793955000				
H	-3.610989000	6.442382000	2.339545000				
H	-2.905372000	6.989974000	0.806078000				
H	-2.078886000	7.330138000	2.342013000				
C	0.351785000	3.770679000	-2.231683000				
H	0.594890000	3.210829000	-3.149317000				
C	1.645876000	3.938605000	-1.425015000				
H	2.377426000	4.525320000	-2.001945000				
H	2.111744000	2.971530000	-1.189292000				
H	1.453252000	4.467923000	-0.480247000				
C	-0.226187000	5.133455000	-2.622714000				
H	-0.447198000	5.745132000	-1.736621000				
H	-1.141142000	5.051825000	-3.225848000				
H	0.513789000	5.686391000	-3.223782000				
C	-2.450068000	2.740852000	-2.183003000				
H	-2.687749000	3.817743000	-2.210234000				
C	-3.544395000	2.014949000	-1.392179000				
H	-4.503991000	2.100136000	-1.926206000				
H	-3.671650000	2.449110000	-0.391301000				
H	-3.301849000	0.948967000	-1.268970000				
C	-2.360603000	2.224136000	-3.623129000				
H	-2.126466000	1.149991000	-3.637939000				
H	-1.596842000	2.749798000	-4.213992000				
H	-3.328711000	2.360976000	-4.129435000				
C	0.526955000	0.908947000	2.533003000				
C	-0.394642000	0.185480000	3.337950000				
C	0.055014000	-0.381126000	4.538218000				
H	-0.661624000	-0.927328000	5.159428000				
C	1.377834000	-0.248132000	4.978174000				

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C	8.401728000	7.917233000	5.519263000	114			
H	8.588597000	8.981724000	5.714754000	UC44P2N5H62			
H	7.983398000	7.808191000	4.507896000	U	9.300718000	3.922078000	6.157086000
H	9.376382000	7.404608000	5.520576000	P	8.134859000	2.816241000	3.589576000
C	5.787513000	8.454550000	9.809493000	P	11.665325000	2.164028000	5.948804000
H	4.762876000	8.237641000	10.146075000	N	7.502684000	5.262624000	5.180899000
H	5.859177000	9.532012000	9.599142000	N	11.281844000	4.822870000	7.319638000
H	6.459679000	8.241938000	10.658050000	N	8.434488000	2.648871000	7.433452000
C	5.294158000	4.232865000	7.083760000	N	7.875555000	1.802130000	8.439070000
H	4.643350000	3.976174000	7.930182000	N	7.167739000	2.124586000	9.343182000
H	6.021862000	3.421055000	6.940941000	C	6.773663000	5.219647000	4.014960000
H	4.681192000	4.271088000	6.168872000	C	5.814425000	6.212093000	3.658713000
C	12.378597000	4.155839000	7.629088000	H	5.622476000	7.027010000	4.359262000
C	13.306597000	4.767954000	8.514005000	C	5.131695000	6.172462000	2.448432000
H	13.222484000	5.840104000	8.698211000	H	4.412785000	6.967140000	2.221460000
C	14.304137000	4.040898000	9.161082000	C	5.342934000	5.145184000	1.513694000
H	14.985672000	4.566187000	9.838462000	C	6.254400000	4.143877000	1.873404000
C	14.442671000	2.657628000	8.974053000	H	6.415396000	3.327801000	1.163912000
C	13.556899000	2.049283000	8.075322000	C	6.956234000	4.142708000	3.088882000
H	13.659364000	0.973731000	7.907671000	C	4.633768000	5.128025000	0.182049000
C	12.551355000	2.751755000	7.386353000	H	4.715647000	4.141898000	-0.298752000
C	15.487784000	1.859831000	9.714259000	H	5.053861000	5.869415000	-0.520076000
H	15.590017000	0.849942000	9.290185000	H	3.561766000	5.359305000	0.288252000
H	15.235692000	1.742794000	10.782307000	C	9.007170000	2.478965000	1.939974000
H	16.476988000	2.343364000	9.669292000	H	8.224951000	2.423111000	1.165586000
C	12.688234000	1.579655000	4.690678000	C	9.922688000	3.661791000	1.606643000
H	12.018540000	1.158051000	3.920875000	H	10.730300000	3.755570000	2.348764000
C	13.242212000	2.908554000	4.174239000	H	9.363918000	4.608085000	1.588330000
H	13.921062000	3.356104000	4.915432000	H	10.391867000	3.520961000	0.618816000
H	12.436192000	3.632379000	3.984560000	C	9.775767000	1.156173000	1.941577000
H	13.807067000	2.760655000	3.238893000	H	10.329641000	1.035556000	0.995701000
C	13.828588000	0.588687000	4.941008000	H	9.113283000	0.286996000	2.054890000
H	14.427056000	0.466741000	4.021073000	H	10.504322000	1.123426000	2.763204000
H	13.472347000	-0.409743000	5.231452000	C	7.046630000	1.268945000	3.795987000
H	14.506409000	0.955564000	5.725646000	H	7.786273000	0.492006000	4.060268000
C	11.228543000	0.185824000	6.805053000	C	6.114958000	1.462962000	4.996687000
H	12.229657000	-0.256627000	6.937808000	H	5.376298000	2.252161000	4.788253000
C	10.519522000	0.190479000	8.161062000	H	6.676279000	1.743078000	5.899508000
H	9.512829000	0.622428000	8.078402000	H	5.564809000	0.530353000	5.202016000
H	11.072355000	0.779867000	8.904918000	C	6.258305000	0.806835000	2.566849000
H	10.424130000	-0.841008000	8.539519000	H	5.753898000	-0.148341000	2.789883000
C	10.458986000	-0.661989000	5.784450000	H	6.888603000	0.646914000	1.679877000
H	10.316497000	-1.685716000	6.168450000	H	5.478103000	1.536307000	2.306469000
H	10.981407000	-0.737475000	4.819469000	C	7.233664000	6.328389000	6.084408000
H	9.461148000	-0.236487000	5.595960000	C	7.871582000	7.587052000	5.923720000
C	11.341605000	6.277182000	7.227602000	C	7.603145000	8.615007000	6.833194000
C	12.038947000	7.125041000	6.323838000	H	8.099873000	9.580869000	6.696311000
C	12.039775000	8.507865000	6.533848000	C	6.725966000	8.439716000	7.910363000
H	12.577998000	9.145981000	5.824641000	C	6.104091000	7.194824000	8.054627000
C	11.380139000	9.095755000	7.621025000	H	5.404151000	7.038977000	8.881970000
C	10.711804000	8.247170000	8.512481000	C	6.329937000	6.137635000	7.163452000
H	10.197924000	8.678526000	9.377759000	C	8.800321000	7.823956000	4.761533000
C	10.681319000	6.857832000	8.343366000	H	9.234399000	8.831775000	4.809030000
C	12.767119000	6.538315000	5.146360000	H	8.273909000	7.708872000	3.801410000
H	13.251229000	7.326692000	4.553125000	H	9.628162000	7.097480000	4.752856000
H	12.075174000	5.981187000	4.493299000	C	6.485200000	9.547149000	8.905554000
H	13.533358000	5.816886000	5.465904000	H	5.488268000	9.465577000	9.362619000
C	11.361896000	10.592480000	7.807243000	H	6.566381000	10.537533000	8.433313000
H	12.255766000	11.062441000	7.370934000	H	7.224545000	9.513805000	9.723162000
H	11.318407000	10.864393000	8.872487000	C	5.591815000	4.835671000	7.326812000
H	10.483240000	11.049230000	7.319927000	H	4.834177000	4.918315000	8.117755000
C	9.966750000	5.994396000	9.350089000	H	6.273775000	4.012365000	7.595871000
H	9.722691000	6.573605000	10.251411000	H	5.096497000	4.544904000	6.388674000
H	10.574437000	5.126511000	9.641241000	C	12.410105000	4.163197000	7.765564000
H	9.015588000	5.602065000	8.950509000	C	13.297745000	4.715823000	8.734834000
				H	13.089289000	5.713347000	9.125799000
				C	14.402166000	4.016324000	9.207516000
³ xii-TS				H	15.042982000	4.489037000	9.959716000
				C	14.706248000	2.720970000	8.756461000

C	13.855215000	2.178459000	7.785558000	C	7.074602000	4.253792000	3.068466000
H	14.072248000	1.169593000	7.423778000	C	4.439356000	5.102571000	0.408783000
C	12.739896000	2.859096000	7.272335000	H	3.403301000	4.762938000	0.560138000
C	15.880225000	1.947403000	9.304016000	H	4.900049000	4.449211000	-0.343763000
H	16.048003000	1.023984000	8.730381000	H	4.385799000	6.117579000	-0.013008000
H	15.727053000	1.655700000	10.357224000	C	9.506931000	3.469382000	1.741292000
H	16.811479000	2.536253000	9.267048000	H	8.744952000	3.371912000	0.950984000
C	12.815861000	2.203354000	4.424639000	C	10.058805000	4.899500000	1.695935000
H	12.171450000	1.825581000	3.613648000	H	10.842365000	5.049569000	2.455407000
C	13.163853000	3.661758000	4.110249000	H	9.271001000	5.648430000	1.855963000
H	13.790513000	4.091581000	4.905430000	H	10.514891000	5.096208000	0.714288000
H	12.263732000	4.288662000	4.025860000	C	10.598201000	2.427853000	1.485756000
H	13.717718000	3.732555000	3.159828000	H	11.039321000	2.599646000	0.492228000
C	14.083691000	1.346529000	4.471252000	H	10.214348000	1.398948000	1.499772000
H	14.624009000	1.424822000	3.512164000	H	11.410454000	2.506387000	2.218954000
H	13.867946000	0.281909000	4.640223000	C	7.942481000	1.436533000	3.306604000
H	14.765250000	1.690289000	5.262631000	H	8.863940000	0.850253000	3.469366000
C	11.604955000	0.324678000	6.376170000	C	7.005533000	1.209614000	4.500175000
H	12.645705000	-0.037765000	6.431626000	H	6.086374000	1.803952000	4.393936000
C	10.936070000	0.124185000	7.739829000	H	7.474010000	1.475478000	5.460855000
H	9.906591000	0.511650000	7.740308000	H	6.713522000	0.150338000	4.554775000
H	11.486442000	0.639957000	8.538181000	C	7.285932000	0.978167000	2.001243000
H	10.904848000	-0.950842000	7.983790000	H	7.069874000	-0.099525000	2.060913000
C	10.874619000	-0.463368000	5.284383000	H	7.922556000	1.135892000	1.120190000
H	10.809016000	-1.526807000	5.567010000	H	6.329959000	1.493423000	1.836356000
H	11.383297000	-0.408615000	4.310694000	C	7.023469000	5.901934000	6.412676000
H	9.848518000	-0.086006000	5.157685000	C	7.504352000	7.236519000	6.516105000
C	11.076594000	6.137209000	7.824606000	C	7.095286000	8.019405000	7.600265000
C	11.674468000	7.252473000	7.182066000	H	7.454702000	9.049441000	7.670151000
C	11.469601000	8.536708000	7.696932000	C	6.221914000	7.531734000	8.580700000
H	11.944179000	9.387048000	7.195169000	C	5.718067000	6.231475000	8.431481000
C	10.689843000	8.761814000	8.838314000	H	4.997855000	5.852366000	9.161803000
C	10.108127000	7.652732000	9.461052000	C	6.072826000	5.412793000	7.355073000
H	9.503901000	7.801093000	10.361915000	C	8.367154000	7.831699000	5.432836000
C	10.284215000	6.346993000	8.983185000	H	8.452522000	8.917171000	5.566745000
C	12.561091000	7.050377000	5.981822000	H	7.944072000	7.636863000	4.437471000
H	12.899692000	8.015144000	5.579043000	H	9.394124000	7.431685000	5.439196000
H	12.040198000	6.500834000	5.183269000	C	5.823416000	8.382095000	9.756822000
H	13.447035000	6.449610000	6.239878000	H	4.782754000	8.193875000	10.053645000
C	10.463915000	10.159564000	9.358503000	H	5.934705000	9.451958000	9.536404000
H	11.350111000	10.793547000	9.205682000	H	6.453872000	8.156584000	10.632105000
H	10.228995000	10.153798000	10.432865000	C	5.365542000	4.099258000	7.157773000
H	9.619980000	10.647572000	8.842442000	H	5.042634000	3.675819000	8.117345000
C	9.699381000	5.179659000	9.736774000	H	5.986488000	3.364853000	6.633050000
H	9.127836000	5.528085000	10.607363000	H	4.462627000	4.253871000	6.545368000
H	10.493714000	4.502626000	10.087187000	C	12.430356000	4.012994000	7.645275000
H	9.025516000	4.554736000	9.125973000	C	13.373001000	4.643681000	8.483061000
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UC44P2N5H62

U	9.330962000	4.200210000	6.229577000	C	13.558776000	1.898494000	8.089705000
P	8.559315000	3.214987000	3.346484000	H	13.632715000	0.818157000	7.946947000
P	11.369635000	1.868667000	6.242481000	C	12.547541000	2.615622000	7.434667000
N	7.457603000	5.089294000	5.312999000	C	15.564342000	1.730028000	9.635548000
N	11.372538000	4.709803000	7.034513000	H	15.536307000	0.670095000	9.350950000
N	8.402699000	2.949366000	7.798793000	C	15.452229000	1.787365000	10.729040000
N	7.836986000	2.602631000	8.817530000	H	16.564918000	2.118994000	9.394115000
N	7.299122000	2.257221000	9.777691000	C	12.441410000	1.524047000	4.720212000
C	6.683058000	5.083439000	4.146150000	H	11.709170000	1.187796000	3.966570000
C	5.538633000	5.894213000	3.983723000	C	13.079535000	2.829533000	4.237216000
H	5.219286000	6.540069000	4.803148000	H	13.816486000	3.194671000	4.965995000
C	4.828153000	5.891241000	2.788282000	H	12.337254000	3.625088000	4.084045000
H	3.952258000	6.538450000	2.692926000	C	13.604486000	2.665846000	3.284215000
C	5.212968000	5.088316000	1.701278000	C	13.507983000	0.437250000	4.884712000
C	6.341987000	4.277391000	1.871688000	H	14.046835000	0.314944000	3.932428000
H	6.654506000	3.652845000	1.032224000	H	13.088969000	-0.542484000	5.147654000
C	11.024974000	0.149822000	0.149822000	C	14.251346000	0.717209000	5.644252000
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H	12.017865000	-0.318659000	7.014779000	H	5.970664000	1.486671000	4.431077000
C	10.369993000	0.175896000	8.301164000	H	7.357286000	1.297455000	5.528094000
H	9.336198000	0.537059000	8.242409000	H	6.706627000	-0.113787000	4.654292000
H	10.919602000	0.807700000	9.011273000	C	7.258541000	0.678568000	2.088307000
H	10.342824000	-0.845199000	8.709780000	H	7.154979000	-0.414552000	2.165682000
C	10.198416000	-0.673396000	5.922616000	H	7.870333000	0.886454000	1.200422000
H	10.061439000	-1.693369000	6.311504000	H	6.251788000	1.084219000	1.922519000
H	10.679046000	-0.759841000	4.938033000	C	7.343065000	6.215466000	6.133545000
H	9.198031000	-0.238537000	5.784285000	C	7.957129000	7.485268000	5.925819000
C	11.306365000	6.134002000	7.197565000	C	7.704862000	8.512337000	6.833447000
C	11.996236000	6.989765000	6.290343000	H	8.157637000	9.491738000	6.658800000
C	11.937356000	8.368931000	6.488819000	C	6.867894000	8.332235000	7.946257000
H	12.478395000	9.022137000	5.798495000	C	6.258204000	7.086459000	8.120801000
C	11.222308000	8.941817000	7.553873000	H	5.573436000	6.941346000	8.961103000
C	10.557623000	8.085950000	8.435261000	C	6.449375000	6.025207000	7.225086000
H	10.012036000	8.510932000	9.281705000	C	8.773391000	7.751434000	4.687957000
C	10.587361000	6.692094000	8.287060000	H	9.241978000	8.741748000	4.736230000
C	12.808595000	6.428318000	5.155069000	H	8.137997000	7.712450000	3.789624000
H	13.349292000	7.228183000	4.634343000	H	9.571945000	7.010660000	4.531017000
H	12.175542000	5.917657000	4.412306000	C	6.631511000	9.454049000	8.920744000
H	13.538766000	5.688224000	5.510548000	H	5.669439000	9.342244000	9.437574000
C	11.175164000	10.435923000	7.729034000	H	6.645798000	10.431319000	8.419142000
H	12.171096000	10.883689000	7.602766000	H	7.418441000	9.472483000	9.692100000
H	10.794020000	10.714833000	8.719665000	C	5.609562000	4.784235000	7.371157000
H	10.519446000	10.898780000	6.974039000	H	5.487389000	4.512942000	8.428049000
C	9.883007000	5.819861000	9.296576000	H	6.030590000	3.929614000	6.831914000
H	9.754220000	6.358951000	10.244043000	H	4.602630000	4.971446000	6.964959000
H	10.434939000	4.893088000	9.499027000	C	12.411787000	4.012599000	7.761169000
H	8.862581000	5.546674000	8.968075000	C	13.324216000	4.633009000	8.641287000
				H	13.170450000	5.674049000	8.929375000
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³ xiii-TS				C	14.404387000	3.924820000	9.157931000
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114				H	15.088284000	4.431060000	9.844146000
UC44P2N5H62				C	14.630265000	2.577474000	8.829879000
U	9.327945000	4.152295000	6.212436000	C	13.733376000	1.973190000	7.938339000
P	8.420299000	3.015928000	3.403214000	H	13.894956000	0.925896000	7.674108000
P	11.476349000	1.959055000	6.171222000	C	12.645163000	2.666007000	7.390785000
N	7.576007000	5.175622000	5.178935000	C	15.789609000	1.816659000	9.417023000
N	11.276294000	4.662387000	7.255061000	H	15.856063000	0.801743000	9.003816000
N	8.396616000	2.894785000	7.327503000	H	15.693824000	1.728604000	10.510141000
N	7.599028000	1.953346000	8.340400000	H	16.743871000	2.327037000	9.218400000
N	6.987800000	2.235999000	9.265974000	C	12.511581000	1.781457000	4.602439000
C	6.670357000	5.030506000	4.126250000	H	11.784927000	1.390063000	3.870626000
C	5.543824000	5.867037000	3.960168000	H	12.969286000	3.169627000	4.142090000
H	5.346161000	6.651712000	4.691931000	H	13.665905000	3.614147000	4.866824000
C	4.695634000	5.708336000	2.870503000	H	12.125027000	3.864601000	4.014981000
H	3.834272000	6.373799000	2.769186000	H	13.490576000	3.099748000	3.175678000
C	4.925156000	4.725162000	1.892913000	C	13.695703000	0.813676000	4.673930000
C	6.046387000	3.901392000	2.060319000	H	14.178216000	0.757997000	3.685965000
H	6.249644000	3.150706000	1.294643000	H	13.397014000	-0.207087000	4.946644000
C	6.910035000	4.026271000	3.157910000	H	14.455026000	1.159991000	5.388610000
C	4.000341000	4.566907000	0.714962000	C	11.220564000	0.193597000	6.751444000
H	3.001763000	4.232172000	1.036159000	H	12.232155000	-0.243504000	6.787911000
H	4.384503000	3.830550000	-0.003120000	C	10.619388000	0.141106000	8.158517000
H	3.863300000	5.520120000	0.183081000	H	9.596453000	0.538383000	8.166679000
C	9.282733000	3.288548000	1.748604000	H	11.216292000	0.708212000	8.884785000
H	8.489316000	3.120452000	1.001528000	H	10.577219000	-0.904557000	8.498216000
C	9.739328000	4.747630000	1.634415000	C	10.382139000	-0.607982000	5.750330000
H	10.548083000	4.970519000	2.348449000	H	10.303511000	-1.652109000	6.087821000
H	8.914543000	5.450854000	1.812144000	H	10.822197000	-0.622329000	4.742914000
H	10.134324000	4.940052000	0.625715000	H	9.361022000	-0.206669000	5.683178000
C	10.429113000	2.315289000	1.466860000	C	11.068785000	6.030457000	7.630075000
H	10.788013000	2.461577000	0.436802000	C	11.634983000	7.073264000	6.845596000
H	10.129868000	1.262893000	1.563016000	C	11.491294000	8.392504000	7.277823000
H	11.281275000	2.496943000	2.134173000	H	11.944374000	9.192433000	6.685311000
C	7.867003000	1.214151000	3.389686000	C	10.814148000	8.717695000	8.463178000
H	8.813504000	0.677966000	3.577266000	C	10.256430000	7.676401000	9.213415000
C	6.926190000	0.961322000	4.574674000	H	9.735008000	7.910439000	10.145244000
				C	10.367754000	6.335960000	8.827597000
				C	12.446183000	6.765143000	5.614534000

H	12.766937000	7.689405000	5.118497000	H	4.773471000	7.986816000	10.272401000
H	11.888081000	6.166075000	4.877849000	H	5.788402000	9.337901000	9.703969000
H	13.343542000	6.181251000	5.868790000	H	6.464428000	8.101482000	10.779983000
C	10.697114000	10.150494000	8.909009000	C	5.460759000	3.999718000	7.281656000
H	11.672048000	10.657590000	8.872931000	H	4.747405000	3.803678000	8.091508000
H	10.309735000	10.224783000	9.933094000	H	6.183057000	3.174576000	7.239423000
H	10.019035000	10.716235000	8.250647000	H	4.906284000	3.996721000	6.330578000
C	9.821254000	5.246669000	9.715075000	C	12.410874000	4.078178000	7.501241000
H	9.282018000	5.678080000	10.567037000	C	13.352448000	4.778963000	8.285297000
H	10.632370000	4.612251000	10.103858000	H	13.296810000	5.866206000	8.350229000
H	9.125952000	4.569836000	9.191407000	C	14.342047000	4.098836000	8.988198000
				H	15.050126000	4.674520000	9.589934000
				C	14.445906000	2.698411000	8.953507000
^{1xiv}				C	13.520599000	2.007980000	8.160268000
				H	13.580594000	0.917769000	8.121301000
112				C	12.520384000	2.666025000	7.430806000
UC44P2N3H62				C	15.506189000	1.975690000	9.741005000
U	9.275598000	3.995330000	6.336557000	H	15.455938000	0.890622000	9.582677000
P	8.557388000	3.254324000	3.414457000	H	15.396620000	2.164279000	10.819824000
P	11.336365000	1.812913000	6.327912000	H	16.513992000	2.313644000	9.456569000
N	7.488551000	5.108741000	5.420047000	C	12.395576000	1.325940000	4.837194000
N	11.355758000	4.735597000	6.826958000	H	11.652419000	1.084558000	4.058476000
N	8.400752000	2.637499000	7.061015000	C	13.214792000	2.538711000	4.377996000
C	6.703740000	5.119320000	4.269945000	H	14.014308000	2.761108000	5.098151000
C	5.547923000	5.924937000	4.138215000	H	12.603028000	3.445683000	4.273232000
H	5.234843000	6.552345000	4.974283000	H	13.686446000	2.327453000	3.407064000
C	4.815803000	5.931104000	2.957899000	C	13.302091000	0.108412000	5.043176000
H	3.930275000	6.568426000	2.888688000	H	13.861373000	-0.083629000	4.114667000
C	5.189947000	5.148919000	1.850713000	H	12.744726000	-0.805751000	5.283859000
C	6.327821000	4.343575000	1.988917000	H	14.042793000	0.287545000	5.835704000
H	6.633139000	3.735234000	1.135208000	C	10.903591000	0.202142000	7.177185000
C	7.078442000	4.304343000	3.172979000	H	11.849100000	-0.359918000	7.252317000
C	4.395419000	5.180549000	0.572039000	C	10.346447000	0.420740000	8.587962000
H	3.353734000	4.868563000	0.742604000	H	9.404548000	0.985053000	8.552913000
H	4.826295000	4.514515000	-0.186956000	H	11.054562000	0.956222000	9.234476000
H	4.360519000	6.196183000	0.149179000	H	10.142535000	-0.556871000	9.050105000
C	9.552635000	3.638274000	1.867218000	C	9.921902000	-0.590039000	6.302946000
H	8.838475000	3.516293000	1.036133000	H	9.712924000	-1.563340000	6.770892000
C	10.008509000	5.101341000	1.893729000	H	10.314614000	-0.787617000	5.294632000
H	10.726932000	5.279751000	2.708942000	H	8.969097000	-0.050275000	6.209676000
H	9.164492000	5.792491000	2.021584000	C	11.260880000	6.153970000	6.999376000
H	10.513811000	5.355229000	0.950019000	C	11.943185000	7.037221000	6.120861000
C	10.726327000	2.682168000	1.647119000	C	11.877133000	8.408062000	6.373892000
H	11.213815000	2.911712000	0.687602000	H	12.410308000	9.090979000	5.706695000
H	10.416437000	1.628899000	1.614301000	C	11.168070000	8.935949000	7.466285000
H	11.484317000	2.794768000	2.432545000	C	10.506878000	8.045738000	8.318277000
C	7.970836000	1.470938000	3.218941000	H	9.959523000	8.436189000	9.179880000
H	8.870813000	0.889017000	3.486922000	C	10.539510000	6.661950000	8.109175000
C	6.874778000	1.168662000	4.249137000	C	12.765623000	6.508329000	4.977880000
H	5.957731000	1.728280000	4.013560000	H	13.223589000	7.330251000	4.414248000
H	7.180543000	1.426909000	5.271936000	H	12.156812000	5.913671000	4.280882000
H	6.628562000	0.096921000	4.219929000	H	13.567896000	5.847200000	5.338089000
C	7.519373000	1.059916000	1.812627000	C	11.113014000	10.422106000	7.698053000
H	7.333984000	-0.024905000	1.800454000	H	12.091251000	10.891103000	7.522941000
H	8.260833000	1.274196000	1.031923000	H	10.792871000	10.659887000	8.720671000
H	6.574235000	1.549426000	1.541342000	H	10.400874000	10.899815000	7.005684000
C	7.052922000	5.877151000	6.545237000	C	9.844015000	5.726577000	9.068215000
C	7.462536000	7.237357000	6.652880000	H	9.602602000	6.238925000	10.008415000
C	7.031682000	7.986601000	7.749948000	H	10.459047000	4.849021000	9.313274000
H	7.332285000	9.035399000	7.820479000	H	8.857443000	5.377602000	8.690899000
C	6.202398000	7.444371000	8.741486000				
C	5.755887000	6.125913000	8.580572000				
H	5.052199000	5.711135000	9.307219000				
C	6.129253000	5.332479000	7.489384000				
C	8.252600000	7.892833000	5.551964000				
H	8.412924000	8.954570000	5.773875000				
H	7.717616000	7.818598000	4.593511000				
H	9.237969000	7.428139000	5.405193000				
C	5.780112000	8.263494000	9.931251000				

N	1.911336	-1.035379	-1.239841	H	-2.438047	7.223525	1.954616
N	0.316615	1.663997	1.096196	C	-0.230693	3.478264	-2.614849
N	-1.428252	-0.940668	-0.726536	H	-0.001428	2.819383	-3.469409
H	-1.136315	-0.808019	1.995272	C	1.093607	3.924317	-1.985230
C	2.338954	-2.350748	-1.482830	H	1.676464	4.499424	-2.719569
C	3.239677	-2.671031	-2.523399	H	1.707967	3.071846	-1.665145
H	3.642927	-1.872420	-3.148013	H	0.916747	4.572116	-1.114979
C	3.607965	-3.989123	-2.768717	C	-1.038551	4.678308	-3.116960
H	4.303062	-4.199753	-3.585733	H	-1.289940	5.366814	-2.297828
C	3.101418	-5.052994	-2.003189	H	-1.965458	4.387747	-3.628508
C	2.223578	-4.730209	-0.960102	H	-0.430451	5.243891	-3.839684
H	1.817409	-5.544296	-0.355557	C	-2.886427	2.203548	-2.061957
C	1.847675	-3.409564	-0.676757	H	-3.224842	3.240378	-2.224551
C	3.484619	-6.478615	-2.300096	C	-3.813356	1.533776	-1.042452
H	3.102755	-7.166510	-1.534432	H	-4.835516	1.500161	-1.448637
H	4.577151	-6.596855	-2.349503	H	-3.848011	2.083871	-0.092386
H	3.082046	-6.803164	-3.272326	H	-3.493463	0.501344	-0.841656
C	1.765126	-3.310052	2.267075	C	-2.897465	1.459123	-3.403317
H	1.154604	-2.866795	3.072518	H	-2.580341	0.414727	-3.269694
C	3.088539	-2.540470	2.192710	H	-2.249010	1.928567	-4.156988
H	3.636818	-2.651435	3.139888	H	-3.919616	1.446702	-3.809663
H	2.934083	-1.466702	2.019472	C	1.070853	1.201370	2.215188
H	3.726107	-2.932537	1.387612	C	0.471463	0.260596	3.091922
C	2.003848	-4.788159	2.588450	C	1.198897	-0.189885	4.200730
H	2.612176	-5.275961	1.813835	H	0.729289	-0.895574	4.891416
H	1.072610	-5.356137	2.712987	C	2.495016	0.265878	4.465372
H	2.561838	-4.865831	3.534326	C	3.061963	1.205245	3.587847
C	-0.611011	-4.243433	0.711772	H	4.066034	1.586018	3.794959
H	-0.103078	-5.204934	0.894859	C	2.379297	1.691768	2.470857
C	-1.331614	-4.318976	-0.637672	C	-0.962375	-0.169216	2.889644
H	-2.101645	-5.103989	-0.592177	H	-1.635115	0.695835	2.800886
H	-0.644248	-4.569038	-1.456596	H	-1.303484	-0.785278	3.731635
H	-1.823142	-3.366091	-0.877045	C	3.268443	-0.233854	5.655779
C	-1.592078	-3.979446	1.861163	H	3.773728	0.590694	6.178074
H	-2.145164	-3.043485	1.694277	H	4.051873	-0.942713	5.343283
H	-1.096783	-3.924682	2.841491	H	2.617501	-0.749921	6.373032
H	-2.331000	-4.792827	1.910713	C	2.977913	2.770852	1.611234
C	2.451809	0.006858	-2.055201	H	4.048936	2.887660	1.817470
C	3.664365	0.649628	-1.682633	H	2.488088	3.737151	1.810019
C	4.191419	1.625964	-2.530458	H	2.841885	2.567171	0.540700
H	5.131095	2.111283	-2.252163	=====	=====	=====	=====
C	3.574035	1.976378	-3.741879	1xv-TS	=====	=====	=====
C	2.392208	1.316153	-4.096363	=====	=====	=====	=====
H	1.916418	1.552251	-5.052389	112	=====	=====	=====
C	1.815490	0.333045	-3.281831	UC44P2N3H62	=====	=====	=====
C	4.420598	0.214144	-0.457204	U	0.292159	-0.110097	-0.350156
H	5.260148	0.890825	-0.255643	P	1.092779	-2.783443	0.809981
H	4.827014	-0.799714	-0.597254	P	-0.786809	2.578583	-1.342696
H	3.781505	0.171981	0.434896	N	2.205746	-0.986289	-1.203894
C	4.172009	3.034032	-4.630040	N	0.095029	1.506512	1.248188
H	5.264098	2.929380	-4.695540	N	-1.450766	-0.697464	-0.493359
H	3.970244	4.041197	-4.231096	H	-2.047238	-0.136072	1.860995
H	3.758654	2.989226	-5.645887	C	2.683349	-2.298197	-1.384975
C	0.612476	-0.437256	-3.767214	C	3.553246	-2.650687	-2.437561
H	0.179481	0.037890	-4.656442	H	3.881994	-1.887803	-3.144474
H	-0.194881	-0.532951	-3.020640	C	3.981820	-3.965460	-2.592645
H	0.895233	-1.467134	-4.036247	H	4.652949	-4.207358	-3.420802
C	-0.456246	2.831923	1.231928	C	3.565276	-4.987686	-1.723488
C	-0.502612	3.563153	2.438730	C	2.688306	-4.634714	-0.688355
H	0.099764	3.235629	3.287624	H	2.324846	-5.421814	-0.023406
C	-1.315159	4.685427	2.560933	C	2.244229	-3.318421	-0.506465
H	-1.328714	5.226103	3.510851	C	4.041249	-6.404607	-1.904168
C	-2.123717	5.131766	1.502147	H	3.497916	-7.098843	-1.249992
C	-2.069114	4.407219	0.304163	H	5.113647	-6.494386	-1.670569
H	-2.698793	4.732726	-0.527039	H	3.909434	-6.740900	-2.942940
C	-1.248193	3.282139	0.143643	C	2.113694	-2.920989	2.389725
C	-3.014942	6.335622	1.655510	H	1.543651	-2.320012	3.116425
H	-3.776125	6.169868	2.433239	C	3.479723	-2.256673	2.171092

H	4.000869	-2.159196	3.134692		H	-3.306672	2.322486	-4.172723
H	3.392809	-1.252445	1.735349		C	0.535682	0.840706	2.433201
H	4.108681	-2.863527	1.505100		C	-0.396257	0.146489	3.256889
C	2.281576	-4.341669	2.938171		C	0.061018	-0.401529	4.461686
H	2.836101	-4.983093	2.238326		H	-0.655930	-0.919697	5.104596
H	1.326072	-4.826701	3.175894		C	1.389002	-0.270501	4.888462
H	2.868211	-4.300473	3.869014		C	2.285410	0.425517	4.063376
C	-0.227254	-4.105442	0.915438		H	3.319515	0.558958	4.392472
H	0.296957	-5.041273	1.170802		C	1.890399	0.981193	2.844919
C	-0.944053	-4.287727	-0.426594		C	-1.862642	0.090834	2.919755
H	-1.684317	-5.096776	-0.337535		H	-2.334658	1.066184	3.119754
H	-0.249586	-4.556323	-1.234121		H	-2.372463	-0.659337	3.537009
H	-1.483625	-3.371801	-0.708560		C	1.847100	-0.867235	6.192091
C	-1.218335	-3.759831	2.034620		H	2.616881	-0.244951	6.668403
H	-1.768818	-2.839357	1.792278		H	2.289844	-1.864216	6.033239
H	-0.729108	-3.624334	3.009491		H	1.012482	-0.988174	6.894849
H	-1.953652	-4.571103	2.140191		C	2.864356	1.789158	2.027318
C	2.250128	-0.099518	-2.317375		H	3.839567	1.842891	2.526921
C	3.349096	0.755308	-2.587665		H	2.496116	2.813755	1.871493
C	3.288376	1.562649	-3.725128		H	3.026952	1.357921	1.026618
H	4.140023	2.208757	-3.956418		=====			
C	2.177112	1.565217	-4.591097		1xvi			
C	1.086472	0.748206	-4.286702		=====			
H	0.219177	0.737339	-4.950868		112			
C	1.099729	-0.106088	-3.167138		UC44P2N3H62			
C	4.576074	0.741464	-1.717277		U	0.869762	0.218211	0.123916
H	5.063904	1.724875	-1.707183		P	1.733397	-2.636853	0.742953
H	5.313110	0.013901	-2.092830		P	-0.239040	2.660434	-1.305188
H	4.337277	0.444760	-0.688124		N	3.070899	-0.235778	-0.269776
C	2.180827	2.432379	-5.822413		N	0.073060	1.866691	1.456924
H	2.980923	2.125485	-6.512898		N	0.182377	-0.725661	-1.394504
H	2.369206	3.486230	-5.567361		H	-0.175674	-1.264891	-2.192124
H	1.227973	2.373513	-6.363286		C	3.833993	-1.382161	-0.534233
C	-0.021258	-1.022542	-2.841833		C	5.116347	-1.331491	-1.124757
H	-0.818583	-0.994103	-3.595321		H	5.558986	-0.364269	-1.366601
H	-0.991173	-0.890542	-1.753044		C	5.816490	-2.498926	-1.410475
H	0.311489	-2.061273	-2.695803		H	6.803670	-2.421994	-1.873598
C	-0.526772	2.751062	1.401918		C	5.285106	-3.768023	-1.127813
C	-0.637342	3.401677	2.652500		C	4.029925	-3.813331	-0.504996
H	-0.207529	2.936176	3.540549		H	3.612004	-4.791774	-0.258202
C	-1.295184	4.621038	2.765602		C	3.310187	-2.654055	-0.188602
H	-1.364688	5.093766	3.748787		C	6.035923	-5.025256	-1.477875
C	-1.880133	5.252957	1.654666		H	5.574997	-5.910648	-1.020563
C	-1.748505	4.616676	0.413489		H	7.081944	-4.973593	-1.142314
H	-2.197635	5.092104	-0.461160		H	6.055096	-5.184889	-2.567488
C	-1.073889	3.397005	0.266285		C	2.241067	-3.093750	2.506116
C	-2.617126	6.558125	1.798207		H	1.286534	-3.050417	3.056239
H	-3.516512	6.440550	2.422252		C	3.164779	-2.015292	3.078976
H	-2.935343	6.950413	0.823436		H	3.404913	-2.250007	4.126745
H	-1.988405	7.320530	2.282034		H	2.698980	-1.020905	3.060474
C	0.369048	3.756221	-2.257007		H	4.111976	-1.969746	2.522644
H	0.652636	3.178028	-3.150742		C	2.854115	-4.486624	2.677659
C	1.630335	3.983040	-1.413231		H	3.812363	-4.571715	2.146343
H	2.373134	4.547336	-1.996596		H	2.192863	-5.294670	2.337852
H	2.100523	3.038577	-1.104876		H	3.056734	-4.660562	3.745742
H	1.399981	4.564175	-0.508847		C	0.811678	-4.164316	0.150843
C	-0.236513	5.090033	-2.704820		H	1.534930	-4.986705	0.278228
H	-0.508294	5.719695	-1.846379		C	0.436731	-4.084687	-1.331451
H	-1.121275	4.967246	-3.343547		H	0.073962	-5.066591	-1.670084
H	0.512015	5.647555	-3.289063		H	1.290182	-3.802607	-1.962517
C	-2.438169	2.696258	-2.224949		H	-0.371723	-3.358239	-1.488504
H	-2.668919	3.774216	-2.263373		C	-0.414023	-4.468258	1.020656
C	-3.539534	1.988602	-1.428511		H	-1.172992	-3.679032	0.927954
H	-4.497867	2.094103	-1.958864		H	-0.164498	-4.585768	2.083840
H	-3.658902	2.421213	-0.426363		H	-0.876554	-5.408592	0.685735
H	-3.324519	0.916994	-1.312061		C	3.641800	1.035064	-0.601196
C	-2.345271	2.168747	-3.660743		C	4.290747	1.797490	0.411735
H	-2.136773	1.089301	-3.671346		C	4.922711	2.990984	0.058065

H	5.435461	3.563578	0.835859
C	4.949277	3.457736	-1.264837
C	4.305271	2.694448	-2.244792
H	4.331845	3.032115	-3.284859
C	3.651044	1.491737	-1.948644
C	4.378143	1.291919	1.826437
H	4.919426	2.006076	2.459217
H	4.905007	0.327412	1.865214
H	3.388890	1.125642	2.277649
C	5.645316	4.746071	-1.611144
H	6.609013	4.830708	-1.089538
H	5.039167	5.614055	-1.305386
H	5.826784	4.829786	-2.690342
C	3.067485	0.668564	-3.066871
H	2.859969	1.294019	-3.944675
H	2.144850	0.152020	-2.768102
H	3.777633	-0.114607	-3.377400
C	-0.904022	2.865258	1.353680
C	-1.652399	3.326940	2.456580
H	-1.474275	2.900864	3.444724
C	-2.631507	4.300471	2.287098
H	-3.197869	4.636864	3.159325
C	-2.923546	4.846643	1.025553
C	-2.196284	4.362377	-0.071582
H	-2.441022	4.742980	-1.065945
C	-1.197154	3.391645	0.071491
C	-3.979085	5.907636	0.862524
H	-4.887513	5.658669	1.429514
H	-4.259021	6.039751	-0.190888
H	-3.622217	6.880344	1.236547
C	0.868539	4.061247	-1.907759
H	1.584816	3.557762	-2.577858
C	1.642381	4.631248	-0.713192
H	2.379531	5.365481	-1.068964
H	2.183900	3.853692	-0.158078

H	0.964541	5.144866	-0.016886
C	0.154630	5.173297	-2.682598
H	-0.563905	5.709843	-2.047082
H	-0.370620	4.808979	-3.575074
H	0.899827	5.910048	-3.019930
C	-1.486999	2.367145	-2.668719
H	-1.937052	3.350140	-2.885867
C	-2.594012	1.414363	-2.203737
H	-3.322673	1.271981	-3.015613
H	-3.134618	1.806813	-1.331940
H	-2.182403	0.428418	-1.942540
C	-0.784390	1.853201	-3.931368
H	-0.291073	0.889175	-3.740698
H	-0.027711	2.555126	-4.308820
H	-1.523781	1.701222	-4.731458
C	0.157440	1.077529	2.633393
C	-0.510398	-0.192478	2.577280
C	-0.412004	-1.041917	3.708897
H	-0.923085	-2.007771	3.682923
C	0.247990	-0.641764	4.863891
C	0.887429	0.621222	4.886728
H	1.416021	0.928432	5.793436
C	0.865432	1.487976	3.798367
C	-1.124573	-0.580131	1.324775
H	-1.742072	0.190609	0.832292
H	-1.584912	-1.567889	1.280986
C	0.288281	-1.520876	6.085535
H	-0.190998	-1.023163	6.942048
H	1.325546	-1.737105	6.383821
H	-0.227927	-2.474347	5.916365
C	1.525156	2.838480	3.863560
H	2.310209	2.855429	4.630030
H	0.794382	3.622232	4.118295
H	1.960387	3.121499	2.895329

Frequencies

===== 4i =====									
9.409	17.416	20.659	21.332	23.056	26.427	35.715	38.625		
39.549	42.090	42.363	43.714	48.038	51.171	53.636	55.423		
59.104	61.225	62.375	65.730	67.952	69.666	73.749	82.133		
88.592	88.283	90.581	94.863	97.069	103.233	106.195	107.763		
110.266	110.470	114.662	118.669	119.361	124.188	129.643	133.391		
149.978	157.593	171.415	176.238	179.285	185.716	191.905	205.196		
211.082	212.403	214.304	220.670	224.866	225.617	228.584	238.978		
240.082	242.953	252.730	258.111	260.579	268.696	269.146	272.757		
274.540	285.795	286.870	293.276	296.182	296.984	304.686	306.534		
327.440	332.076	352.112	357.079	360.695	361.489	371.847	376.007		
381.891	390.169	403.461	406.640	420.822	424.134	448.209	453.652		
477.162	481.443	490.675	493.137	494.504	499.785	502.610	507.248		
529.683	532.101	536.072	537.303	565.109	566.416	573.541	575.324		
579.270	585.769	587.325	590.094	598.516	599.794	614.955	619.952		
678.052	679.434	698.630	705.053	718.203	719.177	799.504	800.783		
805.337	811.109	813.086	818.359	838.353	841.837	859.360	861.916		
862.168	863.363	868.199	868.572	872.105	872.830	878.902	883.176		
898.366	900.657	903.786	907.137	917.948	919.179	930.895	931.443		
939.999	941.354	944.085	945.807	948.060	949.385	977.731	977.803		
992.690	994.068	999.421	1000.292	1006.164	1010.069	1010.854	1013.247		
1013.658	1014.647	1016.498	1016.722	1017.453	1018.177	1018.399	1018.551		
1019.143	1019.615	1041.993	1042.264	1072.312	1073.998	1096.846	1097.352		
1122.555	1124.680	1139.534	1141.609	1143.267	1144.824	1147.306	1148.547		
1176.732	1179.869	1199.258	1200.386	1218.567	1219.933	1220.779	1224.463		
1224.982	1225.244	1244.088	1249.144	1253.772	1272.507	1282.968	1285.383		
1286.129	1289.548	1291.308	1292.215	1303.369	1304.311	1308.135	1310.905		
1342.294	1343.915	1347.976	1349.317	1356.455	1357.357	1358.123	1359.174		
1359.715	1360.602	1360.952	1362.003	1364.292	1364.718	1365.503	1366.406		
1368.406	1378.418	1382.207	1392.592	1394.444	1397.239	1398.041	1423.524		
1425.637	1428.476	1429.444	1431.092	1433.192	1434.236	1434.279	1435.209		
1435.455	1435.741	1437.719	1437.369	1438.754	1439.221	1440.451	1442.237		
1443.031	1445.823	1446.286	1449.417	1451.331	1451.581	1451.987	1452.846		
1453.046	1454.282	1455.410	1456.963	1458.360	1458.662	1461.271	1463.587		
1465.503	1526.294	1527.085	1547.095	1551.904	1586.672	1587.302	1592.305		
1594.367	2145.401	2922.043	2940.744	2941.032	2946.554	2947.322	2949.163		
2949.339	2950.465	2950.723	2951.403	2952.442	2953.723	2953.910	2954.096		
2955.715	2957.379	2957.975	2959.244	2961.681	2962.042	2998.116	2999.002		
3006.870	3008.384	3009.250	3011.498	3012.051	3012.854	3014.052	3015.143		
3017.374	3018.500	3021.220	3023.108	3024.329	3024.652	3030.262	3031.739		
3032.621	3032.712	3036.036	3038.320	3041.329	3041.493	3042.382	3042.435		
3045.593	3048.463	3050.598	3058.388	3058.738	3059.335	3069.042	3073.095		
3073.202	3073.516	3073.592	3077.113	3081.348	3082.361	3103.599	3110.352		

===== 2i-TS =====									
-168.571	12.776	18.846	19.927	24.607	28.984	30.046	35.140		
36.122	37.562	44.753	45.575	48.085	49.447	50.924	53.412		
54.748	59.978	60.099	65.288	67.323	68.272	70.810	77.000		
85.263	87.985	91.754	93.849	99.122	103.446	105.153	106.330		
111.481	112.912	117.113	119.738	122.319	124.607	128.509	139.143		
146.925	159.883	169.534	174.627	180.363	188.238	191.867	199.242		
204.593	206.603	216.370	220.375	224.459	228.558	231.043	233.020		
237.981	240.727	248.073	253.229	259.816	261.233	266.214	269.393		
269.453	272.737	273.931	286.725	293.314	296.345	298.552	306.558		
307.081	330.914	333.007	349.521	352.771	356.229	359.117	361.828		
375.612	379.150	382.934	392.501	402.988	408.215	422.115	425.422		
450.267	454.688	479.552	483.001	490.677	495.078	495.465	499.441		
503.455	509.112	530.760	533.362	536.611	537.923	563.705	566.648		
575.504	576.082	584.526	589.335	599.603	600.910	617.492	627.801		
663.928	679.968	680.888	700.047	705.705	720.271	720.308	798.605		
801.399	805.158	811.497	817.542	818.128	838.171	842.053	859.213		
863.918	864.645	865.180	867.927	868.312	869.858	873.914	881.849		
883.743	898.702	900.775	904.065	908.451	917.815	918.925	930.902		
933.058	939.902	940.524	943.901	947.273	949.124	949.760	978.276		
978.360	991.612	993.633	998.578	1000.202	1002.744	1009.147	1012.338		
1013.953	1015.353	1015.591	1016.352	1016.750	1017.740	1017.796	1018.412		
1018.631	1020.482	1020.881	1043.055	1043.355	1070.265	1074.103	1095.		

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2ii

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16.096	19.046	19.528	26.091	33.176	34.632	35.428	40.226
41.943	45.741	49.908	52.362	54.062	56.674	60.143	60.602
64.692	65.874	72.790	78.489	79.316	84.605	89.846	95.686
96.577	101.573	105.496	108.145	110.229	112.014	116.196	117.697
118.988	123.055	126.232	128.857	134.271	148.865	158.282	164.618
175.618	182.056	185.981	191.803	204.130	206.015	211.854	215.419
224.445	225.498	230.330	232.284	234.097	235.870	243.789	245.805
252.212	261.714	263.060	269.113	270.166	273.409	275.281	290.966
293.982	294.615	299.085	306.003	308.491	332.890	334.541	352.777
357.959	359.855	362.955	372.506	379.612	384.538	391.473	405.046
407.885	420.476	423.838	451.660	455.503	477.991	482.119	489.789
493.948	498.409	498.925	503.455	509.355	530.174	531.606	536.145
537.675	564.658	566.018	575.267	576.601	584.262	586.867	599.682
600.933	622.799	629.375	678.624	679.544	701.877	706.691	718.490
718.923	799.860	799.896	804.338	808.649	816.311	817.587	837.870
842.217	858.220	863.227	863.603	865.494	868.393	869.933	870.289
874.070	878.818	881.910	899.389	903.292	907.520	911.984	916.093
918.737	920.656	932.101	932.839	940.887	943.972	945.177	948.335
948.737	952.722	977.288	978.489	992.186	997.009	999.363	1000.299
1007.584	1008.614	1010.358	1016.017	1016.081	1016.165	1016.657	1016.992
1018.143	1018.256	1018.636	1019.101	1021.845	1029.425	1041.564	1042.251
1071.054	1072.978	1094.760	1096.463	1123.406	1126.316	1140.672	1142.694
1143.436	1146.719	1148.394	1151.107	1176.912	1181.445	1198.851	1201.332
1218.876	1220.181	1222.233	1223.369	1225.847	1226.151	1242.006	1249.379
1253.494	1272.701	1279.403	1285.029	1286.632	1287.210	1291.002	1291.900
1301.670	1303.088	1307.723	1311.187	1342.189	1342.683	1349.821	1349.138
1355.338	1357.624	1357.704	1360.303	1361.023	1361.188	1361.424	1363.826
1365.066	1365.743	1366.405	1372.019	1382.784	1382.815	1393.122	1395.285
1398.232	1401.755	1425.569	1427.429	1428.728	1430.504	1432.554	1433.737
1433.953	1434.642	1435.321	1437.027	1437.937	1438.199	1438.754	1439.630
1440.852	1442.972	1443.886	1445.305	1445.848	1445.912	1449.111	1451.285
1452.606	1453.305	1453.700	1454.501	1455.716	1456.998	1458.347	1460.996
1462.418	1464.776	1468.725	1470.290	1523.481	1526.853	1546.578	1553.226
1587.252	1587.829	1592.437	1594.414	2906.175	2938.312	2942.767	2945.692
2945.920	2946.452	2947.557	2949.137	2949.205	2949.506	2950.107	2951.668
2952.920	2953.383	2954.183	2958.482	2958.827	2959.151	2960.854	2961.115
2996.244	3001.331	3004.797	3009.474	3009.677	3010.596	3010.796	3015.464
3016.016	3016.727	3016.914	3017.309	3018.938	3020.038	3024.457	3026.044
3026.702	3032.163	3032.664	3035.160	3035.516	3037.288	3040.433	3040.737
3041.145	3041.666	3042.537	3042.675	3046.147	3047.613	3048.821	3055.969
3070.507	3071.664	3072.272	3072.546	3075.239	3077.438	3082.396	3083.159
3105.873	3112.266						

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3iii

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13.345	15.955	18.923	25.061	26.768	29.603	37.536	38.809
46.162	46.464	53.797	56.216	57.436	59.000	62.705	65.801
67.244	68.578	73.045	73.333	76.351	80.929	82.225	87.385
88.405	98.387	98.955	101.129	106.977	110.095	112.484	115.812
117.904	122.027	123.616	140.881	148.902	149.839	154.918	175.708
181.307	183.701	186.476	196.163	201.816	205.803	209.010	210.726
218.873	226.644	227.884	231.217	231.887	240.711	244.401	252.247
253.401	257.442	263.388	267.095	268.181	274.241	277.560	287.991
289.536	291.007	292.110	303.073	304.393	334.446	337.916	347.813
349.598	356.661	357.935	362.613	363.882	382.834	387.067	404.030
406.004	414.698	417.043	442.841	450.831	475.956	476.820	487.936
488.703	496.174	496.959	500.917	502.837	526.301	527.420	532.776
534.825	562.822	563.847	565.185	574.886	575.181	578.608	594.865
597.077	606.351	623.386	673.618	676.128	701.167	705.790	711.597
714.543	787.204	788.412	797.298	800.024	814.932	817.438	830.887
832.519	847.318	849.599	854.054	863.586	865.369	866.854	868.872
869.625	872.694	875.261	876.569	896.195	900.551	905.992	911.191
911.345	916.001	920.210	920.245	939.993	942.813	944.401	948.499
949.355	950.910	971.356	972.541	993.092	995.416	996.468	997.852
998.890	1000.399	1008.065	1009.719	1011.918	1012.600	1013.914	1014.246
1014.531	1014.858	1020.466	1023.495	1028.852	1029.118	1033.399	1034.913
1071.647	1072.738	1093.988	1095.830	1123.193	1123.928	1136.938	1137.893
1141.833	1142.729	1145.526	1149.677	1183.290	1187.504	1194.486	1195.947
1211.043	1213.449	1215.255	1217.475	1218.209	1218.513	1241.541	1244.873
1277.607	1279.222	1280.389	1284.899	1286.585	1291.948	1301.655	1302.583
1304.989	1305.635	1311.330	1312.468	1336.647	1337.573	1342.185	1342.504
1348.958	1350.965	1351.903	1352.891	1355.068	1355.929	1356.576	1358.721
1363.263	1364.009	1367.947	1370.324	1380.761	1385.093	1392.908	1394.753
1400.339	1400.782	1419.565	1422.131	1424.110	1427.010	1427.382	1429.164
1431.951	1431.275	1431.611	1434.078	1434.524	1434.996	1436.611	1436.797
1438.720	1440.796	1441.364	1442.235	1443.442	1444.081	1444.786	1447.541
1449.937	1450.427	1452.901	1453.259	1454.207	1454.488	1456.206	1458.544
1460.813	1461.972	1467.133	1469.744	1505.774	1508.810	1504.786	1508.321
1574.258	1583.254	1590.106	1591.521	2006.590	2922.832	2923.607	2923.872
2925.364	2931.735	2932.771	2933.407	2933.664	2934.684	2935.668	2936.168
2936.461	2938.118	2938.369	2939.686	2943.099	2946.313	2950.575	2950.730
2967.268	2969.504	2986.027	2988.596	2993.281	2994.873	2995.552	2995.721
2995.864	2996.094	2996.904	3001.303	3002.207	3003.727	3005.708	3010.185
3010.846	3013.787	3015.849	3019.862	3024.197	3024.301	3025.447	3027.761
3028.272	3031.311	3032.699	3032.796	3033.859	3034.256	3034.807	3037.742
3052.604	3053.174	3055.431	3055.809	3058.535	3059.282	3067.988	3071.343
3096.579	3098.701						

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3iv

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11.082	16.104	17.009	20.358	21.153	33.486	39.020	41.347
42.506	43.519	49.441	55.020	55.439	58.753	61.995	65.150
67.485	70.217	72.303	75.180	77.792	81.362	82.397	90.344
91.406	98.649	102.336	105.393	107.675	108.989	114.298	116.183
122.133	135.204	138.216	147.623	149.531	157.216	165.753	173.441
183.690	185.716	187.785	192.043	205.777	209.016	209.388	223.098
226.356	228.056	228.383	230.585	235.084	240.397	242.305	249.340
249.452	260.053	261.256	266.856	266.979	268.827	270.944	288.615
289.783	291.589	292.550	303.715	304.470	325.446	332.869	336.883
349.304	352.455	357.679	360.559	363.780	384.948	386.955	404.104
405.974	412.865	415.948	448.617	452.286	477.017	478.592	480.106
487.915	492.651	494.370	494.978	500.729	527.164	527.729	530.264
530.951	558.754	563.356	567.516	575.213	579.896	581.262	596.745
597.954	618.367	623.769	675.941				

42.374	46.154	50.408	51.072	53.801	56.794	59.969	62.926
67.432	68.936	72.745	75.834	83.407	85.729	87.306	89.510
91.883	93.061	99.731	100.614	104.023	109.082	109.453	111.713
116.851	118.899	143.646	153.691	159.841	166.042	166.666	171.774
179.864	181.405	190.020	201.372	204.109	208.543	213.604	219.056
219.559	224.720	225.579	234.199	236.267	238.033	249.686	254.516
256.777	261.476	266.094	270.171	272.781	286.142	288.224	290.980
294.585	298.426	301.930	319.684	324.728	330.080	350.611	354.432
355.036	358.652	364.170	367.972	380.024	384.590	388.175	402.701
404.394	416.169	418.473	442.618	446.024	470.136	472.637	475.622
486.704	489.895	491.149	499.545	506.823	519.104	523.070	528.771
533.023	536.885	559.489	561.098	563.301	572.644	576.498	589.654
590.873	605.742	616.539	624.960	663.471	674.122	676.856	695.487
711.486	712.614	758.116	763.421	783.846	787.478	793.023	811.120
812.963	814.427	829.330	843.810	849.379	850.071	850.742	863.056
866.061	868.039	869.796	872.422	878.412	898.553	900.109	901.960
902.514	903.120	906.327	906.946	915.953	938.060	939.840	945.033
945.143	947.775	951.598	970.692	971.247	973.611	989.553	989.848
994.696	995.833	1000.926	1007.786	1009.722	1010.194	1011.875	1012.845
1013.051	1013.437	1013.850	1015.730	1019.888	1033.807	1037.817	1041.134
1069.555	1071.889	1078.662	1092.541	1093.415	1115.535	1124.390	1129.174
1135.558	1140.473	1140.666	1144.515	1145.600	1165.556	1176.082	1181.579
1193.585	1195.374	1205.358	1208.707	1210.990	1215.059	1222.104	1227.125
1236.216	1236.818	1259.625	1264.507	1285.738	1286.520	1288.202	1290.748
1295.673	1303.580	1304.223	1306.610	1315.045	1323.796	1333.137	1336.947
1338.329	1345.722	1347.423	1350.028	1350.391	1350.765	1351.605	1352.219
1353.105	1354.732	1357.350	1359.364	1362.967	1365.584	1371.202	1378.423
1383.639	1390.707	1394.330	1409.876	1412.319	1412.931	1416.704	1424.575
1427.322	1428.891	1430.047	1431.509	1432.053	1432.767	1434.054	1434.305
1435.337	1436.218	1438.160	1438.965	1439.074	1441.523	1442.666	1443.833
1444.603	1445.878	1446.717	1447.911	1448.713	1450.646	1453.142	1455.020
1455.478	1455.622	1460.203	1461.023	1462.997	1504.783	1511.243	1522.756
1526.134	1559.784	1562.763	1573.480	2898.402	2918.929	2921.257	2922.298
2924.336	2929.820	2930.743	2931.924	2933.423	2933.933	2934.643	2935.332
2938.995	2939.582	2941.042	2943.585	2946.492	2948.160	2963.846	2964.539
2970.858	2978.147	2980.599	2982.450	2987.335	2988.023	2988.227	2995.899
2998.370	3000.940	3001.433	3003.528	3003.733	3009.892	3014.714	3014.760
3015.357	3016.325	3020.319	3021.973	3027.791	3028.361	3029.973	3039.083
3029.271	3029.602	3032.217	3034.592	3035.078	3038.355	3052.222	3052.670
3054.374	3054.979	3055.094	3060.718	3061.380	3066.387	3073.238	3092.874
3100.442	3435.447						

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12.197	19.369	21.319	21.936	25.275	32.627	32.947	34.560
38.854	42.054	42.906	44.420	48.555	51.453	58.474	61.732
65.565	66.654	68.627	73.493	79.810	85.142	88.421	92.440
94.244	97.819	102.828	104.879	106.906	108.300	112.041	114.627
129.011	142.906	148.045	150.902	157.159	159.197	175.810	180.293
184.182	192.023	203.213	206.311	208.201	214.406	217.795	220.482
225.201	226.708	230.769	234.205	236.977	241.989	243.754	254.767
255.066	262.437	265.697	267.965	271.508	288.381	289.927	292.685
297.120	299.495	304.775	326.401	328.344	328.880	351.285	351.087
355.626	357.445	364.276	366.105	382.291	384.960	401.947	403.238
407.238	416.708	423.866	443.257	444.589	473.133	474.414	481.173
485.667	487.961	488.643	496.896	509.467	523.387	526.844	528.585
535.156	559.200	562.900	569.493	571.792	576.452	587.397	589.285
601.662	608.535	623.374	674.811	677.813	692.603	703.567	710.077
714.786	779.528	787.536	790.047	793.087	813.259	815.234	828.379
829.891	843.008	846.749	846.927	852.325	862.535	866.246	867.819
868.892	872.268	873.473	896.625	897.400	899.054	901.632	902.515
911.060	914.777	915.298	924.941	937.078	938.818	944.533	945.852
946.399	967.539	970.328	971.345	986.790	988.338	991.626	992.439
993.586	995.504	1007.689	1008.792	1011.172	1012.522	1012.575	1013.249
1013.526	1013.713	1014.857	1019.563	1031.447	1034.780	1037.806	1069.521
1071.100	1091.507	1093.008	1119.002	1120.339	1130.624	1134.649	1139.201
1140.367	1142.612	1143.966	1154.442	1178.379	1181.282	1193.086	1193.994
1196.514	1204.779	1205.396	1215.514	1215.979	1222.900	1227.215	1244.711
1242.331	1264.862	1269.809	1284.664	1285.644	1292.286	1294.033	1294.968
1296.898	1304.056	1305.679	1308.973	1309.968	1331.461	1335.956	1336.969
1342.110	1343.268	1347.239	1349.842	1350.179	1350.866	1351.931	1352.298
1353.148	1354.474	1355.429	1356.985	1359.166	1370.146	1381.050	1390.311
1392.249	1394.879	1411.622	1412.421	1413.646	1416.665	1427.568	1427.965
1430.520	1430.990	1431.293	1432.150	1432.297	1432.675	1432.930	1433.384
1435.618	1436.125	1436.356	1436.611	1441.975	1442.450	1442.933	1443.617
1444.933	1445.768	1446.243	1449.644	1449.953	1452.001	1452.233	1453.158
1455.892	1456.411	1458.434	1459.802	1502.746	1513.321	1514.599	1524.087
1556.941	1566.964	1571.020	1577.541	2829.650	2847.203	2900.573	2923.135
2924.469	2925.032	2925.284	2929.758	2930.949	2931.772	2931.875	2933.713
2934.261	2934.660	2935.779	2940.203	2941.359	2942.197	2943.155	
2958.761	2967.769	2978.282	2978.930	2983.321	2985.517	2987.180	
2994.609	2994.831	2997.091	2999.957	3000.082	3003.047	3004.154	3010.611
3014.642	3015.128	3015.138	3023.332	3023.834	3026.509	3027.543	3028.881
3029.162	3030.762	3030.166	3030.476	3030.655	3032.260	3033.820	3050.804
3051.435	3053.037	3054.139	3055.436	3058.527	3063.112	3069.626	3094.842
3100.629	3377.112						

2 vii

15.018	18.056	20.883	33.685	34.734	39.398	41.546	42.646
43.900	46.580	52.221	60.579	63.200	64.863	66.007	67.961
71.860	75.037	76.399	84.886	86.905	92.156	94.073	97.366
103.993	104.658	107.232	109.290	110.453	114.462	117.858	124.514
124.923	131.131	143.583	151.917	155.252	162.378	170.359	181.022
185.805	189.290	194.200	209.649	210.766	211.956	217.437	234.430
226.636	226.990	232.330	234.464	236.769	241.488	244.555	256.274
259.784	261.906	269.961	275.021	277.567	294.510	294.727	294.727
298.816	304.818	307.031	329.861	334.360	344.703	355.326	359.831
361.623	363.803	380.486	389.630	389.846	404.074	404.462	410.277
420.834	427.712	437.428	454.330	457.729	479.267	479.628	488.962
492.774	496.279	497.265	509.927	516.225	532.219	533.255	538.463
540.141	556.153	562.851	565.928	568.796	577.990	583.476	584.996
591.311	598.123	607.244	627.172	635.226	681.784	682.986	691.462
704.827	720.206	720.896	734.758	777.364	798.529	800.204	803.248
807.431	816.953	820.701	826.716	840.833	856.733	861.176	862.521
863.168	868.009	870.004	873.120	873.926	882.329	883.685	901.407

261.027	261.490	269.785	271.831	275.706	278.789	295.781	295.920
300.402	305.848	307.810	331.629	335.046	349.306	357.182	360.333
363.113	365.012	385.588	390.456	390.886	403.843	405.064	418.398
421.232	431.099	456.115	456.641	476.129	479.886	485.880	488.057
492.212	496.117	496.955	508.584	515.571	532.937	533.863	539.633
541.074	553.821	565.326	569.940	575.909	583.948	585.324	588.047
593.565	596.651	609.275	623.117	635.134	681.623	683.014	694.764
701.879	718.815	719.126	757.381	790.278	804.969	806.047	808.887
811.062	818.680	830.267	843.059	845.397	864.872	865.371	867.558
869.045	869.454	872.676	872.859	874.264	884.573	885.836	901.890
902.839	906.630	908.197	920.680	932.178	940.395	940.820	940.885
941.559	943.632	945.036	945.381	950.252	981.479	981.772	993.716
996.356	1001.998	1004.247	1009.373	1010.466	1015.367	1016.029	1016.473
1017.293	1017.445	1018.051	1018.408	1018.453	1018.544	1021.220	1038.217
1046.396	1046.635	1070.980	1073.970	1094.286	1097.969	1122.780	1124.307
1140.547	1141.936	1144.394	1144.879	1146.078	1150.826	1170.633	1174.805
1201.331	1201.859	1218.709	1222.970	1225.100	1227.040	1229.204	
1238.552	1252.002	1254.970	1259.182	1277.602	1278.896	1281.667	1283.812
1285.072	1285.411	1307.612	1311.771	1311.988	1319.897	1345.588	1346.094
1305.525	1351.494	1359.925	1360.921	1362.512	1364.778	1364.898	1365.103
1366.511	1367.864	1368.572	1370.606	1371.165	1376.821	1382.216	1382.659
1390.307	1392.665	1394.748	1416.681	1423.301	1426.792	1428.063	1431.750
1432.524	1433.164	1434.583	1435.172	1435.901	1437.052	1438.074	1438.590
1438.866	1440.461	1442.638	1443.919	1444.108	1444.436	1447.922	1449.793
1450.729	1451.823	1452.142	1453.251	1454.452	1454.868	1455.485	1457.002
1458.147	1459.595	1463.355	1463.850	1525.818	1534.481	1536.028	1543.264
1579.530	1581.676	1583.510	1589.908	2954.697	2957.268	2957.804	2958.325
2958.864	2959.018	2959.418	2959.460	2959.790	2961.522	2961.704	2962.165
2962.492	2962.862	2963.024	2963.104	2964.336	2964.633	2965.408	2966.509
3013.575	3017.438	3019.100	3019.235	3020.471	3020.666	3022.048	3025.302
3026.516	3028.403	3029.530	3032.470	3032.655	3034.228	3035.596	3038.449
3043.788	3044.206	3046.263	3046.749	3047.801	3048.023	3049.424	3049.584
3049.693	3050.581	3053.342	3055.106	3056.511	3058.085	3078.605	3083.581
3083.611	3086.366	3089.995	3090.809	3092.046	3092.318	3114.323	3116.380
3117.408	3399.053						

2973.449	3002.881	3009.848	3013.008	3015.444	3016.510	3016.762	3019.206
3019.647	3022.953	3024.279	3024.611	3025.497	3025.517	3029.193	3032.175
3033.068	3035.879	3042.126	3042.933	3043.605	3045.647	3045.876	3046.294
3046.851	3047.947	3049.058	3053.942	3055.151	3055.510	3056.495	3078.175
3079.628	3083.026	3086.165	3086.947	3088.005	3090.525	3092.649	3109.418
3111.884	3404.228						

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-217.029	12.430	19.435	24.937	29.187	32.400	35.356	42.253
45.975	47.842	50.220	52.066	54.691	56.202	61.253	65.188
68.100	68.413	71.248	78.543	82.980	87.000	89.051	90.465
92.854	96.655	100.107	101.916	108.222	112.060	115.889	118.414
119.713	121.444	125.456	142.595	154.303	156.940	168.528	178.532
182.230	189.004	195.348	206.309	208.559	210.835	211.523	214.162
222.692	225.494	226.692	228.733	239.550	241.830	250.740	255.382
258.214	264.784	270.279	272.522	273.142	287.175	291.732	295.919
298.985	303.423	305.351	326.148	331.039	338.355	356.977	358.939
361.847	364.871	385.154	388.762	391.211	399.434	403.999	404.121
424.554	425.798	451.683	455.631	475.394	479.510	481.771	493.148
495.883	498.524	502.176	512.879	523.705	534.453	537.785	538.646
544.532	564.661	565.220	577.698	580.400	591.082	594.291	597.708
589.571	626.562	631.439	661.262	682.384	682.533	693.341	705.570
719.634	720.928	730.556	769.289	794.465	802.301	804.834	811.142
819.464	829.749	839.251	846.939	865.029	865.466	868.700	869.047
871.100	872.936	873.260	875.518	885.660	888.605	899.253	901.740
906.932	909.057	917.664	934.367	938.603	938.953	939.270	940.372
944.450	946.070	946.322	949.493	968.105	981.152	981.500	991.596
1000.671	1001.878	1010.157	1011.082	1012.592	1013.609	1016.049	1016.878
1017.103	1017.497	1018.856	1019.308	1019.608	1020.444	1021.171	1041.448
1046.170	1047.824	1070.874	1073.787	1094.429	1097.527	1124.450	1128.435
1142.588	1143.276	1143.748	1144.041	1147.939	1148.524	1175.753	1179.839
1201.076	1202.464	1219.329	1221.164	1226.324	1227.526	1229.177	1231.713
1237.861	1253.225	1254.874	1277.368	1282.880	1283.839	1285.288	1286.538
1290.551	1299.171	1305.509	1313.360	1313.576	1322.648	1345.327	1346.217
1349.205	1351.483	1360.996	1362.636	1363.038	1364.914	1365.171	1365.866
1366.260	1366.877	1368.760	1369.419	1370.803	1380.492	1383.827	1386.325
1391.207	1393.321	1395.299	1423.394	1423.860	1427.165	1427.252	1428.095
1432.135	1432.785	1434.190	1435.804	1435.922	1436.465	1437.049	1438.059
1438.205	1439.284	1440.768	1441.912	1444.428	1445.550	1446.006	1450.457
1451.486	1451.763	1452.264	1453.064	1453.916	1454.807	1457.209	
1457.833	1458.644	1461.887	1462.933	1516.916	1536.570	1536.941	1546.819
1575.528	1582.912	1585.014	1589.827	2959.331	2959.469	2960.287	2960.412
2956.833	2956.033	2962.592	2962.841	2963.784	2969.392	2974.772	3002.226
3007.702	3015.073	3015.484	3017.759	3019.060	3019.487	3020.764	3023.044
3023.997	3027.424	3029.766	3031.311	3031.747	3031.879	3037.902	
3038.945	3042.673	3044.761	3045.905	3047.601	3048.043	3048.144	3048.687
3053.558	3053.765	3054.128	3054.170	3058.451	3074.973	3080.354	3081.279
3081.821	3087.447	3089.503	3089.723	3094.428	3106.754	3110.131	3114.189
3165.640	3419.156						

1.282	13.042	17.594	22.638	26.875	30.297	36.519	38.770
41.745	42.879	44.996	46.249	48.424	48.678	54.405	57.861
61.185	64.132	65.085	71.138	73.694	81.629	85.438	88.719
91.027	95.766	98.437	99.026	102.965	106.911	107.335	111.040
113.164	113.772	142.413	160.285	168.760	173.266	179.111	
186.456	196.633	201.744	205.594	207.481	211.132	216.704	217.92
220.316	222.997	224.416	229.540	241.934	246.667	248.804	252.709
254.377	267.067	269.879	270.716	272.049	290.312	296.036	297.691
303.124	306.906	331.881	336.528	339.691	357.013	358.461	361.479
371.499	381.544	384.416	385.326	389.495	400.546	403.530	404.916
425.762	428.484	450.680	451.304	463.682	480.951	481.469	486.734
496.508	497.407	501.808	513.069	530.582	537.390	538.964	539.824
544.360	563.265	572.260	574.041	593.067	593.959	597.353	597.831
626.907	628.729	630.627	682.840	683.920	700.224	714.768	720.388
720.849	801.258	804.209	808.708	810.346	823.		

797.887	801.905	810.818	812.478	829.800	833.705	845.641	845.837
848.579	850.431	863.075	863.452	865.607	868.410	871.114	873.588
895.096	898.041	901.190	903.271	904.830	906.924	917.644	918.758
938.326	938.618	943.296	944.810	947.697	948.610	971.647	972.005
991.153	993.126	993.741	994.165	996.011	996.927	1000.180	1000.974
1010.491	1012.730	1013.153	1013.470	1013.711	1015.760	1016.890	1018.643
1018.912	1020.834	1037.041	1038.538	1072.103	1073.135	1094.312	1095.928
1120.313	1121.812	1135.361	1136.884	1139.209	1139.944	1144.442	1145.485
1176.612	1179.188	1193.532	1196.096	1206.468	1207.697	1210.564	1211.797
1219.479	1219.617	1236.333	1239.023	1250.204	1270.742	1284.963	1287.189
1287.984	1290.775	1292.220	1292.949	1303.624	1305.013	1305.215	1308.611
1334.827	1336.247	1338.766	1341.728	1343.150	1350.752	1351.411	1351.509
1352.064	1352.781	1355.142	1356.253	1356.729	1358.803	1359.743	1360.714
1361.379	1365.726	1373.542	1392.713	1393.486	1394.925	1397.343	1417.235
1420.218	1422.401	1426.606	1426.901	1427.659	1430.515	1430.904	1432.272
1432.291	1432.831	1434.696	1434.823	1434.933	1436.268	1437.701	1438.859
1439.939	1441.983	1442.601	1443.223	1444.729	1445.519	1447.286	1448.982
1450.152	1451.913	1452.397	1454.180	1454.819	1458.224	1458.721	1460.032
1463.565	1508.951	1509.324	1513.136	1537.364	1559.560	1564.502	1581.523
1585.016	2127.294	2295.525	2296.407	2298.844	2299.437	2326.616	2333.904
2394.294	2394.869	2395.171	2397.115	2397.465	2397.708	2397.922	2394.283
2943.124	2943.244	2949.192	2949.406	2950.032	2952.650	2976.030	2978.568
2988.979	2990.347	2994.137	2996.867	2997.661	2999.977	3000.500	3001.780
3003.626	3004.754	3006.187	3008.360	3010.116	3014.211	3016.387	3016.743
3018.984	3022.373	3023.735	3023.999	3025.000	3031.269	3031.695	3031.882
3033.367	3039.165	3041.223	3042.257	3044.452	3047.161	3055.528	3057.441
3059.033	3060.447	3061.575	3063.562	3072.170	3072.792	3098.247	3105.655

3xiii-TS

-584.962	14.609	18.402	20.543	25.692	27.590	31.211	34.801
36.615	38.023	42.105	43.964	48.309	52.748	56.251	58.420
61.002	62.317	65.475	66.261	66.691	68.983	76.457	79.232
82.244	84.876	85.617	92.281	94.441	95.293	100.511	104.508
107.741	111.925	112.698	118.071	119.816	121.107	123.304	130.263
136.629	161.891	172.029	173.684	179.820	184.141	190.448	192.994
205.241	210.113	213.687	217.803	219.092	220.612	224.744	229.943
234.635	238.939	240.277	244.341	255.341	257.408	258.476	269.652
271.168	272.466	274.669	287.628	292.024	296.992	300.447	305.665
309.601	323.437	334.828	349.669	355.848	360.086	361.832	363.292
383.665	387.293	390.786	393.056	403.875	407.276	422.029	425.082
452.518	455.398	479.184	482.088	490.304	495.000	497.162	498.224
513.277	514.039	513.344	535.401	536.763	540.419	564.243	565.509
576.781	576.984	589.777	591.665	596.742	598.063	601.880	616.997
627.669	680.825	681.485	696.796	703.618	719.800	720.429	804.661
806.074	807.172	810.837	820.598	821.856	843.933	845.429	865.717
868.979	868.876	869.335	872.379	872.812	873.725	873.969	885.609
887.624	889.838	902.842	906.517	910.366	917.982	919.660	938.925
941.067	941.458	942.428	942.761	945.081	946.004	950.946	981.410
981.485	991.813	995.218	1000.261	1002.367	1009.572	1009.986	1012.456
1013.023	1014.451	1015.498	1017.949	1017.066	1017.242	1018.305	1018.899
1019.253	1019.908	1020.816	1046.762	1047.355	1071.130	1074.822	1096.822
1098.220	1121.865	1123.858	1141.020	1141.457	1143.214	1146.667	1148.246
1150.984	1174.377	1176.315	1202.036	1202.215	1221.643	1222.555	1225.210
1229.011	1229.217	1231.591	1241.040	1250.488	1254.548	1258.559	1279.203
1282.663	1283.953	1285.249	1286.426	1288.864	1308.662	1311.499	1313.969
1315.090	1346.231	1347.112	1351.861	1352.772	1358.746	1359.342	1361.788
1363.700	1365.328	1365.502	1365.785	1368.258	1369.011	1370.528	1372.142
1372.600	1381.220	1382.222	1389.903	1392.110	1392.139	1394.978	1422.275
1425.126	1429.014	1430.161	1432.524	1433.756	1434.088	1434.193	1435.939
1437.087	1437.584	1438.571	1438.839	1439.112	1439.754	1441.363	1441.941
1443.938	1445.298	1445.516	1446.081	1451.070	1451.848	1452.759	1453.367
1454.111	1455.275	1455.872	1456.163	1457.349	1458.470	1459.988	1463.244
1466.920	1536.587	1537.869	1543.836	1545.907	1582.302	1582.562	1590.025
1591.770	1908.607	2042.565	2048.108	2048.417	2049.585	2053.145	2066.253
2095.468	2096.599	2098.168	2098.233	2098.840	2096.331	2096.658	2096.780
2096.878	2096.691	2096.472	2096.518	2096.842	2096.459	3001.598	3006.079
3007.244	3016.316	3016.637	3017.555	3017.652	3019.706	3021.470	3026.636
3028.676	3028.847	3029.333	3030.151	3032.927	3035.716	3036.768	3038.196
3040.724	3041.903	3047.318	3048.391	3049.589	3051.703	3053.946	3054.552
3055.788	3057.064	3057.265	3057.738	3059.542	3077.656	3080.453	3082.012
3085.893	3086.309	3089.799	3090.323	3093.669	3102.608	3113.322	3113.616

3xii-TS

-547.495	16.256	19.739	27.831	29.423	31.787	36.930	38.397
40.988	44.266	45.348	50.253	51.730	56.069	58.819	60.361
63.804	65.015	67.774	70.619	72.651	76.089	79.890	82.206
86.787	89.472	90.194	95.013	99.421	103.644	105.585	107.009
109.531	110.936	111.075	119.680	120.516	124.368	125.643	129.557
129.804	150.273	156.925	171.818	177.486	184.292	187.028	192.858
199.290	208.443	209.678	225.042	226.763	226.860	227.922	229.770
236.832	242.190	244.317	250.088	255.887	258.611	267.417	268.022
271.093	273.297	274.363	288.062	289.595	289.821	292.132	300.626
303.051	303.695	311.564	315.075	354.143	357.020	365.902	365.199
368.099	369.339	382.414	386.312	403.833	406.595	416.888	419.214
443.157	446.619	447.153	457.011	457.732	464.207	464.877	470.700
466.169	474.917	477.447	481.254	484.592	490.030	497.487	498.780
501.917	507.494	508.614	509.154	510.116	513.535	513.886	513.953
520.004	527.832	528.283	528.533	534.735	539.869	540.263	540.360
540.004	544.937	544.983	549.902	550.034	550.244	550.775	550.985
550.004	554.833	554.983	555.992	556.034	556.234	556.535	556.634
565.040	570.444	570.502	570.560	570.612	570.850	571.093	571.237
570.004	574.832	575.004	575.062	575.120	575.360	575.598	575.736
585.004	590.854	591.004	591.154	591.304	591.454	591.604	591.744
600.004	604.891	614.159	634.128	660.978	680.979	701.980	717.701
718.663	804.708	805.256	806.010	812.208	815.429	820.464	842.209
846.648	846.517	846.657	846.757	848.060	868.652	868.964	869.917
874.785	881.264	886.798	891.968	904.197	907.296	911.054	917.030
918.244	939.738	941.688	942.213	943.074	943.871	946.402	947.195
949.626	953.615	981.961	981.994	981.999	981.999	995.658	1000.581
1004.668	1013.413	1013.872	1016.691	1016.102	1016.763	1017.278	1017.495
1070.587	1070.891	1096.742	1096.700	1121.898	1124.058	1142.412	1142.585
1143.454	1146.785	1148.309	1150.003	1173.331	1175.770	1201.444	1201.971
1219.754	1220.738</td						

1072.316	1073.245	1095.175	1095.956	1122.824	1124.999	1142.179	1142.818
1144.683	1144.937	1149.048	1149.600	1174.970	1177.763	1202.314	1202.597
1220.524	1222.244	1226.751	1226.757	1228.488	1228.970	1237.880	1240.679
1254.034	1254.426	1278.547	1278.915	1284.082	1284.952	1285.564	1286.923
1308.437	1308.887	1310.893	1311.227	1347.022	1347.263	1351.636	1352.083
1360.527	1361.967	1363.060	1364.796	1365.082	1365.525	1367.027	1369.016
1369.511	1370.460	1370.642	1374.030	1379.715	1380.170	1391.436	1392.623
1394.618	1396.092	1421.085	1427.836	1429.257	1430.527	1432.324	1433.790
1434.001	1434.196	1435.548	1436.255	1436.911	1437.744	1439.566	1439.964
1440.621	1441.699	1444.582	1444.790	1446.079	1448.922	1450.964	1451.360
1452.825	1453.141	1454.619	1454.449	1455.523	1456.447	1456.602	1458.355
1460.840	1462.568	1465.984	1466.545	1534.519	1535.151	1545.614	1547.594
1582.377	1582.571	1589.439	1589.795	2840.003	2927.134	2950.673	2956.152
2956.372	2957.048	2958.048	2958.691	2959.278	2960.021	2960.223	2960.343
2960.740	2960.994	2961.543	2961.606	2962.491	2962.907	2964.174	2964.932
2991.842	2997.032	3017.329	3018.431	3020.798	3021.992	3023.591	3025.465
3025.728	3025.837	3028.960	3030.059	3030.650	3031.177	3032.578	3032.877
3033.961	3037.418	3042.441	3043.897	3045.444	3048.777	3048.891	3048.929
3049.549	3049.712	3050.765	3053.141	3054.475	3055.468	3059.450	3061.533
3080.001	3082.406	3082.949	3083.845	3089.613	3090.485	3091.814	3092.335
3111.592	3112.187						

1xv-TS

-1245.821	12.239	18.300	22.125	32.179	33.355	34.857	36.455
41.463	42.115	44.753	45.108	51.087	56.008	60.697	63.062
66.219	68.574	70.764	74.812	77.386	79.075	87.165	91.952
97.082	99.175	103.236	106.295	109.140	110.962	113.936	117.284
119.399	123.505	129.733	131.519	154.534	161.541	169.256	180.625
182.939	188.884	197.006	201.384	211.698	211.993	218.646	222.320
223.424	226.598	229.950	230.584	233.170	241.341	245.043	246.610
255.289	263.139	268.474	270.273	271.935	272.277	293.911	297.596
297.931	306.701	308.427	321.164	332.285	336.013	357.057	358.485
360.226	362.724	383.838	390.804	393.978	403.688	404.360	406.336
421.285	422.160	427.046	455.198	457.317	475.787	479.979	487.801
493.099	497.129	498.775	514.551	522.202	532.006	534.236	539.070
540.560	564.545	565.265	575.695	576.912	587.974	591.418	594.347
598.606	617.875	628.856	636.409	682.174	683.803	701.238	705.726
718.580	718.954	795.685	803.487	807.025	810.313	820.665	824.325
839.100	846.361	864.536	865.120	866.071	867.384	868.395	870.107
870.582	872.142	872.937	884.211	886.853	901.041	903.677	910.498
911.195	919.094	933.939	939.128	939.297	939.944	940.908	945.986
946.125	948.382	950.670	981.357	981.550	983.386	994.846	1001.164
1002.963	1012.257	1012.902	1014.078	1014.448	1016.019	1016.695	1017.643
1018.450	1018.938	1019.238	1019.950	1021.856	1022.376	1046.876	1047.601
1052.515	1069.335	1072.240	1091.224	1096.477	1122.248	1125.019	1139.875
1142.679	1142.850	1144.003	1148.045	1149.655	1167.451	1176.172	1180.006
1201.869	1201.889	1219.677	1221.115	1228.330	1228.968	1230.307	1231.065
1244.294	1244.802	1253.581	1254.597	1281.208	1281.948	1283.299	1284.504
1287.577	1289.205	1305.591	1311.041	1312.959	1313.854	1346.886	1347.073
1352.402	1353.152	1359.545	1360.992	1362.808	1363.254	1365.032	1365.384
1368.436	1368.712	1369.612	1371.186	1372.833	1381.253	1381.975	1389.356
1392.115	1392.806	1394.052	1415.031	1426.186	1429.284	1430.399	1432.577
1433.308	1433.708	1433.822	1434.488	1436.308	1437.023	1437.741	1438.629
1438.838	1439.786	1441.160	1444.094	1444.747	1444.888	1448.178	1450.231
1452.112	1452.156	1453.052	1453.575	1453.741	1454.678	1456.164	1456.692

1458.091	1458.967	1463.477	1464.887	1534.480	1536.345	1537.617	1541.306
1578.433	1582.352	1583.418	1588.516	1758.221	2952.962	2954.199	2956.733
2957.475	2958.353	2958.693	2959.429	2960.261	2960.608	2960.651	2961.032
2961.476	2961.869	2962.299	2963.507	2963.923	2964.346	2971.937	2974.717
2978.850	3011.590	3016.730	3018.962	3020.158	3020.652	3021.153	3024.123
3024.887	3025.446	3028.194	3029.473	3030.793	3032.528	3033.532	3035.687
3037.276	3039.063	3039.559	3040.203	3046.492	3048.053	3048.281	3048.901
3049.893	3049.995	3054.957	3055.869	3056.005	3056.007	3057.192	3060.426
3082.203	3082.436	3084.325	3089.659	3089.703	3091.277	3093.818	3094.610
3114.062	3116.170						

1xvi

14.249	18.610	21.861	34.811	35.672	36.875	38.354	42.559
45.844	47.019	51.627	59.934	62.987	63.747	67.244	69.936
73.001	76.820	78.159	85.866	87.674	94.617	97.550	100.028
105.543	108.057	110.382	110.947	111.606	114.248	115.573	118.774
127.595	130.579	147.941	159.995	161.256	167.190	174.782	182.286
186.538	192.136	199.148	207.874	210.908	213.330	218.258	220.901
222.455	231.948	234.508	236.808	238.000	242.081	252.781	257.863
261.026	261.489	269.785	271.831	275.706	278.789	295.781	295.920
300.402	305.849	307.810	331.629	335.047	349.306	357.182	360.332
363.114	365.012	385.588	390.457	390.886	403.843	405.064	418.399
421.232	431.100	456.115	456.642	476.130	479.887	485.881	488.057
492.212	496.118	496.955	508.582	515.570	532.937	533.863	539.634
541.074	553.821	565.326	569.940	575.908	583.948	585.324	588.046
593.568	596.650	609.275	623.118	635.136	681.623	683.014	694.762
701.878	718.816	719.126	757.383	790.278	804.969	806.047	808.888
811.062	818.680	830.266	843.058	845.397	864.872	865.371	867.558
869.045	869.454	872.677	872.858	874.264	884.572	885.835	901.891
902.839	906.631	908.197	920.680	932.179	940.395	940.820	940.884
941.558	943.633	945.036	945.381	950.252	981.479	981.771	993.716
996.357	1001.998	1004.247	1009.373	1010.467	1015.368	1016.030	1016.473
1017.294	1017.446	1018.051	1018.409	1018.453	1018.544	1021.221	1038.217
1046.395	1046.634	1070.981	1073.970	1094.287	1097.969	1122.779	1124.307
1140.547	1141.936	1144.395	1144.880	1146.079	1150.827	1170.633	1174.805
1201.331	1201.859	1218.711	1222.971	1225.101	1226.316	1227.041	1229.205
1285.074	1285.411	1307.611	1311.771	1311.988	1345.591	1346.095	
1350.525	1351.495	1359.925	1360.922	1362.513	1364.778	1364.895	1365.102
1366.513	1367.865	1368.574	1370.607	1371.166	1376.824	1382.216	1382.659
1390.308	1392.666	1394.749	1416.683	1423.304	1426.795	1428.065	1431.752
1432.528	1433.166	1434.582	1435.170	1435.902	1437.053	1438.076	1438.591
1438.867	1440.463	1442.632	1443.920	1444.108	1444.435	1447.922	1449.793
1450.730	1451.824	1452.143	1453.252	1454.453	1455.870	1455.486	1457.003
1458.149	1459.597	1463.557	1463.852	1525.818	1534.481	1536.028	1543.264
1579.531	1581.677</						

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