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Synthesis of Dimeric Indoles from Friedel–Crafts Reaction of Indoles with Ketones Catalysed by a Bronsted Acid Ionic Liquid and Their Interactions with BSA and DNA

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Experimental Section

Materials and Methods

substituted indoles, isatin, substituted isatins, Acenaphthoquinone, Indole, Phenanthrenequinone, cyclohexanone, dibromo alkanes, imidazole, and 2-chloro acetic acid, were acquired from Sigma-Aldrich, and all organic solvents were developed from commercial suppliers and used without any further purification. Analytical thin-layer chromatography (TLC) was performed using 0.25-mm silica gel-coated Kieselgel 60 F254 plates. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) spectra were recorded on a Bruker AVANCE III 400 MHz spectrometer. Chemical shifts and coupling constants are stated in parts per million (ppm) and Hertz (Hz) respectively using tetra-methyl silane (TMS) as an internal standard and the solvent resonance at (DMSO-d₆: ¹H NMR 400 MHz and ¹³C NMR 100 MHz): δ 2.49 and 39.7 ppm; The peak multiplicities are denoted as s (singlet), d (doublet), dd (doublet of doublet), m (multiplet), dt (doublet of triplet), and t (triplet). The FT-IR spectra were recorded utilising the Perkin-Elmer RX-I FTIR spectrometer in ATR mode. The UV-Vis absorption spectra were acquired using the JASCO V-670 spectrophotometer, operating at room temperature, with the solvent being DMSO and acetonitrile. JASCO fluorescence spectrophotometer (FP8200) equipped with a xenon and helium lamp using 1 cm quartz cell was utilized to measure emission fluorescence spectra by excitation at their respective absorption maxima.

General Procedure for the Synthesis of *1,3-bis(carboxymethyl)imidazolium chloride* [BCMIM][Cl] ionic liquid 4.^{1,2}

1 equivalent (5.0 g) of imidazole 1 was reacted with 2 equivalents (13.9 g) of chloroacetic acid 2 in the presence of 1.2 equivalents (3.6 g) of NaOH in acetonitrile under reflux conditions for a duration of 18 hours, resulting in the formation of 3. Subsequently, the crude ionic liquid 3 was subjected to a reaction with cold concentrated hydrochloric acid at ambient temperature for a period of 24 h. The precipitate obtained was filtered and subjected to thorough washing using acetonitrile (3 X 30 mL). The concentration of the cumulative filtrates, followed by dichloromethane and ether wash yielded the desired 1,3-bis(carboxymethyl)imidazolium chloride [BCMIM][Cl] ionic liquid 4 as white solid with 95% yield (14.9 g). The formed product was further characterized by ¹H, ¹³C NMR and FT-IR spectral techniques.

Representative General Procedure for the Synthesis of *1H*,*1''H-[3,3':3',3''-terindol]-2'(1'H)*one 7aa.

To a dried 25-mL round bottom flask, indole **5a** (0.24 g, 2 equiv, 2.04 mmol), isatin **6a** (0.15 g, 1 equiv, 1.02 mmol), and 4 mol% of [BCMIM][Cl] ionic liquid **4** were sequentially added to 5 mL of aqueous ethanol (1:1 ν/ν) and stirred at 80 °C under reflux conditions for 30 min. The progress of reaction was scrutinized by TLC. After, the completion of the reaction the resultant solid precipitate was filtered out and then washed with ether (10 mL X 2) and hexane without any additional column chromatography to obtain the desired product **7aa** in 95% yield (0.35 g). The furnished products were subjected to characterization using ¹H NMR, ¹³C NMR, FT-IR and HRMS spectra techniques and were found to be similar to those reported in the literature.

Representative General Procedure for the Synthesis of 1',1'''-(propane-1,3diyl)bis(([3,3':3',3''-terindolin]-2'-one)) 10aa.

To a dried 25-mL round bottom flask, indole **5a** (0.21 g, 4 equiv, 1.79 mmol), bis-isatin **9a** (0.15 g, 1 equiv, 0.45 mmol), and 4 mol% of [BCMIM][Cl] ionic liquid **4** were sequentially added to 5 mL of aqueous ethanol (1:1 v/v) and stirred at 80 °C under reflux conditions for 1.5 h. The progress of reaction was scrutinized by TLC. After, the completion of the reaction the resultant solid precipitate was filtered out and then washed with ether (10 mL X 2) and hexane without any additional column chromatography to obtain the desired product **10aa** in 94% yield (0.32 g). The furnished products were subjected to characterization using ¹H NMR, ¹³C NMR, FT-IR and HRMS spectra techniques.

General information

UV-Vis and FL studies

The molar extinction coefficient (ϵ) was estimated using Beer-Lambert's law using equation 1.

$$A = \varepsilon cl \qquad \dots \dots (eqn. i)$$

where, A - absorbance, ε - molar adsorption coefficient, *c* - concentration of the sample, and *l* - distance travelled by the light through the sample.

The Stoke's Shift was determined using the following equation (ii):

Computational details

Calculations employing density functional theory (DFT) were executed to gain insight into both the structural and functional characteristics. The computations were carried out using Gaussian 16W software, employing the density functional theory (DFT) methodology.³ The configurations of compounds in the gaseous phase were refined utilizing Becke's threeparameter and Lee–Yang–Parr functional (B3LYP).⁴ Throughout all computations, the B3LYP functional was coupled with the 6-31G (d, p) basis set.⁵ TD-DFT single-point calculations were performed at the B3LYP/6-31G (d, p) level of theory on the optimized configurations in the gaseous phase. The molecular visualization tool Gauss View 6.1 facilitated the determination of electronic structures and frontier molecular orbital architectures.⁶

Molecular docking studies with protein BSA

To investigate binding interactions and affinities, the 3D structures of the produced derivatives 7 were docked with the BSA protein target. This study made use of MGL TOOL 1.5.7 and the AutoDock Vina algorithm (ADT).⁷ The crystal structure of BSA (PDB ID 4F5S) was acquired from the Protein Data Bank (www.rcsb.org/pdb).^{8,9} After obtaining the protein, Gasteiger charges and polar hydrogens were included, while water molecules were removed to avoid unwanted interactions. In addition, we performed optimization of rotatable bonds. The ligands, which were optimized using Gaussian 6.1, were saved in PDB format. AutoDock Tools were subsequently utilized to create distinct files for the protein and ligands. A binding site was delineated by constructing a grid box around the active residue sites of the protein, with a spacing of 0.375 Å. The grid dimensions were set to $80 \times 80 \times 80$ points, with coordinates established at 72.821, 26.360, and 91.719 Å in the X, Y, and Z directions, respectively. The files were converted to pdbqt format in the last stage. By employing an exhaustiveness value of eight, AutoDock produced a total of nine significant conformers for each ligand and protein separately. The orientation of each conformer was evaluated using PyMOL, a molecular graphics application (The PyMOL Molecular Graphics System, Version 2.0, Schrödinger, LLC). The most favorable binding configuration was selected for each docking situation, based on the docked conformation with the lowest energy as calculated by the AutoDock scoring technique. In addition, BIOVIA DSV was used to improve the imaging of the docked ligand complexes for the investigation of numerous molecular interactions.¹⁰

Molecular docking studies with DNA

The binding affinities of the synthesized derivatives **7** for DNA were predicted by performing molecular docking using AUTODOCK 4.2 and MGL TOOL 1.5.7. The DNA structure with the PDB id 1BNA was obtained from the Protein Data Bank (www.rcsb.org/pdb) at a resolution of 1.60 Å.¹¹ The water molecules were removed and Gasteiger charges were incorporated. The synthesized derivatives **7** were generated using ChemDraw 21.0.0 and then converted to PDB format using openbabel. Later, the target (DNA) and ligands were created using AutoDock Tools to generate the necessary files. Subsequently, the ligands were positioned into the DNA constructs using certain grid parameters located at their centers. A total of fifty orientations were produced for each ligand. The results, which include the surface analyses of the graphical representations, are displayed using PyMOL (PyMOL Molecular Graphics System, Version 1.3, Schrodinger, LLC). The binding mode chosen for each docking scenario was the docked conformation with the lowest energy, as determined by the Autodock scoring system.

Protein binding studies

Most proteins found in blood plasma are serum albumin proteins, which play a critical role in the transportation and metabolism of drugs. The ligands' interactions with BSA were investigated by intrinsic tryptophan emission quenching assays. The emission intensity of BSA at a wavelength of 342 nm drops gradually as the concentration of ligands increases, providing evidence that the ligands are interacting with BSA. The ligand solutions were gradually introduced into a solution of BSA (2 μ M) in a 5 mM Tris–HCl/NaCl buffer (pH 7.2). The reduction in the emission signals at 342 nm ($\lambda_{ex} = 295$ nm) was then measured. The quenching constant (K_{BSA}) was determined by applying the Stern-Volmer equation. The Stern-Volmer plots were constructed by plotting the ratio of I₀/I against the concentration of the ligand. The corrected fluorescence data was used, considering the impact of dilution. The data were linearly fitted using equation (iii):

$$I_0/I = 1 + K_{BSA}[Q] = 1 + K_q \tau_0[Q]$$
eqn (iii)

where, I_0 and I - emission intensities of BSA in absence and presence of quencher with concentration [Q], respectively,

Kq - quenching rate constant, and

 $τ_0$ - average lifetime of tryptophan in BSA without quencher (reported as 1 x 10⁻⁸ s). The quenching constant (*K*_{BSA}) was deduced using Origin Pro 2022 software.

For static quenching interactions, the binding constant (K) and the number of binding sites (n) was determined using

the Scatchard equation (iv):⁷

$$\log \frac{I_0 - I}{I} = \log k + n \log[Q] \qquad \dots \qquad \text{eqn (iv)}$$

DNA binding studies

The DNA binding assay was performed by using UV-vis spectroscopy with ligands **7af**, **7ai**, **7aj**, and **7ak**, at concentration 4×10^{-5} M in Tris-HCl buffer (pH 7.2).¹² DNA solution with concentration 2.87×10^{-4} M was prepared. Later, the absorption was recorded by an incremental addition of DNA (20-100 μ M) to each ligand. The intrinsic DNA binding constant (K_b) was determined using the equation eq.(v)

$$\frac{[DNA]}{\varepsilon_{a} - \varepsilon_{f}} = \frac{[DNA]}{\varepsilon_{b} - \varepsilon_{f}} + \frac{[DNA]}{K_{b} (\varepsilon_{a} - \varepsilon_{f})} \qquad \dots eqn (v)$$

Where, [DNA] - concentration of DNA in the base pairs, ε_a - apparent extinction coefficient observed for the ligand, ε_b - extinction coefficient of the ligand when fully bound to DNA, ε_f is the extinction of the ligand in its free form. The liner plot data [DNA]/($\varepsilon_a - \varepsilon_f$) vs. [DNA] was obtained using Origin Lab version 8.5. The intrinsic binding constant (K_b) value is the ratio of slope to the intercept of the linear fit.

Ethidium bromide displacement assay

The EtBr displacement experiments were conducted to elucidate the binding mechanism between each ligand and DNA.¹³ The incorporation of EtBr into DNA results in a strong fluorescence emission because of the generation of EtBr-DNA complex. When the ligand molecule inserts itself between the base pairs of DNA, the amount of binding locations on DNA that are accessible to EtBr reduces, leading to a decrease in the fluorescence intensity. The value of K_{SV} (Stern-Volmer quenching constant) was calculated from the following eq. (vi):

$$I_0/I = 1 + K_{sv}[Q] \qquad \dots eqn (vi)$$

where, I₀ and I - emission intensities of EtBr-DNA in absence and presence of ligand with concentration [Q], respectively.

Spectral characterization data



<u>1,3-bis(carboxymethyl)imidazolium chloride [BCMIM][Cl]</u> 4.^{1,2} White solid; Yield: 95% (14.9011g); mp (°C): 225-227 [226-228];^{1,2} FT-IR (ATR mode, cm⁻¹): 2869, 1730, 1564, 1403, 1171, 753, 652.

¹H NMR (400 MHz, D₂O, ppm) δ 8.93 (s, 1H), 7.56 (d, *J* = 1.4 Hz, 2H), 5.14 (s, 4H). ¹³C NMR (100 MHz, D₂O, ppm) δ 169.97, 138.21, 123.55, 50.36. DEPT-135 NMR (100 MHz, D₂O, ppm) δ 138.2, 123.5, 50.4;



<u>1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7aa. Beige-cream solid; Yield: 95%; mp (°C): >300 [312];^{14,15} FT-IR (ATR, cm⁻¹): 3381, 3312, 1705, 1614, 1467, 1247, 1173, 738, 608, 553; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.86 (s, 2H), 10.50 (s, 1H), 7.28 (d, J = 8.1 Hz, 2H), 7.16 (d, J = 7.8 Hz, 4H), 6.96 – 6.91 (m, 3H), 6.85 (t, J

= 7.5 Hz, 1H), 6.78 (s, 2H), 6.72 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.2, 141.8, 137.4, 135.1, 128.3, 126.18, 125.4, 124.7, 121.9, 121.4, 121.2, 118.7, 114.8, 112.1, 110.0, 53.0.



<u>5'-chloro-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7*ab*. Peachy-pink solid; Yield: 94%; mp (°C): 293-295 [294-296];¹⁶ FT-IR (ATR, cm⁻¹):3347, 1700, 1476, 1171, 1104, 734, 642, 550, 491, 426; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.99 (s, 1H), 8.36 (d, *J* = 8.1 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.90 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.6

Hz, 1H), 7.55 (d, *J* = 6.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.02 – 6.98 (m, 4H), 6.85 (d, *J* = 2.0 Hz, 2H), 6.74 (t, *J* = 7.5 Hz, 2H). ¹³**C NMR (100 MHz, DMSO-d₆, ppm)** δ 203.1, 144.3, 140.1, 137.4, 132.5, 131.9, 130.9, 129.5, 129.3, 126.2, 125.1, 124.6, 122.7, 122.2, 121.3, 121.1, 118.8, 115.3, 114.9, 112.1, 58.1.



<u>5'-fluoro-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7*ac*. Off-white solid; Yield: 95%; mp (°C): 291-293 [289-290];¹⁷ FT-IR (ATR, cm⁻¹): 3436, 3387, 3315, 1695, 1480, 1173, 734, 677, 575, 505, 428;¹H NMR (400 MHz, DMSO-d₆, ppm) δ 11.01 (d, *J* = 1.5 Hz, 2H), 10.64 (s, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H),

7.11 – 6.97 (m, 6H), 6.90 (d, J = 2.4 Hz, 2H), 6.82 (t, J = 7.4 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.1, 158.3 (d, J_{C-F} = 231.6 Hz, *ipso*-C), 138.0, 137.4, 136.8 (d, J_{C-F} = 8.3

Hz), 126.0, 124.9, 121.5, 121.1, 118.8, 114.7 (d, *J*_{C-F} = 23.7 Hz), 114.1, 112.9 (d, *J*_{C-F} = 24.7 Hz), 112.1, 110.8 (d, *J*_{C-F} = 7.9 Hz), 53.6.



<u>5'-bromo-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ad. Beige-cream solid; Yield: 93%; mp (°C): >300 [310-312];¹⁴ FT-IR (ATR, cm⁻¹): 3353, 1690, 1472, 1104, 814, 737, 637, 547, 491, 427; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 11.03 (d, *J* = 1.7 Hz, 2H), 10.77 (s, 1H), 7.44

- 7.42 (m, 1H), 7.38 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 1.8 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H),
7.04 (t, J = 7.3 Hz, 2H), 6.98 (d, J = 8.3 Hz, 1H), 6.90 (d, J = 2.5 Hz, 2H), 6.83 (t, J = 7.5 Hz, 2H).
¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.7, 141.2, 137.5, 137.4, 131.2, 127.8, 125.9, 124.9, 121.6, 120.9, 118.9, 113.9, 113.6, 112.2, 112.2, 53.3.



<u>5'-nitro-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ae. Coral-red solid; Yield: 94%; mp (°C): >300 [293-295];¹⁸ FT-IR (ATR, cm⁻¹): 3382, 1706, 1619, 1533, 1340, 1090, 832, 744, 546; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 11.34 (s, 1H), 11.10 (s, 2H), 8.25 (dd, J =

8.6, 2.2 Hz, 1H), 7.98 (d, *J* = 2.1 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.20 (m, 3H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.97 (d, *J* = 2.2 Hz, 2H), 6.84 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.4, 148.3, 142.7, 137.5, 135.7, 125.9, 125.9, 125.1, 121.7, 120.8, 120.6, 119.0, 113.3, 112.3, 110.4, 53.0.



<u>5'-methyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7af. Apricot-pink solid; Yield: 93%; mp (°C): >300 [321-322];¹⁹ FT-IR (ATR, cm⁻¹): 3377, 3317, 1704, 1488, 1191, 1101, 737, 574, 425; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.94 (d, J = 1.8 Hz, 2H), 10.49 (s, 1H),

7.36 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.05 – 7.00 (m, 4H), 6.89 – 6.78 (m, 5H), 2.19 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.2, 139.4, 137.4, 135.1, 130.7, 128.6, 126.2, 125.9, 124.8, 121.37, 121.3, 118.7, 114.9, 112.0, 109.8, 53.1, 21.3.



<u>5'-methoxy-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ag. Lightbrown solid; Yield: 93%; mp (°C): 292-294 [301-303];^{18,20} FT-IR (ATR, cm⁻¹): 3359, 1685, 1487, 1199, 1016, 787, 740, 590, 424; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.95 (s, 2H), 10.44 (s, 1H),

7.35 (d, J = 8.1 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.02 (t, J = 7.5 Hz, 2H), 6.92 – 6.87(m, 3H), 6.82 – 6.79 (m, 4H), 3.61 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.1, 155.1,

137.4, 136.4, 135.2, 126.1, 124.8, 121.4, 121.2, 118.7, 114.7, 112.6, 112.5, 112.1, 110.3, 55.8, 53.5.



<u>7'-chloro-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ah. Pale-pink solid; Yield: 92%; mp (°C): 290-292 [288-289];²¹ FT-IR (ATR, cm⁻¹): 3414, 1724, 740, 483; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 11.05 (s, 1H), 11.03 (d, J = 1.6 Hz, 2H), 7.37 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.1 Hz, 1H), 7.23 7.19 (m, 3H), 7.03 (t, J = 7.5 Hz, 2H), 6.97 (t,

J = 7.8 Hz, 1H), 6.87 (d, *J* = 2.4 Hz, 2H), 6.82 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.1, 155.1, 137.4, 136.4, 135.2, 126.1, 124.8, 121.4, 121.2, 118.7, 114.7, 112.6, 112.5, 112.1, 110.3, 55.8, 53.5.



<u>2'-oxo-1',2'-dihydro-1H,1"H-[3,3':3',3"-terindole]-5,5"-</u> <u>dicarbonitrile</u> 7ba.Lemom-yellow solid; Yield: 90%; mp (°C): >300 [303-305];²² FT-IR (ATR, cm⁻¹):1720, 1600, 1280, 1010, 831, 776, 410; ¹H NMR (400 MHz, DMSO-d₆, ppm) 11.66 (d, J =

1.5 Hz, 2H), 10.84 (s, 1H), 7.59 – 7.57 (m, 4H), 7.41 (dd, *J* = 8.6, 1.3 Hz, 2H), 7.33 – 7.26 (m, 2H), 7.12 (d, *J* = 2.4 Hz, 2H), 7.08 – 6.99 (m, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 178.7, 141.6, 139.3, 133.6, 129.0, 127.5, 126.2, 125.7, 125.5, 124.3, 122.6, 121.1, 115.5, 113.9, 110.6, 101.1, 52.5.



<u>5,5"-dimethoxy-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ca. Offwhite solid solid; Yield: 88%; mp (°C): 291-293 [290-293];²³ FT-IR (ATR, cm⁻¹): 3386, 3314, 1683, 1474, 1207, 1019, 804, 759, 645;

¹H NMR (400 MHz, DMSO-d₆, ppm) 10.80 (d, *J* = 1.6 Hz, 2H), 10.61 (s, 1H), 7.27 – 7.21 (m, 4H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 2.4 Hz, 2H), 6.72 – 6.70 (m, 4H), 3.53 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 179.3, 152.9, 141.9, 135.0, 132.7, 128.3, 126.6, 125.7, 125.4, 121.9, 114.1, 112.6, 110.9, 109.9, 103.8, 55.6, 53.0.



<u>2,2"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7da. Off-white solid; Yield: 90%; mp (°C): 296-298 [286-287];^{14,21,24} FT-IR (ATR, cm⁻¹): 3394, 1704, 1621, 1471, 1304,1070, 923, 752, 608, 521; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.87 (s, 2H), 10.33 (s, 1H), 7.20 – 6.27 (m, 12H),

3.38 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 179.1, 142.0, 135.3, 134.6, 133.9, 129.5, 127.1, 125.4, 122.2, 120.3, 119.6, 118.6, 110.7, 110.1, 109.9, 76.3, 13.8.



<u>5,5"-dibromo-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ea. White solid; Yield: 93%; mp (°C): >300 [320-321];^{14,21} FT-IR (ATR, cm⁻¹): 3418, 3269, 1713, 1468, 1099, 885, 798, 750, 548, 486; ¹H NMR (400 MHz,

DMSO-d₆, ppm) δ 11.16 (d, *J* = 1.8 Hz, 2H), 10.67 (s, 1H), 7.30 – 7.28 (m, 4H), 7.22 – 7.18 (m, 1H), 7.11 – 7.07 (m, 3H), 6.96 – 6.90 (m, 2H), 6.84 (d, *J* = 2.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.91, 141.68, 136.16, 134.06, 128.74, 127.73, 126.46, 125.35, 124.10, 123.13, 122.30, 114.31, 114.27, 111.53, 110.31, 52.62.



5,5"-dibromo-5'-fluoro-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one 7ec. White solid; Yield: 94%; mp (°C): >300 [332-224];²⁵ FT-IR (ATR, cm⁻¹): 3387, 3306, 1690, 1483, 1452, 1174, 885, 793, 588; ¹H NMR (400 MHz, DMSO-d₆, ppm) 11.28 (d, *J* = 1.8 Hz, 2H), 10.79 (s, 1H),

7.39 – 7.37 (m, 4H), 7.19 – 7.10 (m, 3H), 7.05 – 6.99 (m, 2H), 6.97 (d, J = 2.5 Hz, 2H). ¹³C **NMR (100 MHz, DMSO-d₆, ppm)** 178.9, 158.45 (d, $J_{C-F} = 238.3$ Hz, *ipso-*C), 137.9, 136.2, 135.7 (d, $J_{C-F} = 7.4$ Hz), 127.6, 126.6, 124.2, 122.9, 115.2 (d, $J_{C-F} = 23.4$ Hz), 114.4, 113.7, 112.9 (d, $J_{C-F} = 24.6$ Hz), 111.6, 111.2 (d, $J_{C-F} = 8.5$ Hz), 53.1.



 5,5',5''-tribromo-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one
 7ed.

 Merino-white solid; Yield: 92%; mp (°C): >300 [>300];²¹ FT-IR
 (ATR, cm⁻¹): 3374, 1694, 1453, 1168, 1104, 884, 796, 623, 551, 513.

 ¹H NMR (400 MHz, DMSO-d6, ppm) δ 11.29 (d, J = 1.9 Hz, 2H),

10.91 (s, 1H), 7.47 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.40 7.36 (m, 4H), 7.26 (d, *J* = 1.8 Hz, 1H), 7.18 (dd, *J* = 8.6, 1.8 Hz, 2H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.96 (d, *J* = 2.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.5, 141.1, 136.4, 136.2, 131.6, 127.9, 127.5, 126.7, 124.7, 124.3, 123.3, 122.9, 114.5, 113.9, 113.5, 112.4, 111.7, 52.8.



<u>1,1"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7<i>fa. Biege-white solid; Yield: 91%; mp (°C): >300 [>300];²⁰ FT-IR (ATR, cm⁻¹): 1697, 1470, 1330, 1208, 735, 681, 633, 427; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.64 (s, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.22 (m, 4H), 7.09 (t, *J* = 7.4 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 7.4 Hz, 1H), 6.94

- 6.90 (m, 2H), 6.85 (t, J = 7.5 Hz, 2H), 3.70 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm)
δ 179.0, 141.7, 137.8, 134.9, 128.9, 128.4, 126.5, 125.4, 122.1, 121.6, 121.4, 1189, 113.9, 110.2, 110.1, 52.9, 32.8.



5'-fluoro-1,1"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one7fb.White solid; Yield: 92%; mp (°C): >300 [>300]; 20 FT-IR (ATR, cm $^{-1}$):3365, 1685, 1480, 1179, 865, 795, 746, 673, 594, 432; 1 H NMR (400MHz, DMSO-d₆, ppm) δ 10.66 (s, 1H), 7.39 (d, J = 8.2 Hz, 2H), 7.23 (d,

J = 8.0 Hz, 2H), 7.11 – 7.03 (m, 4H), 6.99 – 6.96 (m, 1H), 6.94 (s, 2H), 6.86 (t, J = 7.5 Hz, 2H), 3.72 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.9, 158.3 (d, $J_{C-F} = 241.5$ Hz, *ipso*-C), 137.9, 137.8, 136.6 (d, $J_{C-F} = 7.4$ Hz), 129.1, 126.3, 121.6, 121.2, 119.0, 114.8 (d, $J_{C-F} = 23.3$ Hz),113.2, 112.9 (d, $J_{C-F} = 24.0$ Hz), 110.9 (d, $J_{C-F} = 8.1$ Hz), 110.3, 53.4, 32.8.



<u>5'-bromo-1,1"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7fd. Ivory-cream solid; Yield: 91%; mp (°C): >300 [325-327];^{24,26} FT-IR (ATR, cm⁻¹): 1715, 1613, 1471, 750, 732, 554, 431; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.71 (s, 1H), 7.34 – 7.31 (m, 3H), 7.24 (d, J = 1.6 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 7.04 – 7.00 (m, 2H), 6.91 –

6.86 (m, 3H), 6.79 (t, *J* = 7.5 Hz, 2H), 3.64 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.5, 141.1, 137.8, 137.3, 131.3, 129.0, 127.8, 126.3, 121.7, 121.2, 119.1, 113.7, 113.1, 112.2, 110.4, 53.1, 32.8.



<u>5,5"-dibromo-1,1"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-2'(1'H)-one</u> 7ga. White solid; Yield: 95%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 3385, 1721, 1468, 1193, 788, 768, 660, 565, 542; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.76 (s, 1H), 7.41 – 7.37 (m, 4H), 7.27 (t, *J* = 7.6

Hz, 1H), 7.22 (dd, *J* = 8.7, 1.8 Hz, 2H), 7.17 (d, *J* = 7.3 Hz, 1H), 7.03 – 6.96 (m, 2H), 6.96 (s, 2H), 3.72 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.7, 141.6, 136.6, 133.9, 130.6, 128.8, 127.9, 125.4, 124.2, 123.2, 122.4, 113.3, 112.7, 111.9, 110.3, 52.5, 33.1. HRMS(ESI): Calcd. for C₂₆H₁₉Br₂N₃O [M+H]⁺ m/z: 547.9973; Found, [M+H]⁺: 547.9972.



<u>5,5"-dibromo-5'-fluoro-1,1"-dimethyl-1H,1"H-[3,3':3',3"-terindol]-</u> <u>2'(1'H)-one</u> 7gc. White solid; Yield: 89%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 3387, 3306, 1690, 1483, 1452, 1174, 885, 793, 588; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.80 (s, 1H), 7.43 (s, 1H), 7.40

-7.39 (m, 3H), 7.24 (dd, J = 8.7, 1.8 Hz, 2H), 7.13 (td, J = 9.1, 2.6 Hz, 1H), 7.04 -6.98 (m, 4H), 3.73 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 178.7, 158.5 (d, $J_{C-F} = 238.7$ Hz, *ipso*-C), 137.8, 136.6, 135.6 (d, $J_{C-F} = 7.6$ Hz), 130.8, 127.7, 124.3, 123.1, 115.3 (d, $J_{C-F} = 23.7$

Hz), 113.2, 112.9, 112.7 (d, $J_{C-F} = 4.4$ Hz), 111.7 (d, $J_{C-F} = 8.2$ Hz), 111.2, 52.9, 33.1. HRMS(ESI): Calcd. for C₂₆H₁₈Br₂FN₃O [M+H]⁺ m/z: 565.9879; Found, [M+H]⁺: 565.9881.



<u>5,5',5''-tribromo-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-</u> <u>one</u> 7gd. White solid; Yield: 93%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 1725, 1471, 1285, 1201, 870, 820, 788, 688, 545; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.92 (s, 1H), 7.45 – 7.37 (m, 5H), 7.25 – 7.23 (m,

3H), 7.01 6.99 (m, 3H), 3.73 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 178.3, 140.9, 136.7, 136.3, 131.7, 130.7, 127.9, 127.7, 124.3, 123.0, 114.1, 112.8, 112.5, 112.4, 111.9, 52.7, 33.1. HRMS(ESI): Calcd. for C₂₆H₁₈Br₃N₃O [M+H]⁺ m/z: 625.9078; Found, [M+H] ⁺: 625.9080.



<u>3,3'-(cyclohexane-1,1-diyl)bis(1H-indole)</u> 7*ai*. Tortilla solid; Yield: 86%; mp (°C): 121-123 [76-78];²⁷ FT-IR (ATR, cm⁻¹): 3406, 2289, 2930, 1454, 1414, 1334, 1099, 738, 581, 493, 456; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.74 (s, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.32

(s, 2H), 7.26 (d, *J* = 8.1 Hz, 2H), 6.90 (t, *J* = 7.4 Hz, 2H), 6.70 (t, *J* = 7.4 Hz, 2H), 2.51 – 2.45 (m, 5H), 1.60 (s, 3H), 1.52 (s, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 137.4, 126.4, 122.6, 122.5, 121.0, 120.5, 117.9, 111.7, 39.0, 37.1, 26.9, 23.1.



<u>3,3'-(cyclohexane-1,1-diyl)bis(5-bromo-1H-indole)</u> 7ei. Darkyellow solid; Yield: 81%; mp (°C): 225-227 [223-224];²⁵ ¹H NMR (400 MHz, DMSO-d₆, ppm) 11.10 (s, 2H), 7.48 (d, J =31.9 Hz, 4H), 7.31 (s, 2H), 7.08 (s, 2H), 2.39 (s, 4H), 1.58 – 1.49

(m, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 136.2, 128.1, 124.3, 123.3, 122.8, 122.0, 113.9, 110.9, 38.7, 37.2, 26.8, 22.9.



<u>3,3'-(cyclohexane-1,1-diyl)bis(1-methyl-1H-indole)</u> 7*fi*. Creamwhite solid; Yield: 92%; mp (°C): 211-213 [206-208];²⁸ FT-IR (ATR, cm⁻¹): 2938, 1484, 1329, 1245, 816, 740, 561, 434; ¹H NMR (400 MHz, DMSO-d₆, ppm) 7.37 (d, J = 8.0 Hz, 2H), 7.30 (s, 2H), 7.27 (d, J = 8.2 Hz, 2H), 6.96 (t, J = 7.5 Hz, 2H), 6.74 (t, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5

2H), 3.74 (s, 6H), 2.42 – 2.40 (m, 4H), 1.58 – 1.49 (m, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 137.7, 127.2, 126.7, 121.6, 121.1, 120.7, 118.1, 109.9, 39.0, 37.2, 32.8, 26.8, 22.9.



2.2-di(1H-indol-3-yl)acenaphthylen-1(2H)-one 7aj. Lemon-yellow solid; Yield: 93%; mp (°C): 241-243 [242-244];¹⁶ FT-IR (ATR, cm⁻¹): 3416, 3357, 1682, 1339, 1101, 778, 737, 555; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 10.99 (s, 1H), 8.36 (d, *J* = 8.1 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.90 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 6.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.02 – 6.98 (m, 4H), 6.85

(d, *J* = 2.0 Hz, 2H), 6.74 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 203.1, 144.3, 140.1, 137.4, 132.5, 131.9, 130.9, 129.5, 129.3, 126.2, 125.1, 124.6, 122.7, 122.2, 121.5, 121.1, 118.8, 115.3, 114.9, 112.2, 58.1.



2,2-bis(5-methoxy-1H-indol-3-yl)acenaphthylen-1(2H)-one 7cj.
Lemon-yellow solid; Yield: 90%; mp (°C): 281-283 [284-286];¹⁶
FT-IR (ATR, cm⁻¹): 3395, 3367, 1698, 1481, 1231, 1028, 777, 613, 512; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.80 (s, 2H), 8.36 (d, J = 8.1 Hz, 1H), 8.02 - 8.00 (m, 2H), 7.89 (t, J = 7.5 Hz, 1Hz, 1Hz)

1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 6.9 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 2H), 6.86 (s, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.42 (s, 2H), 3.40 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 203.2, 152.9, 144.3, 140.2, 132.7, 132.5, 132.2, 130.9, 129.5, 129.3, 126.7, 125.9, 124.5, 122.5, 122.2, 114.7, 112.6, 110.9, 103.7, 58.1, 55.5.



2,2-bis(2-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one7dj.Tortilla-brown solid; Yield: 92%; mp (°C): 291-293 [292-293]; 29 FT-IR (ATR, cm⁻¹): 3383, 3340, 1712, 1459, 1022, 781, 741, 521; ¹HNMR (400 MHz, DMSO-d₆, ppm) 10.84 (d, J = 9.7 Hz, 2H), 8.27 (d,J = 8.1 Hz, 1H), 7.96 – 7.95 (m, 2H), 7.80 (t, J = 7.6 Hz, 1H), 7.60 –7.56 (m, 1H), 7.36 (d, J = 7.0 Hz, 1H), 7.15 – 7.12 (m, 2H), 6.83 – 6.77

(m, 2H), 6.54 – 6.44 (m, 3H), 6.25 (d, *J* = 8.1 Hz, 1H), 1.77 (s, 3H), 1.71 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 202.5, 144.5, 140.3, 135.5, 135.5, 134.2, 134.1, 133.9, 133.8, 133.2, 132.1, 130.8, 129.4, 129.2, 128.1, 127.8, 124.6, 122.8, 122.3, 120.3, 120.2, 120.0, 119.91, 118.5, 118.4, 111.4, 110.9, 110.5, 57.9, 13.89, 13.8.



<u>2,2-bis(5-bromo-1H-indol-3-yl)acenaphthylen-1(2H)-one</u> 7ej. Lightyellow solid; Yield: 91%; mp (°C): >300 [>300];²⁹ FT-IR (ATR, cm⁻¹): 3428, 3338, 1076, 1455, 1093, 782, 663, 605, 460, 418; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 11.28 (s, 2H), 8.39 (s, 1H), 8.06 - 8.04 (m, 2H), 7.92 (t, J = 7.6 Hz, 1H), 7.74 (t, J = 7.6 Hz, 1H), 7.54 (d, J = 6.9 Hz, 1H), 7.37 (d, J = 9.1 Hz, 2H), 7.15 (d, J = 6.3 Hz, 4H), 6.95 (d, J = 2.3 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 202.8, 143.3, 140.0, 136.2, 132.9, 131.5, 130.9, 129.6, 129.5, 127.9, 126.8, 124.9, 124.2, 123.1, 122.9, 122.3, 114.7, 114.4, 111.6, 57.7.



<u>2,2-bis(1-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one</u> 7*fj*. Lightyellow solid; Yield: 87%; mp (°C): >300 [>300];²⁹ FT-IR (ATR, cm⁻¹):1715, 1463, 1330, 977, 785, 735, 560, 431; ¹H NMR (400 MHz, DMSO-d₆, ppm) δ 8.36 (d, J = 8.0 Hz, 1H), 8.01 (d, J = 7.6 Hz, 2H), 7.90 (t, J = 7.5 Hz, 2H), 7.69 (t, J = 7.6 Hz, 1H), 7.56 (d, J = 6.8 Hz, 1H), 7.37 (d, J = 8.1 Hz, 2H), 7.06 (dd, J = 14.6, 7.6 Hz, 6H), 6.88 (s,

3H), 6.79 (t, *J* = 7.4 Hz, 3H), 3.67 (s, 11H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 202.9, 144.2, 139.9, 137.8, 132.6, 131.9, 130.9, 129.6, 129.4, 129.3, 126.6, 124.6, 122.8, 122.2, 121.6, 121.2, 119.0, 114.4, 110.3, 57.9, 32.8.



2,2-bis(5-bromo-1-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one 7gj. Pastel-cream solid; Yield: 94%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 1724, 1473, 1283, 1208, 826, 793, 423; ¹H NMR (400 MHz, DMSO-d₆, ppm) 8.40 (d, J = 8.1 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.94 – 7.90 (m, 1H), 7.76 – 7.72 (m, 1H), 7.53 (d, J = 6.9 Hz, 1H), 7.40

(d, *J* = 8.7 Hz, 2H), 7.21 (dd, *J* = 8.7, 1.8 Hz, 2H), 7.15 (d, *J* = 1.6 Hz), 6.98 (s, 2H), 3.69 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) δ 202.6, 143.1, 139.9, 136.7, 132.9, 131.4, 130.9, 130.9, 129.7, 129.6, 128.0, 124.9, 124.3, 123.2, 123.0, 122.3, 113.7, 112.8, 111.9, 57.6, 33.1. HRMS(ESI): Calcd. for C₃₀H₂₀Br₂N₂O [M+H]⁺ m/z: 583.0021; Found, [M+H]⁺: 583.0026.



<u>10,10-di(1H-indol-3-yl)phenanthren-9(10H)-one</u> 7gk. Yellow solid; Yield: 87%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 3333, 1671, 1560, 1449, 1267, 1102, 733, 630, 459; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.92 (s, 2H), 8.24 (dd, J = 21.3, 7.5 Hz, 2H), 7.72 – 7.65 (m, 2H), 7.46 (t, J = 6.9 Hz, 2H), 7.35 (d, J = 7.7 Hz, 1H), 7.03 (t, J = 7.0 Hz, 1H), 6.93 (t, J = 9.8 Hz, 1H), 6.81 (t, J =

7.1 Hz, 1H), 6.43 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 178.7, 159.6, 157.3, 137.8, 136.6, 135.6, 135.6, 130.8, 127.7, 124.3, 123.1, 115.4, 115.2, 113.2, 112.9, 112.7, 112.7, 111.9, 111.3, 111.2, 52.9, 33.1. HRMS(ESI): Calcd. for C₃₀H₂₀N₂O [M+Na]⁺ m/z: 447.1473; Found, [M+Na]⁺: 447.1475.



10,10-bis(5-methoxy-1H-indol-3-yl)phenanthren-9(10H)-one

7*ck*. Lemon-yellow solid; Yield: 91%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 1720, 1600, 1280, 1010, 894, 831, 776; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.78 (s, 2H), 8.23 (dd, *J* = 24.8, 7.9

Hz, 2H), 7.74 (d, J = 7.6 Hz, 1H), 7.66 (t, J = 7.5 Hz, 1H), 7.47 (t, J = 7.4 Hz, 1H), 7.35 (t, J = 7.4 Hz, 1H), 7.27 – 7.25 (m, 3H), 6.94 (d, J = 7.6 Hz, 1H), 6.71 (d, J = 7.2 Hz, 2H), 6.45 (s, 2H), 6.36 (s, 2H), 3.50 (s, 6H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 196.7, 153.1, 141.3, 136.6, 134.5, 132.7, 130.7, 130.4, 130.2, 129.3, 128.8, 128.3, 127.9, 127.4, 126.8, 124.6, 123.7, 115.1, 112.8, 110.8, 103.8, 57.1, 55.8. HRMS(ESI): Calcd. for C₃₂H₂₄N₂O₃ [M+Na]⁺ m/z: 507.1685; Found, [M+Na]⁺: 507.1685.



 $\frac{1',1'''-(propane-1,3-diyl)bis(([3,3':3',3''-terindolin]-2'-one))}{10aa}.$ Brick-red solid; Yield: 94%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 3402, 1693, 1338, 1090, 734; ¹H NMR (400 MHz, DMSO-d6, ppm) 10.90 (d, J = 1.8 Hz, 4H), 7.28 (d, J = 8.1 Hz, 4H), 7.22 (d, J = 7.0 Hz, 2H), 7.15 – 7.08 (m, 6H), 6.95 – 6.89 (m, 8H), 6.78 (d, J = 2.4 Hz, 2H), 6.69 (t, J = 7.5 Hz, 4H), 1.98 – 1.92 (m, 4H), 1.10 (t, J = 7.1 Hz, 2H). ¹³C NMR (100 MHz, DMSO-d6, ppm) 177.4, 142.2, 137.4, 134.3, 128.5,

126.1, 125.3, 124.8, 122.6, 121.5, 121.1, 118.8, 114.4, 112.1, 60.2, 37.9, 21.2. **HRMS(ESI)**: Calcd. for C₅₁H₃₈N₆O₂ [M+Na]⁺ m/z: 789.2954; Found, [M+Na]⁺: 789.2955.



<u>1',1'''-(butane-1,4-diyl)bis(([3,3':3',3''-terindolin]-2'-one))</u> **10ab**. Sandbrown solid; Yield: 91%; mp (°C): >300; FT-IR (ATR, cm⁻¹): 3363, 1676, 1609, 1359, 1100, 740, 615, 427; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.96 (s, 4H), 7.37 – 7.14 (m, 15H), 7.01 (s, 6H), 6.87 – 6.79 (m, 7H), 3.83 (s, 4H), 1.76 (s, 4H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 177.36, 142.41, 137.40, 134.32, 128.44, 126.12, 125.18, 124.72, 122.49, 121.44, 121.13, 118.80, 114.57, 112.12, 109.30, 52.65, 25.16. HRMS(ESI): Calcd. for $C_{52}H_{40}N_6O_2$ [M+H]⁺ m/z: 781.3291; Found, [M+H]⁺: 781.3291.



<u>1',1'''-(pentane-1,5-diyl)bis(([3,3':3',3''-terindolin]-2'-one))</u> **10ac**. Pale-sand brown **solid**; **Yield**: 85%; **mp** (°C): >300 [>300];²⁴ **FT-IR (ATR, cm⁻¹)**: 3342, 1665, 1607, 1466, 1095, 741, 476; ¹H NMR **(400 MHz, DMSO-d_6, ppm)** 10.97 (s, 4H), 7.36 – 7.27 (m, 9H), 7.16 (d, J = 8.1 Hz, 4H), 7.03 – 6.98 (m, 7H), 6.86 – 6.85 (m, 4H), 6.79 (t, J = 7.4 Hz, 4H), 1.71 – 1.61 (m, 6H), 1.38 – 1.23 (m, 4H). ¹³C NMR (100 MHz, DMSO-d_6, ppm) 177.3, 158.5, 151.1, 142.4, 137.4, 134.3, 128.4, 126.1, 124.8, 121.4, 121.1, 118.8, 114.6, 112.1,

109.3, 52.7, 26.9, 23.9. **DEPT-135 NMR (100 MHz, DMSO-d₆, ppm)** 138.7, 128.5, 124.8, 122.5, 121.4, 121.1, 118.8, 112.1, 109.3, 39.6, 26.9, 23.9.



<u>1',1'''-(hexane-1,6-diyl)bis(([3,3':3',3''-terindolin]-2'-one))</u> **10ad.** Brick-red solid; Yield: 92%; mp (°C): 284-286 [283-285];²⁴ FT-IR (ATR, cm⁻¹): 3359, 1665, 1608, 1464, 1367, 1100, 734, 651 607; ¹H NMR (400 MHz, DMSO-d₆, ppm) 10.95 (s, 4H), 7.34 − 7.30 (m, 8H), 7.16 − 7.14 (m, 6H), 6.99 − 6.98 (m, 6H), 6.84 (s, 4H), 6.75 (s, 4H), 3.70 (s, 4H), 1.59 (s, 4H), 1.32 (s, 4H). ¹³C NMR (100 MHz, DMSO-d₆, ppm) 177.3, 142.5, 137.4, 134.3, 128.4, 126.1,

125.2, 124.8, 122.4, 121.1, 118.7, 114.5, 112.1, 109.3, 52.7, 27.4, 26.6. **DEPT-135 NMR (100 MHz, DMSO-d₆, ppm)** 128.4, 125.2, 124.8, 122.5, 121.4, 121.1, 118.7, 112.1, 109.3, 39.9, 27.4, 26.6.



Fig. S1 ¹H NMR spectrum (400 MHz) of **4** in D_2O .



Fig. S2 13 C NMR spectrum (100 MHz) of 4 in D₂O.



Fig. S3 DEPT-135 spectrum of (100 MHz) 4 in D₂O.



Fig. S4 FT-IR spectrum of 4.



Fig. S5 ¹H NMR spectrum (400 MHz) of 7aa in DMSO-d₆.





Fig. S7 FT-IR spectrum of 7aa.



Fig. S8 ¹H NMR spectrum (400 MHz) of 7ab in DMSO-d₆.





Fig. S10 FT-IR spectrum of 7ab.



Fig. S11 ¹H NMR spectrum (400 MHz) of 7ac in DMSO-d₆.





Fig. S13 FT-IR spectrum of 7ac.



Fig. S14 ¹H NMR spectrum (400 MHz) of 7ad in DMSO-d₆.



Fig. S15 ¹³C NMR spectrum (100 MHz) of 7ad in DMSO-d₆.



Fig. S16 FT-IR spectrum of 7ad.



Fig. S17¹H NMR spectrum (400 MHz) of 7ae in DMSO-d₆.



Fig. S18¹³C NMR spectrum (100 MHz) of 7ae in DMSO-d₆.



Fig. S19 FT-IR spectrum of 7ae.





Fig. S21 ¹³C NMR spectrum (100 MHz) of 7af in DMSO-d₆.



Fig. S22 FT-IR spectrum of 7af.



Fig. S23 ¹H NMR spectrum (400 MHz) of 7ag in DMSO-d₆.



Fig. S24 ¹³C NMR spectrum (100 MHz) of 7ag in DMSO-d₆.



Fig. S25 FT-IR spectrum of 7ag.



Fig. S26 ¹H NMR spectrum (400 MHz) of 7ah in DMSO-d₆.



Fig. S27 13 C NMR spectrum (100 MHz) of 7ah in DMSO-d₆.



Fig. S28 FT-IR spectrum of 7ah.



Fig. S29 ¹H NMR spectrum (400 MHz) of 7ba in DMSO-d₆.



Fig. S30 13 C NMR spectrum (100 MHz) of 7ba in DMSO-d₆.


Fig. S31 FT-IR spectrum of 7ba.



Fig. S32 ¹H NMR spectrum (400 MHz) of 7ca in DMSO-d₆.



Fig. S33 ¹³C NMR spectrum (100 MHz) of 7ca in DMSO-d₆.



Fig. S34 FT-IR spectrum of 7ca.



Fig. S35 ¹H NMR spectrum (400 MHz) of 7da in DMSO-d₆.



Fig. S36 ¹³C NMR spectrum (100 MHz) of 7da in DMSO-d₆.



Fig. S37 FT-IR spectrum of 7da.



Fig. S38 ¹H NMR spectrum (400 MHz) of 7ea in DMSO-d₆.



Fig. S39 ¹³C NMR spectrum (100 MHz) of 7ea in DMSO-d₆.



Fig. S40 FT-IR spectrum of 7ea.



Fig. S41 ¹H NMR spectrum (400 MHz) of 7ec in DMSO-d₆.



Fig. S42 ¹³C NMR spectrum (100 MHz) of 7ec in DMSO-d₆.



Fig. S43 FT-IR spectrum of 7ec.



Fig. S44 ¹H NMR spectrum (400 MHz) of 7ed in DMSO-d₆.



Fig. S45 ¹³C NMR spectrum (100 MHz) of 7ed in DMSO-d₆.



Fig. S46 FT-IR spectrum of 7ed.



Fig. S47 ¹H NMR spectrum (400 MHz) of 7fa in DMSO-d₆.



Fig. S48 ¹³C NMR spectrum (100 MHz) of 7fa in DMSO-d₆.



Fig. S49 FT-IR spectrum of 7fa.



Fig. S50 ¹H NMR spectrum (400 MHz) of 7fb in DMSO-d₆.



Fig. S51 ¹³C NMR spectrum (100 MHz) of 7fb in DMSO-d₆.



Fig. S52 FT-IR spectrum of 7fb.



Fig. S53 ¹H NMR spectrum (400 MHz) of 7fd in DMSO-d₆.



Fig. S54 ¹³C NMR spectrum (100 MHz) of 7fd in DMSO-d₆.



Fig. S55 FT-IR spectrum of 7fd.



Fig. S57 13 C NMR spectrum (100 MHz) of 7ga in DMSO-d₆.



Fig. S58 FT-IR spectrum of 7ga.



Fig. S59 HR-MS spectrum of 7ga.



Fig. S60 ¹H NMR spectrum (400 MHz) of 7gc in DMSO-d₆.



Fig. S61 ¹³C NMR spectrum (100 MHz) of 7gc in DMSO-d₆.



Fig. S62 FT-IR spectrum of 7gc.



Fig. S63 HR-MS spectrum of 7gc.



Fig. S64 ¹H NMR spectrum (400 MHz) of 7gd in DMSO-d₆.





Fig. S66 FT-IR spectrum of 7gd.



Fig. S67 HR-MS spectrum of 7gd.



Fig. S68 ¹H NMR spectrum (400 MHz) of 7ai in DMSO-d₆.



Fig. S69 ¹³C NMR spectrum (100 MHz) of 7ai in DMSO-d₆.



Fig. S70 FT-IR spectrum of 7ai.



Fig. S71 ¹H NMR spectrum (400 MHz) of 7ei in DMSO-d₆.



Fig. S72 ¹³C NMR spectrum (100 MHz) of 7ei in DMSO-d₆.





Fig. S74 ¹³C NMR spectrum (100 MHz) of 7fi in DMSO-d₆.



Fig. S75 FT-IR spectrum of 7fi.



Fig. S76 ¹H NMR spectrum (400 MHz) of 7aj in DMSO-d₆.





Fig. S78 FT-IR spectrum of 7aj.



Fig. S80 ¹³C NMR spectrum (100 MHz) of 7cj in DMSO-d₆.





Fig. S82 ¹H NMR spectrum (400 MHz) of 7dj in DMSO-d₆.



Fig. S83 ¹³C NMR spectrum (100 MHz) of 7dj in DMSO-d₆.



Fig. S84 FT-IR spectrum of 7dj.







Fig. S86 ¹³C NMR spectrum (100 MHz) of 7ej in DMSO-d₆.



Fig. S87 FT-IR spectrum of 7ej.




Fig. S89 ¹³C NMR spectrum (100 MHz) of 7fj in DMSO-d₆.



Fig. S90 FT-IR spectrum of 7fj.



Fig. S91 ¹H NMR spectrum (400 MHz) of 7gj in DMSO-d₆.



Fig. S92 ¹³C NMR spectrum (100 MHz) of 7gj in DMSO-d₆.



Fig. S93 FT-IR spectrum of 7gj.



Fig. S94 HR-MS spectrum of 7gj.



Fig. S95 ¹H NMR spectrum (400 MHz) of 7gk in DMSO-d₆.



Fig. S96 ¹³C NMR spectrum (100 MHz) of 7gk in DMSO-d₆.



Fig. S97 FT-IR spectrum of 7gk.



Fig. S98 HR-MS spectrum of 7gk.



Fig. S99 ¹H NMR spectrum (400 MHz) of 7ck in DMSO-d₆.



Fig. S100 ¹³C NMR spectrum (100 MHz) of 7ck in DMSO-d₆.



Fig. S101 FT-IR spectrum of 7ck.



Fig. S102 HR-MS spectrum of 7ck.



Fig. S103 ¹H NMR spectrum (400 MHz) of 10aa in DMSO-d₆.



Fig. S104 ¹³C NMR spectrum (100 MHz) of 10aa in DMSO-d₆.



Fig. S105 FT-IR spectrum of 10aa.



Fig. S106 HR-MS spectrum of 10aa.





Fig. S108 ¹³C NMR spectrum (100 MHz) of 10ab in DMSO-d₆.



Fig. S109 FT-IR spectrum of 10ab.



Fig. S110 HR-MS spectrum of 10ab.



Fig. S111 ¹H NMR spectrum (400 MHz) of 10ac in DMSO-d₆



Fig. S112 ¹³C NMR spectrum (100 MHz) of 10ac in DMSO-d₆.



Fig. S113 DEPT-135 NMR spectrum (400 MHz) of 10ac in DMSO-d₆



Fig. S114 FT-IR spectrum of 10ac.



Fig. S115 ¹H NMR spectrum (400 MHz) of 10ad in DMSO-d₆.



Fig. S116 ¹³C NMR spectrum (100 MHz) of 10ad in DMSO-d₆.



Fig. S117 DEPT-135 NMR spectrum (400 MHz) of 10ad in DMSO-d₆.



Fig. S118 FT-IR spectrum of 10ad.

Crystal Structure Report for 7gj

A specimen of $C_{30}H_{20}Br_2N_2O$, approximate dimensions 0.190 mm x 0.241 mm x 0.274 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured ($\lambda = 0.71073$ Å). The integration of the data using a triclinic unit cell yielded a total of 55571 reflections to a maximum θ angle of 28.35° (0.75 Å resolution), of which 6063 were independent (average redundancy 9.166, completeness = 99.5%, $R_{int} = 5.16\%$, $R_{sig} = 3.84\%$) and 3605 (59.46%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.9565(7) Å, b = 12.0727(9) Å, c = 12.5432(10) Å, $\alpha = 107.005(3)^{\circ}$, $\beta = 105.112(3)^{\circ}$, $\gamma = 97.415(3)^{\circ}$, volume = 1220.78(17) Å³, are based upon the refinement of the XYZ-centroids of reflections above 20 $\sigma(I)$. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4610 and 0.5690. The final anisotropic full-matrix least-squares refinement on F² with 318 variables converged at R1 = 5.35%, for the observed data and wR2 = 15.77% for all data. The goodness-of-fit was 1.029. The largest peak in the final difference electron density synthesis was 0.695 e⁻/Å³ and the largest hole was -1.084 e⁻/Å³ with an RMS deviation of 0.083 e⁻/Å³. On the basis of the final model, the calculated density was 1.590 g/cm³ and F (000), 584 e⁻.

Table S1a Sample and crystal data for 7gj

CCDC No	2360038			
Identification code	7gj			
Chemical formula	$C_{30}H_{20}Br_2N_2O$			
Formula weight	584.30 g/mol			
Temperature	300(2) K			
Wavelength	0.71073 Å			
Crystal size	0.190 x 0.241 x 0.274 mm			
Crystal system	triclinic			
Space group	P -1			
Unit cell dimensions	a = 8.9565(7) Å	$\alpha = 107.005(3)^{\circ}$		
	b = 12.0727(9) Å	$\beta = 105.112(3)^{\circ}$		
	c = 12.5432(10) Å	$\gamma = 97.415(3)^{\circ}$		
Volume	1220.78(17) Å ³			
Ζ	2			
Density (calculated)	1.590 g/cm ³			
Absorption coefficient	3.347 mm ⁻¹			
F(000)	584			

1.79 to 28.35° Theta range for data collection -11<=h<=11, -16<=k<=16, -16<=l<=16 **Index ranges Reflections collected** 55571 **Independent reflections** 6063 [R(int) = 0.0516] Max. and min. transmission 0.5690 and 0.4610 Full-matrix least-squares on F² **Refinement method** SHELXL-2019/1 (Sheldrick, 2019) **Refinement program** $\Sigma w (F_o^2 - F_c^2)^2$ **Function minimized** 6063 / 0 / 318 Data / restraints / parameters Goodness-of-fit on F² 1.029 **Final R indices** 3605 data; I>2σ(I) R1 = 0.0535, wR2 = 0.1355R1 = 0.1015, wR2 = 0.1577all data $w=1/[\sigma^2(F_o^2)+(0.0645P)^2+1.2110P]$ Weighting scheme where $P = (F_o^2 + 2F_c^2)/3$ 0.695 and -1.084 eÅ⁻³ Largest diff. peak and hole 0.083 eÅ⁻³ **R.M.S.** deviation from mean

Table S1b Data collection and structure refinement for 7gj

Table S1c Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for 7gj

	x/a	y/b	z/c	U(eq)
Br1	0.90861(6)	0.13612(4)	0.94322(4)	0.0835(2)
Br2	0.59175(11)	0.90378(5)	0.09954(7)	0.1374(4)
01	0.0938(3)	0.5957(2)	0.1614(3)	0.0636(7)
N1	0.1285(3)	0.3962(3)	0.4613(3)	0.0503(7)
N2	0.5814(4)	0.4431(4)	0.1880(3)	0.0664(9)
C1	0.1233(4)	0.3826(3)	0.2767(3)	0.0430(7)
C2	0.0687(4)	0.3224(3)	0.3460(3)	0.0478(8)
C3	0.9735(4)	0.2091(3)	0.2975(4)	0.0583(10)
C4	0.9312(5)	0.1549(3)	0.1776(4)	0.0633(10)
C5	0.9800(4)	0.2143(3)	0.1087(3)	0.0556(9)
C6	0.0748(4)	0.3268(3)	0.1553(3)	0.0486(8)
C7	0.2229(4)	0.4952(3)	0.3573(3)	0.0420(7)
C8	0.2204(4)	0.4988(3)	0.4663(3)	0.0469(8)
C9	0.3106(4)	0.5932(3)	0.3283(3)	0.0408(7)
C10	0.1803(4)	0.6463(3)	0.2607(3)	0.0465(8)
C11	0.1855(4)	0.7650(3)	0.3405(3)	0.0504(9)
C12	0.3154(4)	0.7918(3)	0.4419(3)	0.0458(8)
C13	0.3972(4)	0.6990(3)	0.4394(3)	0.0444(8)
C14	0.4192(4)	0.5497(3)	0.2593(3)	0.0459(8)
C15	0.5004(4)	0.6140(3)	0.2037(3)	0.0503(8)
C16	0.6006(4)	0.5439(4)	0.1604(3)	0.0607(11)
C17	0.4730(4)	0.4480(4)	0.2483(3)	0.0561(9)
C18	0.1120(5)	0.3640(4)	0.5615(4)	0.0681(11)
C19	0.0944(5)	0.8472(4)	0.3321(4)	0.0617(10)
C20	0.3616(5)	0.9000(3)	0.5364(4)	0.0600(10)
C21	0.2656(6)	0.9824(4)	0.5239(5)	0.0752(13)
C22	0.1381(6)	0.9554(4)	0.4262(5)	0.0785(13)
C23	0.5290(4)	0.7160(3)	0.5313(3)	0.0549(9)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

C24	0.4976(6)	0.9132(4)	0.6294(4)	0.0699(11)
C25	0.5782(5)	0.8247(4)	0.6263(4)	0.0660(11)
C26	0.4972(5)	0.7225(4)	0.1861(3)	0.0618(10)
C27	0.5949(6)	0.7568(4)	0.1274(4)	0.0819(15)
C28	0.6944(6)	0.6878(6)	0.0866(4)	0.0965(19)
C29	0.6980(5)	0.5813(6)	0.1016(4)	0.0827(16)
C30	0.6674(6)	0.3483(5)	0.1648(5)	0.0989(19)

Table S1d Bond lengths (Å) for 7gj

Br1-C5	1.901(4)	Br2-C27	1.908(5)
O1-C10	1.206(4)	N1-C8	1.371(4)
N1-C2	1.375(5)	N1-C18	1.455(4)
N2-C16	1.362(6)	N2-C17	1.375(5)
N2-C30	1.462(5)	C1-C6	1.393(5)
C1-C2	1.422(5)	C1-C7	1.441(5)
C2-C3	1.383(5)	C3-C4	1.376(6)
С3-Н3	0.930000	C4-C5	1.389(6)
C4-H4	0.930000	C5-C6	1.374(5)
С6-Н6	0.930000	C7-C8	1.362(5)
С7-С9	1.520(4)	С8-Н8	0.930000
C9-C14	1.509(4)	C9-C13	1.522(5)
C9-C10	1.576(5)	C10-C11	1.476(5)
C11-C19	1.374(5)	C11-C12	1.402(5)
C12-C20	1.408(5)	C12-C13	1.413(5)
C13-C23	1.361(5)	C14-C17	1.359(5)
C14-C15	1.434(5)	C15-C26	1.392(6)
C15-C16	1.414(5)	C16-C29	1.391(6)
C17-H17	0.930000	C18-H18A	0.960000
C18-H18	0.960000	C18-H18C	0.960000
C19-C22	1.405(7)	С19-Н19	0.930000
C20-C24	1.403(6)	C20-C21	1.413(6)
C21-C22	1.361(7)	C21-H21	0.930000
C22-H22	0.930000	C23-C25	1.414(5)
С23-Н23	0.930000	C24-C25	1.361(6)
C24-H24	0.930000	С25-Н25	0.930000
C26-C27	1.379(5)	C26-H26	0.930000
C27-C28	1.389(8)	C28-C29	1.357(8)
C28-H28	0.930000	С29-Н29	0.930000
С30-Н30	0.960000	С30-Н30	0.960000
С30-Н30	0.960000		

Table S1e Bond angles (°) for 7gj

C8-N1-C2	108.4(3)	C8-N1-C18	126.1(3)
C2-N1-C18	125.2(3)	C16-N2-C17	108.4(3)
C16-N2-C30	126.5(4)	C17-N2-C30	124.9(4)
C6-C1-C2	118.8(3)	C6-C1-C7	134.8(3)
C2-C1-C7	106.4(3)	N1-C2-C3	129.9(3)
N1-C2-C1	107.9(3)	C3-C2-C1	122.2(4)
C4-C3-C2	117.6(4)	С4-С3-Н3	121.200000
С2-С3-Н3	121.200000	C3-C4-C5	120.6(4)
С3-С4-Н4	119.700000	С5-С4-Н4	119.700000
C6-C5-C4	122.7(4)	C6-C5-Br1	119.3(3)
C4-C5-Br1	118.0(3)	C5-C6-C1	118.0(3)
С5-С6-Н6	121.000000	С1-С6-Н6	121.000000
C8-C7-C1	106.4(3)	C8-C7-C9	125.9(3)
C1-C7-C9	127.7(3)	C7-C8-N1	111.0(3)
С7-С8-Н8	124.500000	N1-C8-H8	124.500000
C14-C9-C7	112.4(3)	C14-C9-C13	112.3(3)
C7-C9-C13	110.5(3)	C14-C9-C10	112.6(3)
C7-C9-C10	106.7(2)	C13-C9-C10	101.8(3)
O1-C10-C11	127.9(3)	O1-C10-C9	124.4(3)
C11-C10-C9	107.8(3)	C19-C11-C12	119.0(4)
C19-C11-C10	133.4(4)	C12-C11-C10	107.6(3)
C11-C12-C20	124.0(3)	C11-C12-C13	113.0(3)
C20-C12-C13	123.0(3)	C23-C13-C12	118.6(3)
C23-C13-C9	132.3(3)	C12-C13-C9	109.2(3)
C17-C14-C15	106.3(3)	C17-C14-C9	126.9(3)
C15-C14-C9	126.5(3)	C26-C15-C16	119.5(4)
C26-C15-C1	133.9(3)	C16-C15-C14	106.6(4)
N2-C16-C29	130.4(4)	N2-C16-C15	108.0(3)
C29-C16-C15	121.6(5)	C14-C17-N2	110.6(4)
C14-C17-H17	124.700000	N2-C17-H17	124.700000
N1-C18-H18	109.500000	N1-C18-H18	109.500000
H18-C18-H18	109.500000	N1-C18-H18	109.500000

H18-C18-H18 109.500000 C11-C19-C22 117.8(4) C22-C19-H19 121.100000 C24-C20-C21 128.4(4) C22-C21-C20 120.7(4) C20-C21-H21 119.700000 C21-C22-H22 118.300000 C13-C23-C25 119.2(4) C25-C23-H23 120.400000 C25-C24-H24 119.600000 C24-C25-C23 122.2(4) C23-C25-H25 118.900000 C27-C26-H26 121.200000 C26-C27-C28 122.5(5) C28-C27-Br2 118.7(4) C29-C28-H28 119.500000 C28-C29-C1 118.0(5) C16-C29-H2 121.000000 N2-C30-H30 109.500000 N2-C30-H30 109.500000 H30-C30-H30 109.500000

H18-C18-H18 109.500000 C11-C19-H19 121.100000 C24-C20-C12 116.4(3) C12-C20-C21 115.2(4) C22-C21-H21 119.700000 C21-C22-C19 123.4(4) C19-C22-H22 118.300000 C13-C23-H23 120.400000 C25-C24-C20 120.7(4) C20-C24-H24 119.700000 C24-C25-H25 118.900000 C27-C26-C15 117.5(4) C15-C26-H26 121.200000 C26-C27-Br2 118.8(4) C29-C28-C27 120.9(4) C27-C28-H28 119.500000 C28-C29-H29 121.000000 N2-C30-H30A109.500000 H30-C30-H30 109.500000 H30-C30-H30 109.500000

Table S1f Torsion angles (°) for 7gj

C8-N1-C2-C3	178.4(3)	C18-N1-C2-C3	5.2(6)
C8-N1-C2-C1	-1.1(4)	C18-N1-C2-C1	-174.3(3)
C6-C1-C2-N1	-178.3(3)	C7-C1-C2-N1	1.6(4)
C6-C1-C2-C3	2.2(5)	C7-C1-C2-C3	-177.9(3)
N1-C2-C3-C4	-179.8(3)	C1-C2-C3-C4	-0.4(5)
C2-C3-C4-C5	-1.5(6)	C3-C4-C5-C6	1.7(6)
C3-C4-C5-Br1	-177.2(3)	C4-C5-C6-C1	0.1(5)
Br1-C5-C6-C1	179.0(2)	C2-C1-C6-C5	-2.0(5)
C7-C1-C6-C5	178.1(3)	C6-C1-C7-C8	178.4(4)
C2-C1-C7-C8	-1.5(3)	C6-C1-C7-C9	0.0(6)
C2-C1-C7-C9	-179.9(3)	C1-C7-C8-N1	0.9(4)
C9-C7-C8-N1	179.3(3)	C2-N1-C8-C7	0.1(4)
C18-N1-C8-C7	173.2(3)	C8-C7-C9-C14	126.1(3)
C1-C7-C9-C14	-55.8(4)	C8-C7-C9-C13	-0.2(4)
C1-C7-C9-C13	177.9(3)	C8-C7-C9-C10	-110.0(4)
C1-C7-C9-C10	68.1(4)	C14-C9-C10-O1	51.7(4)
C7-C9-C10-O1	-72.0(4)	C13-C9-C10-O1	172.2(3)
C14-C9-C10-C11	-128.4(3)	C7-C9-C10-C11	107.8(3)
C13-C9-C10-C11	-8.0(3)	O1-C10-C11-C19	4.9(6)
C9-C10-C11-C19	-174.9(4)	O1-C10-C11-C12	-173.9(3)
C9-C10-C11-C12	6.2(3)	C19-C11-C12-C20	-1.4(5)
C10-C11-C12-C20	177.7(3)	C19-C11-C12-C13	179.2(3)
C10-C11-C12-C13	-1.7(4)	C11-C12-C13-C23	177.7(3)
C20-C12-C13-C23	-1.7(5)	C11-C12-C13-C9	-3.7(4)
C20-C12-C13-C9	176.9(3)	C14-C9-C13-C23	-54.1(5)
C7-C9-C13-C23	72.3(4)	C10-C9-C13-C23	-174.7(4)
C14-C9-C13-C12	127.7(3)	C7-C9-C13-C12	-106.0(3)
C10-C9-C13-C12	7.0(3)	C7-C9-C14-C17	-17.5(5)
C13-C9-C14-C17	107.8(4)	C10-C9-C14-C17	-138.0(4)
C7-C9-C14-C15	170.2(3)	C13-C9-C14-C15	-64.5(4)
C10-C9-C14-C15	49.7(4)	C17-C14-C15-C26	-179.9(4)
C9-C14-C15-C26	-6.3(6)	C17-C14-C15-C16	0.4(4)

C9-C14-C15-C16	174.0(3)	C17-N2-C16-C29	179.0(4)
C30-N2-C16-C29	2.5(7)	C17-N2-C16-C15	-0.5(4)
C30-N2-C16-C15	-177.0(4)	C26-C15-C16-N2	-179.7(3)
C14-C15-C16-N2	0.0(4)	C26-C15-C16-C29	0.8(5)
C14-C15-C16-C29	-179.5(3)	C15-C14-C17-N2	-0.8(4)
C9-C14-C17-N2	-174.3(3)	C16-N2-C17-C14	0.8(4)
C30-N2-C17-C14	177.4(4)	C12-C11-C19-C22	0.7(5)
C10-C11-C19-C22	-178.0(4)	C11-C12-C20-C24	-178.0(3)
C13-C12-C20-C24	1.3(5)	C11-C12-C20-C21	0.8(5)
C13-C12-C20-C21	-179.9(3)	C24-C20-C21-C22	179.0(4)
C12-C20-C21-C22	0.3(6)	C20-C21-C22-C19	-0.9(7)
C11-C19-C22-C21	0.3(7)	C12-C13-C23-C25	0.8(5)
C9-C13-C23-C25	-177.3(3)	C12-C20-C24-C25	-0.1(6)
C21-C20-C24-C25	-178.8(4)	C20-C24-C25-C23	-0.7(7)
C13-C23-C25-C24	0.3(6)	C16-C1-C26-C27	-0.6(5)
C14-C15-C26-C27	179.8(4)	C15-C26-C27-C28	-0.2(6)
C15-C26-C27-Br2	179.1(3)	C26-C27-C28-C29	1.0(7)
Br2-C27-C28-C29	-178.4(4)	C27-C28-C29-C16	-0.8(7)
N2-C16-C29-C28	-179.5(4)	C15-C16-C29-C28	-0.1(6)

Table S1g Anisotropic atomic displacement parameters (Å²) for 7gj

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a*2 U_{11} + ... + 2 h k a* b* U_{12}$]

	U11	U22	U33	U23	U13	U12
Br1	0.0895(4)	0.0714(3)	0.0699(3)	0.0049(2)	0.0237(3)	-0.0010(2)
Br2	0.2022(8)	0.0786(4)	0.1319(6)	0.0224(4)	0.1031(6)	-0.0398(4)
01	0.0586(16)	0.0683(17)	0.0631(18)	0.0296(14)	0.0094(14)	0.0148(13)
N1	0.0447(16)	0.0634(18)	0.0564(18)	0.0345(15)	0.0212(14)	0.0145(14)
N2	0.0491(18)	0.094(3)	0.058(2)	0.0164(19)	0.0206(16)	0.0378(18)
C1	0.0407(17)	0.0462(17)	0.055(2)	0.0261(16)	0.0221(15)	0.0160(14)
C2	0.0381(17)	0.054(2)	0.064(2)	0.0315(18)	0.0214(16)	0.0164(15)
C3	0.050(2)	0.057(2)	0.082(3)	0.040(2)	0.024(2)	0.0115(17)
C4	0.055(2)	0.046(2)	0.087(3)	0.024(2)	0.021(2)	0.0050(17)
C5	0.054(2)	0.049(2)	0.064(2)	0.0162(18)	0.0218(18)	0.0123(17)
C6	0.0478(19)	0.0456(18)	0.060(2)	0.0208(16)	0.0252(17)	0.0135(15)
C7	0.0375(16)	0.0466(17)	0.0520(19)	0.0227(15)	0.0208(15)	0.0163(14)
C8	0.0398(18)	0.055(2)	0.054(2)	0.0241(16)	0.0191(15)	0.0147(15)
C9	0.0375(16)	0.0454(17)	0.0490(18)	0.0212(15)	0.0214(14)	0.0130(13)
C10	0.0413(18)	0.0531(19)	0.057(2)	0.0279(17)	0.0240(17)	0.0107(15)
C11	0.050(2)	0.058(2)	0.065(2)	0.0344(18)	0.0333(18)	0.0202(17)
C12	0.0465(19)	0.0475(18)	0.056(2)	0.0238(16)	0.0284(17)	0.0148(15)
C13	0.0456(19)	0.0459(18)	0.0518(19)	0.0207(15)	0.0259(16)	0.0132(15)
C14	0.0365(17)	0.056(2)	0.0481(19)	0.0164(16)	0.0176(15)	0.0128(15)
C15	0.0326(16)	0.069(2)	0.0411(18)	0.0110(16)	0.0131(14)	0.0004(15)
C16	0.0340(18)	0.095(3)	0.0422(19)	0.008(2)	0.0140(15)	0.0094(19)
C17	0.045(2)	0.071(2)	0.057(2)	0.0213(19)	0.0180(17)	0.0244(18)
C18	0.064(3)	0.095(3)	0.068(3)	0.052(2)	0.030(2)	0.018(2)
C19	0.065(2)	0.071(3)	0.078(3)	0.046(2)	0.038(2)	0.034(2)
C20	0.069(3)	0.052(2)	0.069(3)	0.0199(19)	0.036(2)	0.0181(19)
C21	0.097(4)	0.054(2)	0.088(3)	0.022(2)	0.046(3)	0.031(2)
C22	0.096(4)	0.069(3)	0.102(4)	0.042(3)	0.052(3)	0.048(3)
C23	0.046(2)	0.059(2)	0.062(2)	0.0195(18)	0.0203(18)	0.0149(17)
C24	0.079(3)	0.055(2)	0.065(3)	0.0059(19)	0.026(2)	0.007(2)

C25	0.060(2)	0.065(3)	0.061(2)	0.013(2)	0.014(2)	0.005(2)
C26	0.063(2)	0.060(2)	0.054(2)	0.0081(18)	0.0288(19)	-0.0107(18)
C27	0.080(3)	0.083(3)	0.063(3)	0.003(2)	0.038(2)	-0.029(2)
C28	0.066(3)	0.131(5)	0.063(3)	0.000(3)	0.037(2)	-0.038(3)
C29	0.044(2)	0.127(5)	0.055(3)	0.000(3)	0.0245(19)	0.000(3)
C30	0.074(3)	0.131(5)	0.086(3)	0.009(3)	0.027(3)	0.064(3)

	x/a	y/b	z/c	U(eq)
H3	-0.0606	0.1708	0.3441	0.070000
H4	-0.1307	0.0780	0.1425	0.076000
H6	0.1057	0.3646	0.1072	0.058000
H8	0.2739	0.5624	0.5350	0.056000
H17	0.4409	0.3897	0.2776	0.067000
H18	0.1182	0.4343	0.6246	0.102000
H18	0.1957	0.3260	0.5867	0.102000
H18	0.0113	0.3105	0.5392	0.102000
H19	0.0068	0.8318	0.2665	0.074000
H21	0.2898	1.0559	0.5829	0.090000
H22	0.0767	1.0113	0.4214	0.094000
H23	0.5860	0.6569	0.5315	0.066000
H24	0.5331	0.9832	0.6938	0.084000
H25	0.6686	0.8362	0.6887	0.079000
H26	0.4317	0.7700	0.2131	0.074000
H28	0.7594	0.7151	0.0484	0.116000
H29	0.7637	0.5346	0.0735	0.099000
H30	0.6163	0.2805	0.1776	0.148000
H30	0.7746	0.3757	0.2167	0.148000
H30	0.6677	0.3263	0.0849	0.148000

Table S1h Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²) for 7gj

Table S1i Hydrogen bond distances (Å) and angles (°) for 7gj

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
C4-H4Br2	0.93	2.86	3.705(4)	151.6

Symmetry transformations used to generate equivalent atoms: x-1, y-1, z

S No	Inside	Outside	Doroontogo	S No	Inside	Outside	Domontogo
5. NU	atom	atom	Percentage	5. NU	atom	atom	rercentage
1	All	All	100	37	All	All	100
2	All	Br	10.3	38	Br	All	16.0
3	All	0	2.9	39	0	All	3.3
4	All	N	1.3	40	N	All	1.4
5	All	С	16.3	41	С	All	19.3
6	All	Н	69.1	42	Н	All	59.9
7	Br	All	16.0	43	All	Br	10.3
8	Br	Br	1.6	44	Br	Br	1.6
9	Br	0	0.4	45	0	Br	0.3
10	Br	Ν	0.0	46	N	Br	0.0
11	Br	С	0.4	47	С	Br	0.3
12	Br	Н	13.7	48	Н	Br	8.1
13	0	All	3.3	49	All	0	2.9
14	0	Br	0.3	50	Br	0	0.4
15	0	0	0.2	51	0	0	0.2
16	0	Ν	0.0	52	Ν	0	0.0
17	0	С	0.0	53	С	0	0.0
18	0	Н	0.0	54	Н	0	2.4
19	Ν	All	1.4	55	All	N	1.3
20	Ν	Br	0.0	56	Br	N	0.0
21	Ν	0	0.0	57	0	N	0.0
22	Ν	Ν	0.1	58	N	N	0.1
23	Ν	С	0.3	59	С	N	0.3
24	Ν	Н	1.0	60	Н	N	1.0
25	С	All	19.3	61	All	C	16.3
26	С	Br	0.3	62	Br	C	0.4
27	С	0	0.0	63	0	С	0.0
28	С	N	0.3	64	N	C	0.3
29	С	С	2.3	65	С	С	2.3

Table S2 Interactions of Hirshfeld Surface in percentages for 7gj

30	C	Н	16.4	66	Н	C	13.4
31	Н	All	59.9	67	All	Н	69.1
32	Н	Br	8.1	68	Br	Н	13.7
33	Н	0	2.4	69	0	Н	2.8
34	Н	Ν	1.0	70	Ν	Н	1.0
35	Н	C	13.4	71	C	Н	16.4
36	Н	Н	35.1	72	Н	Н	35.1

Table S3 The charge densities in HOMO, LUMO and electrostatic potential energy surface ofthe synthesized derivatives 7 and 10

	номо	LUMO	Band gap (eV)	ESP
7aa	-5.2425	-0.2519	4.9906	
7ab	-5.3514	-0.5418	4.8096	
7ac	-5.3163	0.4612	4.8551	
7ad	-5.3495	-0.5434	4.8061	
7ae	-5.5098	-2.1263	3.3835	

7af	-5.2265	-0.2288	4.9977	
7ag	-5.1919	-0.2174	4.9745	
7ah	-5.3522	-0.5151	4.8371	
7ba	-5.9756	-1.7951	3.4116	
7ca	-5.0559	-0.2520	4.8039	
7da	-5.0186	-0.3059	4.6600	

7ea	-5.5786	-0.6493	4.9293	
7ec	-5.6491	-0.7219	4.9272	
7ed	-5.6774	-0.7472	4.9302	
7fa	-5.1106	-0.2106	4.8999	
7fb	-5.1827	-0.4188	4.7639	
7fd	-5.2159	-0.5009	4.7149	

7ga	-5.4300	-0.6038	4.8262	
7gc	-5.4981	-0.6732	4.8249	
7gd	-5.5266	-0.6991	4.8276	
7ai	-5.0238	-0.1211	4.9027	
7ei	-5.3642	-0.5099	4.8543	
7fi	-4.8923	-0.0879	4.8044	

7aj	-5.1919	-1.8074	3.3845	
7cj	-5.9756	-1.1946	4.7810	CONTRACTOR OF CO
7dj	-4.9876	-1.8188	3.1688	
7ej	-5.5149	-1.9666	3.5483	
7fj	-5.0638	-1.7717	3.2921	
7gj	-5.3707	-1.9263	5.1781	
7gk	-5.2382	-1.5364	3.7018	
------	---------	---------	--------	--
7ck	-4.9843	-1.4879	3.4964	
10aa	-5.1522	-0.2757	4.8765	
10ab	-5.2053	-0.2800	4.9253	
10ac	-5.1296	-0.2310	4.8986	
10ad	-5.1596	-0.2906	4.8690	

Table S4 Frontier molecular orbitals of HOMO and LUMO of all the synthesized derivatives7 and 10 obtained at B3LYP/6-31G (d,p) level of theory in gas phase

Orbitals	7 aa	7ab	7ac	7ad
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
НОМО-1				
НОМО-2				
номо-з				Contraction of the second

Orbitals	7 ae	7af	7ag	7ah
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
НОМО-1				
НОМО-2				
НОМО-3				

Orbitals	7ba	7ca	7da	7ea
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
HOMO-1				
НОМО-2				
номо-з				

Orbitals	7ec	7ed	7fa	7fb
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
НОМО				
НОМО-1				
НОМО-2				
НОМО-3				

Orbitals	7fd	7ga	7gc	7gd
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
HOMO-1				
НОМО-2				
НОМО-3				

Orbitals	7ai	7ei	7fi	7aj
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
HOMO-1				
НОМО-2				
НОМО-3				

Orbitals	7сј	7dj	7ej	7fj
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
НОМО-1				
НОМО-2				
НОМО-3				

Orbitals	7gj	7gk	7ck	
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
НОМО-1				
НОМО-2				
номо-з				

Orbitals	10aa	10ab	10ac	10ad
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
номо				
HOMO-1				
НОМО-2				
НОМО-3				

S No	Code	Excitation energy/ Oscillator		Kov transitions*
5.110	Coue	Theoretical λ_{abs} (nm)	strength	Key transitions
1	799	266.76	0.0598	H-1→L (51.19%)
1	/ aa	200.70	0.0398	H-1→ L+1 (29.09%)
2	7ab	261.85	0.0501	H-1→L+2 (65.13%)
3	7ac	270.36	0.0399	$H \rightarrow L+2 (51.10\%)$
4	7ad	262.09	0.0485	H-1→L+2 (65.97%)
5	7	207.01	0.1609	H-4→ L (70.64%)
5	/ae	507.91	0.1008	H→ L+1 (25.82%)
6	7af	267.85	0.0549	H-1→L (72.30%)
7	7ag	266.77	0.0504	$H \rightarrow L+2 (75.68\%)$
8	7ah	261.22	0.0501	$H-1 \rightarrow L+2 (59.96\%)$
9	7ba	284.57	0.0478	H-1→L (89.45%)
10	7.00	282.20	0.0472	H-2→L+1 (32.59%)
10	/ca	282.39	0.0475	H-1→ L (37.36%)
11	7da	266.20	0.0546	H→L+3 (50.71%)
12	7ea	267.20	0.0501	H-1→ L+1 (72.76%)
12	7	272.97	0.0674	H-1→L (30.10%)
15	/ec	213.81	0.0674	H-1→ L+1 (62.49%)
14	7ed	273.77	0.0569	H-1→ L (59.04%)
15	760	272 17	0.0775	H-1 →L (62.75%)
15	/1a	273.17	0.0775	H-1 →L+1 (25.65%)
16	7fb	288.70	0.0408	H-1→ L (90.31%)
17	7fd	268 17	0.0615	H-2→ L (22.52%)
17	/1 u	200.17	0.0015	H→ L+3 (35.29%)
18	7ga	272.69	0.0488	H-1→ L+1 (75.17%)
19	7gc	279.67	0.0790	H-1→ L (77.15%)
20	7gd	279.69	0.0785	H-1→ L+1 (86.01%)
21	7 ai	224 50	0.0634	$H-1 \rightarrow L+2 (26.06\%)$
21	/ a i	224.39	0.0054	H→ L+2 (63.58%)
22	7ei	262.62	0.0226	H-2→ L+1 (26.51%)
	701	202.02	0.0220	H→ L+1 (38.07%)
23	7 fi	220.80	0.0569	$H-1 \rightarrow L+2 (28.45\%)$
	/11	227.07	0.0307	H→ L+2 (57.29%)
24	7aj	331.73	0.0691	H-4→ L (91.11%)
25	7cj	334.37	0.0901	H-4→ L (92.91%)
26	7dj	333.84	0.0773	H-4→ L (87.66%)

 Table S5 Theoretical UV-Vis Characteristics of synthesized derivatives

27	7ej	333.68	0.0801	H-4→ L (93.48%)
28	7fj	332.47	0.0805	H-4→ L (93.12%)
29	7gj	334.00	0.0844	H-4→ L (93.45%)
30	7ak	31/1 77	0.0485	H-4→ L (38.46%)
50	/ gK	514.77	0.0485	H-1→ L+1 (36.33%)
				H-5→ L (22.02%)
31	7ck	310.90	0.0481	H-4→ L (40.01%)
				H-1 → L+1 (21.71%)
32	10aa	268.95	0.0237	H→ L+5 (53.77%)
33	10ab	268.08	0.0532	H-2→ L+2 (53.54%)
34	10ac	268.10	0.0471	$H-1 \rightarrow L+4 (60.99\%)$
35	10ad	269.45	0.0212	H→ L+5 (67.95%)

S. No	Ligand	BSA Binding	S. No	Ligand	BSA Binding
	_	aminity (AGbinding)		_	ammity (AGbinding)
1	7aa	-8.7	17	7fd	-8.7
2	7ab	-8.2	18	7ga	-8.0
3	7ac	-8.2	19	7gc	-8.0
4	7ad	-8.4	20	7gd	-7.9
5	7ae	-8.5	21	7ai	-9.4
6	7af	-9.2	22	7ei	-8.8
7	7ag	-8.7	23	7fi	-8.2
8	7ah	-8.2	24	7aj	-10.2
9	7ba	-8.9	25	7cj	-9.1
10	7ca	-8.4	26	7dj	-9.5
11	7da	-9.0	27	7ej	-9.2
12	7ea	-8.3	28	7fj	-9.1
13	7ec	-9.0	29	7gj	-9.4
14	7ed	-9.0	30	7gk	-9.3
15	7fa	-9.7	31	7ck	-8.6
16	7fb	-9.0			

Table S6 Binding affinity of BSA-ligand 7 calculated from Molecular docking studies (kcal mol⁻¹) using AutoDock Vina

Table S7 Binding affinity of DNA with ligand 7 calculated from Molecular docking studies (kcal mol⁻¹) using AutoDock Vina

S No	Ligond	BSA Binding	S No	Ligand	BSA Binding
5. NU	Liganu	affinity ($\Delta G_{binding}$)	5. NU	Ligaliu	affinity ($\Delta G_{binding}$)
1	7aa	-8.2	17	7fd	-7.7
2	7ab	-8.9	18	7ga	-7.3
3	7ac	-8.9	19	7gc	-7.3
4	7ad	-8.9	20	7gd	-7.3
5	7ae	-8.6	21	7ai	-8.3
6	7af	-8.7	22	7ei	-8.3
7	7ag	-8.2	23	7fi	-7.0
8	7ah	-8.6	24	7aj	-8.7
9	7ba	-8.8	25	7cj	-7.9
10	7ca	-8.6	26	7dj	-7.5
11	7da	-8.2	27	7ej	-9.0
12	7ea	-8.8	28	7fj	-7.8
13	7ec	-8.8	29	7gj	-8.0
14	7ed	-8.8	30	7gk	-8.6
15	7fa	-7.7	31	7ck	-8.1
16	7fb	-7.7			

	Conventional Hydrogen Bonding	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-cation	Pi-anion	Pi-Pi T- shaped/ Pi- Pi stacked	Pi- Sigma	Alkyl/ Pi-Alkyl	Amide-Pi Stacked
7aa	LYS116, GLU140	-	-	-	-	PHE133	-	LEU122	-
7ab	-	-	-	-	-	-	LEU397, GLU540	LYS396 ALA405, VAL408, LYS544	-
7ac	GLU540	-	-	-	-	-	LEU397	LYS396 ALA405, VAL408, LYS544	-
7ae	ARG217, LYS221, LYS294, PRO446	-	-	-	-	-	-	ALA341	-
7af	SER109, LEU112, ARG144	-	-	GLU424, ARG458	ARG185, GLU424, ARG458	-	-	LYS114, LEU115	-
7ag	THR52	-	GLU45, PHE49	-	ASP72, GLU73	-	-	LEU46	-
7ah	PRO420	-	ASP111	-	GLU424	-	ILE522	LYS114, VAL423, LEU462	-
7ba	GLU45, THR52, LYS64	-	GLY61	GLU73	ASP72, GLU73, LYS76	PHE49	-	-	-
7ca	-	-	GLU16	LYS20	-	-	VAL40	LEU24, VAL43, LYS131	-
7da	SER428		-	GLU424, LYS431	GLU424, ARG427	-	_	LEU189, ILE522	VAL423
7fa	ARG458	-	-	LYS431	-	-	LEU189, ALA193	ARG196	-

Table S8 The binding site residues of BSA with derivatives 7 as determined from Autodock Vina

	Conventional Hydrogen Bonding	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-cation	Pi-anion	Pi-Pi T- shaped/ Pi- Pi stacked	Pi- Sigma	Alkyl/ Pi-Alkyl	Amide-Pi Stacked
7fb	LYS131	-	-	LYS20	-	-	VAL40	LEU24, LYS132	-
7ai	-	PHE133	-	-	GLU125	TYR137	LEU115	PRO117, LEU122, LYS136	-
7fi	-	_	_	-	ASP72, GLU73	PHE49	-	LEU46, PHE49, HIS59, LYS64, LEU69	-
7aj	-	-	-	LYS116	GLU125	TYR160	LEU115	PRO117, LEU122, LYS136	-
7cj	SER109, LEU112	-	PRO110, GLU519	GLU424	HIS145, GLU424, ARG458	-	ARG144	LYS114, LEU115, LEU189, ILE522	-
7dj	-	-	-	-	GLU45, ASP72, GLU73	PHE49	-	LEU46	
7fj	-	-	-	-	GLU45, ASP72, GLU73	PHE49	-	LEU46, LEU69	-
7gk	-	GLU339	TYR340	-	-	TYR340	VAL380, SER442	MET445, PRO446	-
7ck	_	GLU339	TYR340, GLN384, SER442	-	-	-	VAL380	MET445, PRO446	-

	Conventional Hydrogen Bonding	Van der Waals	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-Pi T- shaped/ Pi-Pi stacked	Pi- Sigma	Alkyl/ Pi-Alkyl
7aa	Gua4, Cyt23	Gua2, Cyt3, Ade5,	-	-	-	-	-
		Ade6, Gua22, Gua24					
7ab	Gua4, Gua22, Cyt23,	Gua2, Cyt3, Ade5,	Gua4, Gua22	-	-	-	-
	Gua24	Ade6	,				
7ac	Gua4, Gua22, Cyt23,	Gua2, Cyt3, Ade5,	Gua4, Gua22	-	-	_	_
	Gua24	Ade6					_
7ae	Gua4, Gua22, Cyt23,	Gua2, Cyt3, Ade5,	Gua4 Gua22	_	_	_	_
740	Gua24	Ade6	Guar, Gua22				
7af	Gua4, Gua22, Cyt23,	Gua2, Cyt3, Ade5,	Gua?2				
7 а1	Gua24	Ade6	Guazz	-	_	-	-
7.9.0	Ade5 Ade6 Cut23	Thy7	Gua4,	Cyt21,			Ade5 Ade6
/ ag	Ade5, Ade6, Cyt25	Tity /	Gua22	Thy20,		_	Aucs, Auco
7ah	Gua4, Cyt23	Gua2, Cyt3, Ade5, Ade6	Gua22	-	-	-	-
7ha	Gua4 Ade5 Ade6 Cvt23	Thy7 Thy20 Cyt21	_	Ade5,	_	_	_
7.04	Guu+, Mue3, Mue0, Cyt25	111y7, 111y20, Cyt21		Gau22			
7ca	Gua4, Gua22, Cyt23,	Gua? Cyt3 Ade5	_	Gua2, Cyt3,	_	_	_
7Ca	Gua24	Guaz, Cyts, Aucs	_	Ade6	_	-	-
7da	Gual Guald	Gau2, Cyt3, Ade5,					
/ua	Gua+, Gua2+	Gua22, Cyt23	-	_	_	-	_

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	Conventional Hydrogen Bonding	Van der Waals	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-Pi T- shaped/ Pi-Pi stacked	Pi- Sigma	Alkyl/ Pi-Alkyl
7fa	Gua2, Cyt3	Cyt1, Gua4	Cyt3, Cyt21	Thy20, Gau22	Gua2	Thy20	Cyt21, Gua22
7fb	Gua2, Cyt4	Cyt1, Gua4	Cyt3	Thy20, Gua22	Gua2, Thy20, Cyt21	-	Cyt21, Gua22
7ai	Cyt3, Gua4, Gua22	Gua2, Ade5, Ade6, Cyt21, Gua24	-	Cyt23	-	-	-
7fi	-	Gua4, Thy7, Gua22, Cyt23	-	Ade6, Thy20, Cyt21	-	-	Ade5
7aj	Gua4, Ade5, Ade6, Cyt23	-	Gua22	Gua22	Gua4	-	-
7cj	Gua4, Gua22	Gua2, Ade5, Cyt23	-	Cyt3, Ade5	-	-	-
7dj	Ade4, Ade5	Cyt3, Ade6, Gua22, Cyt23, Gua24	-	-	-	-	-
7fj	-	Cyt3, Ade5, Gua4, Gua24	Gua22	Ade6, Cyt23	-	-	-
7gk	Gua4	Gua2, Cyt3, Ade5, Ade6, Cyt21, Gua22, Gua24	-	Cyt23	-	-	-
7ck	Ade5, Ade6, Gua16, Ade17, Ade18	Thy7, Thy19	Ade18	Thy8	-	-	Gua4, Gua16

Table S10 Cartesian Coordinates of the optimized structures obtained at B3LYP 631-G (d,p) level of theory

Code			Cart	esian Coordinates		
	Center	Atomic	A tom tuno	С	oordinates (Angstror	ns)
	number	number	Atom type	Х	Y	Z
	1	6	С	-0.882828	2.632954	0.301305
	2	6	С	-0.301890	1.533980	-0.352121
	3	6	С	-0.134179	1.577119	-1.728968
	4	6	С	-0.553141	2.711697	-2.438574
	5	6	С	-1.133810	3.790496	-1.771076
	6	6	С	-1.306602	3.766712	-0.381956
	7	6	С	-0.405949	1.153808	2.015767
	8	6	С	0.049541	0.457712	0.682273
	9	1	Н	0.319295	0.745425	-2.255662
	10	1	Н	-0.425121	2.748025	-3.515802
	11	1	Н	-1.456255	4.663150	-2.331280
	12	1	Н	-1.755648	4.605354	0.141649
	13	1	Н	-1.326216	2.999300	2.372261
	14	8	0	-0.303690	0.718660	3.145887
	15	6	С	1.550039	0.207529	0.744913
	16	6	С	2.408019	0.665980	1.715295
	17	6	С	2.368484	-0.491560	-0.224774
	18	1	Н	2.185501	1.199347	2.626670
	19	1	Н	4.509812	0.511296	1.976924
	20	6	С	-0.742556	-0.832155	0.535000
	21	6	С	-0.314452	-2.052454	0.998561
7aa	22	6	С	-2.091884	-1.029723	0.043728
	23	1	Н	0.629795	-2.312516	1.451459
	24	6	С	-2.398012	-2.408431	0.231129
	25	1	Н	-1.213279	-3.974063	1.050794
	26	7	N	-0.946094	2.375558	1.675555
	27	7	N	-1.297081	-2.999143	0.815092
	28	7	N	3.705385	0.316400	1.404299
	29	6	С	3.715627	-0.397218	0.224380
	30	6	С	2.110482	-1.208844	-1.408577
	31	6	С	3.169442	-1.777192	-2.105012
	32	6	С	4.495960	-1.654802	-1.645322
	33	6	C	4,785339	-0.967740	-0.473099
	34	1	Н	2.972701	-2.332050	-3.017582
	35	1	Н	5.303253	-2.109836	-2.211350
	36	1	Н	5.805209	-0.879039	-0.109275
	37	6	C	-3.079435	-0.205027	-0.530300
	38	6	C	-4.300211	-0.758258	-0.894874
	39	6	C	-4.572333	-2.127340	-0.704155
	40	6	C	-3.623899	-2.969906	-0.138996
	41	1	H	-2.892912	0.849970	-0.693051
	42	1	Н	-5.061535	-0.122922	-1.337947
	43	1	Н	-5 536230	-2 529450	-1.001662
	44	1	Н	-3.827167	-4.026161	0.014252
	45	1	Н	1.092329	-1.338850	-1.759398
	Center	Atomic		C	oordinates (Angstror	ns)
	number	number	Atom type	X	Y	Z
	1	6	С	-0.922840	1 746385	1 748207
	2	6	C	-0 327514	1.141241	0.629301
	3	6	C	-0.205277	1.856623	-0 552399
	4	6	C	-0.689533	3 170004	-0.590031
	5	6	C	-1 284786	3.766252	0.519325
	6	6	C	-1 406229	3.048551	1 714443
	7	6	C C	-0.336726	-0.361389	2 / 199/115
7ab	8	6	C	0.100018	-0 286557	0 991201
/ a.9	Q	1	н	0.256281	1 42/11//	_1 430602
	10	1	п u	-1 650557	1.424144	0.454120
	10	1	п u	-1.050557	4.704344	0.434120
	11	1	п u	-1.000400	1.022764	2.303143
	12	1 0	п	-1.309313	1.023704	3./3330/
	13	ð 6		-0.103342	-1.291/93	0.007201
	14	6		2 /81707	-0.4337/0	1 060920
	13	0		2.401/0/	-0.400114	0.20225
	10	1	с u	2.423420	-0.330743	-0.207333
1	1/	1	п	2.207131	-0.+00702	5.02/0/4

	18	1	Н	4.595487	-0.636436	2.100750
	19	6	C	-0.645481	-1 372144	0 231970
	20	6	C	-0.1/6695	-2 632549	0.007601
	20	6	C	-0.140070	1 275277	0.250012
	21	0	U U	-2.008798	-1.5/35//	-0.239913
	22	1	H	0.828537	-3.028405	0.245282
	23	6	C	-2.250511	-2.676980	-0.785605
	24	1	Н	-0.965463	-4.369357	-0.894384
	25	7	Ν	-0.930386	0.843771	2.815381
	26	7	N	-1.099286	-3.414812	-0.604344
	27	7	N	3 780288	-0.567820	1.514346
	28	6	C	3 779825	-0.603301	0.135541
	20	6	C	2 155426	0.587244	1 670826
	29	0	C C	2.133430	-0.387344	-1.070830
	30	0	C	5.213095	-0.677600	-2.300300
	31	6	C	4.548121	-0./26668	-2.1181/4
	32	6	C	4.848281	-0.695011	-0.762289
	33	1	Н	3.008838	-0.716724	-3.632252
	34	1	Н	5.354021	-0.796648	-2.842491
	35	1	Н	5.875337	-0.742173	-0.411336
	36	6	С	-3.055354	-0.434103	-0.316900
	37	6	С	-4.269961	-0.800210	-0.882204
	38	6	C	-4 477844	-2.093300	-1 401134
	20	6	C	2 470180	2.0/3500	1 250620
	39	0		-3.470189	-3.046033	-1.339039
	40	1	H	-2.920177	0.569161	0.070026
	41	1	H	-5.0/6486	-0.074393	-0.92/650
	42	1	Н	-5.438532	-2.347548	-1.838808
	43	1	Н	-3.623789	-4.048196	-1.755190
	44	1	Н	1.132696	-0.583184	-2.032376
	45	17	Cl	-0.543270	4.091294	-2.084745
	Center	Atomic		С	oordinates (Angstro	ms)
	number	number	Atom type	X	Y	Z
	1	6	С	-0.894491	2.318498	1.055804
	2	6	С	-0.306531	1.418019	0.152040
	3	6	C	-0.148216	1,786286	-1.176245
	4	6	C	-0 590783	3 052450	-1 561848
	5	6	C	-1 178211	3 945536	-0.675196
	6	6	C C	-1 335579	3 577328	0.666592
	7	6	C C	-0.385631	0.473348	2 357000
	8	6	C C	0.068044	0.128386	0.801/08
	0	1	<u></u> и	0.000044	1 122259	1.010176
	10	1	11	1 504265	4.015121	-1.910170
	10	1	п	-1.304303	4.913121	-1.034277
	11	1	H	-1./90091	4.201030	1.370048
	12	1	H	-1.324142	2.103001	3.15/25/
	13	8	0	-0.268216	-0.223/16	3.345314
	14	6	C	1.572721	-0.102478	0.882500
	15	6	С	2.431534	0.116920	1.932627
	16	6	С	2.393585	-0.523334	-0.234603
	17	1	Н	2.208141	0.403065	2.948904
	18	1	Н	4.537429	-0.058901	2.137703
	19	6	C	-0.707208	-1.097188	0.435416
7ac	20	6	C	-0.250734	-2.386664	0.563335
	21	6	C	-2.064821	-1.189076	-0.063561
	22	1	Н	0.707586	-2.735122	0.916145
	23	6	С	-2.346786	-2.575468	-0.229304
	24	1	Н	-1.120959	-4.274858	0.140118
	25	7	N	-0.942604	1.733380	2.327761
	26	7	N	-1.224014	-3.273863	0.163092
	27	7	N	3.731039	-0.120917	1,538552
	28	6	C	3 742752	-0 518453	0.217950
	29	6	Č	2 137373	-0.928022	-1 558753
	30	6	C	3 199696	-1 284694	-2 379394
	31	6	C C	4 527846	-1.255801	-1 9093/8
	27	6	C	4 815830	_0 877215	-0.60/100
	22	1	с и	3.004200	1 507625	2 400720
	24	1	<u>п</u>	5.004399	-1.39/023	-5.400720
	34	1	H	5.337701	-1.5398/8	-2.5/4543
	35	1	H	5.83/1//	-0.862692	-0.234166
	36	6	C	-3.0/7149	-0.264658	-0.387826
	37	6	C	-4.298228	-0.729890	-0.858496
	38	6	C	-4.546146	-2.107298	-1.019629
	39	6	C	-3.572996	-3.047587	-0.707234
	40	1	Н	-2.910322	0.800522	-0.277685
	41	1	Н	-5.078663	-0.017595	-1.109512

	42	1	Н	-5.510851	-2.438745	-1.392003
	43	1	Н	-3.757717	-4.111628	-0.825877
	44	1	Ч	1 118749	0.987201	1 927079
	44	1		1.118/49	-0.987201	-1.92/0/9
	45	9	F	-0.442351	3.421428	-2.854801
	Center	Atomic		C	oordinates (Angstro	ns)
	number	number	Atom type	Х	Y	Z
	1	6	C	1 225824	0.090942	1 121719
	1	0	C	1.223834	-0.069642	2.232728
	2	6	С	0.587160	-0.244304	0.991248
	3	6	С	1.167033	-1.044922	0.018632
	4	6	С	2,383216	-1.673126	0.310282
	5	6	C	2.017627	1 51/269	1 520292
	5	0	C	3.017027	-1.314308	1.539382
	6	6	C	2.434213	-0.710480	2.525269
	7	6	С	-0.705905	1.165986	2.437822
	8	6	С	-0.718417	0.560505	0.987445
	0	1	Н	0.607725	1 103332	0.945024
	10	1	11	2.060029	-1.175552	1 721245
	10	1	Н	3.960028	-2.013874	1./31345
	11	1	Н	2.919177	-0.581699	3.487871
	12	1	Н	0.697749	1.030908	3.986981
	13	8	0	-1.555661	1.865450	2.950707
	14	6	C	1 021764	0.247555	0.842052
	14	0	C	-1.931704	-0.347333	0.842932
	15	6	C	-2.787061	-0.722646	1.851161
	16	6	С	-2.376383	-1.041165	-0.348761
	17	1	Н	-2.815422	-0.396842	2.879615
	18	- 1	н	_4 /72000	_2 011505	1 010230
	10	1		0.727200	1 712005	0.002407
	19	6	C	-0.737309	1./13085	-0.003407
	20	6	C	-1.884535	2.246255	-0.539422
	21	6	С	0.356452	2.547759	-0.458997
7ad	22	1	н	-2 905081	1 916015	-0 422447
7 au	22	1	C II	0.21(105	2 55 (012	1 285202
	23	0	L L	-0.216195	5.550815	-1.285292
	24	1	Н	-2.245915	3.891673	-1.828815
	25	7	N	0.460289	0.748840	3.047230
	26	7	N	-1 578945	3 344863	-1 309839
	20	7	N	2 720071	1 615519	1 270007
	27	1	N	-3.720971	-1.013318	1.370997
	28	6	C	-3.500078	-1.829394	0.026421
	29	6	С	-1.966415	-1.065136	-1.695699
	30	6	С	-2.650816	-1.865400	-2.601317
	31	6	C	-3 751522	-2 647816	-2 198808
	20	0	C	4 102085	2.047010	0.891805
	32	6	C	-4.192985	-2.636317	-0.881805
	33	1	Н	-2.336393	-1.885534	-3.640452
	34	1	Н	-4.266331	-3.264041	-2.929729
	35	1	н	-5 046865	-3 230451	-0 568546
	26	6	C	1 751725	2 564125	0.265564
	30	0	C	1.731733	2.304133	-0.203304
	37	6	С	2.513076	3.547272	-0.884180
	38	6	С	1.919725	4.528645	-1.702363
	39	6	С	0.547208	4.545432	-1.913520
	40	1	н	2 234266	1 817354	0 354153
	41	1	TT	2 500010	2 550200	0.726506
	41	1	Н	3.388912	3.339280	-0./30380
	42	1	Н	2.543148	5.282422	-2.173839
	43	1	Н	0.081964	5.300623	-2.540872
	44	1	Н	-1.141260	-0.445265	-2.029753
	45	35	Br	3 197903	_2 780204	-1 022964
	TJ Carta			5.177705	2.700204	1.022704
	Center	Atomic	Atom type	r U	on unnates (Angstrol	115)
	number	number		Х	Y	Z
	1	6	С	-0.963116	1.365545	1.978070
	2	6	С	-0.357783	0.910132	0.789964
	3	6	C	-0 291214	1 753122	-0 303196
	1	2	C C	0.271217	2 020012	0.100100
	4	0		-0.650054	5.058812	-0.160190
	5	6	C	-1.436168	3.490266	0.995026
	6	6	C	<u>-1.5047</u> 80	2.644282	2.100001
	7	6	С	-0.289295	-0.788665	2.477487
	8	6	C	0 139746	-0 526635	0.991065
7ae	0	1	11	0.125000	1 120033	1 020542
	9	1	Н	0.165220	1.460849	-1.258545
	10	1	Н	-1.839766	4.494065	1.026781
	11	1	Н	-1.967983	2.975439	3.023625
	12	1	Н	-1.303166	0.418797	3.866690
	12	0	0	0 107400	1 700200	3 126500
		0	U	-0.10/400	-1./09302	0.001/00/
	1.4	~	<u> </u>		116177415	1 901606
	13	6	C	1.658512	-0.002313	0.001000
	13 14 15	6 6	C C	2.526430	-0.731410	1.959926
	13 14 15 16	6 6 6	C C C	1.658512 2.526430 2.477919	-0.731410 -0.483375	1.959926 -0.287603
	$ \begin{array}{r} 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 17 1 $	6 6 6 1	C C C H	1.658512 2.526430 2.477919 2.311772	-0.731410 -0.483375 -0.880156	1.959926 -0.287603 3.007085
	$ \begin{array}{r} 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 19 \\ 10 \\$	6 6 1	C C C H	1.658512 2.526430 2.477919 2.311772 4.642801	-0.002313 -0.731410 -0.483375 -0.880156 0.786205	1.959926 -0.287603 3.007085

	19	6	С	-0.548432	-1.552698	0.106884
	20	6	С	0.029880	-2.728540	-0.306467
	21	6	С	-1.923786	-1.587068	-0.348262
	22	1	Н	1.038343	-3.080017	-0.152777
	23	6	С	-2.091511	-2.815861	-1.048080
	24	1	Н	-0.694447	-4.374816	-1.430114
	25	7	N	-0.921880	0.358637	2,933350
	26	7	N	-0.885903	-3 484758	-1.000563
	20	7	N	3 827880	-0.684115	1.510966
	27	6	C I	3.827000	0.536220	0.130315
	28	0	C	2 219129	-0.330220	1 666457
	29	0	C C	2.218138	-0.302832	-1.000437
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	35	1	Н	5.936145	-0.493524	-0.397932
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	37	6	С	-4.239302	-1.098324	-0.827998
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	40	1	Н	-2.957808	0.219798	0.276766
	41	1	Н	-5.095491	-0.434879	-0.750813
	42	1	Н	-5.328273	-2,577510	-1.967964
	43	1	Н	-3.398000	-4.134389	-2.170819
	44	1	Н	1.198829	-0 361588	-2 037137
	45	7	N	-0 777472	3 9421/13	-1 331107
	46	8	0	-1 254600	5.072012	-1.331177
	40	0	0	-1.234090	2 522670	-1.201911
	4/	0	0	-0.234645	5.322070	-2.303204
	Center	Atomic	Atom type	v	v v	ns) 7
	number	number	C	A 0.000297	<u>1</u>	1 1 (509)
	1	6	C	-0.909287	2.2/1310	1.165086
	2	6	C	-0.318427	1.412383	0.224111
	3	6	C	-0.1/5683	1.83/519	-1.086615
	4	6	C	-0.623205	3.115925	-1.4/4105
	5	6	С	-1.211625	3.942521	-0.512021
	6	6	C	-1.363124	3.536053	0.820167
	7	6	С	-0.373630	0.385285	2.394037
	8	6	С	0.071683	0.098822	0.913479
	<u>8</u> 9	6 1	C H	0.071683 0.286066	0.098822 1.189331	0.913479 -1.824062
	8 9 10	6 1 1	C H H	0.071683 0.286066 -1.560779	0.098822 1.189331 4.929707	0.913479 -1.824062 -0.802915
	8 9 10 11	6 1 1 1	C H H H	0.071683 0.286066 -1.560779 -1.820228	0.098822 1.189331 4.929707 4.193099	0.913479 -1.824062 -0.802915 1.554033
	8 9 10 11 12	6 1 1 1 1 1	C H H H H	0.071683 0.286066 -1.560779 -1.820228 -1.322023	0.098822 1.189331 4.929707 4.193099 2.035313	0.913479 -1.824062 -0.802915 1.554033 3.262299
	8 9 10 11 12 13	6 1 1 1 1 8	C H H H H O	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227
	8 9 10 11 12 13 14	6 1 1 1 1 8 6	C H H H O C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057
	8 9 10 11 12 13 14 15	6 1 1 1 1 8 6 6	C H H H O C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255
	8 9 10 11 12 13 14 15 16	6 1 1 1 1 8 6 6 6 6	C H H H O C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346
	8 9 10 11 12 13 14 15 16 17	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \end{array} $	С Н Н Н О С С С Н	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297
	8 9 10 11 12 13 14 15 16 17 18	6 1 1 1 1 8 6 6 6 6 1 1	С Н Н Н О С С С С Н Н	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446
	8 9 10 11 12 13 14 15 16 17 18 19	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	С Н Н Н О С С С С Н Н Н С	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H C C C C H H C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H C C C C H H C C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1 198610	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C H H H O C C C C H H C C C H H	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C H H H O C C C C H H C C C H C C H	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.241624
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	С Н Н Н О С С С С С С С С С С С С С	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.04421	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.296795	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H H O C C C C H H C C H H N	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 0.042426	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.629262	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H H O C C C C H H C C C H H C C N	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 1.200625	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 3.286002	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.080704
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 26\\ 27\\ \end{array}$	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H H O C C C C H H C C C H H N N	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 2.74111	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 0.1550(4)	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\end{array}$	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H H O C C C C H H C C C C H H C C C H H N N	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 2.745140	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 0.0155064	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.105002
7af	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H O C C C C H H C C C H H C C H N N N C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.120965	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 0.075452	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 1.60057
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 29\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 29\\ 20\\ 20\\ 27\\ 28\\ 29\\ 29\\ 20\\ 20\\ 27\\ 28\\ 29\\ 20\\ 20\\ 27\\ 28\\ 29\\ 20\\ 20\\ 27\\ 28\\ 29\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20\\ 20$	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H O C C C C H H C C C C H H C C C H N N N C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 -1.12957	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -0.875439	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 21\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 21\\ 21\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 21\\ 21\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 21\\ 21\\ 21\\ 21\\ 21\\ 21\\ 21\\ 21\\ 21\\ 21$	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H O C C C C H H C C C C H H N N N N C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.5000	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 1.627525
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 17\\ \end{array}$	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H O C C C C H H C C C C H H C C C H N N N N	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.15564	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ \end{array}$	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H H O C C C C C H H C C C C C H N N N N N C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C C H C C C C H N N N N C C C C H H C C C C C C C C C C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C H H C C C H N N N C C C H H H H H H H H H H H H H	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C H H C C C H N N N N C C C H H H H H H H H H H H H H	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.280532
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C H H C C C H N N N C C C C H H H C C C C C C C C C C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.74111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549 -3.066223	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045 -0.836473 -0.268400	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.280532 -0.395364
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C C H H C C C C C H H N N C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549 -3.066223 -4.283348	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.8475439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045 -0.836473 -0.268400 -0.724490	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.280532 -0.395364 -0.885197
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C H H C C C C H H N N C C C H H H C C C C H H H C C C C H H H C C C C C C C C C C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549 -3.066223 -4.283348 -4.527129	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045 -0.268400 -0.724490 -2.097856	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.395364 -0.395364 -0.885197 -1.083313
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1$	C H H H O C C C C H H C C C C H H N N N C C C H H H C C C C H H H C C C C H H H C C C C C C C C C C C C C	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549 -3.066223 -4.283348 -4.527129 -3.553515	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045 -0.836473 -0.268400 -0.724490 -2.097856 -3.043607	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.395364 -0.885197 -1.083313 -0.789167
7af	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39\\ 40\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6$	С Н Н Н Н О С С С С С С С С С С С С С	0.071683 0.286066 -1.560779 -1.820228 -1.322023 -0.241787 1.577319 2.442636 2.392676 2.225112 4.550940 -0.699269 -0.240987 -2.053549 0.715760 -2.331376 -1.104431 -0.943426 -1.209625 3.741111 3.745148 2.128886 3.186657 4.518014 4.813681 2.985304 5.324248 5.837549 -3.066223 -4.283348 -4.527129 -3.553515 -2.901780	0.098822 1.189331 4.929707 4.193099 2.035313 -0.345910 -0.125348 0.064858 -0.509255 0.318838 -0.109891 -1.116177 -2.407563 -1.198610 -2.762863 -2.581112 -4.286785 1.639362 -3.286903 -0.155064 -0.513047 -0.875439 -1.204485 -1.184880 -0.843510 -1.488861 -1.447045 -0.836473 -0.268400 -0.724490 -2.097856 -3.043607 0.793673	0.913479 -1.824062 -0.802915 1.554033 3.262299 3.356227 0.887057 1.937255 -0.247346 2.963297 2.123446 0.421454 0.519042 -0.088618 0.869382 -0.291624 0.042742 2.414522 0.089704 1.527525 0.195902 -1.581074 -2.419150 -1.957663 -0.643907 -3.447737 -2.636232 -0.395364 -0.885197 -1.083313 -0.789167 -0.256490

	41	1	Н	-5.064331	-0.007756	-1.121833
	42	1	Н	-5 488942	-2.421952	-1.469584
	43	1	Н	-3 734967	-4 104762	-0.935898
	43	1	11	1 107729	-4.104702	-0.755070
	44	ĺ	П	1.10/728	-0.925607	-1.943437
	45	6	C	-0.468995	3.5/1104	-2.906932
	46	1	H	0.579566	3.545265	-3.224998
	47	1	Н	-1.028503	2.926618	-3.595093
	48	1	Н	-0.832378	4.593671	-3.041418
	Center	Atomic	A tom type	Co	oordinates (Angstro	ms)
	number	number	Atom type	Х	Y	Z
	1	6	C	-1.069557	1.581118	1.760394
	2	6	С	-0.417560	1.059378	0.628697
	3	6	C	-0.388145	1.793421	-0.541701
	4	6	С	-1.016144	3.053459	-0.584153
	5	6	C	-1.665942	3,559196	0.545114
	6	6	C	-1 694212	2 816369	1 736497
	7	6	C	-0.243601	-0.456953	2 483933
	8	6	C C	0.167358	-0.316714	0.971834
	0	1	с и	0.107558	1 /35223	1 /35083
	10	1	п ц	2 152182	1.4532225	-1.455085
	10	1	п	-2.155165	4.520045	0.519690
	11	1	Н	-2.19/842	3.212307	2.013109
	12	1	H	-1.351082	0.790681	3.742552
	13	8	0	0.023774	-1.375634	3.234643
	14	6	C	1.686414	-0.323211	0.872332
	15	6	C	2.566190	-0.287613	1.927157
	16	6	C	2.492826	-0.302826	-0.331238
	17	1	Н	2.363330	-0.327917	2.986284
	18	1	Н	4.685786	-0.223804	2.040143
	19	6	С	-0.464545	-1.469026	0.207268
	20	6	C	0.163329	-2.666342	-0.035991
	21	6	C	-1.824502	-1.613662	-0.272497
	22	1	Н	1.177576	-2.958091	0.188613
	23	6	С	-1.931643	-2.928402	-0.810403
7ag	24	1	Н	-0.474431	-4.472280	-0.950144
8	25	7	N	-0.963916	0.666539	2.818850
	26	7	N	-0.706581	-3 540642	-0.648220
	20	7	N	3 862664	-0.226202	1 /60999
	27	6	C I	3 853174	0.220202	0.082026
	20	0	C	2 219759	-0.238833	1.711201
	29	0	C C	2.218/38	-0.337214	-1./11201
	30	0	C	3.2/1/90	-0.326341	-2.010440
	31	6	C	4.609156	-0.247860	-2.1/9418
	32	6	<u>с</u>	4.91/03/	-0.207504	-0.825368
	33	1	H	3.062486	-0.368550	-3.681191
	34	1	H	5.411391	-0.224949	-2.910936
	35	1	Н	5.946900	-0.156514	-0.483003
	36	6	С	-2.965896	-0.788840	-0.308781
	37	6	С	-4.140695	-1.277121	-0.866179
	38	6	C	-4.215284	-2.579713	-1.397621
	39	6	С	-3.110981	-3.421740	-1.376768
	40	1	Н	-2.932531	0.218978	0.088263
	41	1	Н	-5.020946	-0.641528	-0.894941
	42	1	Н	-5.148242	-2.930947	-1.828401
	43	1	Н	-3.161376	-4.428656	-1.781845
	44	1	Н	1.197129	-0.447402	-2.064174
	45	8	0	-0.932700	3.702008	-1.787384
	46	6	C	-1.545244	4.973751	-1.904394
	47	1	Н	-1.361502	5.305089	-2.927575
	48	1	Н	-2.628651	4.921327	-1.732620
	49	1	Н	-1.109110	5.701439	-1.207039
	Center	Atomic		Сс	oordinates (Angstro	ms)
	number	number	Atom type	X	Y	Ź
	1	6	С	1.667613	-1.658748	0.155133
	2	6	Č	0.639247	-0.916497	-0.448900
		0	C	0.469795	-0.973235	-1 874787
	3	6		0.707/73	-0.713433	-1.024207
	3	6	C C	1 333244	-1 760120	-2 500333
7ah	3 4 5	6 6	C C	1.333244	-1.769129	-2.590333
7ah	3 4 5 6	6 6 6	C C C	1.333244 2.355155 2.523142	-1.769129 -2.502571 -2.448527	-2.590333 -1.988413
7ah	3 4 5 6 7	6 6 6 6	C C C C	1.333244 2.355155 2.523142	-1.769129 -2.502571 -2.448527 0.624522	-2.590333 -1.988413 -0.602634
7ah	3 4 5 6 7	6 6 6 6 6		1.333244 2.355155 2.523142 0.634214	-1.769129 -2.502571 -2.448527 -0.624623	-2.590333 -1.988413 -0.602634 1.936565
7ah	3 4 5 6 7 8	6 6 6 6 6 6	C C C C C C	1.333244 2.355155 2.523142 0.634214 -0.131084	-1.769129 -2.502571 -2.448527 -0.624623 -0.162878	-2.590333 -1.988413 -0.602634 1.936565 0.643406
7ah	3 4 5 6 7 8 9 9	6 6 6 6 6 6 1	C C C C C H	1.333244 2.355155 2.523142 0.634214 -0.131084 -0.322709	-1.769129 -2.502571 -2.448527 -0.624623 -0.162878 -0.413621	-2.590333 -1.988413 -0.602634 1.936565 0.643406 -2.306318

			**	0.00000	0.115005	a FOOOFC							
	11	1	Н	3.022996	-3.11/92/	-2.580876							
	12	1	н	2 307282	-1 880765	2 181211							
	12	1		2.307202	1.000705	2.101211							
	13	8	0	0.385041	-0.323477	3.085580							
	14	6	С	-1.574186	-0.640595	0.731135							
	15	6	C C	2,000509	1 496751	1 692050							
	15	6	C	-2.090508	-1.486/51	1.683050							
	16	6	С	-2.652459	-0.362727	-0.195635							
	17			1 (100(1	1.004720	0.5(0.145							
	17	1	Н	-1.618064	-1.894729	2.563445							
	18	1	Н	-4.013658	-2.339429	1.967761							
	10	1		0.020516	1.250650	0.540020							
	19	6	C	-0.028516	1.350650	0.548920							
	20	6	С	-0.960395	2.215942	1.069184							
	21		Č.	1.0(2024	21(7700	0.050.175							
	21	0	C	1.003834	2.16/799	0.059475							
	22	1	Н	-1.905844	1.992393	1.538738							
	22	6	C	0.702569	2 502422	0.206295							
	23	0	C	0.702308	3.323433	0.300283							
	24	1	Н	-1.048941	4.331257	1.204641							
	25	7	N	1 656361	1 461482	1 533014							
	25	/	19	1.050501	-1.401482	1.555014							
	26	7	N	-0.531497	3.515323	0.922358							
	27	7	Ν	-3.410166	-1.767442	1 400486							
	20		с С	2 70 60 60	1.002012	0.050.000							
	28	6	C	-3./86869	-1.092013	0.258609							
	29	6	С	-2.793390	0.440193	-1.343728							
	20	6	C	4.015974	0.479140	2,002020							
	30	0	C	-4.013874	0.478140	-2.002039							
	31	6	C	-5.118865	-0.266466	-1.538527							
	32	6	C	-5 010084	-1 056832	-0.400465							
	32	U		-3.017704	-1.030032	-0.400403							
	33	1	Н	-4.127615	1.097911	-2.886727							
	34	1	Н	-6.062004	-0.216620	-2 074305							
	25	1	11	5.052004	1 (240/27	2.074505							
	35	1	Н	-5.870186	-1.624967	-0.033567							
	36	6	С	2,305796	1.915788	-0.555876							
	27	~	<u> </u>	2 1000790	2.004050	0.000450							
	3/	0	C	3.122808	2.984059	-0.902450							
	38	6	C	2.735672	4.315402	-0.652884							
	20	6	C	1 520025	4 601902	0.045541							
		0	U	1.320033	4.001805	-0.043341							
	40	1	Н	2.625597	0.901436	-0.763738							
	41	1	Н	4 080523	2 790002	-1 376379							
	12	1	11	2 206650	5 100502	0.027457							
	42	1	Н	3.396659	5.128583	-0.937457							
	43	1	Н	1.215932	5.625667	0.153402							
	44	1	н	-1.963976	1.044504	-1 695281							
	15	17		2,500152	0.065456	0.100202							
	45	1/	CI	3.799155	-3.303430	0.190392							
	Center	Atomic		C	oordinates (Angstron	ns)							
			A A a see Asses a		oor annates (ringstroi								
	number	number	Atom type	X	Y	Z							
	number	number	Atom type	X	<u>Y</u>	Z							
	number 1	number 6	Atom type C	X -1.155520	<u>Y</u> -2.646570	Z 0.431467							
	number 1 2	number 6 6	Atom type C C	X -1.155520 -0.387131	<u>Y</u> -2.646570 -1.492776	Z 0.431467 0.653740							
	number 1 2 2	number 6 6	Atom type C C	X -1.155520 -0.387131	Y -2.646570 -1.492776	Z 0.431467 0.653740							
	number 1 2 3	number 6 6 6 6	Atom type C C C	X -1.155520 -0.387131 -0.199313	Y -2.646570 -1.492776 -1.043086	Z 0.431467 0.653740 1.953606							
	number 1 2 3 4	number 6 6 6 6 6	Atom type C C C C	X -1.155520 -0.387131 -0.199313 -0.784504	Y -2.646570 -1.492776 -1.043086 -1.746587	Z 0.431467 0.653740 1.953606 3.015462							
	number 1 2 3 4 5	number 6 6 6 6 6	Atom type C C C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 1.549860	Y -2.646570 -1.492776 -1.043086 -1.746587 2 887785	Z 0.431467 0.653740 1.953606 3.015462 2.772442							
	number 1 2 3 4 5	number 6 6 6 6 6 6	Atom type C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785	Z 0.431467 0.653740 1.953606 3.015462 2.772442							
	number 1 2 3 4 5 6	number 6 6 6 6 6 6 6	Atom type C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773							
	number 1 2 3 4 5 6 7	number 6 6 6 6 6 6 6	Atom type C C C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860							
	number 1 2 3 4 5 6 7 0	number 6 6 6 6 6 6 6 6 6	Atom type C C C C C C C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 -0.490283	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860							
	number 1 2 3 4 5 6 7 8	number 6	Atom type C C C C C C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669							
	number 1 2 3 4 5 6 7 8 9	number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 1	Atom type C C C C C C C C H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756							
	number 1 2 3 4 5 6 7 8 9 10	number 6 6 6 6 6 6 6 6 6 1	Atom type C C C C C C C C C H H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708							
	number 1 2 3 4 5 6 7 8 9 10	number 6 6 6 6 6 6 6 6 6 6 1 .	Atom type C C C C C C C C C H H H V	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -0.6220 (Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708							
	number 1 2 3 4 5 6 7 8 9 10 11	number 6 6 6 6 6 6 6 6 6 1 1	Atom type C C C C C C C C H H H H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413							
	number 1 2 3 4 5 6 7 8 9 10 11 12	number 6 6 6 6 6 6 6 6 6 1 1 1 1	Atom type C C C C C C C C H H H H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808							
	number 1 2 3 4 5 6 7 8 9 10 11 12 13	number 6 6 6 6 6 6 6 6 6 1 1 1 1	Atom type C C C C C C C C C C H H H H H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809							
	number 1 2 3 4 5 6 7 8 9 10 11 12 13	number 6 6 6 6 6 6 6 6 6 1 1 1 1 1	Atom type C C C C C C C C H H H H H C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.4075	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -0.0046							
	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14	number 6 6 6 6 6 6 6 6 6 1 1 1 1 1 1 1 1 1 8	Atom type C C C C C C C C H H H H H O	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406							
	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	number 6 6 6 6 6 6 6 6 1 1 1 1 8 6	Atom type C C C C C C C C C C C C H H H H O C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094							
	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	number 6 6 6 6 6 6 6 1 1 1 1 8 6	Atom type C C C C C C C C C C C C H H H O C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.270626	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 1.502127							
Tha	$\begin{array}{r} \textbf{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ \end{array}$	number 6 6 6 6 6 6 6 6 6 1 1 1 1 1 8 6 6	Atom type C C C C C C C C C C H H H H O C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.370636	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551 -1.879743	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 -1.502125							
7ba	$\begin{array}{r} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \end{array}$	number 6 6 6 6 6 6 6 6 1 1 1 1 1 1 1 1 8 6 6 6 6	Atom type C C C C C C C C H H H H H H C C C C C C C C C C C C C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.370636 2.566395	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551 -1.879743 -0.092464	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 -1.502125 -0.139794							
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7ba	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ \end{array}$	number 6 6 6 6 6 6 6 1 1 1 1 1 1 1 1 6 6 6 6 6 6 6 6 6 1 6 6 6 6 6 6 6 6 6	Atom type C C C C C C C C C H H H H H H C C C C C C C C C H C C H	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.370636 2.566395 2.043754 4.464073 -0.477460 0.112514 -1.768917 1.070405 -1.871700	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551 -1.879743 -0.092464 -2.674840 -2.160657 0.409148 1.295820 0.972459 1.229620 2.215528	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 -1.502125 -0.139794 -2.154300 -1.735638 -1.060597 -1.927156 -0.720342 -2.419452 -1.412356							
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7ba	$\begin{array}{r} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \end{array}$	number 6 6 6 6 6 6 6 6 6 1 1 1 1 1 1 6 6 6 6 6 6 6 6 1 7 7 6 <td>Atom type C C C C C C C C C C C C C H H O C C C C C H C C H N N N N N N C</td> <td>X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.370636 2.566395 2.043754 4.464073 -0.477460 0.112514 -1.768917 1.070405 -1.871709 -0.491169 -1.210103 -0.714890 3.716288 3.871557 2.451904 3.614036 4.900377 5.037897</td> <td>Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551 -1.879743 -0.092464 -2.160657 0.409148 1.295820 0.972459 1.229620 2.215538 3.176639 -2.912639 2.378508 -1.638827 -0.551508 1.042306 1.669215 1.179603 0.069483 1.691298</td> <td>Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 -1.502125 -0.139794 -2.154300 -1.735638 -1.060597 -1.927156 -0.720342 -2.419452 -1.412356 -2.707364 -0.943152 -1.308143 0.674984 1.137743 0.793527 -0.021793 1.172899</td>	Atom type C C C C C C C C C C C C C H H O C C C C C H C C H N N N N N N C	X -1.155520 -0.387131 -0.199313 -0.784504 -1.549860 -1.746284 -0.490283 0.102912 0.391119 -0.644426 -2.003394 -2.342539 -1.705900 -0.340738 1.620595 2.370636 2.566395 2.043754 4.464073 -0.477460 0.112514 -1.768917 1.070405 -1.871709 -0.491169 -1.210103 -0.714890 3.716288 3.871557 2.451904 3.614036 4.900377 5.037897	Y -2.646570 -1.492776 -1.043086 -1.746587 -2.887785 -3.358028 -2.009458 -0.947184 -0.156430 -1.395926 -3.420666 -4.244679 -3.680722 -2.041393 -0.969551 -1.879743 -0.092464 -2.160657 0.409148 1.295820 0.972459 1.229620 2.215538 3.176639 -2.912639 2.378508 -1.638827 -0.551508 1.042306 1.669215 1.179603 0.069483 1.691298	Z 0.431467 0.653740 1.953606 3.015462 2.772442 1.468773 -1.690860 -0.692669 2.154756 4.032708 3.602413 1.276808 -1.371809 -2.896406 -0.799094 -1.502125 -0.139794 -2.154300 -1.735638 -1.060597 -1.927156 -0.720342 -2.419452 -1.412356 -2.707364 -0.943152 -1.308143 0.674984 1.137743 0.793527 -0.021793 1.172899							

	35	1	Н	6.020662	-0.302313	-0.294909
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	46	7	N	3.425120	3.781356	2.637495
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	2	6	С	-0.540229	-1.460785	0.642837
	3	6	C	-0.283958	-0.979043	1.918752
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	5	6	С	-1.741745	-2.687564	2.845601
	6	6	С	-2.008654	-3.189785	1.565971
	7	6	С	-0.740245	-2.055217	-1.673638
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	9	1	Н	0.378556	-0.134073	2.066196
	10	1	Н	-0.690763	-1.222771	4.022167
	11	1	Н	-2.204517	-3.158428	3.707967
	12	1	Н	-2.668741	-4.040303	1.423821
	13	1	Н	-2.065778	-3.621959	-1.260002
	14	8	0	-0.632742	-2.152069	-2.880243
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	20	6	C	-0.521498	0.379486	-1.141858
	21	6	C	0.122739	1.174863	-2.061746
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	24	6	С	-1.758528	2.280354	-1.527762
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	27	7	N	-0.609949	2.313229	-2.295198
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	39	0	с и	-2.001004	-0 13/1/2	-1.423341
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	40	6	C	-5 047071	0 370764	1 758506
	48	1	н	5 419192	3 452700	1 355086
	49	1	Н	4 457015	4 006055	2 749937
	50	1	Н	5 345452	2.463593	2.840794
	51	1	Н	-4.203676	0.286662	2 455344
	52	1	H	-5.977372	0.447749	2.325787
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	3	6	С	-0.339708	1.554703	-1.903179
	4	6	С	-0.849863	2.625548	-2.650796
	5	6	С	-1.424100	3.725982	-2.011579
	6	6	С	-1.489535	3.794392	-0.614393
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	10	1	Н	-0.798418	2.596974	-3.734651
	11	1	Н	-1.819120	4.547730	-2.601523
	12	1	Н	-1.920995	4.656771	-0.115163
	13	1	Н	-1.208301	3.230993	2.184907
	14	8	0	0.042732	1.094323	3.005955
	15	6	C	1.532936	0.286928	0.342044
	16	6	C	2.623254	0.963353	0.858479
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	20	6	C	-0.499403	-1.745000	0.082105
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	26	7	N	3.780457	0.400203	0.346274
	27	6	С	3.471790	-0.625978	-0.517292
	28	6	С	1.479296	-1.696560	-1.398750
	29	6	С	2.308915	-2.521449	-2.149199
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	32	1	Н	1.867274	-3.270471	-2.799983
	33	1	Н	4.332697	-3.067537	-2.681070
	34	1	H	5.391517	-1.357938	-1.214198
	35	6	C	-3.022506	-0.223452	-0.755409
	36	6	C C	-4.229117	-0.816421	-1.106924
	37	6	C	-4.363373	2 800033	-0.040981
	39	1	н	-2 788636	0.765295	-1 126542
	40	1	Н	-4 915525	-0.275368	-1.751906
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	43	1	Н	0.402059	-1.802789	-1.459967
	44	6	С	0.686677	-2.051836	2.314174
	45	6	С	2.742854	2.122849	1.802549
	46	1	Н	1.050955	-1.144174	2.793716
	47	1	Н	0.410346	-2.762924	3.100732
	48	1	Н	1.503622	-2.491857	1.730967
	49	1	H	3.771310	2.496964	1.820094
	50	1	H	2.100983	2.954569	1.497668
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	1	6	C	1 248654	2 695508	1 05/387
	2	6	C	0 377181	1 604332	0.908309
	3	6	č	0.109126	0.799847	2.007179
	4	6	C	0.716462	1.090616	3.236852
	5	6	С	1.583671	2.176686	3.359459
	6	6	С	1.862951	3.000847	2.262965
	7	6	С	0.596467	2.800256	-1.163156
	8	6	С	-0.118719	1.545001	-0.541546
7ea	9	1	H	-0.562559	-0.046790	1.923609
	10	1	H	0.512156	0.461852	4.097430
	11	1	H	2.051712	2.389280	4.315833
	12	1	H U	2.53/5/2	3.840383	2.334083
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	14	6	C	-1 624884	1.742763	-0 634478
	16	6	č	-2.269867	2.892573	-1.023653
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	17	6	С	-2.663004	0.800859	-0.273277
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	22	6	C	1.571740	-0.441984	-1.162261
	23	1	Н	-1.239094	0.101133	-2.842092
	24	6	C	1 577711	-1 /16023	-2 200621
	24	0		0.142000	-1.410923	-2.200021
	25	1	Н	0.143000	-1.802873	-3.722625
	26	7	N	1.369245	3.361943	-0.171531
	27	7	Ν	0.425903	-1.241375	-2.936415
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	28	1	IN	-3.034402	2.754587	-0.909809
	29	6	C	-3.909422	1.462742	-0.456833
	30	6	С	-2.670159	-0.538745	0.159256
	31	6	C	3 802218	1 1/2980	0.406657
	51	0	C	-3.892218	-1.142980	0.400037
	32	6	C	-5.119015	-0.476527	0.237249
	33	6	С	-5.135101	0.840346	-0.203012
	34	1	н	-6.045888	-0.997215	0.446128
	34	1	11	-0.045888	1.262750	0.440120
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	42	1	Н	2.595717	-3.076314	-3.160959
	43	1	Н	-1.749631	-1.096928	0.274185
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	number	number	Atom type	Х	Y	Z
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	1	0	C C	0.266205	2.092541	0.817012
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	4	6	C	0 684591	1 208447	3 045687
		0	C	1.5(10(0)	2 200 (01	2.152282
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	0	6	C C	0.122192	1 491927	0.722224
	0	0		-0.122102	0.001700	-0.755254
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	10 11 12	1 1 1	H H H	2.006938 2.536089 1.967114	2.509401 3.886492 4.096872	4.113656 2.079583 -0.644692
	10 11 12 13	1 1 1 8	H H H O	2.006938 2.536089 1.967114 0.517630	2.509401 3.886492 4.096872 3.059365	4.113656 2.079583 -0.644692 -2.564876
	10 11 12 13 14	1 1 1 8 6	H H H O C	2.006938 2.536089 1.967114 0.517630 -1.625339	2.509401 3.886492 4.096872 3.059365 1.694058	4.113656 2.079583 -0.644692 -2.564876 -0.839701
	10 11 12 13 14	1 1 1 8 6	H H H O C	2.006938 2.536089 1.967114 0.517630 -1.625339 2.253088	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338	4.113656 2.079583 -0.644692 -2.564876 -0.839701 1.287181
	10 11 12 13 14 15	1 1 1 8 6 6	H H H O C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.755455	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 0.424924
	10 11 12 13 14 15 16	1 1 1 8 6 6 6 6	H H H O C C C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824
	10 11 12 13 14 15 16 17	1 1 1 8 6 6 6 6 1	H H O C C C H	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023
	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \end{array} $	H H O C C C H H	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001
	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ \end{array} $		H H O C C C H H H	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.435064
	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H O C C C H H H C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 0.72575	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064
	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H O C C C C H H H C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570
7ес	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H O C C C H H H C C C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	Н Н О С С С С Н Н Н С С С Н	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C H H C C C C H H C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C H H H C C C H H C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.000320	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 2.047522	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 2.715204
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C H H C C C H H C H H	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\$	H H H O C C C H H C C C H H C H N	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.285570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	H H H O C C C H H C C C H C C H H N N	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	H H H O C C C H H C C H H C C H N N	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619304	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1<170082
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 26\\ 27\\ 26\\ 26\\ 26\\ 26\\ 26\\ 26\\ 26\\ 26\\ 26\\ 26$	$ \begin{array}{c} 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 1\\ 6\\ 1\\ 6\\ 1\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\ 7\\$	H H H O C C C H H C C C H H C C H H C C N N	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 2.00227	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.451022	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.455064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 0.645520
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ \end{array} $	$ \begin{array}{c} 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 1\\ 6\\ 1\\ 7\\ 7\\ 7\\ 7\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\$	H H H O C C C H H C C C C H H C C H N N N C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C H H C C C H C C H N N N C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ \end{array} $	$ \begin{array}{c} 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 1\\ 7\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	H H H O C C C H H C C C H H C C H N N N C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.455064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C H H C C C H N N N C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 22 \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C H C C C H N N N N N	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 5.15220	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 -0.6326	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 0.27550
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C H N N N C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 33\\ 32\\ 33\\ 33\\ 32\\ 33\\ 33\\ 32\\ 33\\ 33$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C C H H H C C C H N N N C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C C H H C C C C H N N N C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.086842 -6.081195	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610
7ec	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ 34 \\ 35 \\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C C H N N N N C C C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671840	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432291	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.90267
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 65\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 2.671849 2.671849	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -0.432281	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.402367
7ec	$ \begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ \end{array} $	$ \begin{array}{c} 1\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 6\\ 1\\ 7\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	H H H O C C C C H H H C C C H H N N C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240	$\begin{array}{r} 4.113656\\ 2.079583\\ -0.644692\\ -2.564876\\ -0.839701\\ -1.287181\\ -0.434824\\ -1.709023\\ -1.458001\\ -1.435064\\ -2.485570\\ -1.266698\\ -2.926417\\ -2.245080\\ -3.715294\\ -0.439076\\ -2.969709\\ -1.170082\\ -0.655038\\ 0.063669\\ 0.336414\\ 0.130189\\ -0.374650\\ 0.361521\\ -0.546610\\ -0.402367\\ -0.544103\\ \end{array}$
7ec	$ \begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C H N N N N C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.086842 -6.08195 2.671849 3.697771 3.678642	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.402367 -0.544103 -1.507377
7ec	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ 34 \\ 35 \\ 36 \\ 37 \\ 38 \\ 38 \\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H C C C C C C C C C C	2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.544103 -1.507377 -2.371119
7ec	$ \begin{array}{r} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 30 \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876 2.73150	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.232512	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.402367 -0.544103 -1.507377 -2.371119 0.230279
7ec	$ \begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39\\ 16 \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	H H H O C C C C H H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876 2.731559	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.333513 -0.530572	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.546610 -0.546610 -0.546610 -0.544103 -1.507377 -2.371119 0.359378
7ec	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ 34 \\ 35 \\ 36 \\ 37 \\ 38 \\ 39 \\ 40 \\ 40 \\ 40 \\ $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C C C H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.086842 -6.08195 2.671849 3.697771 3.678642 2.597876 2.731559 4.508358	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.333513 -3.070008	$\begin{array}{r} 4.113656\\ 2.079583\\ -0.644692\\ -2.564876\\ -0.839701\\ -1.287181\\ -0.434824\\ -1.709023\\ -1.458001\\ -1.435064\\ -2.485570\\ -1.266698\\ -2.926417\\ -2.245080\\ -3.715294\\ -0.439076\\ -2.926417\\ -2.245080\\ -3.715294\\ -0.439076\\ -2.969709\\ -1.170082\\ -0.655038\\ 0.063669\\ 0.336414\\ 0.130189\\ -0.374650\\ 0.361521\\ -0.54610\\ -0.402367\\ -0.544103\\ -1.507377\\ -2.371119\\ 0.359378\\ -1.570539\end{array}$
7ec	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ 34 \\ 35 \\ 36 \\ 37 \\ 38 \\ 39 \\ 40 \\ 41 \\ 41 \\ $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C C H H C C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876 2.731559 4.508358 2.569673	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.333513 -3.070008 -3.273307	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.435064 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.402367 -0.544103 -1.507377 -2.371119 0.359378 -1.570539 -3.122370
7ec	$ \begin{array}{r} 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ 34 \\ 35 \\ 36 \\ 37 \\ 38 \\ 39 \\ 40 \\ 41 \\ 42 \\ 41 \\ 42 \\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 1 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	H H H O C C C C H H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876 2.731559 4.508358 2.569673 -1.79279	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.33513 -3.070008 -3.273307 -1.096682	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -2.485570 -1.26698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.546610 -0.546610 -0.546610 -0.544103 -1.507377 -2.371119 0.359378 -1.570539 -3.122370 0.208380
7ec	$ \begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39\\ 40\\ 41\\ 42\\ 42 \end{array} $	$ \begin{array}{c} 1\\ 1\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 6\\ 1\\ 7\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\$	H H H O C C C C C H H C C C C C C C C C	2.006938 2.006938 2.536089 1.967114 0.517630 -1.625339 -2.253088 -2.677092 -1.821818 -4.294551 0.332680 -0.331919 1.564227 -1.278158 1.557802 0.098360 1.382833 0.392423 -3.619394 -3.913395 -2.704444 -3.935542 -5.152111 -5.148392 -6.086842 -6.081195 2.671849 3.697771 3.678642 2.597876 2.731559 4.508358 2.569673 -1.792729 -2.044672	2.509401 3.886492 4.096872 3.059365 1.694058 2.832338 0.785456 3.727106 3.387713 0.212828 -0.373574 -0.530103 -0.100552 -1.564810 -2.047532 3.299788 -1.438313 2.698732 1.454893 -0.530871 -1.105296 -0.430325 0.863139 -0.926870 1.391943 -0.926870 1.391943 -0.432281 -1.352240 -2.376236 -2.489647 0.333513 -3.070008 -3.273307 -1.09682 2.90927	4.113656 2.079583 -0.644692 -2.564876 -0.839701 -1.287181 -0.434824 -1.709023 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -1.458001 -2.485570 -1.266698 -2.926417 -2.245080 -3.715294 -0.439076 -2.969709 -1.170082 -0.655038 0.063669 0.336414 0.130189 -0.374650 0.361521 -0.546610 -0.544103 -1.507377 -2.371119 0.359378 -1.570539 -3.122370 0.208880 <td< td=""></td<>

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	45	9	F	0.409139	0.480602	4.150138
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	2	6	C C	-0.352499	0.398158	1 568754
	3	6	C	-0.076521	1.477013	0.741879
	4	6	C	-0.698450	2.701262	1.013042
	5	6	С	-1.580494	2.856848	2.079319
	6	6	С	-1.860397	1.771782	2.917263
	7	6	С	-0.568879	-1.649333	2.802707
	8	6	С	0.159049	-1.047729	1.544819
	9	1	Н	0.604462	1.391414	-0.094898
	10	1	Н	-2.048866	3.817494	2.258466
	11	1	H	-2.546541	1.883332	3.750849
	12	0	H	-1.941152	-0.811586	4.143854
	13	6	0 C	-0.402055	-2.770409	1 768367
	15	6	C C	2 292582	-1.472265	2 937366
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	17	1	Н	1.864538	-1.836601	3.858579
	18	1	Н	4.333870	-1.571236	3.509797
	19	6	С	-0.280903	-1.840956	0.325456
	20	6	С	0.406011	-2.913239	-0.191968
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7ed	22	1	H	1.361940	-3.314500	0.107054
	23	6	C	-1.489737	-2.792793	-1.391763
	24	1	H	0.001164	-4.259522	-1./800/6
	25	7	IN N	-1.337421	-0.051/4/	3.335745
	20	7	N	-0.308303	-1.3/3206	-1.220003
	27	6	C	3 948475	-0.912219	1 524070
	29	6	C	2.737622	-0.353418	-0.511306
	30	6	C	3.967041	-0.103810	-1.099661
	31	6	С	5.183538	-0.243527	-0.407678
	32	6	С	5.181771	-0.655474	0.918202
	33	1	Н	6.116853	-0.033731	-0.916291
	34	1	Н	6.114628	-0.775312	1.461060
	35	6	C	-2.643001	-0.904347	-0.380685
	36	6	C	-3.667075	-1.129626	-1.285958
	37	6	C	-3.627603	-2.157872	-2.244068
	38	0	U U	-2.52/840	-3.002770	-2.303429
	40	1	н	-2.718922	-0.094321	-2 929707
	40	1	Н	-2.483699	-3.803268	-3.035896
	42	1	Н	1.826535	-0.261419	-1.088976
	43	35	Br	4.024560	0.442759	-2.937294
	44	35	Br	-5.212850	0.007052	-1.238408
	45	35	Br	-0.326282	4.199660	-0.116377
	Center	Atomic	Atom type	C	oordinates (Angstro	ns)
	number	number	G G	<u>X</u>	Y	Z
	1	6	<u> </u>	0.6/855/	2.865786	-0.441465
	2	6	C	0.2/981/	1./0384/	0.552580
	4	6	C	0.203704	3 126136	2 303149
	5	6	C	0.932276	4 206945	1 516825
	6	6	C	1.010078	4.091581	0.123698
	7	6	С	0.262203	1.209116	-2.002616
	8	6	С	-0.010962	0.574628	-0.591132
7 f9	9	1	Н	-0.109753	1.064702	2.329737
, 1a	10	1	Н	0.475457	3.234055	3.381728
	11	1	H	1.186271	5.152739	1.986221
	12	1	H	1.318493	4.931183	-0.492044
	13	0 0	Н	0.929710	3.112541	-2.561//4
	14	6		-1 470475	0.070757	-3.06/031
	16	6	C	-2.446416	0.428347	-1.442541
	17	6	Č	-2.129353	-0.561703	0.558161
	18	1	H	-2.355065	0.912599	-2.403393
	19	6	С	0.940924	-0.598166	-0.414571
	20	6	С	0.637078	-1.892449	-0.761693

	21	6	С	2.332623	-0.602128	-0.016311
	22	1	Н	-0.297485	-2.294009	-1.123815
	23	6	С	2.785268	-1.948515	-0.136190
	24	7	Ν	0.676282	2,507610	-1.794468
	25	7	N	1.731111	-2.713959	-0.595488
	25	7	N	-3 67/0/9	-0.040737	-1.018957
	20	6	C	3 506225	0.654300	0.206716
	21	0	C	-3.300223	-0.034309	1.7(4522
	28	0	C C	-1./0/845	-1.151015	1./04555
	29	6	C	-2.642084	-1./80438	2.578124
	30	6	C	-4.001509	-1.845235	2.214349
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	32	1	Н	-2.318884	-2.236859	3.509100
	33	1	Н	-4.708466	-2.343858	2.870785
	34	1	Н	-5.496074	-1.346352	0.736480
	35	6	С	3.251532	0.369316	0.424887
	36	6	С	4.551618	-0.013193	0.731739
	37	6	C	4,970139	-1.352579	0.612623
	38	6	C	4 091881	-2 337780	0.178099
	30	1	<u></u> ц	2 052756	1 405578	0.531341
	40	1	11	5.260280	0.725979	1.072601
	40	1	п	5.200389	0.755676	0.0(2070
	41	1	H	5.992601	-1.01956/	0.863079
	42	1	H	4.411109	-3.3/1313	0.083573
	43	1	Н	-0.659815	-1.136564	2.044257
	44	6	С	1.766559	-4.142361	-0.828640
	45	6	С	-4.919868	0.054888	-1.750438
	46	1	Н	0.800985	-4.461793	-1.223628
	47	1	Н	2.542320	-4.399590	-1.558118
	48	1	Н	1.963273	-4.692266	0.098995
	49	1	Н	-5.674556	0.599236	-1.171857
	50	1	Н	-4 743899	0 593487	-2 682862
	51	1	н	-5 315163	-0.938//9	-1 001035
	Conton	Atomia	11	-5.515105	-0.930449	-1.771755
	Center	Atomic	Atom type	v	v N	7
		inuilibei	C	A 0.709/45	1 25(7740	1.000440
	1	6	C	0.708645	2.567740	-1.088448
	2	6	C	0.298377	1.638041	-0.118562
	3	6	C	0.227151	2 (12(1(0))	1 213700
	5	0	C	0.237131	2.020099	1.213790
	4	6	C	0.595630	3.329729	1.536439
	<u>4</u> 5	6 6	C C C	0.237131 0.595630 1.007915	3.329729 4.252480	1.536439 0.583870
	4 5 6	6 6 6	С С С С	0.237131 0.595630 1.007915 1.066656	2.020099 3.329729 4.252480 3.870007	1.536439 0.583870 -0.761943
	4 5 6 7	6 6 6 6	C C C C	0.237131 0.595630 1.007915 1.066656 0.247499	2.020099 3.329729 4.252480 3.870007 0.654696	1.536439 0.583870 -0.761943 -2.306970
	4 5 6 7 8	6 6 6 6 6	C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908	1.213770 1.536439 0.583870 -0.761943 -2.306970 -0.799075
	4 5 6 7 8 9	6 6 6 6 6 6 1	C C C C C H	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611	1.213730 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715
	$ \begin{array}{r} 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 10 \\ 7 \\ 7 \\ 7 \\ 8 \\ 9 \\ 10 \\ 7 \\ $	6 6 6 6 6 1 1	C C C C C H H	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758
	$ \begin{array}{r} $	6 6 6 6 6 1 1 1	C C C C C H H H	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116
	$ \begin{array}{r} $	6 6 6 6 1 1 1 1	C C C C C H H H H	$\begin{array}{c} 0.237131 \\ 0.595630 \\ 1.007915 \\ 1.066656 \\ 0.247499 \\ -0.024967 \\ -0.081110 \\ 1.276138 \\ 1.383970 \\ 0.943954 \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748
	$ \begin{array}{r} $	6 6 6 6 1 1 1 1 1 8	C C C C C H H H H	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.219748 -3.269757
	$ \begin{array}{r} $	6 6 6 6 1 1 1 1 8 6	С С С С С С Н Н Н Н Н О С	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.625612
	$ \begin{array}{r} $	6 6 6 6 1 1 1 1 8 6 6	С С С С С С Н Н Н Н Н О С С	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 2.470504	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052724	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 1.504422
	$ \begin{array}{r} $		С С С С С С Н Н Н Н Н Н Н С С С С	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ 2.157426\end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 0.552011	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.550707
	$ \begin{array}{r} $		C C C C C H H H H H C C C C C C C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ 0.276794\end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.232600	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.621522
	$ \begin{array}{r} $		C C C C C C H H H H H C C C C C C H H C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.022052\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 0.024451	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.02170
7fb	$ \begin{array}{r} $		C C C C C C H H H H H O C C C C C H H H C C C C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.5111\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178
7fb	$ \begin{array}{r} $		C C C C C C H H H H O C C C C H C C C C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.477215
7fb	$ \begin{array}{r} $	$ \begin{array}{c} 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 $	C C C C C H H H H H C C C C C C C C C C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.477215
7fb	$ \begin{array}{r} $	$ \begin{array}{c} 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 1\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\$	C C C C C H H H H H C C C C C H C C H H C C C H H H H H H C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.477215 -0.042010 -0.732355
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 10 \\ \hline & 11 \\ \hline & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline \end{array}$	$ \begin{array}{c} 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C C C C C H H H H H C C C C C H C C C H C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.477215 -0.042010 -0.732355 0.106025
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 22 \\ \hline & 23 \\ \end{array}$	$ \begin{array}{c} 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ $	C C C C C C H H H H H C C C C H C C C H C	$\begin{array}{r} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.042010 -0.732355 0.106025 -2.350805
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \end{array}$	$ \begin{array}{c} 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \end{array} $	C C C C C C H H H H H H C C C C C H C C C H C C C N N	$\begin{array}{r} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.406178 -0.732355 0.106025 -2.350805 -0.168060
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \end{array}$	$ \begin{array}{c} 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 1\\ 6\\ 7\\ 7\\ 7\\ 7\\ 7 \end{array} $	C C C C C C H H H H H H C C C C C H C C C H C C C N N N	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\\ -3.703840\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ \hline & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \end{array}$	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & & $	C C C C C C H H H H H H C C C C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964
7fb	$\begin{array}{r} & 4 \\ & 5 \\ & 6 \\ \hline 7 \\ & 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \end{array}$	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & & $	C C C C C C H H H H H H C C C C C H C C C H C C N N N C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107	1.2137,0 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964 1.856166
7fb	$\begin{array}{r} & 4 \\ & 5 \\ & 6 \\ \hline 7 \\ & 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \end{array}$	$\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$	C C C C C C H H H H H H C C C C C C H C C C N N N C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634	1.2137,00 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964 1.856166 2.780858
7fb	$\begin{array}{r} & 4 \\ & 5 \\ & 6 \\ & 7 \\ & 8 \\ & 9 \\ \hline 10 \\ & 11 \\ & 12 \\ & 13 \\ & 14 \\ & 15 \\ & 16 \\ & 17 \\ & 18 \\ & 19 \\ & 20 \\ & 21 \\ & 22 \\ & 23 \\ & 24 \\ & 25 \\ & 26 \\ & 27 \\ & 28 \\ & 29 \end{array}$		C C C C C C H H H H H C C C C C H C C C N N N C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964 1.856166 2.780858 2.442361
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \end{array}$	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & & $	C C C C C C H H H H H H H C C C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 4.490122	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.477215 -0.042010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964 1.856166 2.780858 2.442361 1.166854
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ & 13 \\ \hline & 14 \\ & 15 \\ & 16 \\ \hline & 17 \\ & 18 \\ & 19 \\ & 20 \\ \hline & 21 \\ \hline & 22 \\ & 23 \\ \hline & 24 \\ & 25 \\ & 26 \\ & 27 \\ \hline & 28 \\ & 29 \\ \hline & 30 \\ \hline & 21 \\ \hline \end{array}$		C C C C C C H H H H H H C C C C C H C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 -4.490123 2.25021	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 2.781719\\ \end{array}$
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 22 \\ \end{array}$		C C C C C C H H H H H H C C C C C C C C	$\begin{array}{r} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\\ -3.703840\\ -3.538989\\ -1.738806\\ -2.680055\\ -4.043724\\ -4.490123\\ -2.359221\\ -2.359221\\ -4.556111\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.59864 1.779226	1.21370 1.536439 0.583870 -0.761943 -2.306970 -0.799075 1.997715 0.895758 -1.522116 -3.219748 -3.269757 -0.635612 -1.594432 0.559797 -2.631523 -0.406178 -0.406178 -0.42010 -0.732355 0.106025 -2.350805 -0.168060 -1.082290 0.238964 1.856166 2.780858 2.442361 1.166854 3.781718 2.18050
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 22 \\ \hline \end{array}$		C C C C C C C H H H H H C C C C C C H C	$\begin{array}{r} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\\ -3.703840\\ -3.538989\\ -1.738806\\ -2.680055\\ -4.043724\\ -4.490123\\ -2.359221\\ -4.756111\\ -5.70456\end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 1.97725	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ -0.01077\\ \end{array}$
7fb	$\begin{array}{c} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ & 13 \\ \hline & 14 \\ & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 33 \\ \hline & 31 \\ \hline \hline & 31 \\ \hline \hline \hline \hline & 31 \\ \hline \hline \hline \hline \hline & 31 \\ \hline $		C C C C C C C H H H H H C C C C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 -4.490123 -2.359221 -4.756111 -5.539429	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 -1.189766	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ -0.90186\\ -0.901867\\ -0.90186\\ -0.901867\\ -0.90186\\ -0.901867\\ -$
7fb	$\begin{array}{c} & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ \hline & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 34 \\ \hline \end{array}$	$\begin{array}{c} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ &$	C C C C C C C H H H H C C C C C C C C C	$\begin{array}{r} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\\ -3.703840\\ -3.538989\\ -1.738806\\ -2.680055\\ -4.043724\\ -4.490123\\ -2.359221\\ -4.756111\\ -5.539429\\ 3.253433\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 -1.189766 0.224271	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ 0.174454\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.17445\\ -0.1744\\ $
7fb	$\begin{array}{c} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ \hline & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 34 \\ \hline & 35 \\ \hline \end{array}$	$\begin{array}{c} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\$	C C C C C C H H H H H C C C C C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 -4.490123 -2.359221 -4.756111 -5.539429 3.253433 4.552023	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 -1.189766 0.224271 -0.120544	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ -0.174454\\ 0.528352\\ \end{array}$
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ \hline & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 34 \\ \hline & 35 \\ \hline & 36 \\ \end{array}$	$\begin{array}{c} & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\$	C C C C C C C H H H C C C C C C C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 -4.756111 -5.539429 3.253433 4.552023 4.939046	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 -1.189766 0.224271 -0.120544 -1.466443	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ 0.174454\\ 0.528352\\ 0.676599\end{array}$
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 34 \\ \hline & 35 \\ \hline & 36 \\ \hline & 37 \\ \hline \end{array}$	$\begin{array}{c} & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ &$	C C C C C C C H H H C C C C C H C C C C	0.237131 0.595630 1.007915 1.066656 0.247499 -0.024967 -0.081110 1.276138 1.383970 0.943954 0.099015 -1.492809 -2.470504 -2.157436 -2.376784 0.903960 0.564406 2.304179 -0.386724 2.725152 0.685464 1.644317 -3.703840 -3.538989 -1.738806 -2.680055 -4.043724 -4.756111 -5.539429 3.253433 4.552023 4.939046 4.030326	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.59864 -1.770226 -1.189766 0.224271 -0.120544 -1.466443 -2.496740	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ 0.174454\\ 0.528352\\ 0.676599\\ 0.468242\\ \end{array}$
7fb	$\begin{array}{r} & 3 \\ & 4 \\ & 5 \\ & 6 \\ \hline & 7 \\ & 8 \\ \hline & 9 \\ \hline & 10 \\ \hline & 11 \\ \hline & 12 \\ & 13 \\ \hline & 14 \\ \hline & 15 \\ \hline & 16 \\ \hline & 17 \\ \hline & 18 \\ \hline & 19 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 20 \\ \hline & 21 \\ \hline & 22 \\ \hline & 23 \\ \hline & 24 \\ \hline & 25 \\ \hline & 26 \\ \hline & 27 \\ \hline & 28 \\ \hline & 29 \\ \hline & 30 \\ \hline & 31 \\ \hline & 32 \\ \hline & 33 \\ \hline & 34 \\ \hline & 35 \\ \hline & 36 \\ \hline & 37 \\ \hline & 38 \\ \end{array}$	$\begin{array}{c} & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\$	C C C C C C C H H H C C C C C H C C C C	$\begin{array}{c} 0.237131\\ 0.595630\\ 1.007915\\ 1.066656\\ 0.247499\\ -0.024967\\ -0.081110\\ 1.276138\\ 1.383970\\ 0.943954\\ 0.099015\\ -1.492809\\ -2.470504\\ -2.157436\\ -2.376784\\ 0.903960\\ 0.564406\\ 2.304179\\ -0.386724\\ 2.725152\\ 0.685464\\ 1.644317\\ -3.703840\\ -3.538989\\ -1.738806\\ -2.680055\\ -4.043724\\ -4.490123\\ -2.359221\\ -4.756111\\ -5.539429\\ 3.253433\\ 4.552023\\ 4.939046\\ 4.030326\\ 2.979873\\ \end{array}$	2.020099 3.329729 4.252480 3.870007 0.654696 0.302908 1.344611 5.255581 4.576901 2.404394 -0.071851 -0.065484 0.052734 -0.536911 0.338600 -0.834431 -2.164014 -0.792800 -2.606715 -2.146398 1.960742 -2.961973 -0.295939 -0.662901 -0.890107 -1.325634 -1.426973 -1.102287 -1.598864 -1.770226 -1.189766 0.224271 -0.120544 -1.466443 -2.496740 1.268051	$\begin{array}{c} 1.21370\\ 1.536439\\ 0.583870\\ -0.761943\\ -2.306970\\ -0.799075\\ 1.997715\\ 0.895758\\ -1.522116\\ -3.219748\\ -3.269757\\ -0.635612\\ -1.594432\\ 0.559797\\ -2.631523\\ -0.406178\\ -0.477215\\ -0.406178\\ -0.477215\\ -0.406178\\ -0.477215\\ -0.042010\\ -0.732355\\ 0.106025\\ -2.350805\\ -0.168060\\ -1.082290\\ 0.238964\\ 1.856166\\ 2.780858\\ 2.442361\\ 1.166854\\ 3.781718\\ 3.186595\\ 0.901867\\ 0.174454\\ 0.528352\\ 0.676599\\ 0.468242\\ 0.072507\\ \end{array}$

	39	1	Н	5.284218	0.663805	0.696475
	40	1	н	5 961164	-1 702840	0.957148
	41	1	Ц	4 325480	3 535630	0.580154
	41	1	11	4.323460	-3.333030	0.300134
	42	1	н	-0.088273	-0.848501	2.123709
	43	9	F	0.540700	3./12882	2.832800
	44	6	C	1.644206	-4.408636	-0.106666
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	47	1	Н	2.395317	-4.827978	-0.784875
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	number	number	~	Δ	Y	L
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	12	1	и	0.705142	0.315548	1 118583
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	13	0	C C	-1.320927	0.29(202	0.00052
	14	0	C	-1./4/409	-0.386292	0.089955
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	Center	Atomic	Atom type	C	oordinates (Angstron	ns)
	number	number	Atom type	X	Y	Z
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	2	6	С	-0.401381	1.677282	-0.930910
	3	6	С	-0.226328	0.946636	-2.097891

	4	6	С	-0.829336	1.389520	-3.283581		
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	9	1	Н	0.369940	0.041351	-2.100313		
	10	1	Н	-0.697795	0.819057	-4.197368		
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	20	6	C	0.173526	-0.451299	2.204095		
	21	6	C	-1.731284	-0.422827	0.998288		
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	23	6	С	-1.799553	-1.473432	1.958944		
	24	7	N	-1.213296	3.418051	0.313610		
	25	7	N	-0.624731	-1.466391	2.683027		
	26	7	N	3.736439	2.312306	0.869590		
	27	6	С	3.880645	1.060273	0.308454		
	28	6	С	2.464084	-0.776463	-0.431486		
	29	6	С	3.625912	-1.458910	-0.756193		
	30	6	С	4.907615	-0.913142	-0.566279		
	31	6	C	5.044102	0.358790	-0.024437		
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	33	1	Н	6.029579	0.785174	0.134228		
	34	6	С	-2.833413	-0.220286	0.145939		
	35	6	C	-3.928835	-1.058229	0.280394		
	36	6	С	-3.985340	-2.098650	1.223665		
	37	6	C	-2.910088	-2.315210	2.075517		
	38	1	Н	-2.835926	0.561257	-0.602003		
	39	1	Н	-4.867464	-2.725111	1.280730		
	40	1	Н	-2.941793	-3.114922	2.808671		
	41	1	Н	1.497253	-1.244592	-0.566977		
	42	6	C	-0.277949	-2.399365	3.736104		
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	4.4	1	н	0 680803	2 110705	1 15379/		
	44	1	11	0.089893	-2.118/05	4.155774		
	44 45	1	H	-1.022958	-2.373837	4.538359		
	44 45 46	1 1 1	H H	-1.022958 -0.209029	-2.118705 -2.373837 -3.423379	4.538359 3.352184		
	44 45 46 47	1 1 1 1	H H H	-1.022958 -0.209029 5.440904	-2.118703 -2.373837 -3.423379 3.457671	4.153754 4.538359 3.352184 0.400655		
	44 45 46 47 48	1 1 1 1 1	H H H H	-1.022958 -0.209029 5.440904 4.398745	-2.118705 -2.373837 -3.423379 3.457671 4.106013	4.538359 4.538359 3.352184 0.400655 1.682398 2.020215		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 52 \\ \end{array} $	1 1 1 1 1 1	H H H H H	-1.022958 -0.209029 5.440904 4.398745 5.454598	-2.118705 -2.373837 -3.423379 3.457671 4.106013 2.720284 -2.720284	4.538359 4.538359 3.352184 0.400655 1.682398 2.020845		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 50 \\ \end{array} $	1 1 1 1 1 35	H H H H H Br	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095	-2.118705 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899	4.538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ \end{array} $	1 1 1 1 1 35 35	H H H H Br Br Br	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700	-2.118705 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363	4.538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905		
	44 45 46 47 48 49 50 51 Center	1 1 1 1 1 35 35 Atomic	H H H H Br Br Atom type	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Ce	-2.118705 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstrop	4.153754 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms)		
	44 45 46 47 48 49 50 51 Center number	1 1 1 1 1 35 35 Atomic number	H H H H Br Br Atom type	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X	-2.118703 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstrop Y 2.856201	4.1538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z		
	44 45 46 47 48 49 50 51 Center number 1	1 1 1 1 1 35 35 Atomic number 6	H H H H Br Br Atom type	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.206177	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstrop Y 2.856201 1.605%C1	4.1538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.672476		
	44 45 46 47 48 49 50 51 Center number 1 2 2	1 1 1 1 1 35 35 Atomic number 6 6	H H H H Br Br C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.202200	-2.118703 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstron Y 2.856201 1.695851 1.057440	4.1538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.805402		
	44 45 46 47 48 49 50 51 Center number 1 2 3 4	1 1 1 1 1 35 35 Atomic number 6 6 6 6	H H H H Br Br C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.812100	-2.118703 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstron Y 2.856201 1.695851 1.057440 1.604859	4.153774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 2.025126		
	44 45 46 47 48 49 50 51 Center number 1 2 3 4	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6	H H H H Br Br C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.500272	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 coordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748972	4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.074120		
	44 45 46 47 48 49 50 51 Center number 1 2 3 4 4 5	1 1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6	H H H H Br Br C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.702459	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 2.305229	4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) 2 0.620687 0.678476 1.895402 3.025136 2.974130 1.74767		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ \hline \begin{array}{r} Center \\ number \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ \end{array} $	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6	H H H H Br Br C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Ca X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485562	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.540922	4.153774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) 2 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 1.564115		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ \hline Center \\ number \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ \end{array} $	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Colspan="2">Colspan="2" Colspan="2">Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2"	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 pordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.264844	4.153774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) 2 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 0.726166		
	$ \begin{array}{r} 44 \\ 45 \\ 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ \hline Center \\ number \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 0 \\ \end{array} $	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 0.200021	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.162317	4.15377 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) 2 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.096469		
7.00	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ Center\\ number\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ \end{array}$	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 1 1	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Colspan="2">Colspan="2" Colspan="2">Colspan="2" Colspan="2"	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 cordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060	4.1538359 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ Center\\ number\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ \end{array}$	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 1 1 1	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Colspan="2">Colspan="2" Colspan="2">Colspan="2" Colspan="2" Colspan="2" <td <="" colspan="2" td="" td<=""><td>-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120</td><td>4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277</td></td>	<td>-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120</td> <td>4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277</td>		-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120	4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \hline$	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 1 1 1 1	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.13094	4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ \end{array}$	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 1 1 1 1 8	H H H H Br Br C C C C C C C C C C C C C C C C C	0.08393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Colspan="2">Colspan="2" Colspan="2">Colspan="2" Colspan="2">Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2" Colspan="2"	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451	4.133774 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \hline$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	H H H H Br Br C C C C C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 cordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643	4.133794 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	H H H H Br Br C C C C C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724 -2.377773	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501	4.133794 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	H H H H Br Br C C C C C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 Co X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724 -2.377773 2.98522	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165	4.133794 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ \end{array}$	1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 1 1 1 8 6 6 1 1 1 1 1 1 1 1 1 1 1 1 1	Н H H H H Br Br C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 CC X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724 -2.377773 -2.598522 -2.036295	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165 3.336457	4.133794 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358 -1.878976		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	Н H H H H H H Br Br C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 CC X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724 -2.377773 -2.598522 -2.036295 0.421357	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165 3.336457 0.063412	4.13374 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ns) Z 0.620687 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358 -1.878976 -1.292697		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ \end{array}$	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ $	Н H H H H H H Br Br C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165 3.336457 0.063412 -0.693316	4.13374 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ms) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358 -1.878976 -1.292697 -2.247849		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ \hline \\ 16\\ 17\\ 18\\ 19\\ 20\\ \end{array}$	$ \begin{array}{r} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 35 \\ 35 \\ Atomic number 6 \\ $	Н H H H H H H Br Br C C C C C C C C C C C C C	0.039393 -1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 X 1.185183 0.396177 0.203200 0.813109 1.599372 1.793458 0.485568 -0.121650 -0.399081 2.051737 2.404635 1.742262 0.328287 -1.639724 -2.377773 -2.598522 -2.036295 0.421357 -0.215288 1.71276	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 cordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165 3.336457 0.063412 -0.693316 -0.553959	4.13374 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ns) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358 -1.878976 -1.292697 -2.247849 -1.087275		
7gc	$\begin{array}{r} 44\\ 45\\ 46\\ 47\\ 48\\ 49\\ 50\\ 51\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 20\\ 21\\ \end{array}$	1 1 1 1 1 1 35 35 Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6	Н H H H H H Br Br C C C C C C C C C C C C C	-1.022958 -0.209029 5.440904 4.398745 5.454598 -5.443095 3.490700 	-2.118/05 -2.373837 -3.423379 3.457671 4.106013 2.720284 -0.795899 -3.229363 oordinates (Angstron Y 2.856201 1.695851 1.057440 1.604858 2.748872 3.395258 2.549823 1.364841 0.163317 3.124060 4.290120 4.130994 2.763451 1.438643 2.462501 0.502165 3.336457 0.063412 -0.693316 -0.553959 -0.549204	4.13374 4.538359 3.352184 0.400655 1.682398 2.020845 -0.871597 -1.485905 ns) Z 0.620687 0.678476 1.895402 3.025136 2.974130 1.747657 -1.564115 -0.726166 1.996468 3.885067 1.687277 -1.019903 -2.750106 -0.798623 -1.344594 -0.257358 -1.878976 -1.292697 -2.247849 -1.087275 -2.683494		

	22	6	C	1767062	1 600202	1 045610
	22	0	C	1.702803	-1.090302	-1.943019
	23	7	N	1.231915	3.320471	-0.701235
	24	7	Ν	0.573879	-1.749973	-2.644035
	25	7	N	2 729245	2 242027	1 170752
	25	/	N	-3.728345	2.242927	-1.1/0/53
	26	6	С	-3.891419	1.044462	-0.506632
	27	6	C	2 502550	0.746066	0.285208
	27	0	C	-2.303330	-0.740000	0.383208
	28	6	C	-3.675682	-1.381104	0.764734
	29	6	C	-4 948626	-0.832550	0.529006
	2)		C	5.065521	0.032550	0.529000
	30	6	C	-5.065531	0.391651	-0.11/056
	31	1	Н	-5.832475	-1.371797	0.848223
	22	1	II	6.044227	0.919926	0.211241
	32	1	п	-0.044227	0.818820	-0.511541
	33	6	C	2.831446	-0.272082	-0.280748
	34	6	C	3 925445	-1 119149	-0.357042
	54		c	3.923443	1.11/14/	0.557042
	35	6	C	3.963758	-2.244348	-1.198408
	36	6	С	2.871910	-2.540004	-2.004150
	27	1		2.840250	0.577.475	0.200005
		1	п	2.649239	0.377473	0.388803
	38	1	Н	4.845281	-2.874036	-1.213658
	30	1	н	2 890083	-3 405527	-2 658764
	37	1	11	2.870083	-3.403327	-2.030704
	40	1	Н	-1.544493	-1.217551	0.559470
	41	6	C	0 207677	-2 776792	-3 598928
	42	6	C	4 700212	2 100704	1 (25570
	42	0	C	-4.798312	3.102784	-1.635572
1	43	1	Н	-0.770913	-2.538460	-4.017807
1	44	1	Ц	0.03/050	-2 822020	-1 117161
1	44	1	п	0.934030	-2.023030	-4.41/101
1	45	1	Н	0.152605	-3.761065	-3.120679
1	46	1	н	-5 414121	3 449678	-0 798698
1	47	1	11	1.264245	2.0725.12	0.100000
1	47	1	Н	-4.364346	5.972542	-2.130/10
	48	1	Н	-5.441718	2,579634	-2.351596
	40	25	D	5 460026	0.747094	0.720779
	49		Br	5.462036	-0.747984	0.732778
	50	35	Br	-3.567890	-3.086623	1.637547
	51	0	Б	0.621520	0.002532	4 215040
-	51	9	Г	0.031329	0.992332	4.213940
	Center	Atomic	A tom tring	C	oordinates (Angstroi	ms)
	number	number	Atom type	X	Y	Z
	1	(C	1 172200	1.0(2)174	2 590170
	1	0	C	-1.1/3300	1.062174	2.580170
	2	6	C	-0.376547	0.771387	1.460917
	3	6	C	-0.216752	1 725795	0.467298
		0	c	-0.210752	1.725775	0.407278
	4	6	C	-0.863999	2.957875	0.615998
	5	6	С	-1.658540	3.241488	1.723879
		6	Č.		2 282216	2 720(71
	(1 0/1/10/2		
	6	0	C	-1.820983	2.282310	2.729671
	<u>6</u> 7	6	C	-1.820983 -0.400747	-1.079755	2.988076
	6 7 8	6 6	C C	-1.820983 -0.400747	-1.079755	2.729671 2.988076
	6 7 8	6 6	C C C	-1.820983 -0.400747 0.191418	-1.079755 -0.646979	2.729671 2.988076 1.596931
	6 7 8 9	6 6 1	C C C H	-1.820983 -0.400747 0.191418 0.394049	-1.079755 -0.646979 1.538623	2.729671 2.988076 1.596931 -0.406355
	6 7 8 9	6 6 1	С С Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798	-1.079755 -0.646979 1.538623 4.203950	2.729671 2.988076 1.596931 -0.406355 1.805432
	6 7 8 9 10	6 6 1 1	С С Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798	-1.079755 -0.646979 1.538623 4.203950	2.729671 2.988076 1.596931 -0.406355 1.805432
	6 7 8 9 10 11	6 6 1 1 1	С С Н Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267	-1.079755 -0.646979 1.538623 4.203950 2.494149	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001
	6 7 8 9 10 11 12	6 6 1 1 1 1 1	С С Н Н Н Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807
	6 7 8 9 10 11 12	6 6 1 1 1 1 1 8	С С Н Н Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 0.210564	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 2.127253	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 2.572478
	6 7 8 9 10 11 12 13	6 6 1 1 1 1 1 8	С С Н Н Н Н О	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478
	6 7 8 9 10 11 12 13 14	6 6 1 1 1 1 1 8 6	С С Н Н Н Н О С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800	2.729871 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ \end{array} $	6 6 1 1 1 1 8 6 6	C C H H H O C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726	2.282316 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 16 \\ 16 \\ 16 \\ 16 \\ 16 \\ 16 \\ 16$	6 6 1 1 1 1 8 6 6	C C H H H H C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 0.622255	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ \end{array} $	6 6 1 1 1 1 1 8 6 6 6	С С Н Н Н О С С С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ \end{array} $		С С Н Н Н Н О С С С Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ \end{array} $		C C H H H C C C C C H C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406	2.282510 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247
	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10$		С С Н Н Н Н О С С С С С С С С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -0.707727	2.729871 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ \end{array} $		С С Н Н Н Н С С С С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ \end{array} $		C C H H H O C C C C H C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ \end{array} $	$ \begin{array}{c} 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C C H H H C C C C C C C C C C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.257222	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 2.062752	2.7298071 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.202675
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ \end{array} $	$ \begin{array}{c} 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	С С Н Н Н Н О С С С С С С С Н Н	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382	2.282316 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ \end{array} $	$ \begin{array}{c} 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C C H H H O C C C C C H C C C H C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ \end{array} $	$ \begin{array}{c} 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	С С Н Н Н Н О С С С С С С С С С С С С С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 6 \\ 7 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 6 \\ 7 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 6 \\ 7 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 6 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 23 \\ 23 \\ 23 \\ 24 \\ 23 \\ 24 \\ 23 \\ 24 \\ 24 \\ 23 \\ 24 \\ 24 \\ 24 \\ 23 \\ 24 \\ 24 \\ 24 \\ 24 \\ 24 \\ 24 \\ 24 \\ 24$		C C H H H C C C C C C H C C C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 0.4227	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -0.038634 -0.02025	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 0.54144
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ \end{array} $		C C H H H O C C C C H C C C H C C N N	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071	2.282316 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ \end{array} $	6 6 1 1 1 1 1 6 6 6 6 6 6 6 7 7 7	C C H H H O C C C C C H C C C H C C N N N	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453
7gd	$ \begin{array}{r} 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 7 \\ 25 \\ 26 \\ 26 \\ 26 \\ 26 \\ 26 \\ 26 \\ 26 \\ 26$	$ \begin{array}{c} 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C C H H H C C C C C C H C C C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 2.055196	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 0.409050	2.7298071 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224000
7gd	$\begin{array}{r} 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \end{array}$	$ \begin{array}{c} 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 6 \\ \end{array} $	C C H H H O C C C C H C C C H C C N N N C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900
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7gd	$\begin{array}{c} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline \end{array}$		C C H H H O C C C C C H C C C H C C N N N C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922
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7gd	$\begin{array}{c} 6\\ \hline 7\\ \hline 8\\ \hline 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 32\\ \hline 33\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 32\\ \hline 33\\ \hline 33\\$	$\begin{array}{c} 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 7\\ 7\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C C H H H C C C C C C C H C C C C H C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -2.76	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -0.871155 -0.87125	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.75075
7gd	$\begin{array}{c} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline \end{array}$	$\begin{array}{c} 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C C H H H C C C C C C C C C H C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -1.259998	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167
7gd	$\begin{array}{r} 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline 35 \\ \end{array}$		C C H H H O C C C C C C H C C C C N N N C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.219638 -0.219638 -1.259998 -2.416499	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906
7gd	$\begin{array}{c} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline 35 \\ \hline 26 \\ \hline \end{array}$		C C H H H C C C C C C C H C C C C H C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 2.723144	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -1.259998 -2.416499 3.206572	$\begin{array}{r} 2.729671 \\ \hline 2.988076 \\ \hline 1.596931 \\ \hline -0.406355 \\ \hline 1.805432 \\ \hline 3.597001 \\ \hline 4.312807 \\ \hline 3.572478 \\ \hline 1.690683 \\ \hline 2.836524 \\ \hline 0.630125 \\ \hline 3.836214 \\ \hline 0.547247 \\ \hline 0.127751 \\ \hline -0.091732 \\ \hline 0.393675 \\ \hline -0.895597 \\ \hline 3.442666 \\ \hline -0.741110 \\ \hline 2.573453 \\ \hline 1.224900 \\ \hline -0.758789 \\ \hline -1.481454 \\ \hline -0.884922 \\ \hline 0.482321 \\ \hline -1.497611 \\ \hline 0.950231 \\ \hline -0.070402 \\ \hline -0.838167 \\ \hline -1.636906 \\ \hline 1.671920 \end{array}$
7gd	$\begin{array}{r} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline 35 \\ \hline 36 \\ \hline \end{array}$		C C H H H O C C C C C C C C H C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 -2.723141	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -1.259998 -2.416499 -3.226572	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906 -1.671880
7gd	$\begin{array}{r} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline 35 \\ \hline 36 \\ \hline 37 \\ \end{array}$		C C H H H O C C C C C C H C C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 -2.723141 -2.819471	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.219638 -0.871155 -1.259998 -2.416499 -3.226572 0.033245	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906 -1.671880 0.521143
7gd	$\begin{array}{c} 6 \\ \hline 7 \\ \hline 8 \\ \hline 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \hline 35 \\ \hline 36 \\ \hline 37 \\ \hline 38 \end{array}$		С С Н Н Н Н О С С С С С С С С С С С С С	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 -2.723141 -2.819471 -4.727812	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -1.259998 -2.416499 -3.226572 0.033245 -2.669228	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906 -1.671880 0.521143 -2.20412
7gd	$\begin{array}{r} 6\\ \hline \\ 7\\ \hline \\ 8\\ 9\\ \hline \\ 10\\ \hline \\ 11\\ \hline \\ 12\\ \hline \\ 13\\ \hline \\ 14\\ \hline \\ 15\\ \hline \\ 16\\ \hline \\ 17\\ \hline \\ 18\\ \hline \\ 19\\ \hline \\ 20\\ \hline \\ 21\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 24\\ \hline \\ 25\\ \hline \\ 26\\ \hline \\ 27\\ \hline \\ 28\\ \hline \\ 29\\ \hline \\ 30\\ \hline \\ 31\\ \hline \\ 32\\ \hline \\ 33\\ \hline \\ 34\\ \hline \\ 35\\ \hline \\ 36\\ \hline \\ 37\\ \hline \\ 38\\ \hline \end{array}$	$\begin{array}{c} 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C C H H H O C C C C C C C C C C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 -2.723141 -2.819471 -4.727812	2.282310 -1.079755 -0.646979 1.538623 4.203950 2.494149 -0.097482 -2.127253 -0.637800 -0.797727 -0.392999 -1.033206 -1.620249 -2.738500 -1.676830 -3.063753 -2.853219 -0.038634 -3.482907 -0.655844 -0.408050 -0.190692 0.004472 0.003367 -0.208470 0.162546 -0.219638 -0.871155 -1.259998 -2.416499 -3.226572 0.033245 -2.669228	2.7298076 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906 -1.671880 0.521143 -2.220412
7gd	$\begin{array}{c} 6\\ \hline \\ 7\\ \hline \\ 8\\ 9\\ \hline \\ 10\\ \hline \\ 11\\ \hline \\ 12\\ \hline \\ 13\\ \hline \\ 14\\ \hline \\ 15\\ \hline \\ 16\\ \hline \\ 17\\ \hline \\ 18\\ \hline \\ 19\\ \hline \\ 20\\ \hline \\ 21\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 24\\ \hline \\ 25\\ \hline \\ 26\\ \hline \\ 27\\ \hline \\ 28\\ \hline \\ 29\\ \hline \\ 30\\ \hline \\ 31\\ \hline \\ 32\\ \hline \\ 33\\ \hline \\ 34\\ \hline \\ 35\\ \hline \\ 36\\ \hline \\ 37\\ \hline \\ 38\\ \hline \\ 39\\ \hline \end{array}$		C C H H H O C C C C C C C C H C C C C C	-1.820983 -0.400747 0.191418 0.394049 -2.149798 -2.438267 -1.691211 -0.210564 1.710204 2.453726 2.661490 2.120302 -0.318406 0.362836 -1.614382 1.357382 -1.621622 -1.182608 -0.403071 3.799978 3.955186 2.560431 3.726988 5.000215 5.123613 5.879494 6.102891 -2.768424 -3.854532 -3.850626 -2.723141 -2.819471 -4.727812 -2.708645	$\begin{array}{r} 2.282316\\ -1.079755\\ -0.646979\\ 1.538623\\ 4.203950\\ 2.494149\\ -0.097482\\ -2.127253\\ -0.637800\\ -0.797727\\ -0.392999\\ -1.033206\\ -1.620249\\ -2.738500\\ -1.676830\\ -3.063753\\ -2.853219\\ -0.038634\\ -3.482907\\ -0.655844\\ -0.408050\\ -0.190692\\ 0.004472\\ 0.003367\\ -0.208470\\ 0.162546\\ -0.219638\\ -0.871155\\ -1.259998\\ -2.416499\\ -3.226572\\ 0.033245\\ -2.669228\\ -4.122543\end{array}$	2.729671 2.988076 1.596931 -0.406355 1.805432 3.597001 4.312807 3.572478 1.690683 2.836524 0.630125 3.836214 0.547247 0.127751 -0.091732 0.393675 -0.895597 3.442666 -0.741110 2.573453 1.224900 -0.758789 -1.481454 -0.884922 0.482321 -1.497611 0.950231 -0.070402 -0.838167 -1.636906 -1.671880 0.521143 -2.220412 -2.284248

	40	1	Н	1.602095	-0.210688	-1.262353
	41	6	С	0.009148	-4.698138	-1.414784
	42	6	C	4.874516	-0.779892	3.538047
	43	1	н	1.003800	-4 977538	-1.064828
	43	1	и и	0.680057	5 518710	1 102027
	44	1	п	-0.060937	-5.516/10	-1.192037
	45	1	H	0.048125	-4.555505	-2.500389
	46	l	Н	5.45/136	0.145800	3.596935
	47	1	H	4.447041	-0.983787	4.520714
	48	1	Н	5.548163	-1.602532	3.273997
	49	35	Br	-0.651476	4.286381	-0.744296
	50	35	Br	-5.439146	-0.176707	-0.817252
	51	35	Br	3.611579	0.275006	-3.377316
	Center	Atomic		C	oordinates (Angstroi	ns)
	number	number	Atom type	X	Y	Z
	1	6	С	-1.475318	0.914115	-0.240970
	2	6	C	-2.453259	1.663154	-0.851167
	3	6	C	-2 118502	-0.323320	0.161000
	4	1	е Н	-2 396980	2 644982	-1 2959/1
		1	и и	4 518740	1 222108	1 240505
	5	1	П	-4.516749	0.070976	-1.240393
	0	0	C	0.900182	0.279870	-0.033931
	1	6	C	1.021010	0.138/9/	-2.018099
	8	6	C	1./4/640	-0.760667	-0.083998
	9	1	H	0.532822	0.695882	-2.804347
	10	6	C	2.335754	-1.469376	-1.175241
	11	1	Н	2.106687	-1.192648	-3.268857
	12	7	N	1.873093	-0.895290	-2.336219
	13	7	N	-3.655624	0.979244	-0.853653
	14	6	C	-3.482768	-0.239959	-0.236544
	15	6	С	-1.688313	-1.497486	0.808209
	16	6	С	-2.599878	-2.518589	1.045173
	17	6	C	-3.946550	-2.404982	0.646956
	18	6	C	-4 404837	-1 265226	-0.001264
	10	1	н	-2 268059	-3 /2/797	1 5/13398
	20	1	- П - Ц	4 635468	3 220657	0.846212
	20	1	П Ц	5 441078	-3.220037	0.315072
	21	I (П	-3.441078	-1.1/2000	-0.515072
7ai	22	0	C	2.076960	-1.203414	1.210/92
	23	6	C	2.942859	-2.275941	1.386853
	24	6	C	3.511302	-2.943744	0.285248
	25	6	C	3.212428	-2.546088	-1.010226
	26	1	Н	1.662857	-0.719663	2.092362
	27	1	Н	3.186905	-2.605910	2.392360
	28	1	Н	4.186179	-3.778158	0.450300
	29	1	Н	3.639842	-3.055137	-1.869839
	30	1	Н	-0.653644	-1.617145	1.108152
	31	6	С	0.207730	1.517566	1.516955
	32	6	С	-0.021545	1.328756	-0.013450
	33	6	С	0.234222	2.720598	-0.668051
	34	6	C	1.616476	3,303096	-0.348195
	35	6	Č	1,809616	3,460615	1.165397
	36	6	C	1,571488	2,126535	1 884602
	37	1	H	-0 584553	2,190637	1 869138
	38	1	н	0.087365	2 661976	-1 752135
	30	1	н	2 39/1866	2.601270	_0 752730
	40	1	и П	2.57+000	3 830020	1 387440
	40	1	п	1 601647	2.037020	2.071647
	41	1		0.52(200	2.20/330	2.9/104/
	42	1	H	-0.526308	5.410287	-0.289227
	43	1	H	1.729829	4.2/1837	-0.850189
	44	1	H	1.100914	4.211823	1.543066
	45	1	Н	2.377995	1.432910	1.623223
	46	1	Н	0.043868	0.574108	2.044564
	Center	Atomic	Atom type	C	oordinates (Angstro	ns)
	number	number	rion type	X	Y	Z
	1	6	С	-2.477864	-1.128242	-0.145513
	2	6	С	-3.802480	-1.486317	-0.054389
	3	6	С	-2.461396	0.321825	-0.117954
7ei	4	1	Н	-4.253704	-2.466543	-0.037297
	5	1	Н	-5.608676	-0.369726	0.094415
	6	6	С	-0.291778	-1.790217	0.861959
	7	6	Č	-0.571904	-2.097280	2.174593
	8	6	Č	1.008313	-1 141355	0 887204
	Q	1	Ч	-1 453860	-2 561118	2 591/82

	10	6	С	1.437814	-1.111109	2.248316
	11	1	н	0.470435	-1 813363	4.003813
	12	7	N	0.453011	1 701000	3 003606
	12	7	IN N	0.455011	-1.701999	0.025264
	13	/	N	-4.604775	-0.363461	0.025264
	14	6	C	-3.811599	0.760471	-0.015148
	15	6	C	-1.443612	1.293684	-0.162419
	16	6	С	-1.807455	2.629817	-0.115381
	17	6	С	-3.145013	3.053226	-0.020964
	18	6	С	-4.164347	2.112428	0.032594
	19	1	Н	-3.371577	4.112286	0.011703
	20	1	н	-5 201931	2 424337	0.109151
	20	1	и и	1 967241	0.565112	0.074872
	21	1	П	2.00020	-0.303113	-0.074675
	22	0	C	3.009030	-0.01/50/	0.542110
	23	6	C	3.4/9/60	-0.005641	1.686010
	24	6	C	2.655137	-0.558273	2.654830
	25	6	C	1.615007	-0.538694	-1.125179
	26	1	Н	4.431229	0.436187	1.956150
	27	1	Н	2.949965	-0.555294	3.700171
	28	1	Н	-0.398286	1.019573	-0.218392
	2.9	6	С	-0.671978	-1.907191	-1.702335
	30	6	C	-1 285437	-2 075356	-0.278660
	21	6	C	1.203437	2.51641	0.194726
	22	0		-1.//0300	-5.551041	-0.104730
	32	0		-0.082/33	-4.383423	-0.4/902/
	33	6	C	-0.100198	-4.3/8/69	-1.883/54
	34	6	C	0.410038	-2.942257	-2.054948
	35	1	Н	-1.502293	-2.011318	-2.412353
	36	1	Н	-2.225082	-3.739837	0.797860
	37	1	Н	0.115666	-4.496427	0.267756
	38	1	Н	0.708543	-5.094477	-2.072534
	39	1	Н	0.741655	-2.776758	-3.087308
	40	1	Н	-2.581031	-3.686529	-0.921759
	41	1	Н	-1.097990	-5.593820	-0.381653
	42	1	Н	-0.880478	-4.582395	-2.631196
	43	1	Н	1.291613	-2.801685	-1.420172
	44	1	Н	-0 299599	-0.888108	-1 838977
	45	35	Br	4 235380	0.757319	-0.970454
	10		ы	1.235500	0.151517	0.970131
	46	35	Br	-0.434767	3 969863	-0 177239
	46 Center	35 Atomic	Br	-0.434767	3.969863	-0.177239
	46 Center number	35 Atomic number	Br Atom type	-0.434767	3.969863 oordinates (Angstron V	-0.177239 ns)
	46 Center number	35 Atomic number	Br Atom type	-0.434767 Co X 1.473021	3.969863 oordinates (Angstron Y 0.687495	-0.177239 ns) <u>Z</u>
	46 Center number	35 Atomic number 6	Br Atom type C	-0.434767 Co X 1.473021 2.542304	3.969863 oordinates (Angstron Y 0.687495	-0.177239 ns) 2 0.081978 0.750251
	46 Center number 1 2	35 Atomic number 6 6	Br Atom type C C	-0.434767 CC X 1.473021 2.543294	3.969863 oordinates (Angstron Y 0.687495 1.233133 0.601626	-0.177239 ns) 2 0.081978 0.750351 0.209107
	46 Center number 1 2 3	35 Atomic number 6 6 6 6	Br Atom type C C C	-0.434767 X 1.473021 2.543294 1.930249 2.20215	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.190992	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262500
	46 Center number 1 2 3 4	35 Atomic number 6 6 6 6 1	Br Atom type C C C H	-0.434767 X 1.473021 2.543294 1.930249 2.629215 0.025516	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.09167
	46 Center number 1 2 3 4 5	35 Atomic number 6 6 6 1 6 6 1 6	Br Atom type C C C H C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812	-0.177239 ms) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 0.424697
	46 Center number 1 2 3 4 5 6	35 Atomic number 6 6 6 1 6 6 6 6	Br Atom type C C C C H C C C	-0.434767 Co X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432	-0.177239 ms) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091
	46 Center number 1 2 3 4 5 6 7	35 Atomic number 6 6 6 1 6 6 6 6 6 6	Br Atom type C C C C H C C C C C	-0.434767 Co X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911
	46 Center number 1 2 3 4 5 6 7 8	35 Atomic number 6 6 6 1 6 6 6 6 6 1 1	Br Atom type C C C H C C C C H H	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394
	46 Center number 1 2 3 4 5 6 7 8 9	35 Atomic number 6 6 6 1 6 6 6 1 6 1 6 6 1 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C H C	-0.434767 Co X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949	-0.177239 ms) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533
	46 Center number 1 2 3 4 5 6 7 8 9 10	35 Atomic number 6 6 6 1 6 6 6 1 6 1 6 7 	Br Atom type C C C H C C C C H C C N	-0.434767 Co X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368	-0.177239 ms) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930
	46 Center number 1 2 3 4 5 6 7 8 9 10 11	35 Atomic number 6 6 1 6 6 6 6 1 6 7 7 7	Br Atom type C C C H C C C C H C C N N	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422
	46 Center number 1 2 3 4 5 6 7 8 9 10 11 11 12	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6	Br Atom type C C C H C C C C H C C N N N C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718
	46 Center number 1 2 3 4 5 6 7 8 9 10 11 11 12 13	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 7 7 6 6 6 7 7 6 6 6 7 7 6 6 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C N N C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088
	46 Center number 1 2 3 4 5 6 7 8 9 10 11 11 12 13 14	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 7 7 6 6 6 6 7 7 6 6 6 6 7 7 6 6 6 6 7 7 6 6 6 6 6 6 7 7 7 6 6 6 6 6 7 7 7 6 6 6 7 7 7 7 6 6 6 7 7 7 7 7 6 6 6 7 7 7 7 7 7 7 7 7 7 7 7 7	Br Atom type C C C H C C C C H C C N N C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566
	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C C N N C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	35 Atomic number 6 6 6 1 6 6 6 1 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C C N N C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694	-0.177239 ms) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	35 Atomic number 6 6 6 1 6 6 6 7 7 6 6 7 7 6 6 6 6 6 6 1 1 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C N N C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409	-0.177239 ns) 2 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1 988042
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C H N C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365	-0.177239 ns)
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	35 Atomic number 6 6 1 6 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 1 1 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 1.973880	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	35 Atomic number 6 6 1 6 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C C C C C C C C C H H C C C C H H C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 2.330111	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 0.756970	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 1.555922
	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	35 Atomic number 6 6 1 6 6 6 1 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C C C C C C C C C H H C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 3.245005	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 1.671413	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 -1.555822 1.900128
	46 Center 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 4.027665	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 2.219752	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 -1.555822 -1.809128 0.752920
7fi	46 Center 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 22	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 2.665724	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 2.062200	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 -1.555822 -1.809128 -0.762820 0.0562876
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	35 Atomic number 6 6 6 1 6 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C H C C C C H C C N N C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 1.921410	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 0.2319752	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 -1.555822 -1.809128 -0.762820 0.560876 2.020261
7fi	46 Center number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	35 Atomic number 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 2.415402	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -0.281916	-0.177239 ns)
7fi	$\begin{array}{r} 46\\ \hline \mathbf{Center}\\ \mathbf{number}\\ \hline 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 5\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 5\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10$	35 Atomic number 6 6 1 6 6 6 1 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C C C C C C N N C C C C C C C C C C C C C	-0.434767 Co X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556	-0.177239 ns)
7fi	$\begin{array}{r} 46\\ \hline \mathbf{Center}\\ \mathbf{number}\\ \hline 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 6\\ \end{array}$	35 Atomic number 6 6 6 1 6 6 6 1 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C C H C C N C C N C C C R C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972	-0.177239 ns)
7fi	$\begin{array}{r} 46\\ \hline \mathbf{Center}\\ \mathbf{number}\\ \hline 1\\ \hline 2\\ \hline 3\\ \hline 4\\ 5\\ \hline 6\\ 7\\ \hline 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline \end{array}$	35 Atomic number 6 6 6 1 6 6 6 1 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972 -2.562362	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255582 0.049479 -1.255582 -1.809128 -0.762820 0.560876 -2.391261 -2.837646 -0.992290 1.374863
7fi	$\begin{array}{r} 46\\ \hline \\ \textbf{Center}\\ \textbf{number}\\ \hline \\ 1\\ \hline \\ 2\\ \hline \\ 3\\ \hline \\ 6\\ \hline \\ 7\\ \hline \\ 8\\ 9\\ \hline \\ 10\\ \hline \\ 11\\ \hline \\ 12\\ \hline \\ 8\\ \hline \\ 9\\ \hline \\ 10\\ \hline \\ 11\\ \hline \\ 12\\ \hline \\ 13\\ \hline \\ 14\\ \hline \\ 15\\ \hline \\ 16\\ \hline \\ 17\\ \hline \\ 18\\ \hline \\ 19\\ \hline \\ 20\\ \hline \\ 21\\ \hline \\ 20\\ \hline \\ 21\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 24\\ \hline \\ 25\\ \hline \\ 26\\ \hline \\ 27\\ \hline \\ 28\\ \hline \end{array}$	35 Atomic number 6 6 1 6 6 6 6 7 7 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514 0.307856	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972 -2.562362 -1.593447	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255582 0.049479 -1.555822 -1.809128 -0.762820 0.560876 -2.391261 -2.837646 -0.992290 1.374863 -1.445607
7fi	$\begin{array}{r} 46\\ \hline \mathbf{Center}\\ \mathbf{number}\\ \hline 1\\ \hline 2\\ \hline 3\\ \hline 4\\ \hline 5\\ \hline 6\\ 7\\ \hline 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \end{array}$	35 Atomic number 6 6 1 6 6 6 6 7 7 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C H H H H H H H H H H H H H H	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514 0.307856 -0.064787	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972 -2.562362 -1.593447 1.664086	-0.177239 ns) Z 0.081978 0.750351 -0.398107 1.262599 0.424697 1.773091 -0.224911 2.603394 0.810533 2.020930 0.722422 0.018718 -1.128088 -1.425566 -1.007411 -0.277772 -1.988042 -1.255508 0.049479 -1.555822 -1.809128 -0.762820 0.560876 -2.391261 -2.837646 -0.992290 1.374863 -1.445607 -1.641429
7fi	$\begin{array}{r c c} 46 \\ \hline \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	35 Atomic number 6 6 6 1 6 6 6 7 7 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C H H H H H H H H H H H H H H H H H H	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514 0.307856 -0.064787 0.103312	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972 -2.562362 -1.593447 1.664086 1.333479	-0.177239 ns)
7fi	$\begin{array}{r c c} 46 \\ \hline \mathbf{Center} \\ \mathbf{number} \\ \hline 1 \\ 2 \\ \hline 3 \\ 4 \\ \hline 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 12 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ \end{array}$	35 Atomic number 6 6 6 1 6 6 6 1 6 7 7 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C C C C H C C C C N N C C C C C C C C C C C C C	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514 0.307856 -0.064787 0.103312 0.048096	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.89556 -3.027972 -2.562362 -1.593447 1.664086 1.333479 2.697538	-0.177239 ns)
7fi	$\begin{array}{r} 46\\ \hline \mathbf{Center}\\ \mathbf{number}\\ \hline 1\\ 2\\ 3\\ \hline 3\\ 4\\ 5\\ \hline 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ \end{array}$	35 Atomic number 6 6 6 1 6 6 6 7 7 6 6 7 7 6 6 6 6 6 6 6 6 6 6 6 1 1 1 6 6 6 6 6 6 6 6 6 6 6 6 6	Br Atom type C H H H H H H H H H H H H H	-0.434767 X 1.473021 2.543294 1.930249 2.629215 -0.985940 -1.150220 -1.962089 -0.599363 -2.668796 -2.151828 3.636968 3.284101 1.342630 2.096211 3.436041 4.047141 1.642569 3.999201 5.078786 -2.330111 -3.345095 -4.027665 -3.695734 -1.831440 -3.617402 -4.818140 -4.213514 0.307856 -0.064787 0.103312 0.048096 -1.223756	3.969863 oordinates (Angstron Y 0.687495 1.233133 -0.601626 2.180093 0.395812 0.174432 -0.461363 0.593495 -1.146949 -0.740368 0.383294 -0.749218 -1.651387 -2.780550 -2.897335 -1.884694 -3.591409 -3.792365 -1.973880 -0.756979 -1.671413 -2.319752 -2.063890 -0.281916 -1.889556 -3.027972 -2.562362 -1.593447 1.664086 1.333479 2.697538 3.504918	-0.177239 ns)

	33	6	С	-1.361046	3.798114	-1.161218
	34	6	С	-1.313262	2.498343	-1.974983
	35	1	Н	0.827032	2.231831	-1.936677
	36	1	Н	0.162836	2,539570	1.704092
	37	1	Н	-2.100413	2,944549	0.685948
	38	1	Н	-2.292631	4.340201	-1.363388
	39	1	Н	-1 320256	2 722760	-3.049077
	40	1	Н	0.912327	3 294952	0 306342
	40	1	 Ц	1 100660	4.441168	0.000342
	41	1	и И	0.530502	4.441100	1 476244
	42	1	II	-0.339302	1.019492	1.772290
	43	1	п	-2.220230	0.746477	-1.//2269
	44	1	H	-0.033035	0.746477	-2.235203
	45	0	C	-2.380884	-1.200774	3.322084
	46	0	C	4.929501	0.636016	1.319868
	47	1	H	-3.638212	-0.94/884	3.501651
	48	1	H	-2.468982	-2.286202	3.415182
	49	1	H	-1.979332	-0.720378	4.090798
	50	1	H	4.909691	1.608394	1.815349
	51	1	Н	5.178166	-0.127647	2.066192
	52	1	Н	5.721821	0.650213	0.562201
	Center	Atomic	Atom type	C	oordinates (Angstro	ms)
	number	number	mon type	X	Y	Z
	1	6	С	-1.649137	-1.672157	0.241290
	2	6	С	-0.569564	-0.870696	0.680261
	3	6	C	-0.311620	-0.818664	2.031353
	4	6	C	-1.135529	-1.559649	2.926703
	5	6	С	-2.192656	-2.336957	2.494508
	6	6	С	-2.484622	-2.417663	1.105087
	7	6	С	-0.756830	-0.804097	-1.735600
	8	6	С	0.110614	-0.219859	-0.536109
	9	1	Н	0.507113	-0.230639	2.430181
	10	1	Н	-0.918702	-1.505728	3.989770
	11	1	Н	-2.799341	-2.886071	3.209278
	12	8	0	-0.549065	-0.584080	-2.911578
	13	6	С	1.549713	-0.695158	-0.677605
	14	6	С	2.013704	-1.632012	-1.569520
	15	6	С	2.685300	-0.316902	0.139396
	16	1	Н	1.489861	-2.139825	-2.364662
	17	1	Н	3.926130	-2.496691	-1.896301
	18	6	С	0.001141	1.294758	-0.577720
	19	6	С	0.874215	2.106913	-1.260951
	20	6	С	-1.052375	2.156628	-0.077522
	21	1	Н	1.778057	1.839795	-1.786400
	22	6	С	-0.727711	3.482143	-0.487072
	23	1	Н	0.931187	4.199863	-1.608774
7aj	24	7	N	0.446674	3.414722	-1.206469
- -	25	7	N	3.354469	-1.872988	-1.351171
	26	6	С	3.797465	-1.080308	-0.313649
	27	6	С	2.889329	0.598212	1.189765
	28	6	С	4.151936	0.712501	1.757550
	29	6	С	5.233077	-0.065662	1.297492
	30	6	C	5.070913	-0.968293	0.253960
	31	1	H	4.312539	1.418845	2.566691
	32	1	Н	6.208823	0.045901	1.760835
	33	1	Н	5.903358	-1.564264	-0.109714
	34	6	C	-2.233212	1,966413	0.666997
	35	6	Č	-3.026415	3,063040	0.978899
	36	6	Č	-2.675257	4.363822	0.567347
	37	6	Č	-1 520965	4 589439	-0 171143
	38	1	H	-2.525671	0.976958	0.997612
	39	1	н	-3 937022	2,915642	1 552153
	40	1	Н	-3 315933	5 200770	0.828780
	41	1	Н	-1 2450/15	5 5889/0	-0 495766
	12	1	н Н	2 07/612	1 225826	1 53/821
	12	6	C	_1 820365	-1 658664	-1 156/78
	43	6	C	-1.020303	-1.050004	-1.130470
	44	6	C	-3.522040	-3.100421	_0.907359
	46	6	C	-2 83/020	_2 380886	-1 7/2202
	40	1	ч	-2.034920	-2.307000	1 00/706
	47	1	п Ц	-4.170304	-3.731001	-1 3/0502
	40	1	п u	-4.471073	-3.120930	-1.340392
L	49	1	П	-2.9/4080	-2.300/02	-2.010012

	Center	Atomic		C	ordinates (Angstro	ns)
	number	number	Atom type	X	Y	Z
	1	6	С	-1.663766	-1.884468	0.471359
	2	6	C	-0.562236	-1.011238	0.630524
	3	6	C C	-0.208371	-0.645121	1.909558
	5	6	<u> </u>	-2.035564	-2.000449	2.851106
	6	6	C	-2.427148	-2.401457	1.543999
	7	6	С	-0.930812	-1.501269	-1.714070
	8	6	С	0.018765	-0.663923	-0.751124
	9	1	H	0.629503	0.015956	2.098985
	10	1	Н	-0.004202	-0.851475	3 717036
	12	8	0	-0.816616	-1.560915	-2.921527
	13	6	С	1.446581	-1.173824	-0.887690
	14	6	С	1.847933	-2.294354	-1.576692
	15	6	C	2.638346	-0.634894	-0.262742
	16	1	H	3 731634	-2.960297	-2.195482
	18	6	C	-0.107396	0.802474	-1.127281
	19	6	С	0.716510	1.438887	-2.027922
	20	6	С	-1.135870	1.757302	-0.768504
	21	1	H	1.590416	1.057023	-2.532658
	22	6	С	-0.849729	2.952837	-1.4/93/8
	23	7	N	0.736321	2,724262	-2.240911
	25	7	N	3.199565	-2.500717	-1.409900
	26	6	С	3.716127	-1.496277	-0.613021
	27	6	C	2.906693	0.489238	0.533546
7cj	28	6	C	4.209256	0.720721	0.973339
	30	6	C	5.202109	-0.132200	-0.176401
	31	1	Н	6.271100	0.035978	0.969129
	32	1	Н	5.832692	-1.931645	-0.449997
	33	6	C	-2.266569	1.724549	0.077354
	34	6	C	-3.052111	2.866173	0.191268
	35	6	C	-2.740536	4.047842	-0.521174
	37	1	Н	-2.509847	0.826395	0.626363
	38	1	Н	-3.389041	4.907416	-0.391387
	39	1	Н	-1.405741	5.007704	-1.909403
	40	1	Н	2.133442	1.201463	0.796081
	41	6	C	-1.939659	-2.192116	-0.8/48/8
	43	6	C	-3.767878	-3.559857	-0.141340
	44	6	С	-2.988478	-3.030044	-1.198434
	45	1	Н	-4.124214	-3.687638	1.970146
	46	1	H	-4.597832	-4.219473	-0.377439
	4/	1 8	н О	-3.208/19 -4 171290	-3.2/3038	-2.233142
	49	8	0	4.378125	1.843699	1.747786
	50	6	С	-4.552198	1.814667	1.724395
	51	6	С	5.676989	2.146814	2.220161
	52	1	H	-3.770207	1.507336	2.431522
	53	1	H H	-5.447962	2.098060	2.280138
	55	1	H	6,384363	2.316918	1.397131
	56	1	H	5.580450	3.066042	2.800709
	57	1	Н	6.073491	1.354617	2.869666
	Center	Atomic	Atom type	C C	oordinates (Angstroi	ms)
7dj	number 1	number 6		-2 116191	<u>¥</u> -1 245871	0 354204
	2	6	c	-0.889770	-0.707178	0.802631
	3	6	C	-0.671947	-0.625478	2.159364
	4	6	С	-1.699412	-1.047104	3.050920
	5	6	C	-2.911530	-1.544981	2.609004
	6 7	6		-3.155979 -0.894453	-1.669202	1.213588
	8	6	C C	-0.013252	-0.351794	-0.407075

	9	1	Н	0 259969	-0.239006	2 558673
	10	1	н	-1 519728	-0.966973	4 119291
	10	1	и П	2 672222	1 840651	2 200245
	11	1	П	-3.072332	-1.049031	3.322343
	12	8	0	-0.555369	-0.938214	-2.//5968
	13	6	C	1.341070	-1.038516	-0.282434
	14	6	C	1.696736	-2.297615	-0.731751
	15	6	С	2.475048	-0.524455	0.459267
	16	1	Н	3.490062	-3.415955	-0.542808
	17	6	С	0.100873	1.157109	-0.664781
	18	6	C	0.957184	1.721361	-1.597858
	10	6	C	-0.676395	2 245759	-0.095784
	20	6	C C	0.210275	2.243737	0.708062
	20	1	U U	-0.210275	2 725020	-0.708003
	21	1	п	0.772506	2.020071	-2.198009
	22	7	IN N	0.775590	3.069071	-1.001415
	23	1	N C	2.993039	-2.304660	-0.329082
	24	0	C	3.497482	-1.510652	0.398/15
	25	6	C	2.734903	0.656356	1.183643
	26	6	C	3.970644	0.818449	1.799210
	27	6	С	4.968291	-0.172321	1.713616
	28	6	C	4.743281	-1.350890	1.012245
	29	1	Н	4.172103	1.727805	2.357894
	30	1	Н	5.924314	-0.015611	2.204267
	31	1	Н	5.505557	-2.122446	0.946907
	32	6	С	-1.720478	2.366536	0.845874
	33	6	С	-2.236110	3.622116	1.143846
	34	6	С	-1.743369	4.787732	0.527931
	35	6	С	-0.722337	4.710285	-0.410133
	36	1	Н	-2.129857	1.495734	1.339557
	37	1	Н	-3.040364	3.704417	1.869282
	38	1	Н	-2 166806	5 754226	0 784360
	30	1	н	-0.335322	5 599752	-0.899870
	40	1	11 11	1 080821	1 421800	1 257708
	40	6	П	2 105260	1.431690	1.237708
	41	0	C	-2.195209	-1.540450	-1.048550
	42	0	C	-4.318504	-2.181002	0.576407
	43	6	C	-4.397203	-2.265038	-0.80/211
	44	6	<u>с</u>	-3.330534	-1.85/545	-1.645887
	45	1	H	-5.155216	-2.518193	1.1832/5
	46	1	Н	-5.300187	-2.663669	-1.260340
	47	1	Н	-3.401271	-1.948635	-2.725281
	48	6	C	1.979944	1.124453	-2.514374
	49	6	С	0.961577	-3.339845	-1.520481
	50	1	Н	2.946093	1.001385	-2.011604
	51	1	Н	1.648285	0.150547	-2.871364
	52	1	Н	2.131326	1.771134	-3.385984
	53	1	Н	1.465281	-4.308133	-1.434931
	54	1	Н	-0.060449	-3 473172	-1.156310
	55	1	Н	0.893896	-3.078175	-2.580802
	Center	Atomic		C	oordinates (Angstro	ns)
	number	number	Atom type	X	V V	Z
	1	6	C	-1 476926	2 283277	-0.720060
	2	6	C C	-0.430620	1 332220	-0.691297
	3	6	C C	-0.090025	0.709095	-1.870/77
	1	6	C	_0 799//7	1 037/37	_3.061600
		6	C	1 924290	1.057457	-3.001000
	5	0	C	-1.624260	2.629670	-3.064702
	0	0		-2.199608	2.028079	-1.885357
	/	6	C	-0.783632	2.288705	1.510067
	8	6	C	0.116299	1.222032	0.741949
	9	1	H	0.706139	-0.025337	-1.917366
7ej	10	1	H	-0.520051	0.533605	-3.982252
-5	11	1	H	-2.344541	2.183314	-4.012682
	12	8	0	-0.665230	2.570655	2.685224
	13	6	С	1.573914	1.652865	0.811939
	14	6	С	2.047503	2.857027	1.276388
	15	6	C	2.731458	0.922007	0.340440
	16	1	Н	1.509773	3.672559	1.734851
	17	1	Н	3.992463	3.700953	1.397277
	19	6	С	-0.110167	-0.131064	1.393682
i .	18	0				
	19	6	С	0.644067	-0.620063	2.434179
	18 19 20	6 6	C C	0.644067 -1.186173	-0.620063 -1.080455	2.434179 1.192737
	10 19 20 21	6 6 1	C C H	0.644067 -1.186173 1.524079	-0.620063 -1.080455 -0.194286	2.434179 1.192737 2.891026
	$ \begin{array}{r} 18 \\ 19 \\ 20 \\ 21 \\ 22 \end{array} $	6 6 1 6	C C H C	0.644067 -1.186173 1.524079 -0.996484	-0.620063 -1.080455 -0.194286 -2.126295	2.434179 1.192737 2.891026 2.141258
	22	1	TT	0 510 004	2 200027	2 (11572)
-----	---	--	--	--	--	--
	25	1	п	0.318004	-2.360637	5.011572
	24	7	N	0.122057	-1.812183	2.881637
	25	7	N	2 /1//51	2 029591	1 100820
	23	/	IN	5.414451	2.926361	1.109850
	26	6	С	3.865708	1.757221	0.542244
	27	(C	2.027(02	0.259294	0.210491
	21	0	U	2.927603	-0.358384	-0.210481
	28	6	С	4.216731	-0.737593	-0.548295
	20	(C	5 221066	0.009049	0.257117
	29	0	U	5.331066	0.098948	-0.35/11/
	30	6	С	5.161133	1.360701	0.197439
	21	1		6.217(21	0.040550	0.197159
	31	1	Н	6.31/621	-0.248558	-0.639582
	32	1	н	6.01/228	2.013546	0 356922
	32	1	11	0.014220	2.013340	0.330722
	33	6	С	-2.288379	-1.162875	0.319368
	34	6	C	3 127508	2 260132	0.422455
		0	C	-3.127308	-2.200132	0.422433
	35	6	С	-2.926914	-3.291887	1.356253
	26	6	C	1 940566	2 220755	2 220252
		0	U	-1.849300	-3.229733	2.229232
	37	1	Н	-2.485581	-0.397798	-0.418999
	20	1	11	2 (15120	1 1270 12	1 200000
	38	1	п	-3.015130	-4.12/943	1.389809
	39	1	Н	-1.681995	-4.016714	2.958648
	10		11	2 100270	1.040004	0.047(0.4
	40	1	Н	2.100279	-1.043224	-0.347684
	41	6	C	-1 7/1395	2 861066	0.537090
	41	0	C	-1.7+1373	2.801000	0.537070
	42	6	С	-3.222767	3.600461	-1.719716
1	13	6	C	-3 /78016	4 165605	-0.477601
	40	U	Ľ	-3.4/0710	4.103003	-0.477091
1	44	6	C	-2.739580	3.805869	0.674853
	15	1	тт	2 01/007	2 002005	2 570071
1	43	1	п	-3.014297	3.902083	-2.3/99/1
1	46	1	Н	-4.269951	4.904115	-0.387295
1	47		 TT	2.051252	4 057107	1 (2012)
	47	1	H	-2.9513/3	4.25/12/	1.639138
1	48	35	Br	4,506885	-2 479931	-1.299787
1	10			1.500005	2.7////	0.200751
	49	35	Br	-4.635243	-2.388675	-0.759754
	Conton	Atomio		C	oordinatas (Angstro	me)
	Center	Atomic	Atom type	C	of unates (Angsu of	113)
	number	number	intoin type	X	Y	Z
	1	6	C	1 526224	2 052228	0.199046
	1	0	C	-1.320324	-2.033328	0.188040
	2	6	С	-0.644849	-1.092927	0.736742
	2	(C	0.504201	1.052057	2 105466
	3	0	U	-0.504391	-1.053057	2.105466
	4	6	С	-1.247804	-1.964975	2,908680
		6	Č	2,112,402	2,007000	2,260224
	5	6	C	-2.112402	-2.897809	2.369224
	6	6	С	-2.278200	-2.970255	0.958737
	ů Z		C C	0.650505	0.0500.40	1 (00100
	/	6	C	-0.653535	-0.959848	-1.683133
	8	6	C	-0.002586	-0.280255	-0.400280
	8	6	C	-0.002586	-0.280255	-0.400280
	8	6 1	C H	-0.002586 0.162656	-0.280255 -0.346688	-0.400280 2.586439
	8 9	6 1	C H	-0.002586 0.162656	-0.280255 -0.346688	-0.400280 2.586439 2.087147
	8 9 10	6 1 1	C H H	-0.002586 0.162656 -1.125997	-0.280255 -0.346688 -1.918483	-0.400280 2.586439 3.987147
	8 9 10 11	6 1 1 1	C H H H	-0.002586 0.162656 -1.125997 -2.663616	-0.280255 -0.346688 -1.918483 -3.574902	-0.400280 2.586439 3.987147 3.015929
	8 9 10 11	6 1 1 1 2	C H H H	-0.002586 0.162656 -1.125997 -2.663616 0.207200	-0.280255 -0.346688 -1.918483 -3.574902	-0.400280 2.586439 3.987147 3.015929 2.821820
	8 9 10 11 12	6 1 1 1 8	С Н Н Н О	-0.002586 0.162656 -1.125997 -2.663616 -0.397390	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165	-0.400280 2.586439 3.987147 3.015929 -2.831830
	8 9 10 11 12 13	6 1 1 1 8 6	C H H O C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638
	8 9 10 11 12 13	6 1 1 1 8 6	C H H O C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202021	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -0.2200	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638
	8 9 10 11 12 13 14	6 1 1 1 8 6 6	C H H O C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958
	8 9 10 11 12 13 14 15	6 1 1 8 6 6 6	C H H O C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188
	8 9 10 11 12 13 14 15	6 1 1 8 6 6 6 6	C H H C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188
	8 9 10 11 12 13 14 15 16	6 1 1 1 8 6 6 6 6 1	C H H O C C C C H	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441
	8 9 10 11 12 13 14 15 16 17	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H C C C C H C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1 189738	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502
	8 9 10 11 12 13 14 15 16 17	6 1 1 8 6 6 6 6 1 6	C H H O C C C C H H C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.26267	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.15776	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502
	8 9 10 11 12 13 14 15 16 17 18	6 1 1 1 8 6 6 6 1 1 6 6 6	C H H O C C C H C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621
	8 9 10 11 12 13 14 15 16 17 18 19	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H C C C C H C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1 826547	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496
	8 9 10 11 12 13 14 15 16 17 18 19	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C H C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496
76	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ \end{array} $	6 1 1 8 6 6 6 6 6 6 6 6 1 6 6 1 1 1	C H H C C C C C H C C C H C C H	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C H H C C C C H C C C H C C H C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1 501964	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834
7fj	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H O C C C C H C C C H C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 0.02205	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.20973 2.096762	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.326834 -0.2522
7fj	$ \begin{array}{r} 8 \\ 9 \\ $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ \end{array} $	C H H C C C C C H C C C H C C N	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ \end{array} $	C H H O C C C C C C H C C C H C C N N	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.99597
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 51 $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ 6 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7 \\ 7$	C H H O C C C C H C C H C C H C C N N	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 2.74001	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 0.42225	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.9959957 0.027405
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ - \end{array} $	6 1 1 1 8 6 6 6 6 6 6 7 7 6	C H H C C C C C H C C C H C C N N N C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C H C C C H C C N N C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.995957 0.097485 1.568088
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ $	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C H C C C H C C N N C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950957 0.097485 1.568088 2.02000
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H C C C C C H C C C C H C C N N C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C H C C C H C C N N C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ 27 \\ 26 \\ 27 \\ 26 \\ 27 \\ $	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H C C C C H C C C H C C C N N C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.45264	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 1 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C H C C C C C N N C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.959577 0.097485 1.568088 2.238850 1.846557 0.769007
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ \end{array} $	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\$	С Н Н О С С С С С С С С С С С С С	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557 0.769007 3.077174
7fj	$ \begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 29\\ 26 $	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 1\\ 6\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H C C C C C C C H C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.01557	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.00007
7fj	$\begin{array}{r} 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1 \end{array} $	C H H O C C C C C C H C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ \end{array} $	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 7 \\ 7 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	C H H O C C C C C H C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 31 \end{array} $	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\$	C H H C C C C C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328
7fj	$ \begin{array}{r} 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ \end{array} $	$ \begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H C C C C C C H C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H O C C C C C C H C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399881 2.323865	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934920
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 32\\ \hline 33\\ \hline \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 1\\ 1\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline \end{array}$	$ \begin{array}{r} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C C C H C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 6\\ 7\\ 7\\ 7\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H C C C C C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505222	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138662	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ 20\\ \hline 21\\ 22\\ 23\\ \hline 24\\ \hline 25\\ 26\\ \hline 27\\ \hline 28\\ 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C C C H C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.505233 -2.925260	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 27\\ \hline \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 1\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.092512	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.950983 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427209
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\\ \hline 30\end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 2.304056	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.950983 -0.96088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 0.320080
7fj	$\begin{array}{r} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\\ \hline 39\end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 -2.394056	$\begin{array}{r} -0.280255 \\ \hline -0.346688 \\ \hline -1.918483 \\ \hline -3.574902 \\ \hline -0.660165 \\ \hline -0.480941 \\ \hline -1.282218 \\ \hline 0.061070 \\ \hline -1.844934 \\ \hline 1.189738 \\ \hline 2.175794 \\ \hline 1.826547 \\ \hline 2.098383 \\ \hline 3.203973 \\ \hline 3.388630 \\ \hline -1.292725 \\ \hline -0.473937 \\ \hline 0.953762 \\ \hline 1.268654 \\ \hline 0.715979 \\ \hline -0.158084 \\ \hline 1.958446 \\ \hline 0.981282 \\ \hline -0.577524 \\ \hline 1.399481 \\ \hline 2.323865 \\ \hline 3.681122 \\ \hline 4.138663 \\ \hline 0.361525 \\ \hline 1.993512 \\ \hline 4.379362 \\ \hline 5.183865 \\ \hline \end{array}$	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.962633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 -0.320980
7fj	$\begin{array}{c} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\\ \hline 39\\ \hline 40\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 8 \\ 6 \\ 6 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6 \\ 6 \\ 1 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 -2.394056 1.504558	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362 5.183865 1.410509	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.995957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 -0.320980 1.863358
7fj	$\begin{array}{c} 8\\ 9\\ \hline \\ 9\\ \hline \\ 10\\ \hline \\ 11\\ \hline \\ 12\\ \hline \\ 13\\ \hline \\ 14\\ \hline \\ 15\\ \hline \\ 16\\ \hline \\ 17\\ \hline \\ 18\\ \hline \\ 19\\ \hline \\ 20\\ \hline \\ 21\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 22\\ \hline \\ 23\\ \hline \\ 24\\ \hline \\ 25\\ \hline \\ 26\\ \hline \\ 27\\ \hline \\ 28\\ \hline \\ 29\\ \hline \\ 30\\ \hline \\ 31\\ \hline \\ 32\\ \hline \\ 30\\ \hline \\ 31\\ \hline \\ 32\\ \hline \\ 33\\ \hline \\ 34\\ \hline \\ 35\\ \hline \\ 36\\ \hline \\ 37\\ \hline \\ 38\\ \hline \\ 39\\ \hline \\ 40\\ \hline \end{array}$	$ \begin{array}{c} 6\\ 1\\ 1\\ 1\\ 8\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\ 6\\$	C H H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 -2.394056 1.504558 1.504558	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362 5.183865 1.410509 2.041542	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 -0.320980 1.863358 1.918200
7fj	$\begin{array}{c} 8\\ 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\\ \hline 39\\ \hline 40\\ \hline 41\\ \hline \end{array}$	$\begin{array}{c} 6\\ \\ 1\\ \\ 1\\ \\ 1\\ \\ 1\\ \\ 8\\ \\ 6\\ \\ 6\\ \\$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 -2.394056 1.504558 -1.589303	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362 5.183865 1.410509 -2.011542	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 -0.320980 1.863358 -1.218200
7fj	$\begin{array}{c} 8\\ 9\\ \hline 9\\ \hline 10\\ \hline 11\\ \hline 12\\ \hline 13\\ \hline 14\\ \hline 15\\ \hline 16\\ \hline 17\\ \hline 18\\ \hline 19\\ \hline 20\\ \hline 21\\ \hline 22\\ \hline 23\\ \hline 24\\ \hline 25\\ \hline 26\\ \hline 27\\ \hline 28\\ \hline 29\\ \hline 30\\ \hline 31\\ \hline 32\\ \hline 33\\ \hline 34\\ \hline 35\\ \hline 36\\ \hline 37\\ \hline 38\\ \hline 39\\ \hline 40\\ \hline 41\\ \hline 42\\ \end{array}$	$\begin{array}{c} 6 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 6 \\ 6$	C H H O C C C C C C C C C C C C C	-0.002586 0.162656 -1.125997 -2.663616 -0.397390 1.505686 2.202934 2.487305 1.843209 -0.385985 0.369681 -1.612919 1.345055 -1.501964 -0.283865 3.548924 3.749811 2.443245 3.618848 4.853924 4.936509 3.587848 5.756105 5.889305 -2.792644 -3.793585 -3.653316 -2.505233 -2.925260 -4.703590 -4.452989 -2.394056 1.504558 -1.589303 -3.115745	-0.280255 -0.346688 -1.918483 -3.574902 -0.660165 -0.480941 -1.282218 0.061070 -1.844934 1.189738 2.175794 1.826547 2.098383 3.203973 3.388630 -1.292725 -0.473937 0.953762 1.268654 0.715979 -0.158084 1.958446 0.981282 -0.577524 1.399481 2.323865 3.681122 4.138663 0.361525 1.993512 4.379362 5.183865 5.183865 1.410509 -2.011542 -3.857528	-0.400280 2.586439 3.987147 3.015929 -2.831830 -0.433638 -1.305958 0.481188 -2.154441 -0.408502 -0.996621 0.023496 -1.453220 -0.326834 -0.950983 -0.950983 -0.950983 -0.950983 -0.95957 0.097485 1.568088 2.238850 1.846557 0.769007 3.077174 2.389732 0.460328 0.662633 0.934929 0.586461 -0.048512 0.943816 1.427298 0.815399 -0.320980 1.863358 -1.218200 0.230521

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	44	6	С	-2.408447	-2.884999	-1.906037
	45	1	Н	-3.719508	-4.583279	0.769496
	46	1	Н	-3.826114	-4.502864	-1.680047
	47	1	Н	-2.463502	-2.861449	-2.989957
	48	6	С	0.228739	4.651016	-1.440175
	49	6	С	4.582426	-2.006268	-1.716245
	50	1	Н	1.195982	4.481247	-1.915577
	51	1	Н	-0.450283	5.087535	-2.180806
	52	1	H	0.362868	5.369544	-0.623251
	53	1	H	5.108781	-2.706007	-1.057521
	54	1	H	4.123281	-2.573702	-2.527229
	55	1	Н	5.315430	-1.314699	-2.14/300
	number	number	Atom type	v	v	IIS) 7
	1	6	С	-1 421986	2 428491	-0.705596
	2	6	Č	-0.471009	1.383320	-0.762155
	3	6	С	-0.227147	0.795828	-1.982861
	4	6	С	-0.937165	1.253714	-3.130013
	5	6	С	-1.868930	2.271752	-3.069962
	6	6	С	-2.142862	2.903278	-1.825645
	7	6	С	-0.663163	2.247519	1.495883
	8	6	С	0.105883	1.144157	0.643323
	9	1	H	0.493402	-0.006601	-2.094636
	10	1	H	-0.735043	0.7/6676	-4.084562
	11	1 0	П	-2.393200	2.369640	-3.900094
	12	6	C C	1 599617	1 / 30089	0.683938
	13	6	C	2 203268	2 556993	1 190492
	15	6	C	2.666990	0.622626	0.137334
	16	1	Н	1.759906	3.394549	1.707951
	17	6	С	-0.231690	-0.215344	1.230377
	18	6	С	0.500776	-0.832689	2.217213
	19	6	C	-1.399061	-1.044652	1.022766
	20	1	Н	1.432723	-0.518626	2.662927
	21	6	C	-1.277793	-2.152056	1.912135
	22	7	N	-0.110690	-1.995621	2.631226
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	25	6	C	3 965077	-0.037808	-0.464023
7	20	6	C	5 157382	-0.396218	-0.687752
gi	28	6	C	5.122099	0.844414	-0.063378
3	29	1	H	6.098710	-0.817205	-1.020317
	30	1	Н	6.038251	1.403213	0.099749
	31	6	С	-2.531529	-0.976509	0.189032
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	35	1	H	-2.6/8450	-0.158429	-0.502923
	27	1	H U	-4.100506	-3.830000	1.139303
	37	1	л Н	-2.11/134	-4.013299	-0 620350
	39	6	C	-1 591840	2 959159	0 588154
	40	6	C	-3.062817	3.956522	-1.574462
	41	6	C	-3.226144	4.474659	-0.296798
	42	6	С	-2.490302	3.984719	0.809141
	43	1	Н	-3.648321	4.359673	-2.396716
	44	1	Н	-3.939792	5.278245	-0.140842
	45	1	Н	-2.628830	4.400773	1.802161
	46	6	C	0.399101	-2.921154	3.622609
	47	6		4.520271	3.526526	1.412487
	48	1	H	1.3190/6	-2.515/33	4.045983
	49	1	H U	-0.324316	-3.000/98	4.432975
	50	1	п И	5.076246	-3.071200	0.556076
	52	1	H	3,980641	4.347117	1.887349
	53	1	Н	5.234934	3.115895	2.134543
	54	35	Br	-5.019956	-1.916874	-0.860048
	55	35	Br	4.069327	-2.833786	-1.733294
	1	1		1		

	Center	Atomic	Atom type	Co	oordinates (Angstroi	ns)
	number	number	Atom type	Х	Y	Z
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	2	6	С	-2.384927	3.074975	-2.776997
	3	6	С	-2.350311	4.064503	-1.789605
	4	6	С	-1.609505	3.877701	-0.626086
	5	6	С	-0.884850	2.693217	-0.408282
	6	6	С	-0.954921	1.689629	-1.397080
	7	6	С	-0.038824	2.482137	0.788190
	8	6	С	0.463981	1.196325	1.090678
	9	6	С	0.115891	-0.032140	0.226695
	10	6	С	-0.246494	0.394166	-1.224056
	11	6	С	0.303819	3.555078	1.631579
	12	6	С	1.087033	3.368883	2.764915
	13	6	С	1.554958	2.092472	3.076350
	14	6	С	1.244964	1.023637	2.238720
	15	8	0	-0.041630	-0.345806	-2.172158
	16	6	С	1.268272	-1.020002	0.193785
	17	6	С	2.580575	-0.790340	-0.369600
	18	6	С	3.343411	-1.968840	-0.147447
	19	7	Ν	2.531632	-2.859398	0.525528
	20	6	С	1.290916	-2.285524	0.723310
	21	6	С	3.189189	0.289177	-1.032713
	22	6	С	4.507751	0.170215	-1.452303
	23	6	С	5.241786	-1.011019	-1.224201
	24	6	С	4.670854	-2.095304	-0.568775
	25	1	Н	2.637771	1.205769	-1.217780
7gk	26	1	Н	4.983244	0.999577	-1.967401
_	27	1	Н	6.270582	-1.075502	-1.566053
	28	1	Н	5.234889	-3.006733	-0.390947
	29	1	Н	2.782179	-3.798962	0.784590
	30	1	Н	1.337478	4.217451	3.394654
	31	1	Н	-0.029150	4.557534	1.386948
	32	1	Н	2.169836	1.930345	3.956696
	33	1	Н	-1.610330	4.660989	0.123456
	34	1	Н	-2.904864	4.988572	-1.926210
	35	1	Н	-2.960647	3.224908	-3.685113
	36	1	Н	-1.686714	1.097265	-3.313386
	37	6	С	-1.174625	-0.668741	0.760786
	38	6	С	-1.910078	-1.793921	0.211209
	39	6	С	-1.885259	-0.244175	1.859528
	40	6	С	-3.046982	-1.989831	1.043278
	41	1	Н	-1.674715	0.568096	2.537877
	42	1	Н	-3.678593	-0.919358	2.771459
	43	7	N	-3.001821	-1.031017	2.034759
	44	1	Н	1.622009	0.032638	2.465144
	45	1	Н	0.505058	-2.832318	1.221151
	46	6	С	-1.724998	-2.659471	-0.885032
	47	6	С	-3.983750	-3.003861	0.817806
	48	6	С	-2.654745	-3.665991	-1.112457
	49	6	С	-3.772575	-3.839226	-0.271482
	50	1	Н	-0.873438	-2.527774	-1.541430
	51	1	Н	-2.519819	-4.333779	-1.958252
	52	1	Н	-4.480177	-4.636843	-0.477900
	53	1	Н	-4.842919	-3.132292	1.470305
	Center	Atomic	Atom type	Co	oordinates (Angstro	ns)
	number	number	Atom type	Х	Y	Z
	1	6	С	0.801850	2.121179	2.832861
	2	6	C	0.940194	3.405791	3.342820
	3	6	С	0.537295	4.495205	2.564268
	4	6	С	-0.011125	4.297388	1.300422
	5	6	C	-0.168899	3.005152	0.770448
7ek	6	6	С	0.271677	1.916829	1.552446
/ (K	7	6	C	-0.800550	2.752274	-0.544305
	8	6	C	-0.713596	1.476387	-1.145737
	9	6	C	0.074356	0.324667	-0.490807
	10	6	С	0.173023	0.522248	1.047828
	11	6	C	-1.519726	3.762757	-1.208848
	12	6	С	-2.106896	3.542813	-2.449485
	13	6	С	-1.991884	2.290879	-3.053291
	14	6	С	-1.303985	1.272538	-2.397753

	15	6	С	0.262190	-0.431147	1.805268
	16	6	С	-0.568692	-1.016862	-0.792048
	17	6	С	-1.880805	-1.455931	-0.368719
	18	6	С	-2.077302	-2.758300	-0.904778
	19	7	N	-0.940517	-3.082485	-1.624199
	20	6	C	-0.044799	-2.036240	-1.547724
	21	6	C	-2.899679	-0.875529	0.397856
	22	6	C	-4.074896	-1.591053	0.620684
	23	6	C	-4.250894	-2.885345	0.085399
	24	6	C	-3.250414	-3.4/64/8	-0.683003
	25	1	H	-2.804564	0.115056	0.828417
	26	1	H	-5.166844	-3.434439	0.265087
	27	1	H	-3.391581	-4.472039	-1.094261
	28	1	н	-0.709590	-3.938347	-2.088175
	29	1	п	-2.0380/1	4.341729	-2.955956
	31	1	Н	-1.041900	2 101792	-0.739020
	32	1	Н	-0.305528	5 163774	0 719041
	32	1	Н	0.651624	5 506655	2 943750
	34	1	Н	1 364618	3 562752	4 329666
	35	1	Н	1.105919	1 248334	3 400441
	36	6	C	1.533175	0.384880	-0.964973
	37	6	Č	2.642521	-0.449235	-0.543372
	38	6	Č	2.050734	1.287635	-1.868691
	39	6	С	3.788619	0.005500	-1.243675
	40	1	Н	1.551082	2.078516	-2.406361
	41	1	Н	3.996585	1.590791	-2.653420
	42	7	N	3.395756	1.063830	-2.041784
	43	1	Н	-1.227779	0.291552	-2.853134
	44	1	Н	0.917257	-2.098394	-2.032786
	45	6	C	2.766718	-1.535311	0.349579
	46	6	C	5.045317	-0.589048	-1.079793
	47	6	C	4.018406	-2.117994	0.514998
	48	0	U U	5.148909	-1.030410	-0.197440
	49 50	1	п	6.098500	-1.6//5/6	0.894028
	51	1	H	5 915310	-0.232576	-0.028229
	52	8	0	-5 021771	-0.948263	1 382445
	53	8	0	4.272565	-3.170237	1.357313
	54	6	C	-6.232412	-1.623864	1.661718
	55	6	С	3.193540	-3.668220	2.131265
	56	1	Н	-6.823863	-0.942976	2.276641
	57	1	Н	-6.794265	-1.857089	0.746809
	58	1	Н	-6.064426	-2.554619	2.220534
	59	1	Н	2.393337	-4.074378	1.498629
	60	1	Н	3.607089	-4.469217	2.746534
	61	1	Н	2.766635	-2.892743	2.779673
	Center	Atomic	Atom type	Co	ordinates (Angstroi	ns)
	number	number	C	A 2.916272	<u> </u>	L 1 212550
	2	6	C C	-2.810373	0.740130	-1.313530
	3	6	C C	-4 685631	-0.305893	-2 267941
	4	6	C	-4.191204	-0.606997	-3.545421
	5	6	C	-3.018574	-1.346347	-3.691983
	6	6	С	-2.310820	-1.800860	-2.572226
	7	6	С	-3.093401	-1.387519	0.971540
	8	6	С	-4.292929	-0.596124	0.347690
	9	1	Н	-5.601889	0.263123	-2.162890
10aa	10	1	Н	-4.726227	-0.259934	-4.423746
1000	11	1	Н	-2.643039	-1.574594	-4.685106
	12	1	Н	-1.398854	-2.376553	-2.689966
	13	8	0	-2.884755	-1.588148	2.154333
	14	6	C	-3.396248	-1.280942	0./30101
	15	6	C	-5.709505	-2.400237	0./3/680
	17	1	н	-4 934725	-3.099037	1 823282
	18	1	H	-7.376341	-3,659328	1.980244
	19	6	C	-4.211934	0.835474	0.853829
	20	6	C	-4.957866	1.343799	1.889006
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	21	6	C	-3.263275	1.867651	0.485806

23	6	С	-3.513447	2.979043	1.339473
24	1	Н	-4.957238	3.218123	2.884887
25	7	N	2 287790	1 837251	0.059722
25	7	N	4.552200	2 629206	2 177026
20	/	IN N	-4.552290	2.028390	2.17/030
27	/	N	-/.0364/4	-2.83/34/	1.509262
28	6	С	-7.821931	-1.861218	0.934016
29	6	С	-7.520792	0.277761	-0.176385
30	6	С	-8.902275	0.365442	-0.291422
31	6	С	-9.742551	-0.654639	0.197522
32	6	С	-9.213465	-1.777933	0.820370
32	1		0 3/15030	1 238765	0.761166
24	1	11	-9.343039	0.559209	-0.701100
34	1	п	-10.819111	-0.538598	0.092947
35	1	H	-9.85/0/1	-2.562376	1.208/30
36	6	C	-2.220559	1.975045	-0.455109
37	6	С	-1.474912	3.145382	-0.515814
38	6	С	-1.749431	4.231216	0.338707
39	6	С	-2.774319	4.164288	1.274030
40	1	Н	-1.999165	1.157246	-1.131278
41	1	Н	-0.659614	3,226540	-1.228070
42	1	н	-1.145250	5 130536	0.266300
42	1	п Ц	2 080100	4.007500	1.027569
4.5	1	11	-2.707177	1.007000	0.520070
44	1	Н	-0.890860	1.08/298	-0.528870
45	6	<u> </u>	-1.020583	-2.510173	0.176847
46	6	C	0.187198	-1.588452	-0.048499
47	6	С	1.516189	-2.302162	0.237812
48	6	С	3.366264	-0.780323	0.928102
49	6	С	4.432362	0.124833	0.218319
50	6	С	4.292753	-0.337750	-1.227415
51	6	С	3.223149	-1.240460	-1.327530
52	1	Н	-0.962547	-3.394828	-0.470315
53	1	Н	-1.051690	-2.852737	1.214699
54	1	Н	0.100253	-0.716749	0.607845
55	1	Н	0.184406	-1.214615	-1.078360
56	1	Н	1 597042	-3 229299	-0 343745
57	1	н	1 589129	-2 562109	1 297251
58	7	N	2 668694	-1.465831	-0.056731
59	8	0	3 1/2973	-0.855091	2 120657
60	6	<u>с</u>	3.065675	1 561460	0.467010
61	6	C C	2.062028	2 115277	1 729/19
62	0	C	2 260000	2.115277	0.411252
62	0	<u> </u>	3.302222	2.340410	-0.411555
03	0	U U	3.048404	3.077572	0.400010
64	l	H	3.288931	3.9/496/	2.491331
65	6	C	5.829338	-0.13/108	0.751684
66	6	C	6.466180	-1.424920	0.926/58
67	6	C	6.773010	0.807322	1.073274
68	6	С	7.794574	-1.177069	1.369422
69	6	С	5.059217	-0.046216	-2.343853
70	6	С	4.721394	-0.623129	-3.576785
71	6	С	3.633102	-1.491727	-3.670168
72	6	С	2.869733	-1.820837	-2.542556
73	1	Н	2.039029	-2.514398	-2.620532
74	1	Н	3.376357	-1.932581	-4.628953
75	1	Н	5.309554	-0.394792	-4.459985
76	1	Н	5.907751	0.626216	-2.259819
77	7	N	3,431258	3,382010	1.690354
78	6	C	3.031221	2.617461	-1.780892
79	6	r r	2,455737	4,839599	-0 103351
80	6	C C	2.435770	3 767601	_2 282725
<u>81</u>	6	C C	2.450277	4 872506	1 457772
01 92	1	ц Ц	2.132032	1 785580	-1.431113
02	1	11	2 195409	2.916024	-2.442755
0.0	1	п	2.103498	5.010034	-3.337408
05	1	н	1.092211	5./39804	-1.883913
80	1	H	2.23/922	5.082889	0.546205
86	1	H	4.281276	1.009817	2.03864/
8/	/	N	7.952085	0.191458	1.442688
88	1	H	8.783318	0.668665	1.749385
89	1	H	6.691186	1.883102	1.066349
90	6	С	8.699569	-2.205728	1.649309
91	6	С	6.055272	-2.759247	0.756963
92	6	С	6.950402	-3.784862	1.031471
93	6	С	8.259920	-3.512037	1.474715

	94	1	Н	5.051782	-2.989987	0.415160
	95	1	Н	8.936752	-4.335481	1.682353
	96	1	Н	9.708986	-1.991555	1.989248
	97	1	Н	6.638019	-4 816927	0.903024
	Center	Atomic		C	ordinates (Angstro	ns)
	number	number	Atom type	X	V	Z
	1	6	C	3 274553	-1 358898	0.670027
	2	6	C	4 670576	-1 212513	0.611539
	2	6	C	5 475372	2 034581	1 386115
	3	6	C C	1 991442	2.034581	2 210610
		0	C	4.001442	-2.995574	2.219019
	5	0	C	3.493899	-3.121482	2.2/0/64
	6	6	C	2.666238	-2.302221	1.492654
	1	6	C	3.592325	0.316809	-0.876259
	8	6	<u> </u>	5.018634	-0.100303	-0.380661
	9	1	Н	6.554777	-1.943673	1.34/420
	10	1	Н	5.507739	-3.637691	2.828722
	11	1	Н	3.042826	-3.865571	2.920652
	12	1	Н	1.587110	-2.405974	1.534106
	13	8	0	3.327014	1.159256	-1.715490
	14	6	C	5.818525	-0.629898	-1.562840
	15	6	С	5.330870	-0.878241	-2.823108
	16	6	С	7.208996	-1.036137	-1.576998
	17	1	Н	4.350457	-0.677731	-3.227108
	18	1	Н	6.213132	-1.671865	-4.584248
	19	6	С	5.667710	1.121241	0.252416
	20	6	С	6.461275	2.009539	-0.431742
	21	6	С	5.488658	1.670317	1.581810
	22	1	Н	6.807214	1.962299	-1.452741
	23	6	С	6.225023	2.889391	1.624189
	24	1	Н	7.397351	3.832564	0.120142
	25	7	Ν	2.658760	-0.445628	-0.200631
	26	7	Ν	6.801350	3.065573	0.383873
	27	7	Ν	6.318103	-1.428864	-3.613213
	28	6	С	7.482076	-1.535322	-2.881598
	29	6	С	8.260517	-1.010339	-0.640993
	30	6	С	9.512104	-1.487248	-1.009236
	31	6	С	9.750476	-1.990326	-2.303806
10ab	32	6	С	8.740417	-2.016629	-3.257240
	33	1	Н	10.324918	-1.467140	-0.289291
	34	1	Н	10.739434	-2.356676	-2.562562
	35	1	Н	8.921659	-2.394645	-4.259562
	36	6	С	4.791927	1.278020	2.741919
	37	6	С	4.849678	2.080215	3.874461
	38	6	С	5.591632	3.277732	3.889196
	39	6	С	6.289441	3.696859	2.763877
	40	1	Н	4.220729	0.357257	2.758768
	41	1	Н	4.313805	1.777408	4.769358
	42	1	Н	5.618403	3.881507	4.791452
	43	1	Н	6.861947	4.620298	2.766444
	44	1	Н	8.101885	-0.598451	0.349896
	45	6	С	1.225797	-0.275090	-0.391383
	46	6	С	0.588130	0.624485	0.680202
	47	6	С	-1.764122	-0.409618	0.750348
	48	6	С	-3.909777	-0.591692	-0.502787
	49	6	С	-5.384483	-0.083372	-0.343000
	50	6	С	-5.341635	0.501019	1.064597
	51	6	С	-4.028455	0.442228	1.555054
	52	1	Н	0.762890	-1.267314	-0.415778
	53	1	Н	1.098795	0.178596	-1.378028
	54	1	Н	1.101686	1.591272	0.652832
	55	1	Н	0.776102	0.201108	1.675706
	56	1	Н	-1.568373	-0.790681	1.761079
	57	1	Н	-1.526064	-1.203642	0.038463
	58	7	N	-3.192474	-0.173822	0.608348
	59	8	0	-3.445015	-1.211345	-1.440679
	60	6	С	-5.580153	0.950980	-1.452713
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	62	6	С	-5.620481	2.401523	-1.416096
	63	6	С	-5.717022	2.840387	-2.770141
	64	1	Н	-5.755860	1.719015	-4.576759
	65	6	C	-6.377797	-1.229428	-0.431111

	66	6	C	-6 30/1609	-2 501915	0.25/1899
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	0/	0	Ľ	-7.578347	-1.219201	-1.098193
	68	6	C	-7.495203	-3.213945	-0.057945
	69	6	С	-6.359929	0.985731	1.869176
	70	6	С	-6.052570	1 456095	3.154049
	71	6	Č	1 736862	1 /20588	3 618302
	71	0	C	-4.730802	1.420300	3.018392
	12	6	C	-3./02416	0.904955	2.826920
	73	1	Н	-2.685719	0.863672	3.203161
	74	1	Н	-4.506825	1.787948	4.614185
	75	1	Н	-6 840925	1 846510	3 789823
	76	1	II	7 291744	1.010310	1 501044
	/0	1	п	-7.381744	1.002434	1.301944
		7	N	-5.718994	1.718282	-3.570802
	78	6	С	-5.575929	3.392066	-0.412550
	79	6	С	-5.786725	4.188777	-3.133708
	80	6	C	-5 639333	4 732303	-0.770431
	00	0	C C	5.057555	5 122250	2.116(40
	<u> 81</u>	0	U 	-3.747201	3.132339	-2.110049
	82	1	Н	-5.489600	3.119186	0.630866
	83	1	Н	-5.603071	5.490246	0.006637
	84	1	Н	-5.795372	6.189039	-2.362131
	85	1	Н	-5 862675	4 484317	-4 176539
	86	1	и и	5 567642	0.280702	2 217501
	00	1	п	-3.307042	-0.389792	-3.21/391
	8/	1	N	-8.252332	-2.403/52	-0.8/8524
	88	1	Н	-9.141707	-2.647535	-1.281239
	89	1	Н	-8.006972	-0.447966	-1.719076
	90	6	С	-7.756687	-4 497455	0 431721
	01	6	Č	-5 361548	-3 115070	1 000380
	02	0	C	-5.501540	-3.1130/7	1.077307
	92	0	C	-3.01091/	-4.588014	1.590588
	93	6	С	-6.802136	-5.075101	1.259437
	94	1	Н	-4.443893	-2.602861	1.368354
	95	1	Н	-6.973065	-6.070549	1.658322
	96	1	н	-8 672794	-5 022474	0 175901
	07	1	и П	4 801634	1 866418	2 242444
	97	Í	П	-4.891034	-4.600416	2.242444
	98	6	C	-0.918/39	0.845632	0.479643
	99	1	H	-1.252765	1.650143	1.144410
	100	1	Н	-1.116681	1.188037	-0.543355
	Center	Atomic		C	oordinates (Angstro	ms)
	number	number	Atom type	X	Y	Z
	number 1	number 6	C Atom type	X 4.077401	Y -1.663192	Z 1.511218
	number 1 2	number 6	C	X 4.077401 5.109574	Y -1.663192 -0.749155	Z 1.511218 1.241594
	number 1 2 2	number 6 6	C C	X 4.077401 5.109574	Y -1.663192 -0.749155	Z 1.511218 1.241594
	number 1 2 3	number 6 6 6 6	C C C C	X 4.077401 5.109574 5.837401	Y -1.663192 -0.749155 -0.212495	Z 1.511218 1.241594 2.293146
	number 1 2 3 4	number 6 6 6 6 6 6	C C C C C	X 4.077401 5.109574 5.837401 5.527983	Y -1.663192 -0.749155 -0.212495 -0.588808	Z 1.511218 1.241594 2.293146 3.608332
	number 1 2 3 4 5	number 6 6 6 6 6	C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109	Z 1.511218 1.241594 2.293146 3.608332 3.859035
	number 1 2 3 4 5 6	number 6 6 6 6 6 6	C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040
	number 1 2 3 4 5 6 7	number 6 6 6 6 6 6 6	Atom type C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1 529597	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553
	number 1 2 3 4 5 6 7 8	number 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Atom type C C C C C C C C C C C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.210802	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547125	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 0.271400
	number 1 2 3 4 5 6 7 8	number 6	Atom type C C C C C C C C C C C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644067	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 -0.496755	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104755
	number 1 2 3 4 5 6 7 8 9	number 6 6 6 6 6 6 6 6 6 1	Atom type C C C C C C C C C H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761
	number 1 2 3 4 5 6 7 8 9 10	number 6 6 6 6 6 6 6 6 1	Atom type C C C C C C C C C H H H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218
	number 1 2 3 4 5 6 7 8 9 10 11	number 6 6 6 6 6 6 6 6 1 1	Atom type C C C C C C C C C H H H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810
	number 1 2 3 4 5 6 7 8 9 10 11 12	number 6 6 6 6 6 6 6 6 6 6 6 6 6 1 1 1 1 1	Atom type C C C C C C C C H H H H H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997
	number 1 2 3 4 5 6 7 8 9 10 11 12 13	number 6 6 6 6 6 6 6 6 6 1 1 1 1 8	Atom type C C C C C C C C H H H H H O	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803
	number 1 2 3 4 5 6 7 8 9 10 11 12 13	number 6 6 6 6 6 6 6 1 1 1 8	Atom type C C C C C C C C C C C H H H H H O C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125
	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14	number 6 6 6 6 6 6 6 6 1 1 1 8 6	Atom type C C C C C C C C C H H H H C C C C C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.921200	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 2.165520	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 1.476178
	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	number 6 6 6 6 6 6 6 1 1 1 8 6 6	Atom type C C C C C C C C C C C C C C H H H O C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.04005	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.25256	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 0.672120
10ac	$\begin{array}{c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \end{array}$	number 6 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 6 6 6 6 6 6	Atom type C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129
10ac	$\begin{array}{c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \end{array}$	number 6 6 6 6 6 6 6 6 1 1 1 8 6 6 6	Atom type C C C C C C C C H H H H H O C C C H H H H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275
10ac	number 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	number 6 6 6 6 6 6 6 6 1 1 8 6 6 6 1	Atom type C C C C C C C C H H H H O C C C H H H H H H H H H H H H H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292
10ac	$\begin{array}{c} \textbf{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ \end{array}$	number 6 6 6 6 6 6 1 1 1 6 6 6 6 6 6 1 1 1 1 6 6 1 1 6 6 1 6	Atom type C H H O C H H C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ \end{array}$	number 6 6 6 6 6 6 1 1 8 6 6 6 1 1 6 6 6 6 6 6 6 6 6 6	Atom type C C C C C C C C C H H H C C C C H H C C H H C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409007	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1 917063
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ \end{array}$	number 6 6 6 6 6 6 1 1 1 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Atom type C C C C C C C C C H H H C C C C C C C C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781001	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931
10ac	$\begin{array}{c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline \end{array}$	number 6 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 6 6 6 6 6 6 1 1	Atom type C C C C C C C C C C C C C H H O C C C H H C C C C C C U	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.04467	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015720	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 2.639238
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 22 \\ 22 \\ 22 \\ 22 \\ 22$	number 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 6 6 6 6 1 1 6 6 1 1	Atom type C C C C C C C C C C C H H O C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.002020	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -0.0251
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ \end{array}$	number 6 6 6 6 6 6 6 1 1 8 6 6 6 6 6 6 1 1 8 6 6 1 1 6 6 1 6 6 6 6 6 6	Atom type C C C C C C C C C H H H O C C C C C C C C C H C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ \end{array}$	number 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 6 6 6 6 1 6 6 1 6 6 1 6 1 1	Atom type C H C H	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395
10ac	$\begin{array}{c c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \end{array}$	number 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 6 6 1 6 6 1 6 1 6 1 7	Atom type C H N	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.015730 2.888080 3.241054 -2.088429	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883
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10ac	$\begin{array}{c c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline \end{array}$	number 6 6 6 6 6 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 1 6 1 7 7 7 6 6 6	Atom type C H C C H N N N N C C C C C C C C C C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.088429 2.628641 -2.276162 -1.162411 0.904318	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113
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10ac	$\begin{array}{r} \textbf{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ \end{array}$	number 6 6 6 6 6 6 6 6 6 6 6 6 1 1 1 1 6 6 6 6 6 1 7 7 7 6	Atom type C H N N N N C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186 9.610200 10.565806 10.188778	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.088429 2.628641 -2.276162 -1.162411 0.904318 1.245494 0.388544 -0.823470	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113 -0.139430 -0.721083 -1.285680
10ac	$\begin{array}{c} \text{number} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \\ 25 \\ 26 \\ 27 \\ 28 \\ 29 \\ 30 \\ 31 \\ 32 \\ 33 \\ \end{array}$	number 6 6 6 6 6 6 6 1 1 1 1 1 6 6 6 6 1 1 7 7 6 6 1 7 7 6 6 1 6 6 1 6 <td>Atom type C H N N N N C</td> <td>X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186 9.610200 10.565806 10.188778 9.933140</td> <td>Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.088429 2.628641 -2.276162 -1.162411 0.904318 1.245494 0.3823470 2.192789</td> <td>Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113 -0.139430 -0.721083 -1.285680 0.282127</td>	Atom type C H N N N N C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186 9.610200 10.565806 10.188778 9.933140	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.088429 2.628641 -2.276162 -1.162411 0.904318 1.245494 0.3823470 2.192789	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113 -0.139430 -0.721083 -1.285680 0.282127
10ac	$\begin{array}{c} \textbf{number} \\ \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline 5 \\ \hline 6 \\ \hline 7 \\ \hline 8 \\ 9 \\ \hline 10 \\ \hline 11 \\ \hline 12 \\ \hline 13 \\ \hline 14 \\ \hline 15 \\ \hline 16 \\ \hline 17 \\ \hline 18 \\ \hline 19 \\ \hline 20 \\ \hline 21 \\ \hline 22 \\ \hline 23 \\ \hline 24 \\ \hline 25 \\ \hline 26 \\ \hline 27 \\ \hline 28 \\ \hline 29 \\ \hline 30 \\ \hline 31 \\ \hline 32 \\ \hline 33 \\ \hline 34 \\ \end{array}$	number 6 6 6 6 6 6 6 6 1 1 1 1 1 1 6 6 6 6 6 1 6 6 7 7 6 6 6 1 7 7 6 <td>Atom type C H N N N C</td> <td>X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186 9.610200 10.565806 10.188778 9.933140</td> <td>Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.276162 -1.162411 0.904318 1.245494 0.388544 -0.823470 2.192789</td> <td>Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.947803 -0.804125 -1.9476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113 -0.139430 -0.721083 -1.285680 0.282127 0.734527</td>	Atom type C H N N N C	X 4.077401 5.109574 5.837401 5.527983 4.499400 3.756035 4.113675 5.219892 6.644007 6.093906 4.266951 2.958232 3.838851 6.573427 6.831390 7.848096 6.141910 8.613284 4.849578 5.294869 3.887482 6.004657 3.821752 4.867374 3.484970 4.689111 8.181705 8.832388 8.264186 9.610200 10.565806 10.188778 9.933140	Y -1.663192 -0.749155 -0.212495 -0.588808 -1.496109 -2.049890 -1.529597 -0.547135 0.486577 -0.169533 -1.781497 -2.757410 -1.775270 -0.995274 -2.165539 -0.323728 -2.922795 -3.029478 0.851251 1.409097 1.781091 1.015730 2.888080 3.241054 -2.276162 -1.162411 0.904318 1.245494 0.388544 -0.823470 2.192789	Z 1.511218 1.241594 2.293146 3.608332 3.859035 2.809040 -0.786553 -0.271490 2.104761 4.434218 4.880810 3.007997 -1.947803 -0.804125 -1.947803 -0.804125 -1.9476178 -0.652129 -1.816275 -2.243292 -0.743343 -1.917063 -0.185931 -2.628238 -1.080534 -2.899395 0.310883 -2.120788 -1.734130 -1.246626 -0.103113 -0.139430 -0.721083 -1.285680 0.282127 0.734527

SI152

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Center number	Atomic number		X	Y	Z
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0	6	C C	-0.000003968	-0.000005393	-0.000006265
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11	1	Н	0.00000261	-0.000000464	0.000000139
12	1	Н	0.00000639	-0.000000341	0.000000303
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1/	1	H	-0.000001821	-0.000001435	-0.000002707
10	6	Г	-0.000000723	0.000003399	0.000005719
20	6	C	0.000003014	0.000000539	0.000013301
21	6	č	0.000007652	0.000000476	0.000006380
22	1	Н	0.00000695	-0.000001015	0.00000456
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25	7	N	-0.000000941	-0.000015074	0.000001031
26	7	N	-0.000001823	-0.000003516	0.000002395
27	1	N	-0.000001184	-0.000000838	-0.000002194
28	6	C	0.000005945	-0.000000903	-0.000001/64
30	6	C	0.000002593	0.000005940	0.00000137
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33	1	Н	-0.000000503	-0.000000457	0.00000072
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42	1	Н	-0.000000129	0.00000846	-0.000003023
43	1	Н	0.00000023	0.000000002	-0.000002437
44	1	Н	-0.000000639	0.000000728	0.000001907
45	6	C	0.000017986	0.000014953	0.000000427
46	6	C	-0.000013184	-0.000017208	-0.000008583
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54	1	Н	0.000006116	0.000003600	0.000004015
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56	1	H	0.000003996	-0.000000484	-0.000006842
57	1	H	0.000003205	0.000011671	-0.000002453
<u> </u>	/ o	N	-0.000015047	-0.000015345	0.000007802
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75	1	Н	-0.00000625	0.000001182	0.000000539
76	1	Н	-0.000000175	-0.000000722	-0.000000485
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79	6	С	-0.00000688	0.000003388	-0.000004073
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12	12 25 1.0	12 25 1.0	12 25 1.0	12 25 1.0
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21 23 1.0 27 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0
22 24 2.0 37 1.0	22	22	22	22
23	23 26 1.0 39 1.0	23 26 1.0 39 1.0	23 26 1.0 39 1.0	23 26 1.0 39 1.0
24 27 1.0 40 1.0	24 26 1.0	24 26 1.0	24 26 1.0	24 26 1.0
25 27 1.0	25	25	25	25
26	26	26	26	26
27	27 28 1.0	27 28 1.0	27 28 1.0	27 28 1.0
28 29 1.0	28 32 1.0	28 32 1.0	28 32 1.0	28 32 1.0
29 33 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0
30 31 2.0 45 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0
31 32 1.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0
32 33 2.0 35 1.0	32 35 1.0	32 35 1.0	32 35 1.0	32 35 1.0
33 36 1.0	33	33	33	33
34	34	34	34	34
35	35	35	35	35
36	36 37 2.0 40 1.0	36 37 2.0 40 1.0	36 37 2.0 40 1.0	36 37 2.0 40 1.0
37 38 2.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0
38 39 1.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0
39 40 2.0 43 1.0	39 43 1.0	39 43 1.0	39 43 1.0	39 43 1.0
40 44 1.0	40	40	40	40
41	41	41	41	41
42	42	42	42	42
43	43	43	43	43
44	44	44	44	44
45	45	45	45	45 46 1.5 47 1.5
				46
				47
7af	7ag	7ah	7ba	7ca
1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 26 1.0	1 2 2.0 6 1.0 26 1.0
2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0
3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0
4 5 1.0 45 1.0	4 5 1.0 45 1.0	4 5 1.0 10 1.0	4 5 1.0 10 1.0	4 5 1.0 10 1.0
5 6 2.0 10 1.0	5 6 2.0 10 1.0	5 6 2.0 11 1.0	5 6 2.0 11 1.0	5 6 2.0 11 1.0
6 11 1.0	6 11 1.0	6 45 1.0	6 12 1.0	6 12 1.0
7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 14 2.0 26 1.0	7 8 1.0 14 2.0 26 1.0
8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 15 1.0 20 1.0	8 15 1.0 20 1.0
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12 25 1.0	12 25 1.0	12 25 1.0	12	12
13	13	13	13 26 1.0	13 26 1.0
14 15 2.0 16 1.0	14 15 2.0 16 1.0	14 15 2.0 16 1.0	14	14
15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 16 2.0 17 1.0	15 16 2.0 17 1.0
16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 18 1.0 28 1.0	16 18 1.0 28 1.0
17	17	17	17 29 2.0 30 1.0	17 29 2.0 30 1.0
18 27 1.0	18 27 1.0	18 27 1.0	18	18
19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 28 1.0	19 28 1.0
20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 21 2.0 22 1.0	20 21 2.0 22 1.0
21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0 22	21 23 1.0 27 1.0	21 23 1.0 27 1.0
22	22	23 26 1.0 39 1.0	22 24 2.0 36 1.0	22 24 2.0 36 1.0
23 26 1.0 39 1.0	23 26 1.0 39 1.0	24 26 1.0	23	23
24 26 1.0	24 26 1.0	25	24 27 1.0 39 1.0	24 27 1.0 39 1.0

Table S11 Z matrix of the optimized structures obtained at B3LYP 631-G (d,p) level of theor

	25	26	25 27 1.0	25 27 1.0
26	26	27 28 1.0	26	26
27 28 1.0	27 28 1.0	28 32 1.0	27	27
28 32 1.0	28 32 1.0	29 30 2.0 44 1.0	28 29 1.0	28 29 1.0
29 30 2.0 44 1.0	29 30 2.0 44 1.0	30 31 1.0 33 1.0	29 33 1.0	29 33 1.0
30 31 1.0 33 1.0	30 31 1.0 33 1.0	31 32 2.0 34 1.0	30 31 2.0 43 1.0	30 31 2.0 43 1.0
31 32 2.0 34 1.0	31 32 2.0 34 1.0	32 35 1.0	31 32 1.0 44 1.0	31 32 1.0 45 1.0
32 35 1.0	32 35 1.0	33	32 33 2.0 34 1.0	32 33 2.0 34 1.0
33	33	34	33 35 1.0	33 35 1.0
34	34	35	34	34
35	35	36 37 2.0 40 1.0	35	35
30 37 2.0 40 1.0	30 37 2.0 40 1.0	37 38 1.0 41 1.0	30 37 2.0 40 1.0	30 37 2.0 40 1.0
37 38 1.0 41 1.0	37 38 1.0 41 1.0	38 39 2.0 42 1.0	37 38 1.0 43 1.0	37 38 1.0 44 1.0
39 /3 1 0	39 /3 1 0	40	39 42 1 0	39 42 1 0
40	<i>4</i> 0	40	40	40
40	40	42	40	40
42	42	43	42	42
43	43	44	43	43
44	44	45	44 46 3.0	44 47 1.0
45 46 1.0 47 1.0 48 1.0	45 46 1.0		45 47 3.0	45 46 1.0
46	46 47 1.0 48 1.0 49 1.0		46	46 48 1.0 49 1.0 50 1.0
47	47		47	47 51 1.0 52 1.0 53 1.0
48	48			48
	49			49
				50
				51
				52
				53
7da	7ea	7ec	7ed	7fa
1 2 2.0 6 1.0 24 1.0	1 2 2.0 6 1.0 26 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 24 1.0
2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0
3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0
4 5 1.0 10 1.0	4 5 1.0 10 1.0	4 5 1.0 45 1.0	4 5 1.0 45 1.0	4 5 1.0 10 1.0
562.0111.0	562.0111.0	5 6 2.0 10 1.0	5 6 2.0 10 1.0	562.0111.0
6 12 1.0 7 8 1 0 14 2 0 24 1 0	6 12 1.0 7 8 1 0 14 2 0 2C 1 0	0 11 1.0	0 11 1.0 7 8 1 0 12 2 0 25 1 0	6 12 1.0
781.0142.0241.0	7 8 1.0 14 2.0 20 1.0 8 15 1 0 20 1 0	7 8 1.0 15 2.0 25 1.0 8 14 1 0 10 1 0	781.0132.0251.0	7 8 1.0 14 2.0 24 1.0
0	0	0	0	0
10	9	10	10	10
10	10	10	10	10
12	12	12 25 1 0	12 25 1.0	12
	12 26 1 0	12 20 110	13	
13 24 1.0	1.3 26 1.0	1.5	1.7	13 24 1.0
13 24 1.0 14	13 26 1.0 14	13	14 15 2.0 16 1.0	13 24 1.0 14
13 24 1.0 14 15 16 2.0 17 1.0	13 26 1.0 14 15 16 2.0 17 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0	13 24 1.0 14 15 16 2.0 17 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0 22 24 2.0 36 1.0 22	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 22 20 1 0 20 1 0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 22
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0 23 25 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0 22 24 2.0 36 1.0 23 10 20 1 0 20 1 0	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 23 25 1.0 38 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0 23 25 1.0 24	$\begin{array}{c} 13 \ 26 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 28 \ 1.0 \\ 17 \ 29 \ 2.0 \ 30 \ 1.0 \\ 18 \\ 19 \ 28 \ 1.0 \\ 20 \ 21 \ 2.0 \ 22 \ 1.0 \\ 21 \ 2.3 \ 1.0 \ 27 \ 1.0 \\ 22 \ 24 \ 2.0 \ 36 \ 1.0 \\ 23 \\ 24 \ 27 \ 1.0 \ 39 \ 1.0 \\ 25 \ 27 \ 1.0 \\ 39 \ 1.0 \end{array}$	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 23 25 1.0 38 1.0 24 25 44 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0 23 25 1.0 24 25 26 27 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0 22 24 2.0 36 1.0 23 24 27 1.0 39 1.0 25 27 1.0 26	13 14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 23 25 1.0 38 1.0 24 25 44 1.0 26 27 1.0 45 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0 23 25 1.0 24 25 26 27 1.0 27 31 1.0	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 24\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1\ 0\end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 23 25 1.0 38 1.0 24 25 44 1.0 26 27 1.0 45 1.0 27 31 1.0
13 24 1.0 14 15 16 2.0 17 1.0 16 26 1.0 45 1.0 17 27 2.0 28 1.0 18 26 1.0 19 20 2.0 21 1.0 20 25 1.0 44 1.0 21 22 2.0 35 1.0 22 25 1.0 38 1.0 23 25 1.0 24 25 26 27 1.0 27 31 1.0 28 20 2.0 43 1.0	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0 22 24 2.0 36 1.0 23 24 27 1.0 39 1.0 25 27 1.0 26 27 28 20 1.0	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 28\ 21\ 10\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 20 10	13 24 1.0 14 15 16 2.0 17 1.0 16 18 1.0 26 1.0 17 27 2.0 28 1.0 18 19 20 2.0 21 1.0 20 22 1.0 25 1.0 21 23 2.0 35 1.0 22 23 25 1.0 38 1.0 24 25 44 1.0 26 27 1.0 45 1.0 27 31 1.0 28 20 2.0 43 1.0
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 25 \ 1.0 \ 44 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 20 \ 0 \ 32 \ 1.0 \end{array}$	13 26 1.0 14 15 16 2.0 17 1.0 16 18 1.0 28 1.0 17 29 2.0 30 1.0 18 19 28 1.0 20 21 2.0 22 1.0 21 23 1.0 27 1.0 22 24 2.0 36 1.0 23 24 27 1.0 39 1.0 25 27 1.0 26 27 28 29 1.0 29 3.1 0	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 28\ 32\ 1.0\\ 28\ 32\ 1.0\\ 29\ 30\ 2\ 0\ 42\ 1\ 0 \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 32 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0	13 24 1.0 14 $15 16 2.0 17 1.0$ $16 18 1.0 26 1.0$ $17 27 2.0 28 1.0$ 18 $19 20 2.0 21 1.0$ $20 22 1.0 25 1.0$ $21 23 2.0 35 1.0$ 22 $23 25 1.0 38 1.0$ 24 $25 44 1.0$ $26 27 1.0 45 1.0$ $27 31 1.0$ $28 29 2.0 43 1.0$ $29 3.0 1.0 32 1.0$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.5 \ 1.0 \ 44 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2 \ 0 \ 33 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2 \ 0 \ 33 \ 1.0 \\ 30 \ 31 \ 2 \ 0 \ 30 \ 31 \ 0 \ 30 \ 30 \ 30 \ 30 \$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2\ 0\ 43\ 1\ 0 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 28\ 32\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 10\ 43\ 1\ 0\end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 2.0 21 1.0 20 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 2.0 30 2.0 42 1.0 29 30 2.0 42 1.0 30 31 1 0	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2 \ 0 \ 33 \ 1.0 \end{array}$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.5 \ 1.0 \ 44 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1 \ 0 \end{array}$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1\ 0\ 44\ 1\ 0 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 28\ 32\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2\ 0\ 33\ 1\ 0\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 2.0 21 1.0 20 2.0 21 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 31 31 32 2.0 33 1.0	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1 \ 0 \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 28\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 38\ 1.0\\ 23\ 25\ 1.0\\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\end{array}$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ \end{array}$	$ \begin{array}{c} 14 \\ 15 \\ 14 \\ 15 \\ 17 \\ 1.0 \\ 27 \\ 1.0 \\ 17 \\ 18 \\ 27 \\ 1.0 \\ 19 \\ 20 \\ 2.0 \\ 21 \\ 1.0 \\ 20 \\ 21 \\ 1.0 \\ 21 \\ 22 \\ 23 \\ 26 \\ 1.0 \\ 25 \\ 26 \\ 27 \\ 28 \\ 1.0 \\ 25 \\ 26 \\ 27 \\ 28 \\ 1.0 \\ 25 \\ 26 \\ 27 \\ 28 \\ 1.0 \\ 29 \\ 30 \\ 2.0 \\ 42 \\ 1.0 \\ 30 \\ 31 \\ 1.0 \\ 43 \\ 1.0 \\ 31 \\ 31 \\ 22 \\ 32 \\ 31 \\ 0 \\ 32 \\ 41 \\ 0 \end{array} $	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \end{array}$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 28 \ 1.0 \\ 20 \ 2.5 \ 1.0 \ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \end{array}$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \\ 33\ 35\ 1.0 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 26 1.0 38 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0 33 1.0 33 33 33 33 34 1.0 33 1.0	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \end{array}$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 25 \ 1.0 \ 41 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \\ 34 \end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 4\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 5\ 1.0\\ 34\end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 28\ 32\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\\ 34\end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 26 1.0 38 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 31 32 2.0 33 1.0 33 34 34	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \\ 34 \end{array}$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.0 \ 21 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \\ 34 \\ 35 \ 36 \ 2.0 \ 39 \ 1.0 \end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 24\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 51\ 1.0\\ 34\\ 35\end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 26 1.0 23 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 31 32 2.0 33 1.0 32 34 1.0 33 34 35 36 2.0 39 1.0	$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 18 \ 1.0 \ 26 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 25 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 25 \ 1.0 \ 38 \ 1.0 \\ 24 \\ 25 \ 44 \ 1.0 \\ 26 \ 27 \ 1.0 \ 45 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \\ 34 \\ 35 \ 36 \ 2.0 \ 39 \ 1.0 \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 24\\ 25\\ 25\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ \end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 24\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 35\ 1.0\\ 34\\ 35\\ 36\ 37\ 2.0\ 40\ 1.0\\ \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 26 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 28 32 1.0 23 33 1.0 33 34 1.0 31 32 2.0 33 1.0 33 34 35 36 2.0 39 1.0 35 36 2.0 39 1.0 36 37 1.0 44 1.0	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 38\ 1.0\\ 23\ 25\ 1.0\\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ \end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 4\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 35\ 1.0\\ 34\\ 35\\ 36\ 37\ 2.0\ 40\ 1.0\\ 37\ 38\ 1.0\ 45\ 1.0\\ \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 26\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ \end{array}$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 31 32 2.0 33 1.0 32 34 1.0 33 34 35 36 2.0 39 1.0 36 37 1.0 44 1.0 37 38 2.0 40 1.0	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 38\ 1.0\\ 23\ 25\ 1.0\\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ \end{array}$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 2.7\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \\ 33\ 35\ 1.0 \\ 34 \\ 35 \\ 36\ 37\ 2.0\ 40\ 1.0 \\ 37\ 38\ 1.0\ 45\ 1.0 \\ 38\ 39\ 2.0\ 41\ 1.0 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 35\ 1.0\\ 22\\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ \end{array}$	$ \begin{array}{c} 14 \\ 15 \\ 14 \\ 15 \\ 10 \\ 15 \\ 17 \\ 10 \\ 10 \\ 28 \\ 20 \\ 29 \\ 10 \\ 20 \\ 20 \\ 21 \\ 20 \\ 20 \\ 21 \\ 20 \\ 20 \\ 20 \\ 20 \\ 20 \\ 20 \\ 20 \\ 20$	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 24\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 35\ 1.0\\ 34\\ 35\\ 36\ 37\ 2.0\ 40\ 1.0\\ 37\ 38\ 1.0\ 45\ 1.0\\ 38\ 39\ 2.0\ 41\ 1.0\\ 39\ 42\ 1.0\\ \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 35\ 1.0\\ 22\\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\end{array}$	14 15 2.0 16 1.0 $15 17 1.0 27 1.0$ $16 28 2.0 29 1.0$ 17 $18 27 1.0$ $19 20 2.0 21 1.0$ $20 22 1.0 26 1.0$ $21 23 2.0 35 1.0$ 22 $23 26 1.0 38 1.0$ $24 26 1.0$ 25 26 $27 28 1.0$ $29 30 2.0 42 1.0$ $30 31 1.0 43 1.0$ $31 32 2.0 33 1.0$ $32 34 1.0$ 33 34 $35 36 2.0 39 1.0$ $36 37 1.0 44 1.0$ $37 38 2.0 40 1.0$ $38 41 1.0$ 39	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ \end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 4\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 35\ 1.0\\ 34\\ 35\\ 36\ 37\ 2.0\ 40\ 1.0\\ 37\ 38\ 1.0\ 45\ 1.0\\ 38\ 39\ 2.0\ 41\ 1.0\\ 39\ 42\ 1.0\\ 40\\ \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 31\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\\ 40\\ \end{array}$	14 15 2.0 16 10 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 28 32 1.0 23 34 1.0 30 31 1.0 43 1.0 31 32 2.0 33 1.0 32 34 1.0 33 34 35 36 2.0 39 1.0 36 37 1.0 44 1.0 37 38 2.0 40 1.0	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ \end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 38\ 1.0\\ 23\ 25\ 1.0\\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 1\end{array}$	$\begin{array}{c} 13\ 26\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 28\ 1.0\\ 17\ 29\ 2.0\ 30\ 1.0\\ 18\\ 19\ 28\ 1.0\\ 20\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 21\ 2.0\ 22\ 1.0\\ 22\ 4\ 2.0\ 36\ 1.0\\ 23\\ 24\ 27\ 1.0\ 39\ 1.0\\ 25\ 27\ 1.0\\ 26\\ 27\\ 28\ 29\ 1.0\\ 29\ 33\ 1.0\\ 30\ 31\ 2.0\ 43\ 1.0\\ 31\ 32\ 1.0\ 44\ 1.0\\ 32\ 33\ 2.0\ 34\ 1.0\\ 33\ 35\ 1.0\\ 34\\ 35\\ 36\ 37\ 2.0\ 40\ 1.0\\ 37\ 38\ 1.0\ 45\ 1.0\\ 38\ 39\ 2.0\ 41\ 1.0\\ 39\ 42\ 1.0\\ 40\\ 41\\ 1\end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 31\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\\ 40\\ 41\\ 1\end{array}$	14 15 2.0 16 10 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 28 32 1.0 23 34 1.0 30 31 1.0 43 1.0 31 32 2.0 33 1.0 32 34 1.0 33 34 35 36 2.0 39 1.0 36 37 1.0 44 1.0 39 40 41 41 41	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 1\end{array}$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 38\ 1.0\\ 23\ 25\ 1.0\\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \\ 33\ 35\ 1.0 \\ 34 \\ 35 \\ 36\ 37\ 2.0\ 40\ 1.0 \\ 37\ 38\ 1.0\ 45\ 1.0 \\ 38\ 39\ 2.0\ 41\ 1.0 \\ 39\ 42\ 1.0 \\ 40 \\ 41 \\ 42 \\ 42 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 31\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42$	14 15 2.0 16 1.0 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 30 31 1.0 43 1.0 33 34 35 36 2.0 39 1.0 33 34 1.0 37 38 2.0 40 1.0 39 40 41 42 42 41 42 42	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42\\ 42$
$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 26\ 1.0\ 45\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\ 26\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 25\ 1.0\ 44\ 1.0\\ 21\ 22\ 2.0\ 35\ 1.0\\ 22\ 25\ 1.0\ 24\\ 25\\ 26\ 27\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 44\ 41\ 42\\ 43\\ 44\ 44\ 44\ 44\ 44\ 44\ 44\ 44\ 44\ 44$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \\ 33\ 35\ 1.0 \\ 34 \\ 35 \\ 36\ 37\ 2.0\ 40\ 1.0 \\ 37\ 38\ 1.0\ 45\ 1.0 \\ 38\ 39\ 2.0\ 41\ 1.0 \\ 39\ 42\ 1.0 \\ 40 \\ 41 \\ 42 \\ 43 \\ 44 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 31\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 43\\ 44\\ 45\\ 43\\ 44\\ 45\\ 45\\ 45\\ 45\\ 45\\ 45\\ 45\\ 45\\ 45$	$\begin{array}{c} 13\\ 14 \ 15 \ 2.0 \ 16 \ 1.0 \\ 15 \ 17 \ 1.0 \ 27 \ 1.0 \\ 16 \ 28 \ 2.0 \ 29 \ 1.0 \\ 17 \\ 18 \ 27 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 22 \ 1.0 \ 26 \ 1.0 \\ 21 \ 23 \ 2.0 \ 35 \ 1.0 \\ 22 \\ 23 \ 26 \ 1.0 \ 38 \ 1.0 \\ 24 \ 26 \ 1.0 \\ 25 \\ 26 \\ 27 \ 28 \ 1.0 \\ 29 \ 30 \ 2.0 \ 42 \ 1.0 \\ 30 \ 31 \ 1.0 \ 43 \ 1.0 \\ 31 \ 32 \ 2.0 \ 33 \ 1.0 \\ 32 \ 34 \ 1.0 \\ 33 \\ 34 \\ 35 \ 36 \ 2.0 \ 39 \ 1.0 \\ 36 \ 37 \ 1.0 \ 44 \ 1.0 \\ 37 \ 38 \ 2.0 \ 40 \ 1.0 \\ 38 \ 41 \ 1.0 \\ 39 \\ 40 \\ 41 \\ 42 \\ 43 \\ 44 \end{array}$	$\begin{array}{c} 13\ 24\ 1.0\\ 14\\ 15\ 16\ 2.0\ 17\ 1.0\\ 16\ 18\ 1.0\ 26\ 1.0\\ 17\ 27\ 2.0\ 28\ 1.0\\ 18\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 22\ 1.0\ 25\ 1.0\\ 21\ 23\ 2.0\ 35\ 1.0\\ 22\\ 23\ 25\ 1.0\ 38\ 1.0\\ 24\\ 25\ 44\ 1.0\\ 26\ 27\ 1.0\ 45\ 1.0\\ 27\ 31\ 1.0\\ 28\ 29\ 2.0\ 43\ 1.0\\ 29\ 30\ 1.0\ 32\ 1.0\\ 30\ 31\ 2.0\ 33\ 1.0\\ 31\ 34\ 1.0\\ 32\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 40\ 1.0\\ 37\ 38\ 2.0\ 41\ 1.0\\ 38\ 42\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 43\\ 44\ 41\ 42\\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\\ 44\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 42\ 43\ 41\ 41\ 41\ 42\ 43\ 41\ 41\ 41\ 42\ 43\ 41\ 41\ 41\ 42\ 41\ 41\ 42\ 41\ 41\ 41\ 41\ 42\ 41\ 41\ 41\ 42\ 41\ 41\ 41\ 41\ 41\ 41\ 41\ 41\ 41\ 41$
$\begin{array}{c} 13 \ 24 \ 1.0 \\ 14 \\ 15 \ 16 \ 2.0 \ 17 \ 1.0 \\ 16 \ 26 \ 1.0 \ 45 \ 1.0 \\ 17 \ 27 \ 2.0 \ 28 \ 1.0 \\ 18 \ 26 \ 1.0 \\ 19 \ 20 \ 2.0 \ 21 \ 1.0 \\ 20 \ 25 \ 1.0 \ 44 \ 1.0 \\ 21 \ 22 \ 2.0 \ 35 \ 1.0 \\ 22 \ 25 \ 1.0 \ 38 \ 1.0 \\ 23 \ 25 \ 1.0 \\ 24 \\ 25 \\ 26 \ 27 \ 1.0 \\ 27 \ 31 \ 1.0 \\ 28 \ 29 \ 2.0 \ 43 \ 1.0 \\ 29 \ 30 \ 1.0 \ 32 \ 1.0 \\ 30 \ 31 \ 2.0 \ 33 \ 1.0 \\ 31 \ 34 \ 1.0 \\ 32 \\ 33 \\ 34 \\ 35 \ 36 \ 2.0 \ 39 \ 1.0 \\ 36 \ 37 \ 1.0 \ 40 \ 1.0 \\ 37 \ 38 \ 2.0 \ 41 \ 1.0 \\ 38 \ 42 \ 1.0 \\ 39 \\ 40 \\ 41 \\ 42 \\ 43 \\ 44 \ 46 \ 1.0 \ 47 \ 1.0 \ 48 \ 1.0 \\ 45 \ 49 \ 1.0 \ 50 \ 1.0 \ 51 \ 1.0 \end{array}$	$\begin{array}{c} 13\ 26\ 1.0 \\ 14 \\ 15\ 16\ 2.0\ 17\ 1.0 \\ 16\ 18\ 1.0\ 28\ 1.0 \\ 17\ 29\ 2.0\ 30\ 1.0 \\ 18 \\ 19\ 28\ 1.0 \\ 20\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 21\ 2.0\ 22\ 1.0 \\ 22\ 4\ 2.0\ 36\ 1.0 \\ 23 \\ 24\ 27\ 1.0\ 39\ 1.0 \\ 25\ 27\ 1.0 \\ 26 \\ 27 \\ 28\ 29\ 1.0 \\ 29\ 33\ 1.0 \\ 30\ 31\ 2.0\ 43\ 1.0 \\ 31\ 32\ 1.0\ 44\ 1.0 \\ 32\ 33\ 2.0\ 34\ 1.0 \\ 33\ 35\ 1.0 \\ 34 \\ 35 \\ 36\ 37\ 2.0\ 40\ 1.0 \\ 37\ 38\ 1.0\ 45\ 1.0 \\ 38\ 39\ 2.0\ 41\ 1.0 \\ 39\ 42\ 1.0 \\ 40 \\ 41 \\ 42 \\ 43 \\ 44 \\ 45 \end{array}$	$\begin{array}{c} 13\\ 14\ 15\ 2.0\ 16\ 1.0\\ 15\ 17\ 1.0\ 27\ 1.0\\ 16\ 28\ 2.0\ 29\ 1.0\\ 17\\ 18\ 27\ 1.0\\ 19\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 21\ 1.0\\ 20\ 2.0\ 31\ 1.0\\ 22\\ 23\ 26\ 1.0\ 38\ 1.0\\ 24\ 26\ 1.0\\ 25\\ 26\\ 27\ 28\ 1.0\\ 29\ 30\ 2.0\ 42\ 1.0\\ 30\ 31\ 1.0\ 43\ 1.0\\ 31\ 32\ 2.0\ 33\ 1.0\\ 32\ 34\ 1.0\\ 33\\ 34\\ 35\ 36\ 2.0\ 39\ 1.0\\ 36\ 37\ 1.0\ 44\ 1.0\\ 37\ 38\ 2.0\ 40\ 1.0\\ 38\ 41\ 1.0\\ 39\\ 40\\ 41\\ 42\\ 43\\ 44\\ 45\end{array}$	14 15 2.0 16 10 14 15 2.0 10 10 15 17 1.0 27 1.0 16 28 2.0 29 1.0 17 18 27 1.0 19 20 2.0 21 1.0 20 22 1.0 26 1.0 21 23 2.0 35 1.0 22 23 26 1.0 38 1.0 24 26 1.0 25 26 27 28 1.0 28 32 1.0 28 32 1.0 29 30 2.0 42 1.0 30 31 1.0 43 1.0 33 34 35 36 2.0 39 1.0 36 37 1.0 44 1.0 37 38 2.0 40 1.0 39 40 41 42 43 44 45	13 24 1.0 14 $15 16 2.0 17 1.0$ $16 18 1.0 26 1.0$ $17 27 2.0 28 1.0$ 18 $19 20 2.0 21 1.0$ $20 22 1.0 25 1.0$ $21 23 2.0 35 1.0$ 22 $23 25 1.0 38 1.0$ 24 $25 44 1.0$ $26 27 1.0 45 1.0$ $27 31 1.0$ $28 29 2.0 43 1.0$ $29 30 1.0 32 1.0$ $30 31 2.0 33 1.0$ $31 34 1.0$ 32 33 34 $35 36 2.0 39 1.0$ $36 37 1.0 40 1.0$ $37 38 2.0 41 1.0$ $38 42 1.0$ 39 40 41 42 43 $44 46 1.0 47 1.0 48 1.0$ $45 49 1.0 50 1.0 51 1.0$

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51				51
7fb	7fd	7ga	7gc	7gd
1 2 2.0 6 1.0 23 1.0	1 2 2.0 6 1.0 23 1.0	1 2 2.0 6 1.0 24 1.0	1 2 2.0 6 1.0 23 1.0	1 2 2.0 6 1.0 23 1.0
2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0
3 4 2.0 9 1.0	342.091.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0
4 5 1.0 45 1.0 5 6 2 0 10 1 0	56201010	4 5 1.0 10 1.0 5 6 2 0 11 1 0	4 5 1.0 51 1.0 5 6 2 0 10 1 0	4 5 1.0 49 1.0 5 6 2 0 10 1 0
6 11 1.0	6 11 1.0	6 12 1.0	6 11 1.0	6 11 1.0
7 8 1.0 13 2.0 23 1.0	7 8 1.0 13 2.0 23 1.0	7 8 1.0 14 2.0 24 1.0	7 8 1.0 13 2.0 23 1.0	7 8 1.0 13 2.0 23 1.0
8 14 1.0 18 1.0	8 14 1.0 18 1.0	8 15 1.0 19 1.0	8 14 1.0 18 1.0	8 14 1.0 18 1.0
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12 23 1.0	12 25 1.0	13 24 1 0	12 25 1.0	12 23 1.0
14 15 2.0 16 1.0	14 15 2.0 16 1.0	13 24 1.0	14 15 2.0 16 1.0	14 15 2.0 16 1.0
15 17 1.0 25 1.0	15 17 1.0 25 1.0	15 16 2.0 17 1.0	15 17 1.0 25 1.0	15 17 1.0 25 1.0
16 26 2.0 27 1.0	16 26 2.0 27 1.0	16 18 1.0 26 1.0	16 26 2.0 27 1.0	16 26 2.0 27 1.0
17	17	17 27 2.0 28 1.0	17	17
18 19 2.0 20 1.0	18 19 2.0 20 1.0	18	18 19 2.0 20 1.0	18 19 2.0 20 1.0
19 21 1.0 24 1.0	19 21 1.0 24 1.0	19 20 2.0 21 1.0	19 21 1.0 24 1.0	19 21 1.0 24 1.0
20 22 2.0 34 1.0	20 22 2.0 34 1.0	20 22 1.0 25 1.0	20 22 2.0 33 1.0	20 22 2.0 55 1.0
22 24 1.0 37 1.0	22 24 1.0 37 1.0	22	22 24 1.0 36 1.0	22 24 1.0 36 1.0
23	23	23 25 1.0 37 1.0	23	23
24 44 1.0	24 43 1.0	24	24 41 1.0	24 41 1.0
25 26 1.0 45 1.0	25 26 1.0 44 1.0	25 42 1.0	25 26 1.0 42 1.0	25 26 1.0 42 1.0
26 30 1.0	26 30 1.0	26 27 1.0 43 1.0	26 30 1.0	26 30 1.0
27 28 2.0 42 1.0	27 28 2.0 42 1.0	27 31 1.0	27 28 2.0 40 1.0	27 28 2.0 40 1.0
29 30 2.0 32 1.0	29 30 2.0 32 1.0	29 30 1.0 51 1.0	29 30 2.0 31 1.0	29 30 2.0 31 1.0
30 33 1.0	30 33 1.0	30 31 2.0 32 1.0	30 32 1.0	30 32 1.0
31	31	31 33 1.0	31	31
32	32	32	32	32
33	33	33	33 34 2.0 37 1.0	33 34 2.0 37 1.0
34 35 2.0 38 1.0	34 35 2.0 38 1.0	34 35 2.0 38 1.0	34 35 1.0 49 1.0	34 35 1.0 50 1.0
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37 41 1 0	37 41 1 0	37 40 1 0	30 39 1.0	37
38	38	38	38	38
39	39	39	39	39
40	40	40	40	40
41	41	41	41 43 1.0 44 1.0 45 1.0	41 43 1.0 44 1.0 45 1.0
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1 2 2.0 3 1.0 32 1.0	1 2 2.0 3 1.0 30 1.0	1 2 2.0 3 1.0 30 1.0	1 2 2.0 6 1.0 43 1.0	1 2 2.0 6 1.0 41 1.0
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$\begin{array}{c} \textbf{7dj} \\ \hline 1 \ 2 \ 2 \ 0 \ 6 \ 1 \ 0 \ 4 \ 1 \ 1 \ 0 \\ 2 \ 3 \ 1 \ 0 \ 8 \ 1 \ 0 \\ 3 \ 4 \ 2 \ 0 \ 9 \ 1 \ 0 \\ 4 \ 5 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 0 \\ 6 \ 4 \ 2 \ 1 \ 0 \\ 1 \ 1 \ 0 \\ 1 \ 1 \ 1 \ 0 \\ 1 \ 1 \ 1 \ 0 \\ 1 \ 1 \ 1 \ 0 \\ 1 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \\ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 0 \ 1 \ 0 \ 0$	$\begin{array}{c} \textbf{7ej} \\ \hline 1 \ 2 \ 2.0 \ 6 \ 1.0 \ 41 \ 1.0 \\ 2 \ 3 \ 1.0 \ 8 \ 1.0 \\ 3 \ 4 \ 2.0 \ 9 \ 1.0 \\ 4 \ 5 \ 1.0 \ 10 \ 1.0 \\ 5 \ 6 \ 2.0 \ 11 \ 1.0 \\ 6 \ 42 \ 1.0 \\ 7 \ 8 \ 1.0 \ 12 \ 2.0 \ 41 \ 1.0 \\ 8 \ 13 \ 1.0 \ 12 \ 2.0 \ 41 \ 1.0 \\ 8 \ 13 \ 1.0 \ 12 \ 2.0 \ 41 \ 1.0 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \ 14 \ 2.0 \ 15 \ 1.0 \\ 14 \ 16 \ 1.0 \ 25 \ 1.0 \\ 15 \ 26 \ 2.0 \ 27 \ 1.0 \\ 16 \\ 17 \ 25 \ 1.0 \\ 18 \ 19 \ 2.0 \ 20 \ 1.0 \\ 19 \ 2.1 \ 0.2 \ 2.0 \ 31 \ 1.0 \\ 20 \ 22 \ 2.0 \ 33 \ 1.0 \\ 21 \\ 22 \ 4 \ 1.0 \ 36 \ 1.0 \\ 23 \ 24 \ 1.0 \\ 24 \\ 25 \ 26 \ 1.0 \\ 26 \ 30 \ 1.0 \\ 27 \ 28 \ 2.0 \ 40 \ 1.0 \\ 28 \ 29 \ 1.0 \ 48 \ 1.0 \\ 29 \ 30 \ 2.0 \ 31 \ 1.0 \\ 30 \ 32 \ 1.0 \\ 31 \\ 32 \\ 33 \ 34 \ 2.0 \ 37 \ 1.0 \end{array}$	$\begin{array}{c} \mathbf{7fj} \\ 1 \ 2 \ 2.0 \ 6 \ 1.0 \ 41 \ 1.0 \\ 2 \ 3 \ 1.0 \ 8 \ 1.0 \\ 3 \ 4 \ 2.0 \ 9 \ 1.0 \\ 4 \ 5 \ 1.0 \ 10 \ 1.0 \\ 5 \ 6 \ 2.0 \ 11 \ 1.0 \\ 6 \ 42 \ 1.0 \\ 7 \ 8 \ 1.0 \ 12 \ 2.0 \ 41 \ 1.0 \\ 8 \ 13 \ 1.0 \ 12 \ 2.0 \ 41 \ 1.0 \\ 8 \ 13 \ 1.0 \ 17 \ 1.0 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \ 14 \ 2.0 \ 15 \ 1.0 \\ 14 \ 16 \ 1.0 \ 23 \ 1.0 \\ 15 \ 24 \ 2.0 \ 25 \ 1.0 \\ 16 \\ 17 \ 18 \ 2.0 \ 19 \ 1.0 \\ 18 \ 20 \ 1.0 \ 22 \ 1.0 \\ 19 \ 21 \ 2.0 \ 32 \ 1.0 \\ 20 \\ 21 \ 22 \ 1.0 \ 35 \ 1.0 \\ 22 \ 48 \ 1.0 \\ 23 \ 24 \ 1.0 \ 49 \ 1.0 \\ 24 \ 81 \ 0 \\ 25 \ 26 \ 2.0 \ 40 \ 1.0 \\ 25 \ 26 \ 2.0 \ 40 \ 1.0 \\ 26 \ 27 \ 1.0 \ 29 \ 1.0 \\ 29 \ 30 \\ 31 \\ 32 \ 33 \ 2.0 \ 36 \ 1.0 \\ 33 \ 41 \ 0 \ 37 \ 1.0 \end{array}$	7gj 1 2 2.0 6 1.0 39 1.0 2 3 1.0 8 1.0 3 4 2.0 9 1.0 4 5 1.0 10 1.0 5 6 2.0 11 1.0 6 40 1.0 7 8 1.0 12 2.0 39 1.0 8 13 1.0 17 1.0 9 10 11 12 13 1.4 2.0 15 1.0 14 16 1.0 23 1.0 15 24 2.0 25 1.0 16 17 18 2.0 19 1.0 18 20 1.0 22 1.0 19 21 2.0 31 1.0 20 21 22 1.0 34 1.0 22 46 1.0 23 24 1.0 47 1.0 24 28 1.0 25 26 2.0 38 1.0 26 27 1.0 55 1.0 27 28 2.0 29 1.0 28 30 1.0 29 30 31 32 2.0 35 1.0 32 31 .0 54 1.0 33 34 2.0 36 1.0	

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69 70 2.0 76 1.0	68 87 1.0 90 1.0	68 87 1.0 90 1.0	
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Fig. S119 Plot of I₀/I vs. concentrations of compounds; Scatchard plot of log ([I₀-I]/I) vs. log [compound] for BSA in the presence of selected ligands.

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