Supporting Information

for

O₂ Chemistry of Dicopper Complexes with Alkyltriamine Ligands. Comparing Synergistic Effects on O₂ Binding

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1) Experimental Section

Materials and synthesis

Reagents and solvents used were of commercially available reagent quality unless otherwise stated. Solvents were purchased from SDS. Pentane and CH₂Cl₂ were distilled over CaH₂ under nitrogen. THF was distilled over Na/benzophenone under nitrogen.

Syntheses of ligands L1 and L2

Ligand L1

Ligand L1 was synthesized as previously described.¹

Ligand L2

Ligand L2 was synthesized in a three step synthetic method analogous to L1 summarized in figure 1.



Figure S1. Synthetic method used for L2 synthesis

SL2.

A solution of N,N-Dimethyldipropylenetriamine (3.6 mL, 20 mmol) in THF (40 mL) is cooled in an ice bath at 0°C and a solution of isopthalaldehyde (1.34 g, 10 mmols) in THF (20 mL) is added dropwise under vigorous stirring. The mixture is left to attain room temperature and it is stirred for further 5 hours. Then, the solvent is removed under reduced pressure and the resultant product is dried under vacuum to obtain 3.87 g (93 %) of a yellow oil corresponding to SL2. FT-IR: 2940 – 2723 (C-H_{sp3}), 1648 (C=N), 1460 (C=C_{arom}) cm⁻¹. ¹H-NMR (CDCl₃, 200 MHz, 298 K) δ, ppm: 8.31, 8.27, 7.75 – 7.64, 7.49 – 7.28, 3.98 – 3.90, 3.76 - 3.66, 3.33 - 3.09, 2.75 - 2.66, 2.35 - 2.28, 2.21 - 2.12, 1.92 -1.82, 1.66 – 1.52. ¹³C-NMR (CDCl₃, 50 MHz, 300 K) δ, ppm: 160.88, 142.97, 142.85, 142.56, 136.53, 129.49, 128.80, 127.40, 127.31, 127.00, 126.43, 126.02, 81.82, 81.63, 81.54, 67.89, 59.74, 58.03, 57.79, 57.68, 52.19, 52.09, 51.86, 51.74, 51.50, 48.38, 48.00, 45.62, 45.49, 45.37, 45.34, 28.07, 27.29, 26.84, 25.554, 24.78, 24.53. The assignation of the NMR spectra of SL2 is complicated due to the existence of an equilibrium between different isomers in solution as shown in Figure 2. ESI-MS (m/z): 417.0 (100) [M+H]⁺.



Figure S2. Solution equilibrium of the different isomers of SL2

HL2.

3.15 g of **SL2** (7.6 mmols) are dissolved in ethanol absolute (75 mL) and 1.14 g of NaBH₄ are slowly added to the stirred mixture directly as a solid. The mixture is stirred for 12 hours and then 10 mL of water are added to destroy the unreacted NaBH₄. The solvent is removed under reduced pressure and a mixture of a yellow oil and a white solid is obtained. This mixture is treated with 75 mL of CH₂Cl₂ and 20 mL of water and the aqueous phase is extracted with 2 x 40 mL of CH₂Cl₂. The organic layers are dried over MgSO₄ and the solvent is removed to dryness to give 3.13 g (98%) of a yellow oil. FT-IR: 3277 (N-H), 2935 – 2765 (C-H_{sp3}), 1460 (C=C_{arom}) cm⁻¹. ¹H-NMR (CDCl₃, 200 MHz, 300 K) δ , ppm: 7.28 – 7.21 (m, 4 H, Ar-H), 3.78 (s, 4H, ArCH₂), 2.73 – 2.62 (m, 12 H, N-CH₂), 2.31– 2.27 (m, 4 H, N-CH₂), 2.21 (s, 12 H, N-CH₃), 1.91 (br.s, 4 H, N-H), 1.75 – 1.63 (m, 8 H, C-CH₂-C). ¹³C-NMR (CDCl₃, 50 MHz, 300 K) δ , ppm: 140.57 (**arC**-CH₂), 128.34, 127.75, 126.56 (**arC**-H), 58.00, 54.01, 48.47, 47.95 (N-CH₂-C), 45.49 (N-(CH₃)₂), 30.30, 28.09 (C-CH₂-C). ESI-MS (m/z): 421.0 (100) [M+H]⁺.

L2.

2.5 g of L2 (5.9 mmols), HCHO (37%, 25 mL) and HCOOH (85%, 20 mL) are refluxed for 24 h. Then, the solution is cooled and the solvent is removed to obtain a residue which is made basic by the addition of an aqueous solution of NaOH 3M until pH > 14 (~ 25 mL). The resultant suspension is extracted with CH₂Cl₂ (3 x 50 mL), the organic phases are dried over MgSO₄ and the solvent is removed under reduced pressure. The product is dried under vacuum to give 2.09 g (98%) of a yellow oil. The product is purified over an alumina column chromatography using dichloromethane:methanol 9:1 as eluent to give 1.31 g of the pure product (46%). FT-IR: 2944 – 2762 (C-H_{sp3}), 1459 (C=C_{arom}) cm⁻¹. ¹H-NMR (CDCl₃, 200 MHz, 300 K) δ , ppm: 7.14 – 7.11 (m, 4 H, Ar-H), 3.39 (s, 4H, ArCH₂), 2.31 – 2.23 (m, 16H, N-CH₂-C), 2.15 – 2.12 (24 H, CH₃), 1.60 – 1.54 (m, 8H, C-CH₂-C). ¹³C-NMR (CDCl₃, 50 MHz, 300 K) δ , ppm: 138.98 (**arC**-CH₂), 129.68, 128.00, 127.59 (**arC**-H), 62.24 (Ar-CH₂), 57.92, 55.83, 55.78, 55.69 (N-CH₂-C), 45.46 (N-(CH₃)₂), 42.25, 42.16 (N-CH₃), 25.58, 25.26 (C-CH₂-C). ESI-MS (m/z): 477.2 (100) [M+H]⁺.

Syntheses of complexes.

[Cu¹₂(L1)](CF₃SO₃)₂ (1(CF₃SO₃)₂). A solution of Cu(CH₃CN)₄CF₃SO₃ (160 mg, 0.42 mmols) in THF (1.5 mL) is added dropwise to a stirred solution of L1 (117 mg, 0.21 mmols) in THF (1 mL). The reaction mixture is stirred for 1 hour to allow the complete precipitation of a fine solid which corresponds to 1(CF₃SO₃)₂. The solvent is decanted and the precipitate is dried under vacuum to yield 170 mg (82 %) of a pale-yellow powder. Anal. Calcd for $C_{36}H_{58}Cu_2F_6N_6O_6S_2$ (MW = 976.10 g/mol): C, 44.30; H, 5.99; N, 8.61; S, 6.57 %. Found: C, 44.25; H, 6.06; N, 8.90; S, 6.98 %. FT-IR: 2863 (C-H_{sp3}), 1475 (C=C_{arom}), 1247, 1222, 1151, 1026, 634 (CF₃SO₃) cm⁻¹.

[Cu¹₂(L1)](BArF)₂ (1(BArF)₂). To a vigorous stirred mixture of 1(CF₃SO₃)₂ (154 mg, 0.16 mmols) in CH₂Cl₂ (1.5 mL) is added a solution of NaBArF (279 mg, 0.31 mmols) in CH₂Cl₂. The mixture is stirred for 2 hours and then filtered through celite to remove the precipitated NaCF₃SO₃. The colorless filtrate is layered with pentane and after 5 days white crystals suitable for X-Ray analysis appear. The liquid is decanted and the crystalline material is dried under vacuum to yield 167 mg (44 %). Anal. Calcd for C₉₈H₈₂B₂Cu₂F₄₈N₆ (MW = 2404.38 g/mol): C, 48.95; H, 3.44; N, 3.50 %. Found: C, 49.20; H, 3.62; N, 3.40 %. FT-IR: 2857 (C-H_{sp3}), 1473 (C=C_{arom}), 1609, 1353, 1272, 1113, 901, 670 (BArF) cm⁻¹.

[Cu¹₂(L2)](CF₃SO₃)₂ (2(CF₃SO₃)₂). A solution of Cu(CH₃CN)₄CF₃SO₃ (157 mg, 0.42 mmols) in THF (1.5 mL) is added dropwise to a stirred solution of L2 (99.5 mg, 0.21 mmols) in THF (1 mL). The reaction mixture is stirred for 1 hour to allow the complete precipitation of a fine solid which corresponds to $2(CF_3SO_3)_2$. The solvent is decanted and the precipitate is dried under vacuum to yield 156 mg (83 %) of a pale-yellow powder. Anal. Calcd for $C_{30}H_{56}Cu_2F_6N_6O_6S_2$ ·2H₂O (MW = 938.05 g/mol): C, 38.41; H, 6.45; N, 8.96; S, 6.84 %. Found: C, 38.62; H, 6.65; N, 9.11; S, 6.81 %. FT-IR: 2976 - 2800 (C-H_{sp3}), 1471 (C=C_{arom}), 1254, 1224, 1143, 1027, 635 (CF₃SO₃) cm⁻¹.

[Cu¹₂(L2)](BArF)₂ (2(BArF)₂). To a vigorous stirred mixture of 2(CF₃SO₃)₂ (88 mg, 0.098 mmols) in CH₂Cl₂ (1.5 mL) is added a solution of NaBArF (173 mg, 0.20 mmols). The mixture is stirred for 2 hours and then filtered through celite to remove the precipitated NaCF₃SO₃. The colorless filtrate is layered with pentane and after 5 days pale-orange crystals appear. The liquid is decanted and the crystalline material is dried under vacuum to yield 197 mg (87 %). Anal. Calcd for C₉₂H₈₀B₂Cu₂F₄₈N₆ (MW = 2330.30 g/mol): C, 47.42; H, 3.46; N, 3.61 %. Found: C, 47.39; H, 3.69; N, 3.54 %. FT-IR: 2973 - 2869 (C-H_{sp3}), 1465 (C=C_{arom}), 1612, 1354, 1273, 1109, 884, 668 (BArF) cm⁻¹.

[Cu¹₂(L2)](SbF₆)₂ (2(SbF₆)₂). A solution of Cu(CH₃CN)₄SbF₆ (77.4 mg, 0.17 mmols) in THF (1 mL) is added dropwise to a stirred solution of L2 (39.8 mg, 0.08 mmols) in THF (1 mL). The reaction mixture is stirred for 1 hour to allow the complete precipitation of a fine white solid which corresponds to $2(SbF_6)_2$. The solvent is decanted, the precipitate is dried under vacuum and the compound is redissolved in CH₂Cl₂. Slow diethyl ether diffusion over this solution affords 64.5 mg of white crystals suitable for X-Ray analysis (72 %). Anal. Calcd for C₂₈H₅₆Cu₂F₁₂N₆Sb₂·H₂O (MW = 1111.41 g/mol): C, 30.26; H, 5.44; N, 7.56 %. Found: C, 30.21; H, 5.29; N, 7.12 %. FT-IR: 2975 - 2850 (C-H_{sp3}), 1464 (C=C_{arom}), 652 (SbF₆) cm⁻¹.

2) Crystal data for $1(BArF)_2$ and $2(SbF_6)_2$

| Compound | 1(BArF) ₂ | 2(SbF ₆) ₂ |
|-----------------------------------|---|---|
| Empirical formula | C98 H82 B2 Cu2 F48 N6 | C28 H56 Cu2 F12 N6 Sb2 |
| Formula weight | 2404.40 | 1075.37 |
| Temperature | 100(2) K | 100(2) K |
| Wavelength | 0.71073 Å | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic |
| Space group | P 21/n | P21/c |
| Unit cell dimensions | | |
| а | 13.073(5)Å | 16.264(4) Å |
| alpha | 90° | 90° |
| b | 27.978(12) Å | 15.169(4) Å |
| beta | 96.633(7)° | 103.776(4)° |
| С | 13.464 Å | 17.642(5) Å |
| gamma | 90° | 90° |
| Volume | 4891(3) Å ³ | 4227(2) Å ³ |
| Density (calculated) | 1.633 Mg/m ³ | 1.690 Mg/m ³ |
| Absorption coefficient | 0.578 mm ⁻¹ | 2.337 mm ⁻¹ |
| F(000) | 2424 | 2136 |
| Cell formula units_Z | 2 | 4 |
| Crystal size | 0.5 x 0.5 x 0.2 mm | 0.08 x 0.05 x 0.02 mm |
| Theta range for data collection | 2.42 to 27.97° | 2.04 to 28.34 ° |
| Limiting indices | -17<=h<=17, -36<=k<=36, - | -21<=h<=21, -20<=k<=20, - |
| | 17<=I<=17 | 23<=I<=23 |
| Reflections collected | 69618 | 62969 |
| Independent reflections | 11668 [R(int) = 0.0488] | 10415 [R(int)= 0.0351] |
| Completeness to theta | 99.1% (theta = 27.97°) | 98.7% (theta = 28.21°) |
| Refinement method | Full-matrix least-squares on F ² | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 11668 / 30 / 749 | 10415 / 0 / 587 |
| Goodness-of-fit on F ² | 1.163 | 1.076 |
| Final R indices [I>2sigma(I)] | R1 = 0.0510, wR2 = 0.1057 | R1 = 0.0305, wR2 = 0.0772 |
| R indices (all data) | R1 = 0.0716, wR2 = 0.1345 | R1 = 0.0370, wR2 = 0.0797 |
| Largest diff. peak and hole | 0.801 and -0.667 e.Å ⁻³ | 1.403 and -0.872 e.Å ⁻³ |

Table S1. Crystal data for $1(BArF)_2$ and $2(SbF_6)_2$

| 1(BArF) ₂ | 2(SbF ₆) ₂ |
|-----------------------|-----------------------------------|
| Cu1-N1 2.007 (3) | Cu1-N1 1.990 (3) |
| Cu1-N2 2.192 (2) | Cu1-N2 2.120 (3) |
| Cu1-N3 1.999 (3) | Cu1-N3 1.986 (3) |
| N1-Cu1-N2 100.98 (10) | Cu2-N4 1.974 (2) |
| N2-Cu1-N3 102.50 (10) | Cu2-N5 2.100 (3) |
| N3-Cu1-N1 156.52 (10) | Cu2-N6 1.973 (3) |
| | N1-Cu1-N2 105.59 (11) |
| | N2-Cu1-N3 105.08 (10) |
| | N3-Cu1-N1 148.84 (11) |
| | N4-Cu2-N5 104.95 (12) |
| | N5-Cu2-N6 104.34 (15) |
| | N4-Cu2-N6 150.62 (13) |

Table S2. Selected bond lengths (Å) and angles (°) for $1(BArF)_2$ and $2(SbF_6)_2$.

3) Stopped-flow kinetic measurements for the reaction of 2(BArF)₂ with O₂

Kinetic measurements were performed using a Hi-Tech Scientific (Salisbury, Wiltshire, UK) SF-43 multi-mixing anaerobic cryogenic stopped-flow instrument combined with a Hi-Tech Scientific Kinetascan diode array rapid scanning unit. All manipulations of the copper(I) complexes and their solutions were done inside a Vacuum Atmospheres or MBraun glove-box filled with argon. Copper(I) solutions of known concentration were placed in Hamilton gastight syringes and loaded into the stopped-flow mixing unit. Saturated solutions of O₂ in acetone (8 mM) were prepared by bubbling dry O₂ gas through argonsaturated acetone in a syringe at 293 K for 15 min. Solutions of O₂ with smaller concentrations were prepared by diluting the 8 mM O₂ solution with argonsaturated acetone using graduated gas-tight syringes. The solutions of copper(I) complex in acetone and O₂ in acetone were separately cooled to a low temperature (193-243 K) and mixed in a 1:1 volume ratio. The mixing cell (1 cm) was maintained to ± 0.1 K, and the mixing time was ~5-10 ms. Concentrations of all reagents are reported at the onset of the reaction (after mixing) and corrected for the 1:1 dilution. No correction for the temperature contraction of solvent was applied in this work. Dioxygen was always taken in large excess to the copper(I) complex. In all kinetic experiments, a series of 5 -7 shots gave standard deviations within 5%, with overall reproducibility within 10%. Data analysis was performed with the IS-2 Rapid Kinetics Software (Hi-Tech Scientific) for kinetic traces at a single wavelength or with the Specfit program (BioLogic Science Instruments, Grenoble, France) for global fitting of the spectral changes acquired in a diode array mode.



Figure S3. Eyring plot for the reaction of $2(BArF)_2$ with O_2 in a temperature range from -80°C to -50°C. $k_{ox} = k(obs)/[O_2]$, $[O_2] = 0.004$ M. $\Delta H^{\ddagger} = 9.5 \pm 2 \text{ kJ} \cdot \text{mol}^{-1}$, $\Delta S^{\ddagger} = -175 \pm 10 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$.



Figure S4. Variation of k(obs) with O_2 concentration (ranging from 0.00075 to 0.004 M) for the reaction of **2(BArF)**₂ with O_2 at -80°C. The plot shows a first order dependence in O_2 concentration.

4) Computational details

All geometry optimizations calculations have been performed at the B3LYP level,² using the standard 6-31G* basis set³ with the Gaussian03 package.⁴ The geometry optimizations were performed without any symmetry constraints, and the nature of the extrema was checked by analytical frequency calculations. The energies discussed throughout the text are electronic energies without any ZPE corrections.

Table S3. Main geometrical parameters of the DFT calculated structures

 (distances in Angstroms and angles in degrees)

| | $[Cu_2(\mu-\eta^2:\eta^2-O_2)(L1)]^{2+}$ | [Cu ₂ (µ-O) ₂ (L1)] ²⁺ | $[Cu_2(\mu-\eta^2:\eta^2-O_2)(L2)]^{2+}$ | $[Cu_2(\mu-O)_2(L2)]^{2+}$ |
|---------|--|---|--|----------------------------|
| Cu1…Cu2 | 3.603 | 2.810 | 3.636 | 2.831 |
| 01-02 | 1.443 | 2.230 | 1.438 | 2.227 |
| Cu1-N1 | 2.326 | 4.784 | 2.087 | 2.014 |
| Cu1-N2 | 2.026 | 2.008 | 2.044 | 2.001 |
| Cu1-N3 | 2.101 | 1.998 | 2.319 | 2.714 |
| Cu2-N4 | 3.303 | 3.647 | 2.430 | 4.500 |
| Cu2-N5 | 2.013 | 2.005 | 2.056 | 2.014 |
| Cu2-N6 | 2.016 | 2.011 | 2.029 | 1.998 |
| Cu1-O1 | 2.039 | 1.793 | 2.006 | 1.810 |
| Cu1-O2 | 1.892 | 1.794 | 1.938 | 1.805 |
| Cu2-O1 | 1.894 | 1.798 | 1.929 | 1.790 |
| Cu2-O2 | 1.942 | 1.789 | 1.978 | 1.800 |

Table S4. XYZ coordinates and energies of the calculated $[Cu_2(\mu-\eta^2:\eta^2-O_2)(L2)]^{2+}$ and $[Cu_2(\mu-O)_2(L2)]^{2+}$ isomers of **3**.

| [Cu | ₂ (μ-η ² :η ² -O ₂)(L | 2)] ²⁺ E=-48 | 59.722917 a. u. | [C | u ₂ (µ-O) ₂ (L2)] ²⁺ | E= -4859 | .7364318 a. u. |
|-----|--|-------------------------|-----------------|----|---|-------------|----------------|
| Cu | -1.83866600 | -0.49542700 | -0.09246600 | Cu | -0.45413000 | -1.52805100 | -0.23941200 |
| Cu | 1.79655500 | -0.49456700 | -0.16558000 | Cu | 2.11338500 | -0.37218900 | 0.05386700 |
| N | -2.48631400 | -2.08942600 | -1.27305400 | N | -1.32433700 | -2.26164400 | -1.88124900 |
| N | -2.90381800 | 1.49303200 | -0.62969600 | Ν | -4.31571800 | 0.63679400 | 0.58880200 |
| N | 3.05077200 | 1.54411300 | 0.25209600 | Ν | 1.44917400 | 2.23874000 | -0.27616000 |
| N | 2.81459500 | -1.34730600 | -1.69951300 | Ν | 3.67364800 | -0.47268100 | -1.21466800 |
| N | -2.89632800 | -0.87946900 | 1.61447200 | Ν | -1.77298500 | -2.07823600 | 1.18042300 |
| N | 2.55041700 | -1.50853900 | 1.45641700 | Ν | 3.08918800 | 0.08357900 | 1.74043300 |
| 0 | -0.05744600 | -0.45988200 | -0.85474700 | 0 | 0.61873500 | -0.78622900 | 0.98684900 |
| 0 | 0.03446800 | -0.17869000 | 0.55246500 | 0 | 1.04503600 | -1.16455900 | -1.16613600 |
| С | 2.70334200 | 1.78092700 | 1.68332400 | С | 0.83400600 | 2.43165400 | 1.05820200 |
| С | 3.16792100 | 0.70218900 | 2.67330900 | С | 1.79799600 | 2.29898800 | 2.24477400 |
| С | 2.43136400 | -0.64119800 | 2.67447100 | С | 2.20273000 | 0.88429900 | 2.66737400 |
| Н | 3.14714200 | 2.73745300 | 2.00440700 | Н | 0.35567600 | 3.42082000 | 1.11484600 |
| Н | 1.61707300 | 1.89632700 | 1.74248300 | Н | 0.04044800 | 1.68948500 | 1.16670400 |
| Н | 2.99112400 | 1.11843000 | 3.67319500 | Н | 1.27138200 | 2.70157300 | 3.11983000 |

| H 1.36105300 -0.45312200 2.80482900 H 1.3076300 0.27975400 2.81958800 C 4.17331500 -1.83444800 1.29021400 C 4.28845800 0.32652500 -0.854066800 C 4.2190420 -27249090 0.04353400 C 5.36671900 0.17496690 0.55407700 H 4.79864000 0.9552090 1.1350200 H 4.464913900 1.7816300 -1.04863000 H 4.50283900 -2.38593000 -2.13856400 H 5.66844400 0.03892200 -1.54864700 H 3.590670 -3.6122700 -0.1717400 H 5.62599800 -0.86118500 0.62378300 H 4.5359300 -2.261500 0.14747400 H 5.62599800 -0.86118500 0.62378300 H 4.5359300 -2.24725900 0.17174700 H 6.30732200 0.73203100 0.66225900 H 4.63569300 -2.247256900 2.11487500 H 4.35404700 0.25125100 H 4.4276100 0.14275100 H 4.437437400 0.788498500 2.233565100 H 4.319402600 2.247476700 0.62996600 C -3.6795100 0.873499900 1.39554100 C -3.16671800 2.24776700 0.62996600 C -3.6755740 -0.36721600 2.67334100 H 4.30564200 1.16245500 1.32657400 H -4.0220200 -0.16333000 2.934545100 H -4.30564200 1.16245500 1.39507700 C -3.21557400 -0.36721600 2.67394100 H -4.30564200 1.1624500 1.33507700 H -4.0220200 -1.39826200 2.7762400 H -3.2145100 0.254137600 0.94645300 H -1.5708860 -1.59998400 3.22265200 H -3.365130700 0.08614700 3.33704600 H -1.5708800 -1.59998400 3.22265200 H -3.3745100 3.56099100 0.3660500 H -2.81599900 1.52555720 1.734539400 C -3.8848400 2.53134500 -0.92924700 C -3.18355500 -3.37825200 -0.52514200 H -4.22173400 0.74514500 -0.9420400 C -3.18355500 -3.378258200 -0.52514200 C -3.35204100 -3.58480700 0.89021600 H -2.81599900 1.52555720 1.734239400 C -3.35204100 -3.58480700 0.89021600 H -2.8159900 -1.56595500 0.72497100 H -4.2072600 -3.5444000 0.57635900 H -2.2177761100 -2.64923300 0.71247100 H -4.2072600 -3.44164000 C -3.71635000 H -2.24923800 0.41674900 0.4168400 C -1.3525001 -7.5460800 -1.37119100 H -3.30434300 -0.45765100 H -2.24924800 0.57635900 H -2.24953800 0.42651000 H -4.26143300 0.11761900 -2.32645200 C -3.30643100 -1.476771000 -1.42805700 H -3.555500 -0.35648000 -3.5714900 H -2.24953800 H -2.29758400 -2.29758400 -2.29758400 -2.29758400 -2.29758400 -2.29758400 -2.29758400 -2.29758400 -2.29758 | Н | 4.25219800 | 0.56144100 | 2.62641000 | Н | 2.66887500 | 2.95152600 | 2.12996900 |
|--|--------|-------------|-------------------|--------------|--------|--------------|-------------|-------------|
| H 2.7665300 1.22603400 3.5429500 0.833900 3.6325600 C 4.1731500 1.83444800 -1.20074200 C 5.36671900 0.17496900 0.8430660 C 4.27984000 2.27429090 -1.15502200 H 4.464913900 1.761300 1.56480700 H 4.50289300 -2.1856400 H 6.68118500 0.82737300 H 5.62599800 -0.86118500 0.66259000 0.73935000 2.3578300 H 4.3546900 -2.7425600 1.41762800 H 4.20363300 1.81490100 1.37751800 H 4.3341600 0.37434000 2.41008300 C -1.87654400 -1.05336000 2.25386500 C -3.31671800 2.24778700 0.62896800 C -3.21557400 -0.3474600 3.9874900 3.9874900 3.9874900 3.2265200 H -3.0453100 0.26465300 H -1.023010 0.42643300 1.3387600 H -3.21557400 -0.3672300 0.3262200 <td< td=""><td>Н</td><td>1.36105300</td><td>-0.45312200</td><td>2.80482900</td><td>н</td><td>1.30736300</td><td>0.27975400</td><td>2.81958800</td></td<> | Н | 1.36105300 | -0.45312200 | 2.80482900 | н | 1.30736300 | 0.27975400 | 2.81958800 |
| C 4,17331500 1.83444800 1.29021400 C 4.8845800 0.32862500 0.85407700 C 3.93904000 2.03429400 1.29743200 C 4.6049000 0.738146000 1.9584770 H 78864000 0.93527000 -1.13856400 H 6.8614500 0.82378300 H 5.24275100 -0.17742500 H 6.30732200 0.73203100 0.66625900 H 4.3589300 -1.2061600 1.42755100 H 4.87437400 0.793203000 2.59382100 C -3.18431600 0.37474700 6.2269800 C -3.6722100 0.774200 6.2898600 C -3.91672300 1.49426100 1.72566300 C -3.6722100 0.8721600 2.4782400 H -4.1214700 0.74533000 2.9986700 H -3.04143300 2.9999400 3.38574600 H -2.21734100 0.75433000 2.99824700 1.43252800 -1.7262030 2.13857800 H -3.26137000 0.28663700 H <td>Н</td> <td>2.76635300</td> <td>-1.22603400</td> <td>3.54429500</td> <td>н</td> <td>2.73580900</td> <td>0.93938800</td> <td>3.62635600</td> | Н | 2.76635300 | -1.22603400 | 3.54429500 | н | 2.73580900 | 0.93938800 | 3.62635600 |
| C 4.21904200 -2.72490900 0.04353400 C 5.36671900 0.17496900 0.58407700 H 4.78684000 -0.95320900 -1.13502200 H 6.4913900 1.37613300 1.54684700 H 5.5267100 -3.61227900 -0.17174300 H 5.62599800 0.7320300 0.56625900 H 4.53589300 -1.2365000 1.4475700 H 4.6373200 0.7320310 0.66625900 H 4.53649600 2.47478700 0.62898600 C -3.8749900 2.59382100 2.32557400 -3.91671800 2.57394100 0.36625900 2.4778700 0.62898600 C -3.8749900 3.2857600 -3.91671800 2.27784100 1.72680300 C -3.21557400 -0.34662300 1.522857200 2.77624000 3.22857200 H -3.0414300 0.3605300 H -1.0230100 0.3665300 1.37088100 1.32285200 2.7752400 3.22857200 H -3.0453100 0.5826800 H -1.0230100 0.35257200 1.322285200 | С | 4.17331500 | -1.83444800 | -1.29021400 | С | 4.88845800 | 0.32652500 | -0.85406600 |
| C 3.93904000 -2.03429400 1.29743200 C 4.6049000 0.78146000 1.40683000 H 4.76864000 0.93502200 H 4.64913900 1.36164700 H 5.6559800 1.2074300 H 5.6559800 0.86118500 0.82378300 H 5.325700 0.17782800 H 4.20363300 1.73203100 0.36625900 H 4.33940600 0.274256900 2.11487500 H 4.87437400 0.73993600 2.59382100 C 3.16671800 2.24777700 0.62808800 C 3.67929100 0.8749900 1.86554100 C 3.91672300 1.49426100 1.72566300 C 3.67929100 0.8721600 2.1387400 H 4.90564200 1.15273000 2.49663300 H 4.3008100 3.839400 2.36557200 1.385564100 3.3874600 H -21731400 0.5454200 1.217510800 1.4338500 3.9265200 2.77751400 2.4353300 1.78423300 1.78423300 1.78423300 | С | 4.21904200 | -2.72490900 | -0.04353400 | С | 5.36671900 | 0.17496900 | 0.58407700 |
| H 4.79864000 0.95320900 -1.13502200 H 6.46413000 1.75713300 -1.76863000 H 4.65289300 -2.3856400 H 5.68844400 0.0382200 -1.54864700 H 4.53589300 -2.18765400 H 4.56589300 -2.18765400 -1.5586400 -1.6585000 2.274256900 2.1487500 H 4.87437400 0.79893600 2.3558610 2.25586500 C -3.67629100 0.27675400 2.5758400 2.25586500 C -3.67724100 0.27675400 2.57584100 1.72668030 C -3.876929100 0.37649900 3.857600 2.277624000 3.2557400 -3.77624000 3.22585200 2.277824000 3.22858200 2.277824000 3.22858200 2.27782400 3.22858200 2.277824000 3.22858200 2.27782400 3.22858200 2.77824000 3.22858200 2.27782400 3.22858200 2.77824000 3.22858200 2.77824000 3.22858200 2.27782400 3.22858200 2.27782400 3.22858200 2.21782400 3.22858200 2.21782400 3.22858200 | С | 3.93904000 | -2.03429400 | 1.29743200 | С | 4.40649000 | 0.78146000 | 1.60058300 |
| H 4.60283900 -2.38563000 -2.13856400 H 5.68844400 0.03822200 -1.54864700 H 5.24275100 -3.11344500 0.01782800 H 5.0289800 0.86625800 H 4.6358300 1.20601600 1.42755100 H 4.2035300 1.84940100 1.31751800 C -3.13431600 0.274256900 2.11487500 H 4.87437400 0.79893600 2.59382100 C -3.16471800 2.24776700 6.6289800 C -3.87629100 0.87949900 1.88554100 G -3.91672300 1.49426100 1.7256300 C -3.21557400 -0.36721600 2.67394100 H -4.90564200 1.16249500 1.39667300 H -1.1023010 -3.0662300 2.13857600 H -2.20183400 2.56998100 1.02616600 H -2.81599600 1.5325580 1.7353400 C -3.84484400 -2.3145700 C -2.1776100 2.61533300 1.178423300 C -3.84484400 -2.5663700 H -2.2185600 3.73784700 0.5226400 | н | 4.79864000 | -0.95320900 | -1.13502200 | н | 4.64913900 | 1.37613300 | -1.04863000 |
| H 3.59065700 -3.61227900 -0.17174300 H 5.62599800 -0.86118500 0.82378300 H 4.63589300 -1.20601600 1.42755100 H 4.20363300 1.81490100 2.5286500 C -3.13431600 0.274256900 2.11487500 H 4.87437400 0.78998000 2.25986500 C -3.16671800 2.24778700 0.62866800 C -3.6722100 0.87914900 2.25986500 H 4.90564200 1.64249500 1.35067700 H -3.04148300 -0.01450600 2.67384100 H -4.0220600 1.9992200 2.77524000 H -3.04148300 -0.3662300 2.13857600 H -3.6153000 0.75433000 2.80466300 H -1.15706800 1.33854100 H -2.214751100 2.5557200 0.36633300 H -3.73455100 3.2255200 H -3.21424900 0.57613900 H -3.2135500 2.48923800 0.22819910 C -4.187048040 1.38440300 C -3.13152300 2.28819910 0.452555720 H < | Н | 4.60283900 | -2.38593000 | -2.13856400 | н | 5.68844400 | 0.03892200 | -1.54864700 |
| H 5.24275100 -3.11344500 0.071782800 H 6.30732200 0.73203100 0.66625900 H 4.13840600 -2.74265900 2.11487500 H 4.2035300 1.8193600 2.329832100 C 3.16671800 2.24778700 0.68296800 C -3.87929100 0.87949900 1.89554100 C 3.91672300 1.44226100 1.72566300 C -3.87929100 0.87949900 1.89554100 H 4.90564200 1.16249500 1.39507700 H -4.0220600 -1.0929200 2.737624000 H -3.65130700 0.08614700 3.33704600 H -1.5708800 1.5998400 3.22265200 H -2.20133400 2.5698100 0.48208400 C -3.1635500 -3.37852300 -0.5251720 H -4.2100900 -3.21424900 0.48208400 C -3.1635500 -3.37852300 -0.52614200 C -4.2120400 -3.21424900 0.48208400 C -3.1635500 -3.7852300 -0.52614200 | н | 3.59065700 | -3.61227900 | -0.17174300 | н | 5.62599800 | -0.86118500 | 0.82378300 |
| H 4.63589300 -1.20601600 1.42755100 H 4.20363300 1.81490100 1.31751600 C -3.13431600 0.274266900 2.11487500 C -1.87664400 -1.05336000 2.59382100 C -3.16671800 2.24778700 0.62896800 C -3.61292100 0.87949900 1.89554100 C -3.16672300 1.49426100 1.72566300 C -3.61292100 0.01450600 2.67384100 H 4.01504200 1.69249500 1.39507700 H -4.01202000 -1.6992200 2.77524000 H -3.6131700 0.08614700 3.3704600 H -1.57008800 1.5998400 3.22255200 H -3.24531450 0.99264700 C 2.77761100 2.61533300 -1.78233040 C -4.19362200 -2.79730400 0.48204400 C -3.16335000 2.39828700 1.73533940 C -4.19362200 -2.3446400 -1.57018900 -3.31852300 0.72514200 C -4.2149800 -1.5719900 -3.31852300 0.7253300 1.78633800 H -4. | н | 5.24275100 | -3.11344500 | 0.01782800 | н | 6.30732200 | 0.73203100 | 0.66625900 |
| H 4.13940600 -2.74256900 L1487500 H 4.87437400 0.79893600 2.32596500 C -3.16671800 2.24778700 0.62896800 C -3.87029100 0.8794900 1.2955400 H -4.12105400 2.23117600 1.51233200 H -3.04148300 -0.01450600 3.6991900 H -4.12105400 2.23117600 3.52157400 -0.36721600 2.67394100 H -2.14731400 0.75433000 2.68463300 H -1.1023010 -3.0662300 2.13857600 H -3.65130700 0.08614700 3.33704600 H -1.5708800 1.5998400 3.22265200 H -3.20183400 2.56998100 1.02616600 H -2.81599600 1.5325580 1.73539400 C -3.18424400 -2.817970400 A42026400 -3.16533300 -1.17423300 1.78423300 C -4.21209900 -1.57184000 -3.3145200 -3.8484400 -2.8159800 -1.8763300 1.49227900 -3.7027800 -0.82743300 -8.65236300 -1.8263200 H -4.20279800 -3.27424800 < | Н | 4.63589300 | -1.20601600 | 1.42755100 | н | 4.20363300 | 1.81490100 | 1.31751600 |
| C -3.13431600 0.37434000 2.41005300 C -1.87605400 -1.05336000 2.32596500 C -3.3671800 2.24778700 0.62896800 C -3.36724900 2.87949900 2.67394100 H -4.12105400 2.2317600 2.51233200 H -3.04148300 -0.0165080 3.69919900 H -3.05130700 0.6814700 3.33704600 H -1.5708800 -1.59998400 2.25557200 H -3.25134500 0.99264700 C -2.77761100 -2.41533300 -1.57539400 C -3.8484400 -2.57130400 0.4208400 C -3.1352500 -1.7823300 C -4.19362200 -2.7794000 -1.5761900 H -3.03433300 -2.4823800 0.71237100 H -4.0729800 -3.21424900 0.5718300 H -3.03433300 -2.4823800 0.71237100 H -5.572300 -1.5761900 H -3.2088300 -2.8199100 H.35674100 -2.8199100 H -5.572300 | Н | 4.13940600 | -2.74256900 | 2.11487500 | Н | 4.87437400 | 0.79893600 | 2.59382100 |
| C -3.16671800 2.24778700 0.62896800 C -3.67292100 0.87949900 1.89554100 H -4.12105400 2.23117600 2.5123200 H -3.04148300 -0.01450800 3.6919900 H -4.0220200 -1.05998400 -2.07624000 H -4.0220200 -1.05998400 2.27652700 H -3.65130700 0.06614700 3.33704600 H -1.167088100 1.43485400 2.55557200 H -3.26133100 1.0603900 0.38603300 H -4.37088100 1.4348500 2.226153300 -1.5739400 C -3.16135500 -3.37852300 0.52514200 C -3.13152300 -1.7539400 H -4.02709800 -5.1783000 H -3.3088300 -2.99828700 0.52514200 H -4.52729800 -5.178300 H -3.2027800 -1.6548400 0.38941500 2.36653700 H -3.30267800 0.422200 H -4.52729800 -1.57480800 -3.37191000 H -2.28639200 -1.65955 | С | -3.13431600 | 0.37434000 | 2.41006300 | С | -1.87605400 | -1.05336000 | 2.32596500 |
| C -3.91672300 1.49426100 1.72566300 C -3.21557400 -0.36721600 2.67394100 H -4.90564200 1.16249500 1.39507700 H -3.04148300 -0.01450600 3.69919900 H -2.04731400 0.75433000 2.69466300 H -1.10220100 -0.30662300 2.77624000 H -3.65130700 0.08614700 3.33704600 H -1.57008800 -1.59998400 3.22265200 H -3.73453100 3.16003900 0.38603300 H -4.37088100 1.43485400 2.55557200 C -3.88484400 -2.53134500 -0.99264700 C -2.77761100 -2.6153300 -0.52514200 C -4.21200900 -1.56184400 1.36440300 C -3.13152300 -2.48923800 0.71237100 H -4.08724600 -3.44164000 -1.57619900 H -3.03433300 -3.19165800 -0.65236300 H -4.62143800 -1.8548400 0.15778300 H -3.3028300 -2.89928700 0.65236300 H -4.62143800 -1.8548400 0.9572800 H -3.63088300 -2.99828700 0.65236300 H -4.62143800 -1.354840700 0.89021600 H -2.56639200 -1.30267800 0.465236300 H -4.62143800 0.354840700 0.89021600 H -2.56639200 -1.306960 0.40561000 H -3.3628400 0.252149500 0.04416400 C -2.29828700 -1.48209700 0.4862100 C -1.13159500 4.63864300 0.01712100 C -1.05876300 4.15097000 -1.42507760 C -1.02432700 4.50415400 -0.57635900 C -3.32541300 4.04754900 0.84922100 C -1.02473100 3.19187400 -1.04064400 C -3.27545200 2.67327500 -0.65926200 C -1.034109600 3.34451800 -0.47493600 C -0.91215400 2.738666700 -1.4764700 C -2.18198000 2.40689600 -1.60261700 C -4.51691500 1.90366080 -1.34645500 C -2.18198000 2.40689600 -1.60261700 C -4.51691500 1.90366080 -0.34761400 D 0.253673300 0.2379400 0.41838800 H -0.21922900 4.72681700 -1.8548500 H -2.8450500 1.77699200 -2.43451500 C -0.4027700 0.56581200 -1.49645500 C -2.18198000 2.40689600 -0.63921000 H -3.68027700 0.50568000 -1.34645500 C -2.18198000 2.404890 0.30975400 H -2.4016400 5.8512920 -1.49323100 H -2.85566300 -1.6767300 0.25368900 -1.36486500 C -2.18198000 2.2068500 -0.6392000 H -4.33824700 4.54876100 -2.8548500 H -2.28438000 -2.28348100 C -2.38512900 -1.49261900 -2.9455300 C -2.18198000 2.26433200 -0.023493700 H -2.60532200 2.270707000 H -1.56545700 -2.26483400 -2.2848500 H -2.5666500 -0.3717000 -2.2455500 C -2.28453900 -2.8465200 -2.84766000 -2.276560 | С | -3.16671800 | 2.24778700 | 0.62896800 | С | -3.67929100 | 0.87949900 | 1.89554100 |
| H 4.12105400 2.51233200 H -3.04148300 -0.01450600 3.69919900 H -2.14731400 0.75433000 2.69466300 H -1.10230100 -0.30662300 2.13857600 H -3.073453100 3.16003900 0.36603300 H -1.5708800 -1.52998400 2.2265200 H -2.20183400 2.56998100 1.02616600 H -2.81599600 1.53255800 0.52557200 C -4.19362200 -2.79730400 0.4820400 C -3.16335500 -3.37852300 0.52514200 C -4.2100900 -1.56144000 1.37191000 H -3.03433300 -3.19165800 -2.68199100 H -4.02728000 -3.27424900 0.51783000 H -3.30433300 -3.19165800 -2.68199100 H -4.5572300 -1.56480800 -1.371100 H -3.3463100 -0.4273800 -1.82095700 1.4622100 C -1.13159500 -6.3846700 0.9526800 H -3.6563700 -1.66563500 0.44662100 C -1.13159500 -6.3846300 0.1771100 C | С | -3.91672300 | 1.49426100 | 1.72566300 | С | -3.21557400 | -0.36721600 | 2.67394100 |
| H -4.90564200 1.16249500 1.39507700 H -4.0220600 -1.0992200 2.77624000 H -3.65130700 0.08614700 3.33704600 H -1.10230100 0.30662300 2.13857600 H -3.73453100 3.6003900 0.38603300 H -4.37088100 1.43485400 2.2265200 H -2.20183400 2.56998100 1.02616600 H -2.81599600 1.53255800 1.73533400 C -4.1362200 -2.79730400 0.48208400 C -3.1633500 -3.37852300 -0.52514200 H -4.0273900 -3.21424900 0.51783000 H -3.03433300 -3.18165800 -2.86199100 H -5.20729800 -3.24424900 0.51783000 H -2.2078900 -1.627800 -0.65238300 H -4.527300 -1.5490500 0.89526800 H -3.6308300 -2.9828700 1.6429200 C -1.3159500 -0.3524000 0.45364300 0.1712100 C -2.28189600 4.7559700 -1.280 | Н | -4.12105400 | 2.23117600 | 2.51233200 | н | -3.04148300 | -0.01450600 | 3.69919900 |
| H -2.14731400 0.75433000 2.69466300 H -1.10230100 -0.3062300 2.13857600 H -3.73453100 3.16003900 0.33604300 H -1.57008800 1.5325800 1.73539400 C -2.20183400 2.56998100 1.02616600 H -2.81599600 1.5325800 1.73539400 C -4.19362200 -2.5730400 0.48208400 C -3.18335500 -3.3782300 0.71237100 H 4.08724600 -3.44164000 -1.57610900 H -3.03433300 -3.19165800 -2.68199100 H -6.52723800 -1.754980800 -1.37191000 H -3.03433400 -1.67700 -1.82095700 H -3.5524100 -3.58480700 0.89221800 0.95526800 H -3.66749500 -1.65595500 0.48962100 C -1.0315900 4.50415400 -0.57635900 C -3.27545202 2.67327500 -1.28007600 C -1.02432700 4.50415400 -0.57635900 C -3.38581300 4.04759700 -1.28007600 C -1.20432700 4.5217400 -0.5673500 <td>н</td> <td>-4.90564200</td> <td>1.16249500</td> <td>1.39507700</td> <td>н</td> <td>-4.02202600</td> <td>-1.09929200</td> <td>2.77624000</td> | н | -4.90564200 | 1.16249500 | 1.39507700 | н | -4.02202600 | -1.09929200 | 2.77624000 |
| H -3.85130700 0.08614700 3.33704600 H -1.57008800 -1.5999800 3.22265200 H -2.20183400 2.56998100 1.02616600 H -2.81589600 1.43485400 2.55557200 C -3.88484400 -2.53134500 -0.99264700 C -2.17761100 -2.61533300 -1.78423300 C -4.1200900 -1.56184400 1.38440300 C -3.1633500 -3.37852300 -0.52514200 H -4.0273900 -3.21424900 0.51783000 H -4.20273900 -3.70267800 -0.65238300 H -4.5272300 -1.37191000 H -3.3304400 -1.8709500 -1.82095700 H -3.55204100 -3.58480700 0.89021600 H -2.56639200 -1.6771000 -1.47209700 -1.4759700 -1.48209700 C -1.3159500 4.63864300 -0.01712100 C -2.2718600 -2.759500 -2.880700 -4.806700 -1.75952600 C -1.20432700 4.50415400 -0.5765200 C -3.0587300 H -2.5663920 -4.7599700 -1.48007700 <tr< td=""><td>Н</td><td>-2.14731400</td><td>0.75433000</td><td>2.69466300</td><td>н</td><td>-1.10230100</td><td>-0.30662300</td><td>2.13857600</td></tr<> | Н | -2.14731400 | 0.75433000 | 2.69466300 | н | -1.10230100 | -0.30662300 | 2.13857600 |
| H -3.73453100 3.16003900 0.38603300 H -4.37088100 1.4348400 2.5572200 H -2.8183400 -2.56998100 1.02616600 H -2.81599600 1.53255800 -1.75339400 C -4.19362200 -2.79730400 0.48208400 C -2.77761100 -2.61533300 -1.78423300 H -4.08724600 -3.41464000 -1.57619900 H -3.03433300 -3.19165800 -2.6193300 0.71237100 H -4.62143800 -1.3749800 2.36653700 H -3.6088300 -2.99828700 1.5425200 H -4.5572300 -1.75480800 -0.37526800 H -3.66749500 -1.6771000 -1.82095700 H -3.36843700 0.42221800 0.95526800 H -3.66749500 -1.6587500 0.4982100 C -1.120432700 4.5844300 0.01712100 C -1.05876300 4.15997000 -1.42807600 -1.82095700 C -1.20432700 4.5844300 0.055268200 C -2.9129600 4.15997000 -1.42807600 -1.82097600 -1.47507700 C </td <td>н</td> <td>-3.65130700</td> <td>0.08614700</td> <td>3.33704600</td> <td>н</td> <td>-1.57008800</td> <td>-1.59998400</td> <td>3.22265200</td> | н | -3.65130700 | 0.08614700 | 3.33704600 | н | -1.57008800 | -1.59998400 | 3.22265200 |
| H -2.20183400 2.5699100 1.02216600 H -2.81599600 1.5325800 1.73539400 C 3.8484400 -2.55134500 0.9224700 C 2.77761100 -2.8153300 -1.7823300 C 4.19362200 -2.79730400 0.48208400 C -3.13152300 -3.37852300 -0.52514200 H -4.221200900 -1.56184400 1.57619300 H -3.03433300 -3.19165800 -2.88199100 H -5.20729800 -3.2142400 0.5178300 H -4.2623700 -2.8623800 -3.6308300 -2.99828700 -0.65236300 H -4.52572300 -1.75480807 0.95226800 H -3.66749500 -1.8709700 -1.8209700 C -0.13524000 5.22149500 -0.04416400 C -2.29188600 -1.6771000 -1.8209700 -1.2807600 C -1.3159500 4.6384300 -0.01712100 C -3.0576300 4.5759260 -1.7579700 -1.2807600 C -2.7390500 2.78440800 -0.5425500 | Н | -3.73453100 | 3.16003900 | 0.38603300 | н | -4.37088100 | 1.43485400 | 2.55557200 |
| C -3.88484400 -2.5313400 -0.99264700 C -2.7761100 -2.6133300 -1.78423300 C -4.19362200 -2.79730400 0.48208400 C -3.16335500 -3.37852300 -0.5254200 H -4.08724600 -3.4416400 -1.57610900 H -3.03433300 -3.19165800 -2.68199100 H -4.62143800 -1.75480800 -1.37191000 H -3.63088300 -2.99828700 1.54623200 H -4.55572300 -1.75480800 -1.37191000 H -3.63088300 -2.99828700 1.54623200 H -4.89687000 -0.82921800 0.95526800 H -3.663084300 -1.67959700 -1.28007600 C -1.13159500 4.63864300 0.01712100 C -1.05876300 4.15097000 -1.2807700 C -1.20432700 4.50416400 0.37654500 C -3.38581300 4.04754900 -0.81294900 C -2.18198000 2.78440800 -0.47635500 C -3.38581300 4.04754900 -1.8229490 C -2.18198000 2.78440800 -0.6281700 C< | Н | -2.20183400 | 2.56998100 | 1.02616600 | н | -2.81599600 | 1.53255800 | 1.73539400 |
| C -4.19362200 -2.79730400 0.48208400 C -3.16335500 -3.3782300 -0.52514200 H -4.08724600 -3.44164000 -1.57610900 H -3.03433300 -2.48923800 0.71237100 H -4.02729800 -3.21424900 0.51783000 H -3.63083300 -2.9928707 0.56236300 H -4.55572300 -1.75480800 -1.37191000 H -3.3637400 -2.9928707 0.4523200 H -4.56572300 -1.5480800 -1.37191000 H -3.36749500 -1.66795500 0.4962100 C -0.13524000 5.22149500 -0.04416400 C -2.29189600 4.7599700 -1.82095700 C -1.02173100 3.19187400 -1.04064400 C -3.27545200 2.05366900 -1.4455500 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.48645500 C -2.18198000 2.40689600 -1.6021700 -4.51691500 1.9036600 -1.476490 | С | -3.88484400 | -2.53134500 | -0.99264700 | С | -2.77761100 | -2.61533300 | -1.78423300 |
| C -4.21200900 -1.56184400 1.38440300 C -3.13152300 -2.484923800 0.71237100 H -4.6274600 -3.44164000 -1.57610900 H -3.03433300 -3.19165800 -2.68199100 H -5.572300 -1.75480800 -1.3791000 H -3.63088300 -2.98282700 -0.65236300 H -3.55204100 -3.58480700 0.89021600 H -3.63088300 -2.98282700 -1.86595500 0.48967100 C -0.13524000 5.22149500 0.095526800 H -3.66749500 -1.65595500 0.48962100 C -1.20432700 4.50415400 -0.57635900 C -3.27545200 2.67327500 -0.5526200 C -1.20432700 4.50415400 -0.47493600 C -9.21215400 2.78666700 -1.19429200 C 2.73900500 2.78440800 -0.64622500 C 0.40627300 2.85312900 -1.48232100 H -2.8189600 1.77699700 -1.84645500 H -2.40146400 5.3812900 -1.4142020 C 2.73900500 2.78440800 -0.6390 | С | -4.19362200 | -2.79730400 | 0.48208400 | С | -3.16335500 | -3.37852300 | -0.52514200 |
| H -4.08724600 -3.44164000 -1.57610900 H -3.03433300 -3.19165800 -2.68199100 H -5.20729800 -3.21424900 0.51783000 H -4.20273900 -3.70267800 -0.65236300 H -4.55572300 -1.75480800 -1.37191000 H -3.34034400 -1.67771000 -1.82095700 H -3.55204100 -5.22149500 -0.95266800 H -3.66749500 -1.55595500 0.48962100 C -1.03524000 5.22149500 -0.04416400 C -2.29189600 4.17599700 -1.2807700 C -1.02432700 4.63864300 0.01712100 C -3.38581300 4.04754900 -0.5129400 C -1.02173100 3.9187400 -0.47635500 C -3.27645200 2.67327500 -0.55926200 C 2.73900500 2.78440800 -0.5422500 C 0.40627300 2.05366900 -1.34645500 C -2.18198000 2.40689600 -1.60261700 C -4.51691500 1.99360600 -0.4761400 H -2.28073300 6.23704400 0.30975400 H </td <td>С</td> <td>-4.21200900</td> <td>-1.56184400</td> <td>1.38440300</td> <td>С</td> <td>-3.13152300</td> <td>-2.48923800</td> <td>0.71237100</td> | С | -4.21200900 | -1.56184400 | 1.38440300 | С | -3.13152300 | -2.48923800 | 0.71237100 |
| H -5.20729800 -3.21424900 0.51783000 H -4.20273900 -3.70267800 -0.65236300 H -4.55572300 -1.75480800 -1.37191000 H -3.6308300 -2.9828700 1.56432200 H -4.55572300 -1.75480800 -1.37191000 H -3.6308300 -2.98683200 -3.0169600 -0.40561000 H -3.55204100 -3.28480700 0.05256800 H -3.66749500 -1.56595500 0.4892100 C -0.13524000 5.22149500 -0.04416400 C -2.29189600 4.77599700 -1.28007600 C -1.02173100 3.19187400 -1.04064400 C -3.37545200 2.67327500 -0.55926200 C -1.34109600 3.34451800 -0.47493600 C -0.91215400 2.05666700 -1.44645500 C -2.81198000 2.40689600 -1.60261700 C -4.51691500 1.90360600 -0.14761400 H -2.8273900 0.24843500 H -2.43854700 -1.4848500 H -2.8459600 3.1673900 -2.033243700 H -5.8623700 <td>Н</td> <td>-4.08724600</td> <td>-3.44164000</td> <td>-1.57610900</td> <td>Н</td> <td>-3.03433300</td> <td>-3.19165800</td> <td>-2.68199100</td> | Н | -4.08724600 | -3.44164000 | -1.57610900 | Н | -3.03433300 | -3.19165800 | -2.68199100 |
| H -4.62143800 -1.83941500 2.36653700 H -3.63088300 -2.99828700 1.54623200 H -3.55204100 -3.5480700 0.89021600 H -3.366749500 -1.82995700 0.43962100 H -3.3624000 -5.22149500 -0.9526800 H -3.66749500 -1.65595500 0.48962100 C -0.13524000 5.22149500 -0.04416400 C -2.29189600 4.77599700 -1.28007600 C -1.02173100 3.19187400 -0.57635900 C -3.38581300 4.04754900 -0.81294900 C -1.24132000 4.50415400 -0.57635900 C -0.91215400 2.78666700 -1.19429200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.4761400 H -2.6886100 -6.3370400 0.41838800 H -2.21922900 4.72681700 -1.85488500 H -2.8189600 1.7699200 -2.43451500 H -5.6867700 2.5820000 0.43131400 H -2.8666700 -1.65973700 2.29455300 H | Н | -5.20729800 | -3.21424900 | 0.51783000 | н | -4.20273900 | -3.70267800 | -0.65236300 |
| H -4.55572300 -1.75480800 -1.37191000 H -3.34034400 -1.67771000 -1.82095700 H -3.55204100 -3.58480700 0.89021600 H -2.58639200 -4.30169600 -0.48962100 C -0.13524000 5.22149500 -0.04116400 C -2.29189600 4.7559700 -1.28007600 C -1.3159500 4.63864300 0.01712100 C -1.05876300 4.15097000 -1.28007600 C -1.20432700 4.50415400 -0.57635900 C -3.38581300 4.04754900 -0.81294900 C -1.2173100 3.19187400 -1.04064400 C -3.327545200 2.67327500 -0.55926200 C 2.18198000 2.7846800 -0.47493600 C -0.91215400 2.0536600 -1.34645500 H -2.8373300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.4923100 H -2.92093600 3.11779900 -2.03293700 H -5.16963700 2.5820000 0.43131400 H -2.8637200 -1.06653200 C -2.03364400 | Н | -4.62143800 | -1.83941500 | 2.36653700 | н | -3.63088300 | -2.99828700 | 1.54623200 |
| H -3.55204100 -3.58480700 0.89021600 H -2.58639200 -4.30169600 -0.40561000 H -4.89687000 0.522149500 -0.04416400 C -2.2189600 4.77599700 -1.28007600 C -1.13159500 4.63864300 0.01712100 C -1.05876300 4.04754900 -0.81294900 C -1.20432700 4.50415400 -0.57635900 C -3.38581300 4.04754900 -0.5526200 C -1.34109600 3.34451800 -0.47493600 C -3.7545200 2.67327500 -0.5526200 C 2.73900500 2.78440800 -0.64622500 C -0.40627300 2.05366900 -1.4929200 C 2.18496000 -5.6021700 H -2.40146400 5.83512900 -1.49323100 H -2.8450600 -6.3902000 H -4.33824700 4.58476100 -0.65918100 H -2.2681600 2.63837200 -0.2605300 H -5.08123700 1.0564200 0.45760200 H -2.36566300 -2.7780800 -1.58807100 H -5.08123700 1.05668200 | Н | -4.55572300 | -1.75480800 | -1.37191000 | Н | -3.34034400 | -1.67771000 | -1.82095700 |
| H -4.89687000 -0.82921800 0.95526800 H -3.66749500 -1.56595500 0.48862100 C -0.13524000 5.22149500 -0.0416400 C -2.29189600 4.77599700 -1.28007600 C -1.2173100 3.19187400 -0.57635900 C -3.38581300 4.04754900 -0.81294900 C -1.02173100 3.19187400 -0.47493600 C -3.27545200 2.78666700 -1.19429200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.34645500 C -2.18198000 2.40688600 -1.60261700 C -4.51691500 1.90360600 -1.4761400 H -0.28373300 6.23704400 0.30975400 H -2.40146400 5.8312900 -1.48548500 H -2.18450600 4.96988200 -0.63902000 H -4.33824700 4.54876100 -0.65918100 H -2.84519600 1.7699200 -2.43451500 H -5.16963700 2.32757900 -2.2945500 C 0.25681600 2.5638700 -1.0605300 C | Н | -3.55204100 | -3.58480700 | 0.89021600 | Н | -2.58639200 | -4.30169600 | -0.40561000 |
| C -0.13524000 5.22149500 -0.04416400 C -2.29189600 4.77599700 -1.28007600 C 1.13159500 4.63864300 0.01712100 C -1.05876300 4.1509700 -1.47507700 C -1.24422700 4.50415400 -0.57635900 C -3.3581300 4.04754900 -0.81294900 C -1.24173100 3.19187400 -1.04064400 C -3.27545200 2.67327500 -0.55926200 C -1.34109600 2.34451800 -0.47493600 C -0.91215400 2.78666700 -1.34645500 C -2.18198000 2.78440800 -3.6425500 C -4.4616400 5.83512900 -1.4364500 H -0.28373300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.48548500 H -2.18450600 3.11573900 -2.00329300 H -5.16963700 2.5820000 0.43131400 H -2.85861600 2.64337200 -1.28349700 H -5.88123700 1.65074700 -1.05484600 | Н | -4.89687000 | -0.82921800 | 0.95526800 | н | -3.66749500 | -1.56595500 | 0.48962100 |
| C 1.13159500 4.63864300 0.01712100 C -1.05876300 4.15097000 -1.47507700 C -1.20432700 4.50415400 0.57635900 C -3.38581300 4.04754900 -0.55226200 C 1.34109600 3.19187400 -1.04064400 C -3.38581300 4.04754900 -0.55926200 C 2.73900500 2.78440800 -0.6422500 C 0.40627300 2.05366070 -1.19429200 C -2.18198000 2.40689600 -1.60261700 C -4.51691500 1.90360600 -0.474933100 H -0.6642100 5.20739400 0.41838800 H -0.2192290 4.72681700 -1.85488500 H -2.92093600 3.1573900 -2.03029300 H -5.16963700 2.58200000 0.43131400 H -1.85189600 1.77699200 -2.43451500 H -5.08123700 1.65074700 -1.05484600 C 0.25861600 2.63337200 -1.0065300 C -2.03364400 2.9658200 -0.55425500 H 3.44184400 3.57170800 0.23493700 H | C | -0.13524000 | 5.22149500 | -0.04416400 | C | -2.29189600 | 4.77599700 | -1.28007600 |
| C -1.20432700 4.50415400 -0.57635900 C -3.38581300 4.04754900 -0.81294900 C -1.02173100 3.19187400 -1.04064400 C -3.27545200 2.67327500 -0.55926200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.19429200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.4464500 H -0.28373300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.49323100 H -2.18450600 4.96988200 -0.63902000 H -4.33824700 4.54876100 -0.65918100 H -2.18450600 1.7699200 2.43451500 H -5.08123700 1.65074700 -1.05484600 C 0.25861600 2.63837200 -1.00605300 C 2.03364400 2.0326500 -0.75760200 H 2.97933100 2.54539600 -1.5807100 H 0.88082700 2.3275790 -2.9455300 H 2.97058400 -2.238181100 C 4.00714400 | C | 1.13159500 | 4.63864300 | 0.01712100 | C | -1.05876300 | 4.15097000 | -1.47507700 |
| C -1.02173100 3.19187400 -1.04064400 C -3.27545200 2.67327500 -0.55926200 C 1.34109600 3.34451800 -0.47493600 C -0.91215400 2.78666700 -1.19429200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.34645500 C -2.81198000 2.40689600 -1.60261700 C -4.51691500 1.90360600 -0.14761400 H -0.26373300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.49323100 H -2.18450600 4.96988200 -0.63902000 H -4.33824700 4.54876100 -0.65918100 H -2.82693600 3.11573900 -2.00329300 H -5.0812370 1.65074700 -1.05484600 C 0.25861600 2.65863200 0.75760200 L.3384400 3.57170800 -2.23818100 C -2.03364400 2.32757900 -2.29455300 H 2.497933100 2.54538000 -1.58807100 H 0.18679800 0.98441000 -1.39932000 H 2.497033100 | C | -1.20432700 | 4.50415400 | -0.57635900 | C | -3.38581300 | 4.04754900 | -0.81294900 |
| C 1.34109600 3.34451800 -0.47493600 C -0.91215400 2.78666700 -1.19429200 C 2.73900500 2.78440800 -0.54622500 C 0.40627300 2.05366900 -1.34645500 C -2.18198000 2.40689600 -1.60261700 C -4.51691500 1.90360600 -0.14761400 H -0.922373300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.49323100 H -2.18450600 4.96988200 -0.63902000 H -5.16963700 2.5820000 0.43131400 H -2.29293600 3.11573900 -2.00329300 H -5.16963700 2.58268200 -0.75760200 H -1.85189600 1.77699200 -2.43451500 H -5.08123700 1.65074700 -1.05484600 C 0.25861600 2.63837200 -1.00605300 C -2.03364400 2.03275790 -2.29455300 H 2.97933100 2.54539600 -1.5807100 H 0.19679800 0.98441000 -1.39922000 C 2.202161400 -2.48348000 -2.23818100 C | C | -1.021/3100 | 3.1918/400 | -1.04064400 | C | -3.27545200 | 2.67327500 | -0.55926200 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | 1.34109600 | 3.34451800 | -0.4/493600 | C | -0.91215400 | 2.78666700 | -1.19429200 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | 2.73900500 | 2.78440800 | -0.54622500 | C | 0.40627300 | 2.05366900 | -1.34645500 |
| H -0.2837300 6.23704400 0.30975400 H -2.40146400 5.83512900 -1.49323100 H 1.96642100 5.20739400 0.41838800 H -0.21922900 4.72681700 -1.85488500 H -2.18450600 4.96988200 -0.63902000 H -4.33824700 4.54876100 -0.65918100 H -2.29093600 3.11573900 -2.00329300 H -5.16963700 2.5820000 0.43131400 H -1.85189600 1.77699200 -2.43451500 H -5.08123700 1.65074700 -1.05484600 C 0.25861600 2.63837200 -1.00605300 C -2.03364400 2.06568200 -0.75760200 H 2.97933100 2.54539600 -1.58807100 H 0.19679800 0.98441000 -1.39932000 H 0.40707300 1.64343000 -2.23818100 C 4.00714400 -1.9261900 -2.29455300 C 2.02161400 -2.48348000 -2.23818100 C -1.18088300 -1.24630400 -2.97058400 H 2.55566300 -2.96411200 -3.08852900 H | C | -2.18198000 | 2.40689600 | -1.60261700 | C | -4.51691500 | 1.90360600 | -0.14/61400 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | н | -0.28373300 | 6.23704400 | 0.30975400 | н | -2.40146400 | 5.83512900 | -1.49323100 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | н | 1.96642100 | 5.20739400 | 0.41838800 | н | -0.21922900 | 4.72681700 | -1.85488500 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | н | -2.18450600 | 4.96988200 | -0.63902000 | н | -4.33824700 | 4.54876100 | -0.65918100 |
| H -1.8189600 1.77699200 -2.43451500 H -5.08123700 1.05074700 -1.05484600 C 0.25861600 2.63837200 -1.00605300 C -2.03364400 2.06568200 -0.75760200 H 3.44184400 3.57170800 -0.23493700 H 0.88082700 2.32757900 -2.29455300 H 2.97933100 2.54539600 -1.5807100 H 0.19679800 0.98441000 -1.39932000 H 0.40707300 1.64343000 -2.23818100 C 4.00714400 -1.92611900 -1.29264900 C -2.38033900 -1.71961900 -2.23806300 C -1.18088300 -1.24630400 -2.97058400 H 2.55566300 -2.96411200 -3.06852900 H 4.78667400 -2.09171300 -2.04553000 H 1.83777600 -3.22944200 -1.46390800 H 4.36976400 -2.20959600 -0.33104000 H -2.60532200 -2.58043200 -3.35219600 H -1.59253700 -1.65173300 -3.90190500 H 1.06493400 -2.10876500 -2.60208800 H <td></td> <td>-2.92093600</td> <td>3.115/3900</td> <td>-2.00329300</td> <td></td> <td>-5.16963700</td> <td>2.58200000</td> <td>0.43131400</td> | | -2.92093600 | 3.115/3900 | -2.00329300 | | -5.16963700 | 2.58200000 | 0.43131400 |
| C0.258616002.63837200-1.00003300C-2.03844002.00586200-0.7760200H3.441844003.57170800-0.23493700H0.880827002.32757900-2.29455300H2.979331002.54539600-1.58807100H0.196798000.98441000-1.39932000H0.407073001.64343000-1.40903400H-1.937037001.00076300-0.55425500C2.02161400-2.48348000-2.23818100C4.00714400-1.92611900-1.29264900C-2.38033900-1.71961900-2.70806300C-1.18088300-1.24630400-2.97058400H2.55566300-2.96411200-3.06852900H4.78667400-2.9097600-0.33104000H-3.08374400-0.91979700-2.94092900H-1.72767600-0.34022300-2.70070000H-3.08374400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.91888100H-0.12804800-1.00776300-3.10323700C2.97636700-0.36302200-2.80576600C3.2333300-0.02625500-2.56941900H3.580471000.4793070-2.47002400H2.36588200-0.60797800-2.87470100H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.4855 | | -1.85189600 | 1.77699200 | -2.43451500 | | -5.08123700 | 1.05074700 | -1.05484600 |
| H3.441644003.57170800-0.23493700H0.080827002.32737900-2.29435300H2.979331002.54539600-1.58807100H0.196798000.98441000-1.39932000H0.407073001.64343000-1.40903400H-1.937037001.00076300-0.55425500C2.02161400-2.48348000-2.23818100C4.00714400-1.92611900-1.29264900C-2.38033900-1.71961900-2.70806300C-1.18088300-1.24630400-2.97058400H2.55566300-2.96411200-3.06852900H4.78667400-2.90171300-2.04553000H1.83777600-3.22944200-1.46390800H4.36976400-2.29059600-0.33104000H-3.08374400-0.91979700-2.94092900H-1.72767600-0.34022300-2.70070000H-2.60532200-2.58043200-3.35219600H-1.59253700-1.65173300-3.90190500H1.06493400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.91888100H-0.12804800-1.00776300-3.10323700C2.97636700-0.3632200-2.47002400H2.966655001.03010200-2.53347800H3.46896800-0.82835500-3.66958100H4.05010100-0.1717400-3.28601600H1.993890000.00361900-3.1143800H2.36588200-0.60797800-2. | | 0.20001000 | 2.03037200 | -1.000000000 | | -2.03304400 | 2.00000200 | -0.75760200 |
| H2.979331002.3433900-1.38807100H0.196730000.9441000-1.3932000H0.407073001.64343000-1.40903400H-1.937037001.00076300-0.55425500C2.02161400-2.48348000-2.23818100C4.00714400-1.92611900-1.29264900C-2.38033900-1.71961900-2.70806300C-1.18088300-1.24630400-2.97058400H2.55566300-2.96411200-3.06852900H4.78667400-2.09171300-2.04553000H1.83777600-3.22944200-1.46390800H4.36976400-2.29059600-0.33104000H-3.08374400-0.91979700-2.94092900H-1.72767600-0.34022300-2.70707000H-2.60532200-2.58043200-3.35219600H-1.59253700-1.65173300-3.90190500H1.06493400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.80576600C3.2333000-0.02625500-2.56941900H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.4785900H-1.5945700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200 | | 3.44104400 | 3.5/1/0600 | -0.23493700 | | 0.00002700 | 2.32/3/900 | -2.2940000 |
| H0.407073001.04343000-1.40903400H-1.937037001.00070300-0.53423300C2.02161400-2.48348000-2.23818100C4.00714400-1.92611900-1.29264900C-2.38033900-1.71961900-2.70806300C-1.18088300-1.24630400-2.97058400H2.55566300-2.96411200-3.06852900H4.78667400-2.209171300-2.04553000H1.83777600-3.22944200-1.46390800H4.36976400-2.29059600-0.33104000H-3.08374400-0.91979700-2.94092900H-1.72767600-0.34022300-2.70070000H-2.60532200-2.58043200-3.35219600H-1.59253700-1.65173300-3.90190500H1.06493400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.91888100H-0.12804800-1.00776300-3.10323700C2.97636700-0.36302200-2.80576600C3.2333000-0.02625500-2.56941900H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.8455900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.8355500H0.52585100-3.19455400 <td></td> <td>2.97933100</td> <td>2.34339000</td> <td>-1.30007100</td> <td></td> <td>0.19079000</td> <td>0.96441000</td> <td>-1.39932000</td> | | 2.97933100 | 2.34339000 | -1.30007100 | | 0.19079000 | 0.96441000 | -1.39932000 |
| C2.02101400-2.48348000-2.23818100C4.00714400-1.92011900-1.23204900C-2.38033900-1.71961900-2.70806300C-1.18088300-1.24630400-2.97058400H2.55566300-2.96411200-3.06852900H4.78667400-2.09171300-2.04553000H1.83777600-3.22944200-1.46390800H4.36976400-2.29059600-0.33104000H-3.08374400-0.91979700-2.94092900H-1.72767600-0.34022300-2.70070000H-2.60532200-2.58043200-3.35219600H-1.59253700-1.65173300-3.90190500H1.06493400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.91888100H-0.12804800-1.00776300-3.10323700C2.97636700-0.36302200-2.80576600C3.23333000-0.02625500-2.56941900H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.87470100C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-0.53868600-2.88652400-1.23291900H0.52585100-3.194554 | | 2 02161400 | 2 4 9 2 4 9 0 0 0 | 2 22212100 | | -1.93703700 | 1.00070300 | 1 20264000 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Č | 2.02101400 | 1 71061000 | 2 70806300 | | 4.007 14400 | 1 24630400 | 2 07059400 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | ц | 2 55566300 | 2 06/11200 | 3 06852000 | | -1.10000300 | 2 00171300 | 2.97050400 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | и Ц | 2.33300300 | 3 220//200 | 1 46300800 | | 4.76007400 | 2 20050600 | -2.04333000 |
| H-3.06374400-0.91979700-2.34092900H-1.72707000-0.34022300-2.70070000H-2.60532200-2.58043200-3.35219600H-1.59253700-1.65173300-3.90190500H1.06493400-2.10876500-2.60208800H3.10810700-2.47626000-1.56912000H-1.36721500-1.37124000-2.91888100H-0.12804800-1.00776300-3.10323700C2.97636700-0.36302200-2.80576600C3.23333000-0.02625500-2.56941900H3.580471000.47930700-2.47002400H2.966655001.03010200-2.53347800H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.87470100C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.8130200-0.60222700 | и Ц | 3 08374400 | 0.01070700 | 2 04002000 | н Ц | 1 72767600 | -2.23033000 | 2 70070000 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | н | -2 60532200 | -2 580/3200 | -2.3+032300 | н | -1.50253700 | -0.5+022500 | -2.70070000 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | н | 1 06493400 | -2.000+0200 | -2 60208800 | н | 3 10810700 | -2 47626000 | -0.50150500 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | н | -1 36721500 | -1 37124000 | -2.00200000 | н | -0 12804800 | -2.47020000 | -3 10323700 |
| H3.580471000.47930700-2.47002400H2.966655001.03010200-2.53347800H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.87470100C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.69555300H-0.85965100-3.85391400-3.21957300H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.38130200-0.60222700 | C | 2 97636700 | -0.36302200 | -2.81576600 | Ċ | 3 23333000 | -0.02625500 | -2 56941900 |
| H3.46896800-0.82835500-3.66958100H4.05010100-0.17174000-3.28601600H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.87470100C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.69555300H-0.85965100-3.85391400-3.21957300H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.38130200-0.60222700 | н | 3.58047100 | 0.47930700 | -2.47002400 | н | 2.96665500 | 1.03010200 | -2.53347800 |
| H1.993890000.00361900-3.11143800H2.36588200-0.60797800-2.87470100C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.69555300H-0.85965100-3.85391400-3.21957300H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.38130200-0.60222700 | н | 3 46896800 | -0.82835500 | -3 66958100 | н | 4 05010100 | -0 17174000 | -3 28601600 |
| C-1.55458700-3.22166500-1.03708300C-0.52666600-3.47008300-2.24855900H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.69555300H-0.85965100-3.85391400-3.21957300H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.38130200-0.60222700 | H | 1,99389000 | 0.00361900 | -3.11143800 | н | 2.36588200 | -0.60797800 | -2.87470100 |
| H-1.61371600-3.56314700-0.00344400H-0.65737200-4.25380200-1.50017600H-1.79847000-4.06688900-1.69555300H-0.85965100-3.85391400-3.21957300H-0.53868600-2.88652400-1.23291900H0.52585100-3.19455400-2.30359700C-4.201443001.18966500-1.28358500C2.323560003.38130200-0.60222700 | C | -1.55458700 | -3.22166500 | -1.03708300 | C | -0.526666600 | -3.47008300 | -2.24855900 |
| H -1.79847000 -4.06688900 -1.69555300 H -0.85965100 -3.85391400 -3.21957300 H -0.53868600 -2.88652400 -1.23291900 H 0.52585100 -3.19455400 -2.30359700 C -4.20144300 1.18966500 -1.28358500 C 2.32356000 3.38130200 -0.60222700 | Ĥ | -1.61371600 | -3.56314700 | -0.00344400 | Ĥ | -0.65737200 | -4.25380200 | -1.50017600 |
| H -0.53868600 -2.88652400 -1.23291900 H 0.52585100 -3.19455400 -2.30359700 C -4.20144300 1.18966500 -1.28358500 C 2.32356000 3.38130200 -0.60222700 | H | -1.79847000 | -4.06688900 | -1.69555300 | H | -0.85965100 | -3.85391400 | -3.21957300 |
| C -4.20144300 1.18966500 -1.28358500 C 2.32356000 3.38130200 -0.60222700 | H | -0.53868600 | -2.88652400 | -1.23291900 | H | 0.52585100 | -3.19455400 | -2.30359700 |
| | С | -4.20144300 | 1.18966500 | -1.28358500 | С | 2.32356000 | 3.38130200 | -0.60222700 |

| Н | -4.02506000 | 0.80654600 | -2.29094400 | Н | 1.78802200 | 4.34249800 | -0.58496400 |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Н | -4.76399800 | 0.44417400 | -0.72205400 | Н | 3.14986700 | 3.45378100 | 0.10993000 |
| Н | -4.82300500 | 2.09279600 | -1.37366900 | н | 2.75403500 | 3.24880400 | -1.59935400 |
| С | -2.05002400 | -1.75312700 | 2.47132300 | С | 3.29397000 | -1.24814500 | 2.38862400 |
| Н | -1.82149100 | -2.68972000 | 1.96248900 | н | 3.94642200 | -1.87603400 | 1.78159000 |
| Н | -1.11657300 | -1.23640100 | 2.69439400 | н | 3.75349300 | -1.11961300 | 3.37550400 |
| Н | -2.56466400 | -1.98468800 | 3.41346900 | н | 2.32647800 | -1.73661800 | 2.49719500 |
| С | 1.63577200 | -2.66370400 | 1.65779800 | С | -1.03284200 | -3.26879300 | 1.70717000 |
| Н | 0.61172400 | -2.30159100 | 1.71597400 | н | -0.07012600 | -2.94188600 | 2.09917300 |
| Н | 1.71198900 | -3.36115900 | 0.82260300 | н | -1.61028300 | -3.75058900 | 2.50441300 |
| Н | 1.88916100 | -3.20342200 | 2.58080500 | н | -0.86292000 | -4.00058900 | 0.91425900 |
| С | 4.52492100 | 1.41616300 | 0.12751600 | С | -5.64716400 | 0.02897900 | 0.76310100 |
| Н | 4.89215200 | 0.49719600 | 0.57702800 | н | -6.09182500 | -0.16921600 | -0.21685700 |
| Н | 4.80894900 | 1.41944900 | -0.92752100 | н | -5.58349300 | -0.92016000 | 1.30143800 |
| Н | 5.03894800 | 2.26112900 | 0.61007000 | Н | -6.33350000 | 0.68536400 | 1.32468700 |

Table S5. XYZ coordinates and energies of calculated $[Cu_2(\mu-\eta^2:\eta^2-O_2)(L1)]^{2+}$ and $[Cu_2(\mu-O)_2(L1)]^{2+}$.

| l | [Cu ₂ | (μ-η²:η²-O ₂)(L | 1)] ²⁺ E=-5089 |).5483291 a. u. | [0 | Cu ₂ (µ-O) ₂ (L1)] ² | + | E=-5089 | .5736771 a.u. |
|---|------------------|-----------------------------|---------------------------|-----------------|----|---|------|----------|---------------|
| | Cu | 1.93580400 | 0.13140800 | -0.44666700 | Cu | 0.20425900 | 1.4 | 0349100 | -0.20233000 |
| | Cu | -1.53188500 | -0.83884500 | -0.31027700 | Cu | -0.43246500 | -1.3 | 32597200 | -0.00479400 |
| | Ν | 2.85285600 | -2.00102400 | -0.30171400 | Ν | 4.37282000 | -0.5 | 7710000 | -1.46150500 |
| | Ν | 2.42186700 | 1.55052200 | 1.02396500 | Ν | 0.36792000 | 2.7 | 4434400 | 1.26946000 |
| | Ν | -3.54470800 | 1.76856900 | -0.55278900 | Ν | -4.06942000 | -1.1 | 4412000 | -0.20583900 |
| | Ν | -2.64483800 | -1.56608100 | 1.20572500 | Ν | -0.26834900 | -2.5 | 57561300 | 1.56268800 |
| | Ν | 3.01003300 | 0.76824100 | -2.04259900 | Ν | 0.85771400 | 2.4 | 7565500 | -1.76909000 |
| | Ν | -2.46837400 | -1.36798400 | -2.01226500 | Ν | -0.88339800 | -2.6 | 3615300 | -1.45400800 |
| | 0 | 0.26266100 | -0.38129600 | 0.27367300 | 0 | 0.00584700 | 0.0 | 8771100 | 1.00067900 |
| | 0 | 0.05027800 | -0.21327700 | -1.14336900 | 0 | -0.21532900 | -0.0 | 1501600 | -1.21581500 |
| | С | -2.94766600 | 2.01954700 | -1.88502500 | С | -3.83416200 | -0.7 | 7326100 | -1.61693400 |
| | С | -3.21676600 | 0.97209300 | -2.98229100 | С | -3.18250900 | -1.8 | 2915400 | -2.52893900 |
| | С | -2.36863600 | -0.30465700 | -3.07566100 | С | -1.65536800 | -1.9 | 8718900 | -2.59179700 |
| | Н | -3.32496300 | 2.98323100 | -2.27347800 | Н | -4.79836800 | -0.5 | 0551300 | -2.08853700 |
| | Н | -1.86686400 | 2.13803200 | -1.74690000 | Н | -3.21819300 | 0.1 | 3219600 | -1.62050800 |
| | Н | -2.99754300 | 1.48160500 | -3.92978900 | Н | -3.42329100 | -1.5 | 1015400 | -3.55177100 |
| | Н | -4.28285700 | 0.73926200 | -3.05119600 | Н | -3.68011600 | -2.7 | 9855100 | -2.43453300 |
| | Н | -1.31155500 | -0.02911900 | -3.11994700 | Н | -1.18867200 | -1.0 | 1335500 | -2.74505100 |
| | Н | -2.61791200 | -0.78802900 | -4.03187900 | Н | -1.43854000 | -2.6 | 0474400 | -3.47343500 |
| | С | -4.02839100 | -1.88747400 | 0.70821000 | С | -1.13832200 | -3.7 | 9607600 | 1.44941900 |
| | С | -4.10259200 | -2.69516900 | -0.59097700 | С | -0.98484400 | -4.6 | 60647800 | 0.16731800 |
| | С | -3.86621500 | -1.86673900 | -1.85666200 | С | -1.57111100 | -3.8 | 9853900 | -1.04597400 |
| | Н | -4.54024700 | -0.93325600 | 0.56179100 | Н | -2.17405400 | -3.4 | 5252200 | 1.53641900 |
| | Н | -4.55908800 | -2.41814000 | 1.50946800 | Н | -0.92881100 | -4.4 | 2989800 | 2.32013900 |
| | Н | -3.45653600 | -3.57991300 | -0.55714200 | Н | 0.04383700 | -4.9 | 4075600 | 0.00269100 |
| | Н | -5.12260700 | -3.09094900 | -0.66213200 | Н | -1.56586900 | -5.5 | 52623500 | 0.30381000 |
| | Н | -4.52961900 | -1.00343800 | -1.83338600 | Н | -2.60314700 | -3.6 | 3970600 | -0.81996100 |
| | Н | -4.13036400 | -2.45428200 | -2.74725900 | Н | -1.57590100 | -4.5 | 7051700 | -1.91491100 |
| | С | 3.15416300 | 2.26352600 | -1.99801700 | С | 0.78237800 | 3.9 | 6478400 | -1.60369200 |
| | С | 2.81497500 | 2.87603300 | 0.46208500 | С | 0.45106500 | 4.1 | 9031500 | 0.88480000 |
| | С | 3.77077900 | 2.84036200 | -0.72477200 | С | 1.35579800 | 4.5 | 0059300 | -0.29863700 |
| | Н | 4.02130300 | 3.88443800 | -0.94808800 | Н | 1.40281900 | 5.5 | 9199800 | -0.38890600 |
| | Н | 4.72625700 | 2.36889400 | -0.47546400 | Н | 2.38833000 | 4.1 | 7483900 | -0.13602400 |
| | Н | 2.15254500 | 2.68634500 | -2.13084800 | Н | -0.27321600 | 4.2 | 4611400 | -1.67664900 |
| | Н | 3.74946700 | 2.56672700 | -2.87067700 | Н | 1.29833900 | 4.4 | 1521800 | -2.46091900 |
| | Н | 3.25358300 | 3.48206800 | 1.26855900 | Н | 0.77186900 | 4.7 | 4773700 | 1.77396400 |
| | Н | 1.90003400 | 3.37956500 | 0.14675600 | Н | -0.55913300 | 4.5 | 1739400 | 0.63600000 |
| | С | 4.26444600 | -2.00991400 | -0.79804400 | С | 4.10050500 | 0.3 | 3202700 | -2.57785700 |
| | С | 4.51257300 | -1.33865300 | -2.15020700 | С | 2.62115300 | 0.7 | 8878700 | -2.66241400 |

| C 4.38796600 | 0.18333100 | -2.17157900 | С | 2.32265700 | 2.06956900 | -1.87709800 |
|-------------------|------------|-------------|-----|--------------|-------------|-------------|
| H 4.61670500 - | 3.05183800 | -0.85513500 | Н | 4.31225800 | -0.21897300 | -3.49824000 |
| H 5.55902800 - | 1.55021700 | -2.40299500 | Н | 2.37945700 | 0.96152600 | -3.71675600 |
| H 4.81806400 | 0.56506300 | -3.10870800 | Н | 2.85910700 | 2.90450900 | -2.34591700 |
| H 4.87918300 - | 1.50991200 | -0.04123900 | Н | 4.77764100 | 1.20478900 | -2.59092800 |
| H 3.93559000 - | 1.80418200 | -2.95474600 | Н | 1.99232900 | -0.02816600 | -2.30339900 |
| H 4.99365600 | 0.58720400 | -1.35763200 | Н | 2.69752000 | 1.98792300 | -0.85417200 |
| C -0.63011000 | 5.01008500 | 1.93058300 | С | -4.13813700 | 3.71198800 | 0.59020800 |
| C -1.78354600 | 4.63954500 | 1.24511500 | С | -4.72453300 | 2.48186900 | 0.28463400 |
| C 0.35728800 | 4.06067000 | 2.18608200 | С | -2.88688700 | 3.76004300 | 1.20441100 |
| C 0.22328900 | 2.74254500 | 1.72449400 | С | -2.18943900 | 2.57195500 | 1.48349600 |
| C -1.97022900 | 3.31612300 | 0.82005400 | С | -4.07667900 | 1.28376100 | 0.60913600 |
| C -3.35452100 | 2.95947300 | 0.30804100 | С | -4.79973000 | -0.03996500 | 0.46596600 |
| C 1.31987700 | 1.74923100 | 2.06018300 | С | -0.84650700 | 2.56778800 | 2.18093000 |
| H -0.50833900 | 6.03069500 | 2.28038700 | Ĥ | -4.67110800 | 4.63337600 | 0.37596000 |
| H -2.56403200 | 5.37575200 | 1.06917700 | н | -5.71092800 | 2.45590200 | -0.17114900 |
| H 1.23973900 | 4.34673900 | 2,75269200 | H | -2.48046700 | 4,72284800 | 1,50294200 |
| H 1.81425100 | 2.10157800 | 2,97515900 | H | -0.78614100 | 3.36919400 | 2,92774300 |
| H 0.91294200 | 0 75891000 | 2 26889000 | H | -0 70045800 | 1 61680200 | 2 69014900 |
| C -0 95050000 | 2 38476500 | 1 03885200 | C | -2 81078200 | 1.34806500 | 1 19716700 |
| H -3 77597500 | 3 84739900 | -0 19644800 | н | -5 76127700 | 0 13864000 | -0.04772800 |
| H -3 98224200 | 2 80201100 | 1 19476400 | н | -5.05331000 | -0.39632000 | 1 47200000 |
| H _1 08135900 | 1 36909300 | 0.69252400 | н | -2 30517500 | 0.42832100 | 1 46106800 |
| C 3 57901700 | 0.96467200 | 1 75185800 | Ċ | 1 58566700 | 2 36941000 | 2 04994500 |
| H 3 26147100 | 0.00407200 | 2 25275700 | й | 1.56311000 | 1 30284300 | 2.04004000 |
| H / 38082000 | 0.04000100 | 1 06000600 | н | 2 48280300 | 2 50710600 | 1 47165200 |
| H 3 96253500 | 1 66323500 | 2 50857500 | н | 1 61772000 | 2.007 10000 | 2 98384100 |
| C = 2.02614100 = | 2 78707300 | -1 24804900 | C | 5 32628500 | -1 64073900 | -1 79436800 |
| H 0 98067700 - | 2 72520800 | -0.96658400 | н | 5 39791100 | -2 33698100 | -0.95284200 |
| H 2 11281100 - | 2 38573200 | -2 25662600 | н | 4 97447400 | -2.00000100 | -2 66534400 |
| H 2 33868100 - | 3 84198100 | -1 27118900 | н | 6 34012700 | -1 26284900 | -2 01002100 |
| C = 2.78074500 | 0.47130100 | 2 21119600 | Ċ | -0 70416000 | -1.20204300 | 2 79825800 |
| H _3 19714600 | 0.47784000 | 1 71973300 | н | -0.70410000 | -1.55158100 | 2 68875700 |
| H -3 44615600 - | 0.40704000 | 3 02692000 | н | -0.61760800 | -2 53430100 | 3 65796600 |
| H _1 80378300 _ | 0.70021400 | 2 62349300 | н | -0.017060000 | -2.00400100 | 2 95295100 |
| C -5 00766200 | 1 59288800 | -0.65162600 | C | -0.07304000 | -2 32661700 | -0.09387300 |
| H _5 50281800 | 2 46456400 | -1 11251700 | н | -5 91453500 | -2 18069100 | -0 59627900 |
| H -5 27058200 | 0 71284600 | -1 23795700 | н | -4 47887700 | -3 21520400 | -0 52553300 |
| H _5 /2773100 | 1 46122700 | 0 3/072000 | н | -5.13647400 | -2 53/61300 | 0.02000000 |
| $C_{-1} 61107200$ | 2 40007800 | -2 47281300 | Ċ | 0 47259000 | -2.00401000 | -2 00094800 |
| H _1 97155600 _ | 2 88831100 | -2.47201000 | н | 0.39030100 | -3 66372000 | -2.00004000 |
| H -0 58621200 - | 2 14938900 | -2 58672800 | н | 0.93171600 | -2.03000000 | -2.35860000 |
| H _1 63027000 _ | 3 31578800 | -1 74647100 | н | 1 10751900 | -3 38791600 | -1 23031200 |
| C = 2.23029300 | 0.46113800 | -3 27621100 | Ċ | 0.09168800 | 2 14635000 | -3.00612000 |
| H 1 24682800 | 0.40110000 | -3 20187300 | н | -0 93446700 | 2.14000000 | -2 88675300 |
| H 2 74836400 | 0.82926200 | -4 16285800 | н | 0.53440700 | 2.40000000 | -3.87036200 |
| H 2 09812300 - | 0.61389400 | -3 39171300 | н | 0.07821600 | 1 07180400 | -3 16237600 |
| C -2 09192500 - | 2 80321700 | 1 89938200 | Ċ | 1 17801400 | -3 03550300 | 1 73990000 |
| C 2.88861300 - | 2 72686800 | 1.02533800 | c | 4 70783700 | 0.05678500 | -0 18660500 |
| C = 0.86247500 | 1 97983100 | 4 16945900 | c | 3 70011000 | -0 72458300 | 3 42026900 |
| C = 0.44646700 = | 2 20767100 | 3 74806600 | c | 2 64065500 | -0.72400000 | 3 23901400 |
| C 1 92218100 - | 2 13179900 | 3 27129500 | C C | 4 36718800 | -0.19556800 | 2 31591300 |
| C = 0.69245900 = | 2 63785400 | 2 43628700 | c | 2 24010400 | -1 98057200 | 1 94694800 |
| C = 1.002+00000 = | 2 57190300 | 1 95738500 | C C | 3 98140700 | -0 54570800 | 1 01310000 |
| C = 0.38873200 = | 2 88195700 | 1 58824600 | c c | 2 92542500 | -1 44331700 | 0.84751100 |
| H 1 05928700 - | 1 67429600 | 5 19248700 | н | 4 02255500 | -0 46576500 | 4 42448500 |
| H -1 27136300 - | 2 06206800 | 4 44035500 | н | 2 15479000 | -2 05640500 | 4 10711700 |
| H 2 93646000 - | 1 93385700 | 3 60996600 | н | 5 20996300 | 0 47555400 | 2 46796700 |
| H 0 18154000 - | 3 31228200 | 0.61570300 | н | 2 67280300 | -1 73419800 | -0 16827700 |
| H -2,79203200 - | 3.05437900 | 2,70694500 | н | 1.16555000 | -3.71870400 | 2.59865000 |
| | | | | | | |

| H -2.12185200 -3.61886300 1.17213 | 3400 H 1.42903300 -3.63208300 0.86240900 |
|-----------------------------------|--|
| H 3.77445300 -2.36658900 1.55404 | 4700 H 4.46575700 1.12565500 -0.23901000 |
| H 3.06928900 -3.79364300 0.81548 | 3600 H 5.79442100 0.02411500 0.00116300 |

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