Electronic Supplementary Information (ESI)

Completely preorganized bis-lactam-1,10-phenanthroline ligands with high stability for efficient separation of Am(III) over Eu(III)

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1. Experimental section

1.1 General

The chemicals and reagents used in this work, such as europium nitrate hexahydrate $(Eu(NO_3)_3 \cdot 6H_2O)$, tetraethylammonium nitrate (Et_4NNO_3) , sodium thiosulphate $(Na_2S_2O_3)$, acetic acid, 4-tert-butylaniline, potassium carbonate (K_2CO_3) , potassium iodide (KI), Br₂, anhydrous magnesium sulfate (MgSO₄), Cy₃P·HBF₄, cesium carbonate (Cs_2CO_3) , Pd(OAc)₂, thionyl chloride (SOCl₂), deuterated chloroform (CD₃Cl), triethylamine (NEt₃), N, N-dimethylformamide (DMF), dichloromethane (DCM), petroleum ether (PE), methanol (MeOH), dimethyl sulfoxide (DMSO) with analytical purity (AR) are commercially obtained and directly used without purification. 1,2-dichloroethane (1,2-DCE) with AR purity was used as a diluent in solvent extraction. Methanol with HPLC purity and trichloromethane (CHCl₃) with AR purity were used as the solvents in spectroscopic titration and ESI-MS.

1.2 Organic synthesis

Synthesis of 1: A mixture of 4-tert-butylaniline (5.0 g, 33.5 mmol, 2 eq.), bromoalkanes (25.1 mmol, 1.5 eq), K_2CO_3 (6.9 g, 50.3 mmol, 3 eq.), and KI (0.3 g, 1.6 mmol,

0.1 eq.) in DMF was stirred. The reaction mixture was heated to 80 $^{\circ}$ C for 16 hours.

After finishing, the reaction was quenched with water, and the mixture was extracted with PE (15 mL \times 3). The combined organic layer was washed with brine, dried over MgSO₄, and then concentrated under reduced pressure. The residue was purified via flash column chromatography (DCM: PE, 1:5 to 3:5) to afford intermediate **1**.

R = **n-butyl**: Yield: 52%, light yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 7.24 – 7.17 (m, 2H), 6.61 – 6.51 (m, 2H), 3.10 (t, *J* = 7.0 Hz, 2H), 1.65 – 1.56 (m, 2H), 1.47 – 1.39 (q, *J* = 7.4 Hz, 2H), 1.29 (s, 9H), 0.96 (t, *J* = 7.7 Hz, 3H).

R = 2-ethylhexyl: Yield: 48%, light yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 7.20 (d, J = 8.7 Hz, 2H), 6.57 (d, J = 8.7 Hz, 2H), 3.00 (d, J = 6.2 Hz, 2H), 1.58 – 1.51 (m, 1H), 1.48 – 1.29 (m, 8H), 1.28 (s, 9H), 0.93 – 0.87 (m, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 146.46, 139.67, 126.01, 112.33, 47.22, 39.22, 33.85, 31.61, 31.39, 29.04, 24.55, 23.18, 14.17, 10.99. m/z calculated for [C₁₈H₃₁N + H]⁺ 262.2529, found 262.2502.

Synthesis of **2**: The intermediate **1** (3.0 g, 14.6 mmol, 1.0 eq.) was added to 30 mL glacial acetic acid and then the solution was stirred. Bromine (0.5 mL, 1.0 eq.) solution in 15 mL glacial acetic acid was added dropwise over 20 minutes through a dropping funnel. The reaction mixture was stirred at room temperature for 4 hours. After finishing, the reaction was added sodium thiosulphate to quench excess bromine until the solution was colorless. It was diluted with 100 mL water and extracted with DCM (3×40 mL). The combined organic layer was washed with brine, dried over MgSO₄, and then concentrated under reduced pressure. The residue was purified via flash column chromatography (DCM: PE, 1:5) to afford intermediate **2**.

R = **n-butyl**: Yield: 82%, light yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 7.42 (d, J = 2.2 Hz, 1H), 7.19 (dd, J = 8.5, 2.2 Hz, 1H), 6.58 (d, J = 8.5 Hz, 1H), 4.12 (s, 1H), 3.13 (t, J = 7.0 Hz, 2H), 1.68 – 1.59 (m, 2H), 1.49 – 1.40 (m, 2H), 1.26 (s, 9H),0.96 (t, J = 7.4 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 142.86, 140.61, 129.33, 125.28, 110.91, 109.53, 43.72, 33.88, 31.45, 20.29, 13.91. m/z calculated for [C₁₄H₂₂BrN + H]⁺ 284.1008, found 284.0986.

R = 2-ethylhexyl: Yield: 86%, light yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 7.43 (s, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 6.58 (d, *J* = 8.5 Hz, 2H), 3.04 (d, *J* = 6.0 Hz, 2H), 1.64 – 1.58 (m, 1H), 1.48 – 1.29 (m, 8H), 1.27 (s, 9H), 0.95 – 0.88 (m, 7H). ¹³C NMR (126 MHz, CDCl₃) δ 143.02, 140.46, 129.33, 125.31, 110.83, 109.63, 47.08, 38.90, 33.91, 31.48, 31.33, 28.98, 24.59, 23.11, 14.12, 11.00. m/z calculated for [C₁₈H₃₀NBr + H]⁺ 340.1634, found 340.1581.



Scheme S1 Synthetic routes for 1 and 2.

1.3 Solvent extraction

The distribution ratio (D) was calculated as equation S1:

 $D = C_{org}/C_{aq}$ S1 The separation factor (*SF*) was calculated as equation S2:

$$SF = D_{Am}/D_{Eu}$$
 S2

2 Result and discussion

2.1 Organic synthesis



Fig. S1 ¹H spectrum of L1 in CDCl₃.



Fig. S2 ¹H spectrum of L2 in CDCl₃.



Fig. S3 The ESI-HRMS result of L1.



Fig. S4 The ESI-HRMS result of L2.



Fig. S5 The UV-Vis absorption spectra of (a) L1 and (b) L2 in 1,2-DCE before and after 24 hours of exposure to 1 M nitric acid.

2.2 ESI-MS results



Fig. S6 ESI-MS spectrum of the complex solution.

2.3 Single-crystal X-ray diffraction

CCDC number

| Table S1. Structural refinement parameters for L1 | |
|---|--|
| Identification code L1 | |

2390588

| Empirical formula | $C_{44}H_{50}C_{16}N_4O_3$ |
|---------------------------------------|---------------------------------------|
| Formula weight | 895.58 |
| Temperature/K | 302.0 |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 16.465(10) |
| b/Å | 14.702(12) |
| c/Å | 18.759(12) |
| α /° | 90 |
| β /° | 92.77(5) |
| γ /° | 90 |
| Volume/Å3 | 4536(5) |
| Ζ | 4 |
| p calcg/cm3 | 1.311 |
| μ / mm-1 | 3.795 |
| F(000) | 1872.0 |
| Crystal size/mm3 | $0.18 \times 0.15 \times 0.12$ |
| Radiation | $CuK\alpha$ ($\lambda = 1.54178$) |
| 2Θ range for data collection/° | 7.644 to 137.31 |
| | $-19 \leqslant h \leqslant 19,$ |
| Index ranges | $-16 \leqslant k \leqslant 17,$ |
| | $-22 \leqslant l \leqslant 21$ |
| Reflections collected | 42015 |
| Independent reflections | 8331 [Rint = 0.0905, Rsigma = 0.0629] |
| Data/restraints/parameters | 8331/348/666 |
| Goodness-of-fit on F2 | 1.058 |
| Final R indexes [I>=2 σ (I)] | R1 = 0.0836, $wR2 = 0.2380$ |
| Final R indexes [all data] | R1 = 0.1262, wR2 = 0.2824 |
| Largest diff. peak/hole / e Å-3 | 0.47/-0.37 |

2.4 DFT calculation details



Fig. S7 Six calculated isomers of L1 (kcal/mol).



Fig. S8 Six calculated isomers of EuL1(NO₃)₃ (kcal/mol).



Fig. S9 Six calculated isomers of AmL1(NO₃)₃ (kcal/mol).



Fig. S10 (a) Optimized structure of $Eu(L1)(NO_3)_3$ and (b) deformation density $\Delta \rho$ between L1 and $Eu(NO_3)_3$ (isosurface = 0.003 a.u.)



Fig. S11 Thermodynamic cycle for calculating the Gibbs free energy of the reaction.



Fig. S12. The bond distances and angles of $AmL1(NO_3)_3$ and $EuL1(NO_3)_3$ (distance Å/ angle deg).

| ML1(NO ₃) ₃ | $E_{\rm int}$ | E _{elest} | Exrep | $E_{ m orb}$ | Ec |
|--|---------------|--------------------|--------|--------------|--------|
| AmL1(NO ₃) ₃ | -93.84 | -100.00 | 100.39 | -70.05 | -24.18 |
| Eu L1 (NO ₃) ₃ | -92.02 | -91.72 | 86.60 | -65.30 | -21.60 |

Table S2. EDA Analysis (kcal/mol) of ML1(NO₃)₃ at the PBE0/6-311G*

Appendix A

Optimized cartesian coordinates of ML1(NO₃)₃

| AmL1(NO ₃) ₃ | | | | | I | $EuL1(NO_3)_3$ | |
|-------------------------------------|-------------|-------------|------------|----|-------------|----------------|------------|
| Am | -0.01061000 | -1.56563311 | 0.43027403 | Eu | -0.02097700 | -1.65957812 | 0.49278504 |

| O 0.09298401 -0.4431103 2.66536519 O 0.01421700 -0.53163604 2.67799219 0.03502707 -3.832901928 0.23992202 O -1.01476607 -3.87346528 0.35421903 0.0512707 -3.832901928 0.23992202 O -1.01476607 -3.87346528 0.0351296 0.6312926 0.63757605 O -1.44587110 -1.49409811 -1.68522612 0.237590922 -1.57803911 -3.5276601 -4.3789282 -0.38847303 N -0.1366004 -2.2471241 -0.6087505 N -0.1275601 -4.3789282 -0.3887303 N -0.59184004 -0.9182307 2.4196411 -5.52026340 -0.8983406 -2.3724802 O -0.0987706 -0.47347505 -0.375652304 -0.8983463 -2.3724825 -0.32874812 0.374852 O -2.4719241 -1.0154100 -0.37574600 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3774852 -0.3 | | | | | | | | |
|---|---------|--------------|-------------|-------------|--------|-------------|-------------|-------------|
| 0 0.27869102 2.5841019 2.67588619 0 0.3381702 2.65237419 2.6884819 0 0.81627706 3.46964525 0.92036606 0.04480006 3.6812226 0.67557005 0 1.4458111 1.43494013 0.0579042 1.5005616 1.725664613 0 0.4501702 1.568404 1.54744013 0 0.6480805 -0.8039066 1.725664613 0 0.4577061 2.41766401 N 0.425790403 -157803911 3.5296424 N 0.41876601 -4.7771231 0.6087505 N 0.427920433 -15400814 2.8274823 0 -4.07957706 -6.6743506 -5.5784452 0 -5.9652504 -9.8954306 -5.274845333 0 -2.4792218 -1.4710101 1.02244008 0 2.44596917 -1.6533812 0.75657105 0 -2.4792218 -1.4710101 1.02244008 0.245945223 -0.522494522 -0.522494522 -0.522494444 0.1021600 0.55073304 0.35743502 0.32745022 | 0 | 0.09298401 | -0.44531103 | 2.66536519 | 0 | 0.01421700 | -0.53163604 | 2.67099219 |
| 0 0.95027207 3.82901928 0.23992202 0. 1.01476607 3.87465228 0.23491903 0 0.8162706 3.4048006 0.94480805 0.64480805 0.691926 0.67857365 0 0.4519100 1.59048041 1.68122612 0.04548085 0.0390666 1.7874413 0.01866061 4.77471231 0.06879505 N 0.21736601 4.78798323 0.39487303 0.04010430 1.48798014 5.75739 1.08331108 0.95924803 1.09780708 2.35288117 0.4010430 1.48798014 5.3275733 0.95952504 0.89853406 5.3274825 0.23007701 5.37156739 1.08331108 0.95952504 0.89853406 5.3274825 0.23007218 1.47190810 1.02244080 0.24599917 1.66358122 0.33774802 0.240792218 1.47191810 1.03240805 0.24599201 0.70051005 0.32075733 0.72159940 0.33774592 0.23748023 0.32276533 0.72159940 0.33774592 0.322776533 0.72159940 0.33 | 0 | 0.27869102 | -2.58413019 | 2.67588619 | 0 | 0.33831702 | -2.65237419 | 2.68846819 |
| 0 0.81627706 3.46964525 0.92036606 0 0.840810006 3.60112926 0.67857005 0 0.458110 1.4342811 3.1447613 0 0.4648100 -1.014411 -1.256561613 0 0.258790402 -1.5864614 3.3479724 0.08037060 -1.37503911 3.35296414 0 0.40103403 -1.47870310 4.3787233 0 0.012376014 -4.3789231 -0.39924803 -1.4780310 4.3272733 0 0.99924803 -1.543005811 4.5444333 0 -0.0103403 -1.47870310 4.37823234 0 0.9995400 -1.45303811 0.35274822 0 2.35288117 0 0.4649256 0.5595234 0.4599510 0.52073340 0.3222302 0 2.45996917 -1.66533812 0.75657105 1.24271614 0.1221308 0.244514118 -1.55823711 1.122123107 1.122123107 1.122123107 1.126205 0.33774502 0.32254062 N.1.22771540 0.224719224 N.02581504 0.07675905 0.32745022 N.12273540 0.22471924505 <td>Ō</td> <td>-0.95027207</td> <td>-3 82901928</td> <td>0 23992202</td> <td>Ō</td> <td>-1 01476607</td> <td>-3 87465228</td> <td>0 35421903</td> | Ō | -0.95027207 | -3 82901928 | 0 23992202 | Ō | -1 01476607 | -3 87465228 | 0 35421903 |
| 0 0 0.205000 2.005000 2.001221 0.01702100 2.001241 0 0.44619304 -0.59664604 -1.84744013 0 0.6448805 -0.8030666 -1.75864613 0 0.0571902 -1.5084211 3.349724 N 0.12736601 +3.780231 3.35296424 N 0.11866601 +2.7471231 -0.60879302 N N 1.12736601 +3.783232 -0.39487303 0 0.30973706 -0.67435405 -3.5784152 0 0.39924803 -1.5430811 -3.5243811 0 0.20673701 -5.3775379 -0.83110 0.0075905 0.3202502 N -1.5230614 -0.8985210 -0.8985210 -0.55205341 -0.8995230 -0.5753130 0 -2.37405223 -0.64405205 0.50449494 -2.32276523 -0.6231504 -0.5973304 2 -3.4710590 0.32086202 N -1.2973499 -0.0527510 N -5.21900023 -0.5275905 -2.31900023 -0.5274504 -0.027757905 -3.2204645 -0. | õ | 0.81627706 | 3 46064525 | 0.02036606 | | 0.84080006 | 3 60312026 | 0.67857605 |
| 0 -1,443,0,110 -1,245,0,011 -1,08,32,012 0 -1,340,3010 -1,001,4411 -1,020,3412 0,025,0190 -1,256,4613 0,039,066 -1,2771,221 -0,087,9505 N -0,273,002 -1,378,0231 -3,35,94424 N -0,118,660 -1,42,771,221 -0,087,9505 N -0,273,002 -1,378,0231 -3,35,94424 N -0,182,030 -1,273,001 -3,371,502,031 -4,537,573 0 -0,399,24,803 -1,078,0708 -2,352,88117 -0,040143 -1,487,050 -3,734,152 0 -0,595,2504 -0,898,5430 -5,327,4382 0 -2,909,2718 -1,471,090 -1,371,510 -3,371,550 -3,714,512 0 -0,595,2504 -0,898,5430 -5,327,4382 0 -2,409,2218 -1,471,090 -1,371,310 -0,320,2500 -1,247,992,118 -1,471,090 -1,371,310 -0,320,2500 -2,44,992,118 -1,427,090 -1,321,310 -0,302,530 -0,24,5992,110 -0,264,152 -0,377,4502 -0,377,4502 -0,370,4503 -0,377,4502 -0,370,4503 -0,377,4502 -0,326,45119 -0,708,510 -0,377,4502 -0,308,9702 -2,469,491 -0,708,5706 -1,91,7191 -0,1091,106 -0,785,386 -1,841,281 -1,021,230,70 -2,264,914,91 -0,774,980 -0,335,2703 -2,264,914,91 -0,632,739,94 -0,349,5100 -3,572,330 +2,326,45119 -0,774,980 -0,353,2703 -2,264,914,91 -0,632,739,94 -0,349,5100 -3,572,733 +0,234,245,31 -0,741,4403 -0,783,840 -0,4572,703 -4,4518,23 -0,741,4403 -0,688,370 -1,521,9801 N +4,556,873 -0,634,4403 -0,373,5400 -0,479,5201 -1,437,0191 -3,038,0722 -0,122,1500 N +4,518,233 -0,741,1403 -0,688,370 -3,598,410 -0,4573,703 -0,398,410 -0,473,7100 -0,773,7802 -3,129,7203 -0,424,724,41 -0,220,411,4103 -0,468,310 -0,478,310 -0,121,41101 C -1,3519,710 -3,142,721 -0,123,500 N +4,512,423 -0,741,1403 -0,688,370 -2,508,413 -0,712,41,513 -0,121,41101 C -1,3519,710 -3,142,721 -0,123,500 N +4,512,423 -0,241,4403 -0,783,840 -0,479,520 C -1,320,825 -1,812,813 -0,121,41101 C -1,3519,710 -3,142,721 -0,123,500 N +4,512,423 -0,241,4403 -0,783,810 -0,373,820 -0,273,820 -0,274,140,82 -0,284,841 -0,273,820 -0,274,140,82 -0,284,441 -0,243,810 -0,273,820 -0,274,140,82 -0,284,511 -0,202,200 -0,273,7800 -0,273,7800 -2,286,969,22 -0,074,140 -2,276,904 +3,412,820 -0,214,4101 -2,214,411,41,410 -2,414,414,7 -2,064,197,15 -1,033,905,00 -2,328,924 -0,214,140 -2,276,900 -1,233,7300 -0,319,820 - | 0 | 1 44597110 | 1 40400911 | -0.92030000 | | 1 24025010 | -5.00512920 | -0.07857005 |
| 0 0.949(15)40 -0.59664004 -1.84/44015 0 0.063700000 -1.758646113 N 0.011866601 -2.7471231 -0.00879505 N -0.12736601 -4.37892332 -0.39487303 N 0.9114040 -0.1826507 -2.4196417 N -0.12359403 -1.54305413 -3.5282811 -4.5443333 0 -0.20673701 -5.3715679 -0.633110 0.02502504 -0.89052266 -0.8095226 0 -0.20673706 -0.67335050 -0.3205204 -0.89052260 -0.6533812 -0.6533812 -0.532120 -0.532120 -0.532120 -0.532120 -0.532120 -0.532120 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.5503304 -0.3774502 -0.325402823 -0.62404905 -0.58043904 -0.6533810 -0.6533810 -0.6533810 -0.6533810 -0.6533810 -0.6533810 -0.6533810 -0.14717501 -0.12757051 -0.45404919 -0.73745702 -0.45419218 -0.166533812 | 0 | -1.4458/110 | -1.49409811 | -1.08322012 | | -1.34035010 | -1.00144411 | -1.02055412 |
| N 0.26371902 -1.59048211 3.34497824 N 0.25704002 -1.57803911 3.35296244 N 0.59184004 -0.91826307 -2.41964017 N 0.43598403 -1.09780708 -2.35288117 0 0.401034 1.48705301 4.5372733 0.03924803 -1.53405811 4.54445333 0 -0.20673701 -5.37156739 -1.08331108 0 0.1912901 -5.52025340 0.8895306 -5.32743825 0 -2.30027418 -1.39907311 0.70027605 0 2.4599617 -1.653538112 0.73875105 0.3202502 N 1.36809510 0.68116205 0.33774502 1.29711609 0.7381105 0.3308502 N 1.36909510 0.68116205 0.33774502 2.300253 0.53227301 0.33225703 0.32275304 0.33774502 0.3273402 2.3040519 0.77867606 1.9247614 0.10124701 C 0.667553806 1.84192813 0.1427101 C 3.4399845 0.35323703 N 4.5451823 0.7414805 | 0 | 0.49619304 | -0.59664604 | -1.84744013 | 0 | 0.64486805 | -0.80390606 | -1./5864613 |
| N -0.11866601 -4.27471231 -0.60879505 N -0.12736601 -4.37892832 -0.39887303 N -0.59184040 -0.91825030 -2.419464017 N -0.43598403 -1.54305811 -2.35288117 O -0.20673701 -5.3757545 -0.67435405 -3.57841526 -0.95952304 -0.89854306 -3.2757311 -0.027305 O -2.4719218 -1.47109810 -0.2265302 N -1.38438710 -0.74937555 0.32065202 N -1.28721409 -0.7001003 0.33774502 C -3.1990023 -0.52129040 .7091505 C -3.1900023 -0.521500 0.5377304 C -3.771606 -1.971840 0.1024701 C -0.67885806 6.3275904 0.30451033 C -2.71666119 0.70679005 0.33774502 0.3263503 N 4.57124633 -0.7187605 0.3603003 A 4.5052733 O.65484405 0.69752705 N 4.54518233 -0.7187802 0.3314322 -0.1055701 C | Ν | 0.26371902 | -1.50848211 | 3.34497824 | N | 0.25709402 | -1.57803911 | 3.35296424 |
| N 0.59184004 -0.91826307 2.21964017 N 0.43992403 -1.9780708 -2.3528117 O -0.20673701 -5.37156739 -1.08331108 O -0.1992901 -5.50205340 -0.59523204 O -0.79857706 -0.67435405 -3.578481256 O -0.99563204 -0.89854304 -0.89563204 -0.89854304 -0.89563204 -0.89854304 -0.89563204 -0.89563204 -0.89563204 -0.85563731 -0.751505 -0.245414118 -1.55823711 -0.75666633 N -1.29711609 -0.78126005 -0.32086202 N -1.29723409 -0.7051005 0.35773304 C -2.3099523 -0.54440220 -0.5089702 C -3.19000923 -0.755705 0.5577315 C -0.66294405 -9.2847164 -0.10124701 C -0.6785330 0.7815905 0.45321703 C -2.61863419 0.8662405 0.3363705 C -3.6634405 -0.6284405 0.9284704 0.49453701 C -3.5192725 N.45518233 -0.7114805 0 | Ν | -0.11866601 | -4.27471231 | -0.60879505 | N | -0.12736601 | -4.37892832 | -0.39487303 |
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| O -0.20673701 -5.37156739 -1.08331108 O -0.19129901 -5.50205340 -0.20783705 O -2.3502716 -0.67453503 -3.57841525 O -0.5955294 -0.89854304 -0.89854304 -3.57743825 O -2.34719218 -1.47109810 1.02540308 O -2.45414118 -1.55823711 1.02123307 N 1.33843710 0.7793705 0.32025302 N -1.29723409 0.068116305 0.35773304 C 3.2379505 0.320286202 N -1.29723409 0.061005 0.33899702 C -3.1909023 -0.6527905 0.5373304 C -0.66278405 1.9284714 0.10124701 C 0.6785306 1.8524313 0.1251980 C -4.663419 0.66862405 0.3532763 N 4.5518233 -0.67191305 0.3512705 A 4.45565713 -0.6548405 0.6985300 C -1.3871813 0.13872731 0.12141101 C 1.4387031 0.77438905 0.45505101 C | 0 | 0.40103403 | -1.48708310 | 4.53725733 | 0 | 0.39924803 | -1.54305811 | 4,54445333 |
| 0 -0.7987706 -0.67434405 -3.57481526 0 -0.39652504 -0.08954306 -3.52743823 0 -2.30027418 -1.59907311 0.70027605 0 -2.45414118 -1.55823111 1.02123307 N 1.38438710 0.74937505 0.3202302 N 1.36809510 0.63854360 0.333774502 C 3.25402823 -0.64408205 0.50843904 C 3.227523 -0.72150905 0.53373344 C 3.2990233 -0.532150904 0.7091505 C -3.19009233 -0.64215100 0.70651005 0.5373341 0.1271201 C -0.66298405 1.92847614 0.10124701 C 0.67853806 0.45570903 N 4.57124633 -0.8711400 0.47919403 N 4.5568733 -0.63548405 0.645709003 N 4.57124633 -0.87114805 0.636240 0.30631003 X 4.5568713 -0.63584051 0.69486301 C 3.5192722 -0.1285102 C 1.3614119 0.66662405 0.30383705 | Õ | -0.20673701 | -5 37156739 | -1.08331108 | Ö | _0 10120001 | -5 50205340 | -0.80952206 |
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| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 0 | -0./983//00 | -0.0/455405 | -3.3/841320 | | -0.39032304 | -0.89834300 | -3.32/43823 |
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| $ \begin{array}{c} c \\ c$ | С | 3.25402823 | -0.64408205 | 0.50843904 | C | 3.22276523 | -0.72150905 | 0.55073304 |
| C 2.7465119 0.70610005 0.30890702 C 2.68604919 0.62275904 0.34951003 C 0.77867606 1.91178914 0.10911601 C 0.76853806 1.84192813 0.14271201 C 2.61914919 0.77439805 0.35323703 C 2.61863419 0.68662405 0.36030003 N 4.60502433 0.7858405 0.045509003 N 4.57124633 0.87716106 0.47919403 N 4.55658733 -0.63548405 0.69752705 N 4.54518233 -0.74114805 0.68583705 C 3.5526626 1.82308613 0.09486301 C 3.51927225 1.74317513 0.12141101 C 1.49617711 3.11085422 -0.11326601 C 1.48701911 3.03806722 -0.08911501 C -3.42012825 1.9058114 0.1145401 C -3.42598525 1.81281313 0.1189201 C 5.46936242 0.30051802 0.26236102 C 5.44273041 0.20222001 0.27737802 C 5.12808937 -2.15272515 0.59963904 C 5.08111037 -2.25044016 0.60781205 C -5.39210540 0.44838703 0.39984703 C -5.38781340 0.3827302 0.39065503 C -5.12022237 -1.94933714 1.04504608 C -5.09841437 -2.06419715 1.01390507 C 2.8889121 3.0410252 -0.11349001 C 2.88035821 2.96365922 -0.0145901 C 0.76280206 4.32580231 -0.33628802 C 0.75008505 4.24980830 -0.31982302 C -2.74709820 3.10270822 -0.12610501 C -2.75999120 3.01482822 -0.11816201 C -4.86234635 1.722274420 1.02904708 H 4.29094531 -2.8159020 1.10004608 H 5.397613144 -2.11769915 1.28659009 H 5.93646241 -2.23113416 -0.23254801 H 4.3390331 -2.7274420 -0.1630717 C -5.4860994531 -2.8159020 1.1004668 H 5.49766231 -2.74709820 3.10270822 -0.21610501 C -5.4826812 -0.211816201 L -4.86234635 1.72224821 0.12648311 1.2865409 H 4.3209094531 -4.8129723 -0.3218202 -0.7759052 H 4.32905931 -2.7274420 1.80904708 H 4.23094531 -2.8159020 1.1004668 H 5.39766221 -0.72915605 5.4727349 -2.87066221 -0.72915605 H -5.95628142 -1.78078213 1.72723812 H -5.93938040 -1.91304614 1.69413112 H 4.3398731 -2.46833518 1.60539311 H 4.31992431 -2.53829219 1.002482904204 H 1.32935954 4.02109129 $-$ | Ċ | -3 19995023 | -0 53229904 | 0 70915505 | Ċ | -3 19000923 | -0 62541504 | 0 70675905 |
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| C -2.61914919 0.77439805 0.35323703 C -2.61863419 0.68662405 0.36030003 N 4.65052433 -0.78585405 0.45509003 N 4.57110160 0.47919403 N 4.53058733 -0.63548405 0.69752705 N 4.54871233 -0.74114805 0.68583705 C 3.53296626 1.82308613 0.09486301 C 3.51927225 1.74317513 0.12141101 C 1.43501711 3.1185422 -0.12252301 C -1.36616210 3.0631722 -0.011898201 C 5.46936242 0.30051802 0.26236102 C 5.44273041 0.2022001 0.27737802 C 5.12002237 -1.94933714 1.04504608 C 5.0871134 -2.20440161 0.607812057 C 2.8789121 3.04102522 -0.11349001 C 2.88035821 2.9064533 -0.32738202 C 0.76280206 4.32580231 -0.33658802 C 0.7590120 3.01482822 -0.0148901 C <td< td=""><td>С</td><td>-0.66298405</td><td>1.92847614</td><td>0.10124/01</td><td>C</td><td>-0.6/195305</td><td>1.85243313</td><td>0.12519801</td></td<> | С | -0.66298405 | 1.92847614 | 0.10124/01 | C | -0.6/195305 | 1.85243313 | 0.12519801 |
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| C 3.53296626 1.82308613 0.09486301 C 3.51927225 1.74317313 0.12141101 C 1.49617711 3.11085422 -0.11326601 C 1.36616210 3.0680722 -0.08511501 C -3.42012825 1.90558114 0.11415401 C -3.46273041 0.20222001 0.27737802 C 5.12808937 -2.15272515 0.59963904 C 5.08111037 -2.25044016 0.60781205 C -5.39210540 0.44838703 0.39984703 C -5.38781340 0.33827302 0.39065503 C -5.3920237 1.94933714 1.04504608 C -5.0881437 -2.06419715 1.0390507 C 0.76280206 4.32580231 -0.33658802 C 0.7508505 4.24980830 -0.31982302 C -0.75150204 4.31120531 -0.12605001 C -2.75999120 3.01482822 -0.11816201 C -4.8624535 1.72922813 0.12605001 C 4.26498935 1.62485812 0.12548801 <tr< td=""><td>Ν</td><td>-4.55658733</td><td>-0.63548405</td><td>0.69752705</td><td>N</td><td>-4.54518233</td><td>-0.74114805</td><td>0.68583705</td></tr<> | Ν | -4.55658733 | -0.63548405 | 0.69752705 | N | -4.54518233 | -0.74114805 | 0.68583705 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | 3.53296626 | 1.82308613 | 0.09486301 | C | 3.51927225 | 1.74317513 | 0.12141101 |
| $ \begin{array}{c} \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$ | Ċ | 1 49617711 | 3 11085422 | -0 11326601 | Ċ | 1 48701911 | 3 03806722 | -0.08911501 |
| C -1.32617012 -0.12252010 C -1.3261702 -0.11845401 C -3.42598525 -1.81281313 -0.11898201 C 5.46936242 -0.30051802 -0.2236102 C 5.44273041 -0.222001 -0.7737802 C 5.1208937 -2.15272515 -0.59963904 C 5.08111037 -2.25044016 -0.60781205 C -5.39210540 -0.44838703 -0.39984703 C -5.38781340 -0.33827302 -0.39065503 C -5.12022237 -1.94933714 -1.04504608 C -5.09841437 -2.06419715 -1.01390507 C -0.5898121 -0.304102522 -0.11349001 C 2.88035821 2.96365922 -0.09145901 C -0.59150204 4.34120531 -0.34211802 C -0.60496504 4.26177330 -0.3738202 C -0.59150204 4.34120531 -0.34211802 C -0.60496504 4.26177330 -0.3738202 C -2.74709820 -0.12070822 -0.12610501 C -2.75999120 -0.11816201 C 4.86234635 1.72922813 -0.12610501 C -4.86698935 1.62485812 -0.12848801 H 4.33990331 -2.72274420 1.08904708 H 4.29094531 -2.81539020 1.10004608 H 5.97613144 -2.11769915 1.28659009 H 5.93646241 -2.23113416 1.28636409 C 5.49613138 -2.80822020 -0.72743105 C 5.42750439 -2.89766221 -0.72915605 H -5.95628142 -1.78078213 1.72723812 H -5.93938040 -1.91304614 1.69413112 C -5.53075941 -2.78521420 -0.16312101 C -5.49440938 -2.8866721 -0.20826002 H -3.4368731 -2.46833518 1.60539311 H -4.31942431 -2.58329219 1.57073212 C -5.53075941 -2.78521420 -0.16612101 H -3.45068257 -0.49428504 H -1.12619108 5.27019638 -0.51609504 H -1.14057508 5.18927438 -0.50669204 H -3.2939524 4.02109129 -0.31376002 H -3.8050824 -2.33309517 -1.23347509 H 5.92888443 -3.78680267 -0.4842300 H 5.85531043 -3.88178728 -0.49902604 H -5.92280443 -3.17875366 -0.31982501 C -5.89253046 -2.34760617 -0.80755806 C 4.97067536 1.61152511 -0.9885601 C -7.64904551 -2.34736017 -0.80735806 C -7.71420752 -0.8774536 -0.34878403 H 5.85531043 -3.881787728 -0.49902604 H 5.31972404 3.7897247 -0.35035203 H 5.73356422 -0.7188107 -0.36035806 | Č | -1 35319710 | 3 1/1320722 | -0.12252301 | Ċ | -1 36616210 | 3 0631/1322 | -0.10655701 |
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| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | -3.42012825 | 1.90558114 | 0.11415401 | | -3.42398323 | 1.81281313 | 0.11898201 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | 5.46936242 | 0.30051802 | 0.26236102 | C | 5.442/3041 | 0.20222001 | 0.27737802 |
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| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | -5.39210540 | 0.44838703 | 0.39984703 | C | -5.38781340 | 0.33827302 | 0.39065503 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | -5.12022237 | -1.94933714 | 1.04504608 | C | -5.09841437 | -2.06419715 | 1.01390507 |
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| $ \begin{array}{c} \mbox{C} 0.59150204 & 4.34120531 & -0.34211802 & C & -0.60496504 & 4.26177530 & -0.32738202 \\ \mbox{C} -2.74709820 & 3.10270822 & -0.12610501 & C & -2.75999120 & 3.01482822 & -0.11816201 \\ \mbox{C} -4.86234635 & 1.72922813 & 0.12605001 & C & -4.86698935 & 1.62485812 & 0.12548801 \\ \mbox{H} & 4.3990331 & -2.72274420 & 1.08904708 & H & 4.29094531 & -2.81539020 & 1.10004608 \\ \mbox{H} & 5.97613144 & -2.11769915 & 1.28659009 & H & 5.93646241 & -2.23113416 & 1.28636409 \\ \mbox{C} & 5.49613138 & -2.80822020 & -0.72743105 & C & 5.42750439 & -2.89766221 & -0.72915605 \\ \mbox{H} & -5.95628142 & -1.78078213 & 1.72723812 & H & -5.93938040 & -1.91304614 & 1.69413112 \\ \mbox{L} & -4.34368731 & -2.46833518 & 1.60539311 & H & -4.31942431 & -2.58329219 & 1.57073212 \\ \mbox{C} & -5.53075941 & -2.78521420 & -0.16312101 & C & -5.49440938 & -2.88668721 & -0.20826002 \\ \mbox{H} & 3.45564825 & 3.94888229 & -0.29157702 & H & 3.45068225 & 3.86771728 & -0.27755902 \\ \mbox{H} & -1.12619108 & 5.27019638 & -0.51609504 & H & -1.14057508 & 5.18927438 & -0.50669204 \\ \mbox{H} & -3.29339524 & 4.02109129 & -0.31376002 & H & -3.31135624 & 3.92921028 & -0.31074502 \\ \mbox{H} & -6.27280043 & -2.24716816 & -0.7659306 & H & -6.23925345 & -2.34760617 & -0.89735806 \\ \mbox{C} & 4.97067536 & 1.61152511 & 0.09486701 & C & 4.95502636 & 1.51834011 & 0.11246301 \\ \mbox{C} & 5.87632941 & 2.66298619 & -0.07224201 & C & 5.8695042 & 2.56105918 & -0.06293300 \\ \mbox{C} & 6.85298047 & 0.11233501 & 0.23865202 & C & 6.82435648 & 0.00174300 & 0.24222902 \\ \mbox{C} & 7.71688154 & 1.17991809 & 0.06913600 & C & 7.24409051 & 2.37353417 & -0.09071801 \\ \mbox{H} & 5.47932137 & 3.6527526 & -0.1982601 & H & 5.47980340 & 3.56678226 & -0.17891201 \\ \mbox{H} & 7.27422652 & -0.87745366 & 0.34878403 & H & 7.23717654 & -0.99185007 & 0.35920603 \\ \mbox{C} & -7.61712152 & 1.36110110 & 0.11541601 & C & -7.61904455 & 1.23533909 & 0.10430101 \\ \mbox{C} & -7.61742152 & 1.36110110 & 0.11541601 & C & -7.61904455 & 1.23533909 & 0.10430101 \\ \mbox{C} & -7.61742152 & 1.36110110 & $ | Ċ | 0 76280206 | 4 32580231 | -0.33658802 | Ċ | 0.75008505 | 4 24980830 | -0.31982302 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | Č | 0.50150204 | 4 34120531 | 0.34211802 | | 0.60496504 | 4 26177530 | 0.31702302 |
| $ \begin{array}{c} \text{C} & -\frac{2}{4}, \frac{4}{6}, \frac{3}{820} & \frac{5}{102}, \frac{102}{20822} & -0.12610501 \\ \text{C} & -\frac{4}{8}, \frac{6698935}{8090331} & \frac{1}{-2}, \frac{2}{7274420} & 1.08904708 \\ \text{H} & \frac{4}{3}, \frac{3}{3990331} & \frac{2}{-2}, \frac{2}{7274420} & 1.08904708 \\ \text{H} & \frac{4}{2}, \frac{2}{9094531} & \frac{2}{-2}, \frac{8}{8}, \frac{1}{8}, \frac{1}{2004608} \\ \text{H} & \frac{5}{-9}, \frac{5}{7613144} & \frac{2}{-2}, \frac{11769915}{11} & 1.28659009 \\ \text{C} & \frac{5}{-4}, \frac{2}{9}, \frac{3}{938040} & \frac{1}{-1}, \frac{1}{2}, \frac{3}{2}, \frac{3}{8}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{1}, \frac{1}{2}, \frac{2}{2}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{1}, \frac{1}{2}, \frac{2}{2}, \frac{1}{6}, \frac{1}{3}, \frac{1}{1}, \frac{1}{2}, \frac{2}{2}, \frac{1}{6}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}$ | C | -0.59150204 | 2 10270922 | -0.34211602 | | 2 75000120 | 4.20177330 | -0.32/36202 |
| $ \begin{array}{c} \mbox{C} = 4.86234035 & 1.72922813 & 0.12605001 & C & 4.86059353 & 1.62483812 & 0.12248801 \\ \mbox{H} = 5.97613144 & -2.11769915 & 1.28659009 & H & 5.93646241 & -2.81539020 & 1.10004608 \\ \mbox{H} = 5.97613144 & -2.11769915 & 1.28659009 & F & 5.93646241 & -2.23113416 & 1.286536409 \\ \mbox{C} = 5.49613138 & -2.80822020 & -0.72743105 & C & 5.42750439 & -2.89766221 & -0.72915605 \\ \mbox{H} & -5.95628142 & -1.78078213 & 1.72723812 & H & -5.9393804 & -1.91304614 & 1.69413112 \\ \mbox{C} & -5.53075941 & -2.78521420 & -0.16312101 & C & -5.49440938 & -2.88668721 & -0.20826002 \\ \mbox{H} & 3.45564825 & 3.94888229 & -0.29157702 & H & 3.45068225 & 3.86771728 & -0.27755902 \\ \mbox{H} & -1.31961810 & 5.27019638 & -0.50689304 & H & -1.30369909 & 5.16762937 & -0.49428504 \\ \mbox{H} & -1.12619108 & 5.27019638 & -0.51609504 & H & -1.14057508 & 5.18927438 & -0.50669204 \\ \mbox{H} & -3.29339524 & 4.02109129 & -0.31376002 & H & -3.31135624 & 3.92921028 & -0.31074502 \\ \mbox{H} & 6.29213144 & -2.24181216 & -1.22697709 & H & 6.22188945 & -2.33309517 & -1.23347509 \\ \mbox{H} & -6.27280043 & -2.24716816 & -0.76659306 & H & -6.23925345 & -2.34760617 & -0.80735806 \\ \mbox{C} & 4.97067536 & 1.61152511 & 0.09486701 & C & 4.95502636 & 1.51834011 & 0.11246301 \\ \mbox{C} & 5.87632941 & 2.66298619 & -0.07224201 & C & 5.8695042 & 2.56105918 & -0.06293300 \\ \mbox{C} & 6.85298047 & 0.11233501 & 0.23865202 & C & 6.82435648 & 0.00174300 & 0.24222902 \\ \mbox{C} & 7.71688154 & 1.17991809 & 0.06913600 & C & 7.69678556 & 1.06112807 & 0.06454300 \\ \mbox{C} & 7.25317453 & 2.48818218 & -0.08893301 & C & 7.24409051 & 2.37353417 & -0.09071801 \\ \mbox{H} & 5.47932137 & 3.66527526 & -0.19082601 & H & 5.47980340 & 3.56678226 & -0.17891201 \\ \mbox{H} & 5.47932137 & 3.66527526 & -0.19082601 & H & 5.47980340 & 3.56678226 & -0.17891201 \\ \mbox{H} & 5.47932137 & 3.66527526 & -0.19082601 & H & 5.47980340 & 3.56678226 & -0.17891201 \\ \mbox{H} & 7.22425054 & -0.67546005 & 0.56984104 & H & 7.21231754 & -0.98051900 & 0.36803203 \\ \mbox{C} & -7.61712152 & 1.36110$ | C | -2.74709820 | 5.102/0822 | -0.12010301 | | -2.73999120 | 5.01462622 | -0.11610201 |
| $ \begin{array}{llllllllllllllllllllllllllllllllllll$ | C | -4.86234635 | 1./2922813 | 0.12605001 | C | -4.86698935 | 1.62485812 | 0.12548801 |
| $ \begin{array}{llllllllllllllllllllllllllllllllllll$ | Н | 4.33990331 | -2.72274420 | 1.08904708 | H | 4.29094531 | -2.81539020 | 1.10004608 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | Н | 5.97613144 | -2.11769915 | 1.28659009 | H | 5.93646241 | -2.23113416 | 1.28636409 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | 5.49613138 | -2.80822020 | -0.72743105 | C | 5.42750439 | -2.89766221 | -0.72915605 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | Н | -5.95628142 | -1.78078213 | 1.72723812 | Н | -5.93938040 | -1.91304614 | 1.69413112 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | Н | -4.34368731 | -2.46833518 | 1.60539311 | н | -4.31942431 | -2.58329219 | 1.57073212 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | -5 53075941 | -2 78521420 | -0.16312101 | C | -5 49440938 | -2 88668721 | -0.20826002 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | ц Ц | 2 45564825 | 2 04882220 | 0.20157702 | ц Ц | 2 45068225 | 2 96771729 | 0.27755002 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | п 11 | 1.210(1010 | 5.94000229 | -0.29137702 | | 1.202(0000 | 5.60771726 | -0.27733902 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | н | 1.31961810 | 5.24239/38 | -0.50689304 | H | 1.30369909 | 5.16/6293/ | -0.49428504 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | Н | -1.12619108 | 5.27019638 | -0.51609504 | H | -1.1405/508 | 5.18927438 | -0.50669204 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | Н | -3.29339524 | 4.02109129 | -0.31376002 | H | -3.31135624 | 3.92921028 | -0.31074502 |
| H5.92888443-3.78680627-0.48342303H5.85531043-3.88178728-0.49902604H-6.27280043-2.24716816-0.76659306H-6.23925345-2.34760617-0.80735806C4.970675361.611525110.09486701C4.955026361.518340110.11246301C5.876329412.66298619-0.07224201C5.869050422.56105918-0.06293300C6.852980470.112335010.23865202C6.824356480.001743000.24222902C7.716881541.179918090.06913600C7.2696785561.061128070.06454300C7.253174532.48818218-0.08893301C7.244090512.37353417-0.09071801H5.479321373.66527526-0.19082601H5.479803403.56678226-0.17891201H7.27422652-0.877453060.34878403H7.23717654-0.991850070.35020603H8.780366620.972092070.06085600H8.758188650.843337060.04777700C-5.741401432.78300220-0.13950001C-5.753566422.67316919-0.13647601C-7.617121521.361101100.11541601C-7.619044551.235339090.10430101C-7.121797492.63964419-0.15226901C-7.132820522.51921118-0.15422701H-5.319720403.75975427-0.35035203H-5.338741363.65458626-0.33923902 <tr< td=""><td>Н</td><td>6.29213144</td><td>-2.24181216</td><td>-1.22697709</td><td>H</td><td>6.22188945</td><td>-2.33309517</td><td>-1.23347509</td></tr<> | Н | 6.29213144 | -2.24181216 | -1.22697709 | H | 6.22188945 | -2.33309517 | -1.23347509 |
| $\begin{array}{llllllllllllllllllllllllllllllllllll$ | Н | 5.92888443 | -3.78680627 | -0.48342303 | H | 5.85531043 | -3.88178728 | -0.49902604 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Н | -6.27280043 | -2.24716816 | -0.76659306 | Н | -6.23925345 | -2.34760617 | -0.80735806 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | С | 4 97067536 | 1 61152511 | 0.09486701 | C | 4 95502636 | 1 51834011 | 0 11246301 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Ċ | 5 87632041 | 2 66208610 | 0.07224201 | | 5 86005042 | 2 56105018 | 0.06203300 |
| C6.832930470.112333010.23863202C6.824336480.001743000.24222902C7.716881541.179918090.06913600C7.696785561.061128070.06454300C7.253174532.48818218-0.08893301C7.244090512.37353417-0.09071801H5.479321373.66527526-0.19082601H5.479803403.56678226-0.17891201H7.27422652-0.877453060.34878403H7.23717654-0.991850070.35020603H8.780366620.972092070.06085600H8.758188650.843337060.04777700C-5.741401432.78300220-0.13950001C-5.753566422.67316919-0.13647601C-6.780110490.292098020.38253203C-6.774468510.171409010.36803203C-7.617121521.361101100.11541601C-7.619044551.235339090.10430101C-7.121797492.63964419-0.15226901C-7.132820522.51921118-0.15422701H-5.319720403.75975427-0.35035203H-5.338741363.65458626-0.33923902H-7.22495054-0.675460050.56984104H-7.21231754-0.800519060.54922704H-8.685130651.177525080.11453201H-8.685592621.043511080.09932201C8.181175573.68783526-0.27419802C8.181651573.56437426-0.28452402 <t< td=""><td>C</td><td>6 95 2090 47</td><td>2.00298019</td><td>-0.07224201</td><td></td><td>6.02425649</td><td>2.30103918</td><td>-0.00293300</td></t<> | C | 6 95 2090 47 | 2.00298019 | -0.07224201 | | 6.02425649 | 2.30103918 | -0.00293300 |
| C7.716881541.179918090.06913600C7.696785561.061128070.06454300C7.253174532.48818218-0.08893301C7.244090512.37353417-0.09071801H5.479321373.66527526-0.19082601H5.479803403.56678226-0.17891201H7.27422652-0.877453060.34878403H7.23717654-0.991850070.35020603H8.780366620.972092070.06085600H8.758188650.843337060.04777700C-5.741401432.78300220-0.13950001C-5.753566422.67316919-0.13647601C-6.780110490.292098020.38253203C-6.774468510.171409010.36803203C-7.617121521.361101100.11541601C-7.619044551.235339090.10430101C-7.121797492.63964419-0.15226901C-7.132820522.51921118-0.15422701H-5.319720403.75975427-0.35035203H-5.338741363.65458626-0.33923902H-7.22495054-0.675460050.56984104H-7.21231754-0.800519060.54922704H-8.685130651.177525080.11453201H-8.685592621.043511080.09932201C-8.019395563.83878828-0.45425703C-8.038793563.71336427-0.45096003 | C | 0.8529804/ | 0.11233301 | 0.23805202 | | 0.82433048 | 0.001/4300 | 0.24222902 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | 7.71688154 | 1.17991809 | 0.06913600 | C | 7.69678556 | 1.06112807 | 0.06454300 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | С | 7.25317453 | 2.48818218 | -0.08893301 | C | 7.24409051 | 2.37353417 | -0.09071801 |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | Н | 5.47932137 | 3.66527526 | -0.19082601 | H | 5.47980340 | 3.56678226 | -0.17891201 |
| H8.780366620.972092070.06085600H8.758188650.843337060.04777700C-5.741401432.78300220-0.13950001C-5.753566422.67316919-0.13647601C-6.780110490.292098020.38253203C-6.774468510.171409010.36803203C-7.617121521.361101100.11541601C-7.619044551.235339090.10430101C-7.121797492.63964419-0.15226901C-7.132820522.51921118-0.15422701H-5.319720403.75975427-0.35035203H-5.338741363.65458626-0.33923902H-7.22495054-0.675460050.56984104H-7.21231754-0.800519060.54922704H-8.685130651.177525080.11453201H-8.685592621.043511080.09932201C8.181175573.68783526-0.27419802C8.181651573.56437426-0.28452402C-8.019395563.83878828-0.45425703C-8.038793563.71336427-0.45096003 | Η | 7.27422652 | -0.87745306 | 0.34878403 | H | 7.23717654 | -0.99185007 | 0.35020603 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Н | 8.78036662 | 0.97209207 | 0.06085600 | Н | 8.75818865 | 0.84333706 | 0.04777700 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | C | -5.74140143 | 2.78300220 | -0.13950001 | C | -5.75356642 | 2.67316919 | -0.13647601 |
| C -7.60712152 1.36110110 0.11541601 C -7.61904455 1.23533909 0.10430101 C -7.12179749 2.63964419 -0.15226901 C -7.13282052 2.51921118 -0.15422701 H -5.31972040 3.75975427 -0.35035203 H -5.33874136 3.65458626 -0.33923902 H -7.22495054 -0.67546005 0.56984104 H -7.21231754 -0.80051906 0.54922704 H -8.68513065 1.17752508 0.11453201 H -8.68559262 1.04351108 0.09932201 C 8.18117557 3.68783526 -0.27419802 C 8.18165157 3.56437426 -0.28452402 C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | č | -6 780110/0 | 0.20200220 | 0 38253203 | | -6 77446851 | 0 17140001 | 0 36803203 |
| C-7.017121321.301101100.11341001C-7.019044551.253539090.10430101C-7.121797492.63964419-0.15226901C-7.132820522.51921118-0.15422701H-5.319720403.75975427-0.35035203H-5.338741363.65458626-0.33923902H-7.22495054-0.675460050.56984104H-7.21231754-0.800519060.54922704H-8.685130651.177525080.11453201H-8.685592621.043511080.09932201C8.181175573.68783526-0.27419802C8.181651573.56437426-0.28452402C-8.019395563.83878828-0.45425703C-8.038793563.71336427-0.45096003 | C C | 7 61710150 | 1 26110110 | 0.115/11/01 | | 7 61004455 | 1 22522000 | 0.10/20101 |
| C -7.12179749 2.65964419 -0.15226901 C -7.13282052 2.51921118 -0.15422701 H -5.31972040 3.75975427 -0.35035203 H -5.33874136 3.65458626 -0.33923902 H -7.22495054 -0.67546005 0.56984104 H -7.21231754 -0.80051906 0.54922704 H -8.68513065 1.17752508 0.11453201 H -8.68559262 1.04351108 0.09932201 C 8.18117557 3.68783526 -0.27419802 C 8.18165157 3.56437426 -0.28452402 C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | Č | -/.01/12132 | 1.30110110 | 0.11341001 | | -/.01904433 | 1.23333909 | 0.10430101 |
| H -5.319/2040 3.75975427 -0.35035203 H -5.33874136 3.65458626 -0.33923902 H -7.22495054 -0.67546005 0.56984104 H -7.21231754 -0.80051906 0.54922704 H -8.68513065 1.17752508 0.11453201 H -8.68559262 1.04351108 0.09932201 C 8.18117557 3.68783526 -0.27419802 C 8.18165157 3.56437426 -0.28452402 C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | C | -/.121/9/49 | 2.03964419 | -0.15226901 | | -/.13282052 | 2.51921118 | -0.15422/01 |
| H-7.22495054-0.675460050.56984104H-7.21231754-0.800519060.54922704H-8.685130651.177525080.11453201H-8.685592621.043511080.09932201C8.181175573.68783526-0.27419802C8.181651573.56437426-0.28452402C-8.019395563.83878828-0.45425703C-8.038793563.71336427-0.45096003 | Н | -5.31972040 | 3.75975427 | -0.35035203 | H | -5.33874136 | 3.65458626 | -0.33923902 |
| H -8.68513065 1.17752508 0.11453201 H -8.68559262 1.04351108 0.09932201 C 8.18117557 3.68783526 -0.27419802 C 8.18165157 3.56437426 -0.28452402 C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | Н | -7.22495054 | -0.67546005 | 0.56984104 | H | -7.21231754 | -0.80051906 | 0.54922704 |
| C 8.18117557 3.68783526 -0.27419802 C 8.18165157 3.56437426 -0.28452402 C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | Η | -8.68513065 | 1.17752508 | 0.11453201 | H | -8.68559262 | 1.04351108 | 0.09932201 |
| C -8.01939556 3.83878828 -0.45425703 C -8.03879356 3.71336427 -0.45096003 | С | 8.18117557 | 3.68783526 | -0.27419802 | C | 8.18165157 | 3.56437426 | -0.28452402 |
| | C | -8.01939556 | 3.83878828 | -0.45425703 | C | -8.03879356 | 3.71336427 | -0.45096003 |

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