Electronic Supplementary Information TYPE

ARTICLE

Evaluating the Cation Binding Strength and Selectivity of Calix[4]pyrroles: A Computational and ESI-MS/MS Study

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Figure S1. Plot of Binding Energies with (--) and without BSSE (•) for all [1+X]⁺ complexes at M052X/6-31g(d) for Li⁺, Na⁺, K⁺ and with effective core potentials and valence basis sets of Hay and Wadt for Rb⁺ and Cs⁺ complexes. 10

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5 Figure S2. AIM topological graph for the parent complex and fragments of [1+Li]⁺ at B3LYP/6-31G* level of theory.



Figure S3. AIM topological graph for the parent complex and fragments of [1+Na]⁺ at B3LYP/6-31G* level of theory.



Figure S4. CID product ion spectra of a) $[1+Li]^+$ (*m*/*z* 435), b) $[1+Na]^+$ (*m*/*z* 451), c) $[1+K]^+$ (*m*/*z* 467), d) $[1+Rb]^+$ (*m*/*z* 513), and e) $[1+Cs]^+$ (*m*/*z* 561) at a collision energy of 30 eV.

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m/z 154

m/z 221



m/z 261

m/z 328



Figure S5. Optimized geometries of **1** showing cation to centroid of pyrrole ring distances of various fragments complexed with Li⁺ ion calculated at M05-2X/TZVP level of theory.



m/z 384

Figure S6. Optimized geometries of **1** showing cation to centroid of pyrrole ring distances of various fragments complexed with Na⁺ ion calculated at M05-2X/TZVP level of theory.



Figure S7. CID dissociation curves for the complexes of CP (1-5) with **a**) Li^+ **b**) Na^+ **c**) K^+ **d**) Rb^+ and **e**) Cs^+ . The 5 $E_{com}^{50\%}$ values were presented in parentheses (eV).

| Table S1: Dihedral angles (| A) between two | adjacent pyrrol | e rings connected | by the methylene grou | up. ^a |
|-----------------------------|----------------|---------------------------------------|-------------------|-----------------------|------------------|
| | .) | · · · · · · · · · · · · · · · · · · · | | | ~r · |

| Complexes | ab | ab' | a′b | a′b′ |
|---------------------------|---------|----------|----------|---------|
| 1 | 127.867 | -127.903 | -127.903 | 127.867 |
| 1-Li+ | 110.721 | -133.897 | -133.897 | 110.721 |
| 1- Na ⁺ | 108.974 | -111.748 | -111.753 | 108.972 |
| 1-K ⁺ | 98.051 | -98.053 | -98.053 | 98.051 |
| $1-Rb^+$ | 96.601 | -96.588 | -96.590 | 96.604 |
| 1- Cs ⁺ | 139.763 | -139.729 | -139.729 | 139.763 |

^a The atoms chosen to measure the dihedral angle is shown as bold ones in Fig.3

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Table S2: Energy components in kcal/mol obtained from LMOEDA technique incorporated in GAMESS software.

| Complex | Elec | Exch | Rep | Pol | Disp | IE |
|--------------------|--------|-------|-------|--------|--------|--------|
| CP-Li ⁺ | -43.47 | -2.36 | 14.61 | -38.09 | -12.79 | -82.09 |
| CP-Na ⁺ | -44.54 | -3.08 | 23.57 | -25.42 | -19.82 | -69.30 |

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Table S3: Electron density (ρ) and Laplacian of electron density (∇^2) at the bond critical points (BCP, R) and cage critical points (CCP, π) obtained for the parent and various fragments of Li, Na and K complexes of 1 obtained at B3LYP/6-31G*//M05-2X/6-31G* level.

| 5 | | | | | | | | | | | | |
|-----------|---------|--------------|---------|--------------|--------|-----------------|--------|-----------------|--------|----------------|--------|-----------------|
| Complexes | π_1 | | π_2 | | | R_a | | $R_{a'}$ | | R _b | | R _{b'} |
| complexes | Р | $ abla^2 ho$ | ρ | $ abla^2 ho$ | ρ | $\nabla^2 \rho$ | ρ | $\nabla^2 \rho$ | ρ | $ abla^2 ho$ | ρ | $\nabla^2 \rho$ |
| Li-154 | 0.0168 | -0.270 | Х | х | 0.0186 | -0.0316 | Х | х | Х | х | Х | х |
| Li-221 | 0.0144 | -0.0217 | -a- | -a- | 0.0229 | -0.0319 | 0.0175 | -0.0255 | х | х | х | Х |
| Li-261 | 0.150 | 0.225 | -a- | -a- | 0.0227 | -0.0314 | 0.0184 | -0.0272 | X | Х | Х | Х |
| Li-328 | -a- | -a- | -a- | -a- | 0.0116 | -0.0136 | 0.0143 | -0.0176 | 0.0128 | -0.0170 | Х | х |
| Li-368 | 0.0114 | -0.0166 | 0.0116 | -0.0163 | 0.0129 | -0.0154 | 0.0135 | -0.0175 | 0.0133 | -0.0169 | х | Х |
| Li-Parent | -a- | -a- | -a- | -a- | 0.0134 | -0.0164 | 0.0134 | -0.0164 | 0.0134 | -0.0164 | 0.0134 | -0.0164 |
| Na-170 | 0.0111 | -0.0163 | X | х | 0.0159 | -0.0199 | Х | х | X | Х | Х | Х |
| Na-237 | -a- | -a- | -a- | -a- | 0.0134 | -0.0161 | 0.0132 | -0.0158 | Х | Х | Х | Х |
| Na-277 | -a- | -a- | -a- | -a- | 0.0125 | -0.0155 | 0.0132 | -0.0160 | Х | х | Х | х |
| Na-344 | 0.0096 | -0.0139 | 0.0097 | -0.0138 | 0.0125 | -0.0147 | 0.0118 | -0.0142 | 0.0123 | -0.0148 | Х | Х |
| Na-384 | 0.0084 | -0.0116 | 0.0084 | -0.0116 | 0.0124 | -0.0147 | 0.0114 | -0.0129 | 0.0114 | -0.0129 | Х | х |
| Na-Parent | 0.0076 | -0.0098 | 0.0076 | -0.0098 | 0.0102 | -0.0135 | 0.0102 | -0.0135 | 0.0126 | -0.0150 | 0.0126 | -0.0150 |
| K-Parent | 0.0089 | -0.0119 | 0.0089 | -0.0119 | 0.0121 | -0.0134 | 0.0129 | -0.0124 | 0.0121 | -0.134 | 0.0129 | -0.0124 |

-a- The corresponding cage critical point is not observed.

^x The corresponding bond critical point is not present.

Table S4: Binding Energies (BE in kcal/mol) of the precursor ions, $[1+X]^+$ where $X^+ = Li$, Na, K, Rb, Cs, and the product ions (fragment ions) computed at B2PLYP/TZVP level of theory.

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| | | Bi | nding En | ergies | | |
|----|------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| | Precursor ion | | Pr | oduct io | 15 | |
| | [1 +Li] ⁺ | <i>m/z</i> 154 | <i>m/z</i> 221 | <i>m/z</i> 261 | <i>m/z</i> 328 | <i>m/z</i> 368 |
| 10 | (-74.24) | (-44.95) | (-61.88) | (-62.79) | (-74.78) | (-74.81) |
| | [1 +Na] ⁺ | <i>m/z</i> 170* | <i>m/z</i> 237 | <i>m/z</i> 277 | <i>m/z</i> 344 | <i>m/z</i> 384 |
| | (-59.55) | (-29.79) | (-46.03) | (-46.06) | (-55.88) | (-55.46) |
| 15 | [1 +K] ⁺ | <i>m/z</i> 186* | <i>m/z</i> 253* | <i>m/z</i> 293* | <i>m/z</i> 360* | <i>m/z</i> 400* |
| | (-46.49) | (-19.59) | (-22.50) | (-29.73) | (-36.73) | (-38.81) |
| | [1 +Rb] ⁺ | <i>m/z</i> 233* | <i>m/z</i> 299* | <i>m/z</i> 339* | <i>m/z</i> 406* | <i>m/z</i> 446* |
| 20 | (-30.34) | (-16.85) | (-25.79) | (-26.61) | (-34.83) | (-35.31) |
| | [1 +Cs] ⁺ | <i>m/z</i> 281* | <i>m/z</i> 347* | <i>m/z</i> 387* | <i>m/z</i> 454* | <i>m/z</i> 494* |
| | (-19.22) | (-12.31) | (-8.55) | (-18.57) | (-19.26) | (-21.91) |
| | * - · · · | | - | | | |

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* Ions are not observed experimentally

| Ср | p-Parent | | | | | | |
|-------------|-----------|-----------|-----------|-------------|-----------|-----------|-----------|
| | | | | 60 c | 0.615437 | 4.420249 | 1.081988 |
| С | 1.633765 | -2.640979 | 1.857749 | Н | -0.143580 | 5.076018 | 1.505450 |
| С | 1.067733 | -2.658081 | 0.608599 | Н | 1.048038 | 3.826768 | 1.884774 |
| 10 N | 1.698667 | -1.698687 | -0.134800 | Н | 1.400912 | 5.029335 | 0.640481 |
| С | 2.658134 | -1.067733 | 0.608489 | С | -0.615486 | 4.420306 | -1.081710 |
| С | 2.640733 | -1.633324 | 1.857837 | 65 н | 0.143518 | 5.076080 | -1.505186 |
| Н | 3.284263 | -1.370564 | 2.677046 | Н | -1.048151 | 3.826860 | -1.884488 |
| С | 3.526351 | 0.00000 | -0.000099 | Н | -1.400924 | 5.029382 | -0.640120 |
| 15 с | 2.658081 | 1.067733 | -0.608599 | С | 4.420306 | 0.615486 | 1.081710 |
| C | 2.640979 | 1.633765 | -1.857749 | H | 3.826860 | 1.048151 | 1.884488 |
| С | 1.067733 | 2.658134 | -0.608489 | 70 н | 5.076080 | -0.143518 | 1.505186 |
| С | 1.633324 | 2.640733 | -1.857837 | Н | 5.029382 | 1.400924 | 0.640120 |
| Н | 3.284719 | 1.371315 | -2.676896 | C | 4.420249 | -0.615437 | -1.081988 |
| 20 H | 1.370564 | 3.284263 | -2.677046 | н | 3.826768 | -1.048038 | -1.884774 |
| N | 1.698687 | 1.698667 | 0.134800 | H | 5.076018 | 0.143580 | -1.505450 |
| Н | 1.414093 | -1.414196 | -1.056319 | 75 н | 5.029335 | -1.400912 | -0.640481 |
| С | 0.00000 | 3.526351 | 0.000099 | | | | |
| C | -1 067733 | 2 658081 | 0 608599 | | | | |
| 25 č | -2.658134 | 1.067733 | 0.608489 | Cp | -T.i | | |
| C | -2.640733 | 1.633324 | 1.857837 | op | | | |
| C | -1.633765 | 2.640979 | 1.857749 | 80 C | -1.396803 | 2.478258 | 1,993140 |
| C | -3 526351 | 0 000000 | -0 000099 | C | -0 745494 | 2 640203 | 0 806278 |
| C | -2 658081 | -1 067733 | -0 608599 | N | -1 421033 | 1 886357 | -0 141552 |
| 30 c | -2.640979 | -1.633765 | -1.857749 | C | -2.557846 | 1.334343 | 0.426573 |
| С | -1.633324 | -2.640733 | -1.857837 | C | -2.543247 | 1.654890 | 1.752178 |
| C | -1.067733 | -2.658134 | -0.608489 | 85 н | -3.269935 | 1.347337 | 2.481812 |
| C | 0.00000 | -3.526351 | 0.000099 | С | -3.455244 | 0.450260 | -0.393007 |
| N | -1.698667 | 1.698687 | -0.134800 | C | -2.640203 | -0.745494 | -0.806278 |
| 35 N | -1.698687 | -1.698667 | 0.134800 | C | -2.478258 | -1.396803 | -1.993140 |
| Н | -3.284263 | 1.370564 | 2.677046 | С | -1.334343 | -2.557846 | -0.426573 |
| Н | -3.284719 | -1.371315 | -2.676896 | 90 с | -1.654890 | -2.543247 | -1.752178 |
| Н | -1.370564 | -3.284263 | -2.677046 | Н | -2.910644 | -1.108826 | -2.933641 |
| Н | -1.414093 | 1.414196 | -1.056319 | Н | -1.347337 | -3.269935 | -2.481812 |
| 40 н | -1.371315 | 3.284719 | 2.676896 | Ν | -1.886357 | -1.421033 | 0.141552 |
| Н | 1.371315 | -3.284719 | 2.676896 | Н | -1.312471 | 2.043811 | -1.130932 |
| Н | -1.414196 | -1.414093 | 1.056319 | 95 с | -0.450260 | -3.455244 | 0.393007 |
| Н | 1.414196 | 1.414093 | 1.056319 | С | 0.745494 | -2.640203 | 0.806278 |
| С | 0.615486 | -4.420306 | -1.081710 | С | 2.557846 | -1.334343 | 0.426573 |
| 45 н | 1.048151 | -3.826860 | -1.884488 | С | 2.543247 | -1.654890 | 1.752178 |
| Н | 1.400924 | -5.029382 | -0.640120 | С | 1.396803 | -2.478258 | 1.993140 |
| Н | -0.143518 | -5.076080 | -1.505186 | 100 с | 3.455244 | -0.450260 | -0.393007 |
| С | -0.615437 | -4.420249 | 1.081988 | С | 2.640203 | 0.745494 | -0.806278 |
| Н | -1.048038 | -3.826768 | 1.884774 | С | 2.478258 | 1.396803 | -1.993140 |
| 50 н | -1.400912 | -5.029335 | 0.640481 | С | 1.654890 | 2.543247 | -1.752178 |
| Н | 0.143580 | -5.076018 | 1.505450 | С | 1.334343 | 2.557846 | -0.426573 |
| С | -4.420249 | 0.615437 | -1.081988 | 105 с | 0.450260 | 3.455244 | 0.393007 |
| Н | -3.826768 | 1.048038 | -1.884774 | Ν | 1.421033 | -1.886357 | -0.141552 |
| Н | -5.076018 | -0.143580 | -1.505450 | Ν | 1.886357 | 1.421033 | 0.141552 |
| 55 н | -5.029335 | 1.400912 | -0.640481 | Н | 3.269935 | -1.347337 | 2.481812 |
| С | -4.420306 | -0.615486 | 1.081710 | Н | 2.910644 | 1.108826 | -2.933641 |
| Н | -5.029382 | -1.400924 | 0.640120 | 110 н | 1.347337 | 3.269935 | -2.481812 |
| Н | -3.826860 | -1.048151 | 1.884488 | Н | 1.312471 | -2.043811 | -1.130932 |
| Н | -5.076080 | 0.143518 | 1.505186 | Н | 1.108826 | -2.910644 | 2.933641 |

Table S5: Cartesian coordinates of the complexes considered in the study at M05-2X/TZVP level of theory

| Н | -1.108826 | 2,910644 | 2,933641 | 60 с | 2.746174 | -0.413815 | 1,953830 |
|-----------------|----------------------|------------------------|----------------------|------------------------|------------------------|----------------------|------------------------|
| Н | 2.043811 | 1.312471 | 1.130932 | С | 2.168968 | 2.786725 | 0.087275 |
| Н | -2.043811 | -1.312471 | 1.130932 | С | 0.809914 | 2.697929 | -0.563486 |
| С | 0.00000 | 4.652342 | -0.452028 | С | 0.416727 | 2.693075 | -1.879103 |
| 5н | -0.545511 | 4.337214 | -1.339599 | С | -1.001001 | 2.510550 | -1.908004 |
| Н | -0.651972 | 5.288377 | 0.141138 | 65 с | -1.434200 | 2.409264 | -0.608779 |
| Н | 0.865054 | 5.231602 | -0.768374 | С | -2.797292 | 2.163282 | -0.008961 |
| С | 1.187156 | 3.971941 | 1.631318 | Ν | 2.537371 | 0.322060 | -0.119935 |
| Н | 1.482982 | 3.163100 | 2.297530 | Ν | -0.320919 | 2.500961 | 0.190455 |
| 10 н | 2.076210 | 4.518049 | 1.326040 | Н | 2.517318 | 1.622031 | 2.860873 |
| Н | 0.543216 | 4.646201 | 2.191591 | 70 н | 1.056144 | 2.850944 | -2.728171 |
| С | 3.971941 | -1.187156 | -1.631318 | Н | -1.625306 | 2.507383 | -2.782839 |
| Н | 3.163100 | -1.482982 | -2.297530 | Н | 2.753136 | 0.371155 | -1.100785 |
| Н | 4.646201 | -0.543216 | -2.191591 | Н | 2.865985 | -1.056561 | 2.806533 |
| 15 н | 4.518049 | -2.076210 | -1.326040 | H | -2.866005 | 1.056329 | 2.806540 |
| С | 4.652342 | 0.00000 | 0.452028 | 75 н | -0.335215 | 2.439466 | 1.194126 |
| Н | 5.288377 | 0.651972 | -0.141138 | Н | 0.335182 | -2.439564 | 1.193924 |
| Н | 4.337214 | 0.545511 | 1.339599 | С | -3.861734 | 2.200327 | -1.108246 |
| H | 5.231602 | -0.865054 | 0.768374 | Н | -3.666702 | 1.477577 | -1.899114 |
| 20 c | -1.187156 | -3.971941 | 1.631318 | H | -4.835368 | 1.982297 | -0.676654 |
| Н | -0.543216 | -4.646201 | 2.191591 | 80 H | -3.893613 | 3.188185 | -1.562604 |
| Н | -1.482982 | -3.163100 | 2.297530 | С | -3.126469 | 3.236762 | 1.030980 |
| Н | -2.076210 | -4.518049 | 1.326040 | Н | -2.405106 | 3.252622 | 1.845396 |
| 25 ··· | 0.000000 | -4.652342 | -0.452028 | Н | -3.127844 | 4.214927 | 0.556594 |
| 23 H | -0.865054 | -5.231602 | -0./683/4 | н 95 а | -4.110312 | 3.050195 | 1.455568 |
| H | 0.545511 | -4.33/214 | -1.339599 | 83 C | 3.223539 | 3.146/90 | -0.962469 |
| H | 0.651972 | -5.288377 | 0.141138 | H | 3.255389 | 2.429109 | -1.780659 |
| U U | -4.052342 | 0.000000 | 1 220500 | н | 3.008342 | 4.125208 | -1.386352 |
| 30 ^H | -4.33/214 | -0.545511 | 1.339399 | н С | 4.204252 2 174227 | 3.1/4914 | -0.494476 |
| л 30 н | -5.231002 | -0 651072 | -0 1/1120 | 00 ^U | 2.1/422/ | J.000J04 | 1.1//303 |
| C II | -3.200377 | 1 187156 | -1 631318 | ло II Ц | 1,954000 | 3 651189 | 1 962997 |
| с н | -3 163100 | 1 482982 | -2 297530 | H II | 3 159590 | 3 917613 | 1 634307 |
| н | -4 646201 | 0 543216 | -2 191591 | C | 3 126429 | -3 236851 | 1 030792 |
| 35 H | -4.518049 | 2.076210 | -1.326040 | Н | 4.110261 | -3.050323 | 1.455426 |
| Li | 0.000000 | 0.000000 | 0.000000 | 95 н | 2.405043 | -3.252780 | 1.845186 |
| | | | | H | 3.127818 | -4.214974 | 0.556320 |
| | | | | С | 3.861767 | -2.200232 | -1.108319 |
| Cp- | -Na | | | Н | 3.893653 | -3.188048 | -1.562768 |
| 40 | | | | Н | 3.666770 | -1.477405 | -1.899124 |
| С | -2.746193 | 0.413653 | 1.953785 | 100 н | 4.835388 | -1.982251 | -0.676672 |
| С | -2.748966 | 0.807421 | 0.646721 | С | -2.174254 | -3.860603 | 1.176911 |
| Ν | -2.537412 | -0.322055 | -0.120044 | Н | -1.451099 | -3.651352 | 1.962638 |
| С | -2.455906 | -1.436656 | 0.691752 | Н | -3.159628 | -3.917753 | 1.633887 |
| 45 c | -2.561083 | -1.004474 | 1.982430 | H | -1.934620 | -4.826172 | 0.738488 |
| Н | -2.517234 | -1.622253 | 2.860665 | 105 c | -3.223511 | -3.146720 | -0.962832 |
| С | -2.168972 | -2.786734 | 0.086971 | Н | -3.255341 | -2.428975 | -1.780966 |
| С | -0.809898 | -2.697880 | -0.563743 | Н | -3.008295 | -4.125103 | -1.386788 |
| co ^C | -0.416674 | -2.692909 | -1.879349 | Н | -4.204238 | -3.174890 | -0.494869 |
| 50 C | 1.434216 | -2.409207 | -0.608946 | Na | -0.000035 | 0.000024 | -0.784681 |
| C | 1.001055 | -2.510378 | -1.908193 | 110 | | | |
| H | -1.056066 | -2.850704 | -2./28449 | | | | |
| H | 1.625384 | -2.50/134 | -2./83010 | | | | |
| N 55 TT | U.32U912 | -2.3009// | U.19U248 | 0 | V | | |
| 55 H | -2.133218 | -0.3/10/2 | -1.100889 | 115 Cp- | L. | | |
| C | 2.191209 2 710016 | -2.1032/9 -0 807/76 | -0.009065 | 110 | _0 712002 | 2 272207 | -2 010114 |
| C | 2./40940 2 /55226 | -U.0U/4/0 1 /26506 | 0.040/34 0 601050 | C | -U./13003 -1 131000 | 2.3/33U/ 2 552022 | -2.019144 -0 730245 |
| C | 2.40000 | 1 004317 | 1 982590 | N | 0 000000 | 2.JJ2922 2 636830 | 0.750245 |
| <u> </u> | | | | ± N | | | |

| С | 1.131920 | 2.552931 | -0.730217 | 60 н | 3.442976 | 3.689913 | -1.655511 |
|-----------------|-----------|-----------|-----------|--------------|-----------|-----------|------------------------|
| С | 0.713934 | 2.373317 | -2.019127 | Н | 4.558512 | 2.654219 | -0.748031 |
| Н | 1.349204 | 2.266545 | -2.879308 | С | 2.673870 | 3.575195 | 0.962679 |
| С | 2.506142 | 2.500283 | -0.112036 | Н | 1.985757 | 3.437338 | 1.796250 |
| 5с | 2.677088 | 1.130151 | 0.503758 | Н | 3.684099 | 3.542406 | 1.364283 |
| С | 3.036408 | 0.714205 | 1.763771 | 65 н | 2.506803 | 4.557965 | 0.528487 |
| С | 2.677086 | -1.130159 | 0.503731 | K | 0.00000 | 0.00000 | 1.408302 |
| С | 3.036407 | -0.714243 | 1.763754 | | | | |
| Н | 3.309210 | 1.352415 | 2.584645 | | | | |
| 10 н | 3.309208 | -1.352475 | 2.584611 | Ср | -Rb | | |
| Ν | 2.454028 | 0.000005 | -0.239088 | 70 | | | |
| Н | -0.000013 | 3.040943 | 0.975524 | С | -0.713667 | -2.331686 | 2.155419 |
| С | 2.506137 | -2.500275 | -0.112095 | С | -1.131510 | -2.534371 | 0.870044 |
| С | 1.131900 | -2.552922 | -0.730245 | N | -0.000010 | -2.630202 | 0.084268 |
| 15 c | -1.131920 | -2.552931 | -0.730217 | C | 1.131567 | -2.534402 | 0.869936 |
| С | -0.713934 | -2.373317 | -2.019127 | 75 c | 0.713851 | -2.331698 | 2.155350 |
| С | 0.713883 | -2.373307 | -2.019144 | Н | 1.349379 | -2.209734 | 3.013289 |
| С | -2.506142 | -2.500283 | -0.112036 | С | 2.507934 | -2.498992 | 0.257347 |
| C | -2.677088 | -1.130151 | 0.503758 | С | 2.710917 | -1.129222 | -0.349812 |
| 20 c | -3.036408 | -0.714205 | 1.763771 | C | 3.205864 | -0.713843 | -1.563242 |
| С | -3.036407 | 0.714243 | 1.763754 | 80 C | 2.710914 | 1.129288 | -0.349670 |
| С | -2.677086 | 1.130159 | 0.503731 | С | 3.205862 | 0.714064 | -1.563152 |
| С | -2.506137 | 2.500275 | -0.112095 | Н | 3.565036 | -1.352091 | -2.350064 |
| AC N | 0.00000 | -2.636830 | 0.056152 | Н | 3.565037 | 1.352413 | -2.349891 |
| 23 N | -2.454028 | -0.000005 | -0.239088 | N 05 | 2.409278 | -0.000011 | 0.364550 |
| Н | -1.349204 | -2.266545 | -2.879308 | 83 H | -0.000060 | -3.070047 | -0.818263 |
| Н | -3.309210 | -1.352415 | 2.584645 | C | 2.507934 | 2.498978 | 0.257666 |
| H | -3.309208 | 1.3524/5 | 2.584611 | C | 1.131490 | 2.534382 | 0.8/00/8 |
| 20 ^H | 0.000013 | -3.040943 | 0.975524 | С | -1.13158/ | 2.534403 | 0.869894 |
| 30 H | 1.349132 | -2.266528 | -2.8/9340 | | -0.713912 | 2.331657 | 2.155315 |
| H | -1.349132 | 2.200520 | -2.8/9340 | 90 C | 0.713605 | 2.331/38 | 2.133449 |
| п u | -2.109227 | -0.000019 | -1 185651 | C | -2.307932 | 2.490997 | -0 3/9901 |
| п | -2 672000 | 2 575216 | -1.103031 | C | -2.710902 | 1.129225 | -0.349901 -1.562241 |
| 35 " | -2.075099 | 3 / 37/08 | 1 796159 | C | -3.205823 | -0 714062 | -1.563249 |
| уу п н | -2 506864 | 4 557978 | 0 528363 | 95 č | -2 710904 | -1 129285 | -0 349754 |
| H | -3 684126 | 3 542405 | 1 364193 |))) () () | -2507934 | -2 498975 | 0 257586 |
| C | -3 569377 | 2 712234 | -1 195739 | N | 0 000018 | 2 630202 | 0 084264 |
| H | -3.505586 | 1.953760 | -1.972738 | N | -2.409281 | 0.000016 | 0.364471 |
| 40 н | -4.558492 | 2.654164 | -0.748148 | Н | -1.349469 | 2.209658 | 3.013227 |
| H | -3.442952 | 3.689863 | -1.655615 | 100 н | -3.564976 | 1.352092 | -2.350173 |
| С | -2.673870 | -3.575195 | 0.962679 | Н | -3.564979 | -1.352412 | -2.349996 |
| Н | -1.985757 | -3.437338 | 1.796250 | Н | 0.000100 | 3.070031 | -0.818275 |
| Н | -3.684099 | -3.542406 | 1.364283 | Н | 1.349020 | 2.209834 | 3.013477 |
| 45 н | -2.506803 | -4.557965 | 0.528487 | Н | -1.349111 | -2.209711 | 3.013418 |
| С | -3.569407 | -2.712279 | -1.195648 | 105 н | -1.968673 | 0.000078 | 1.271236 |
| Н | -4.558512 | -2.654219 | -0.748031 | Н | 1.968640 | -0.000071 | 1.271301 |
| Н | -3.505650 | -1.953816 | -1.972660 | С | -2.665222 | -3.572940 | -0.819720 |
| Н | -3.442976 | -3.689913 | -1.655511 | Н | -1.990329 | -3.415258 | -1.661090 |
| 50 с | 3.569377 | -2.712234 | -1.195739 | Н | -2.473497 | -4.554533 | -0.392784 |
| Н | 3.442952 | -3.689863 | -1.655615 | 110 н | -3.680244 | -3.560983 | -1.210088 |
| Н | 3.505586 | -1.953760 | -1.972738 | С | -3.562185 | -2.730358 | 1.347012 |
| Н | 4.558492 | -2.654164 | -0.748148 | Н | -3.506171 | -1.967588 | 2.120269 |
| С | 2.673899 | -3.575216 | 0.962586 | Н | -4.554253 | -2.689225 | 0.904118 |
| 55 н | 3.684126 | -3.542405 | 1.364193 | Н | -3.416638 | -3.704952 | 1.807894 |
| Н | 1.985778 | -3.437408 | 1.796159 | 115 с | -2.665014 | 3.572807 | -0.820234 |
| Н | 2.506864 | -4.557978 | 0.528363 | Н | -1.990026 | 3.414949 | -1.661495 |
| С | 3.569407 | 2.712279 | -1.195648 | Н | -3.679985 | 3.560856 | -1.210732 |
| Н | 3.505650 | 1.953816 | -1.972660 | Н | -2.473285 | 4.554455 | -0.393428 |

| C | -3 562316 | 2 730604 | 1 346508 | 60 ¤ | 1 861717 | 0 000263 | 1 369155 |
|------------------|-----------------------|------------|------------|-----------------|------------------------|----------------------|------------|
| с ц | -4 554326 | 2 689/55 | 1.0403488 | UU II | _1 861763 | -0.000203 | 1 360117 |
| 11 11 | -3.506442 | 1 067045 | 2 110001 | C | -1.001703 | 2 560510 | -0 669570 |
| п | -3.300442 | 2 705250 | 2.119004 | | 1 001600 | 2 204021 | -0.0000079 |
| 5 C | -3.410779 | 2 720257 | 1 247125 | п | 1.901023 | J.J940ZI 4 550752 | -1.312210 |
| 50 | 3.JUZIJZ 2.41CE02 | 2.730337 | 1.000005 | б 5 ц | 2.440333 | 4.550755 | 1 055200 |
| H | 3.416593 | 3.704950 | 1.808005 | 05 н | 3.000113 | 3.5/3134 | -1.055308 |
| н | 3.506111 | 1.96/585 | 2.120379 | U | 3.559200 | 2.746900 | 1.301630 |
| H | 4.554234 | 2.089222 | 0.904263 | н | 3.512604 | 1.984074 | 2.2/5330 |
| 10 | 2.665261 | 3.572943 | -0.819634 | H | 4.551278 | 2.716789 | 1.05/882 |
| 10 H | 3.680296 | 3.560981 | -1.209968 | 70 ^H | 3.401672 | 3.720477 | 1.960826 |
| H | 1.990396 | 3.415264 | -1.661026 | /0 C | 2.650821 | -3.5/0041 | -0.666611 |
| H | 2.4/3526 | 4.554536 | -0.392705 | H | 1.983159 | -3.395287 | -1.510/49 |
| C | 3.562282 | -2./30594 | 1.346631 | H | 3.66/444 | -3.5/3583 | -1.052/20 |
| H 15 | 3.506384 | -1.96/931 | 2.120003 | Н | 2.4414/8 | -4.551079 | -0.246503 |
| 15 н | 3.416731 | -3.705247 | 1.807387 | 75 | 3.558717 | -2.745801 | 1.503638 |
| Н | 4.554308 | -2.689446 | 0.903643 | / 5 H | 4.551058 | -2.715657 | 1.060478 |
| С | 2.665054 | -3.572803 | -0.820137 | Н | 3.511415 | -1.982528 | 2.276858 |
| Н | 1.990093 | -3.414949 | -1.661422 | Н | 3.401213 | -3.719154 | 1.963319 |
| an ^H | 3.680038 | -3.560849 | -1.210600 | С | -3.559247 | -2.747072 | 1.501258 |
| 20 H | 2.473312 | -4.554452 | -0.393336 | H | -3.401738 | -3.720699 | 1.960355 |
| Rb | 0.000006 | -0.000016 | -1.665695 | 80 H | -3.512669 | -1.984329 | 2.275041 |
| | | | | H | -4.551313 | -2.716908 | 1.057485 |
| - | - | | | С | -2.649721 | -3.569461 | -0.669009 |
| Cp- | Cs | | | H | -3.666096 | -3.573042 | -1.055763 |
| 25 | | 0 001 15 1 | | H O <i>F</i> | -1.981592 | -3.393887 | -1.512612 |
| C | 0.713988 | 2.281454 | 2.308725 | 83 H | -2.440356 | -4.550748 | -0.249488 |
| С | 1.131187 | 2.521198 | 1.028541 | С | -3.558761 | 2.745623 | 1.503847 |
| Ν | -0.000131 | 2.643503 | 0.249801 | Н | -3.511477 | 1.982266 | 2.276986 |
| 20 ° | -1.130972 | 2.521033 | 1.029197 | Н | -3.401263 | 3.718926 | 1.963635 |
| 30 C | -0.713012 | 2.281390 | 2.309146 | | -4.551092 | 2.715529 | 1.060663 |
| H | -1.348527 | 2.134507 | 3.163206 | 90 C | -2.650819 | 3.5/0090 | -0.666297 |
| C | -2.506518 | 2.498401 | 0.415266 | H | -1.983137 | 3.395426 | -1.510438 |
| C | -2.730983 | 1.128830 | -0.186590 | H | -3.66/433 | 3.5/3669 | -1.052430 |
| 25 0 | -3.324313 | 0./13/48 | -1.355962 | H | -2.441489 | 4.551084 | -0.246082 |
| 330 | -2.730947 | -1.128623 | -0.18/352 | 05 US | 0.000035 | 0.000139 | -1.802081 |
| C II | -3.324262 | -0.712760 | -1.336439 | 95 | | | |
| п | -3.743740 | 1.352204 | -2.112323 | т : | 1 = 4 | | |
| H | -3./43041 2.27100/ | -1.350705 | -2.113283 | <u>гт</u> _ | 154 | | |
| /0 ^{IN} | -2.371004 | -0.000119 | -0 6499230 | C | -2 100166 | -0 262021 | _0 007400 |
| ч 0 п | -0.000401 | -2 409625 | -0.040003 | 100° | -2.490100 -1.120271 | -0.303921 | -0.007400 |
| C | -2.300413 | -2.490023 | 1 028258 | 100 C | -1.139271 | 1 /0424 | -0.014072 |
| C | 1 120020 | -2.521350 | 1 020250 | C | 1 120201 | 1.490555 | -0.014676 |
| C | 0 712950 | -2 281627 | 2 308924 | C | 0 711957 | 1 / 90619 | 0.014070 |
| 45 č | -0.712000 | -2 281764 | 2 308486 | н | -1 352896 | 2 352711 | 0.121369 |
| ч у С | 2 506497 | -2 498465 | 0 415062 | 105 H | 1 352759 | 2.352834 | 0.121305 |
| C | 2 730977 | -1 128832 | -0 186645 | N | 0.000040 | -0 603447 | -0 030545 |
| C | 3 324345 | -0 713629 | -1 355955 | C | 2 498188 | -0 363851 | -0 087322 |
| C | 3 324306 | 0.712878 | -1 356300 | н | 0 000110 | -1 581408 | -0 264320 |
| 50 č | 2 730955 | 1 128621 | -0 187169 | C | 2 738586 | -1 667504 | 0.023150 |
| C | 2 506397 | 2 498562 | 0 413848 | 110 H | 3 745194 | -2 047070 | -0 053725 |
| N | 0.000115 | -2.643544 | 0.249530 | H | 1.963705 | -2.401159 | 0.193651 |
| N | 2.371786 | 0.000048 | 0.499284 | C | 3.585710 | 0.647363 | -0.299983 |
| H | 1.348447 | -2.134816 | 3.163010 | н | 3.417650 | 1.203846 | -1.220630 |
| 55 н | 3.743800 | -1.352008 | -2.112373 | H | 3.620012 | 1.363399 | 0.520658 |
| H | 3.743711 | 1.350901 | -2.113045 | 115 н | 4.549957 | 0.154562 | -0.361064 |
| H | 0.000462 | -3.091247 | -0.648394 | C | -2.738594 | -1.667684 | 0.021626 |
| H | -1.350096 | -2.135063 | 3.162183 | Ĥ | -3.745247 | -2.047096 | -0.055406 |
| Н | 1.350016 | 2.134627 | 3.162415 | Н | -1.963725 | -2.401613 | 0.190990 |

| С | -3.585754 | 0.647505 | -0.298863 | 60 с | 2.321788 | -0.317258 | -1.740730 |
|------------------|------------------------|-----------------------|-----------------------|-------------|-----------------------|-----------------------|------------------------|
| Н | -3.619839 | 1.362717 | 0.522503 | С | 1.492163 | 0.836752 | -1.829655 |
| Н | -3.417974 | 1.204891 | -1.219017 | С | 3.276849 | -1.641003 | 0.294875 |
| Н | -4.550008 | 0.154749 | -0.360197 | N | 1.738662 | 0.306717 | 0.297004 |
| 5 Li | 0.000177 | 0.377514 | 1.869855 | Н | 2.778812 | -0.837303 | -2.562380 |
| | | | | 65 н | 1.678212 | 0.346882 | 1.300645 |
| | | | | Н | 1.185307 | 1.331286 | -2.733261 |
| Li- | 221 | | | Н | -1.873452 | 0.632408 | -1.318975 |
| 10 | | | | С | 3.101670 | -1.740290 | 1.783778 |
| 10 C | 2.454138 | -2.241383 | -0.789251 | H | 2.060710 | -1.922559 | 2.056052 |
| С | 2.596681 | -0.805303 | -1.004556 | 70н | 3.697443 | -2.556896 | 2.176944 |
| С | 2.841769 | -0.105676 | -2.145878 | Н | 3.428318 | -0.825120 | 2.279783 |
| С | 2.716779 | 1.406575 | -0.473640 | С | 4.113279 | -2.423395 | -0.378636 |
| 1 C | 2.910988 | 1.286354 | -1.811073 | H | 4.688090 | -3.181079 | 0.130646 |
| 15 H | 2.954418 | -0.527975 | -3.127593 | H 76 | 4.257098 | -2.326542 | -1.443661 |
| Н | 3.075409 | 2.095165 | -2.499797 | /3 C | -0.408445 | 3.058934 | -1.164681 |
| N | 2.456376 | 0.123602 | 0.039091 | Н | 0.409105 | 3.667884 | -1.544528 |
| С | 2.518206 | 2.611026 | 0.416103 | Н | -0.815499 | 2.487706 | -1.99/583 |
| 20° | 1.075205 | 2.51/61/ | 0.85//1/ | Н | -1.18/468 | 3./1694/ | -0./88918 |
| 20 C | -1.135957 | 2.209857 | 0.502934 | 20 T | 0.631411 | 3.032092 | 1.102169 |
| C | -0.887705 | 1.910385 | 1.820074 | о0 н 11 | -0.100972 | 3.009544 | 1 020022 |
| C N | 0.507992 | 2.104244 | 2.0445/3 | H | 1 422600 | 2.440990 | 1.930022 |
| IN | 1 625104 | 2.557405 | -0.070701 | п | 1.433000 2.016006 | J.002040 1.700041 | 1 594060 |
| 25 ^п | -1.023194 | 2 016270 | 2.J40127 _1 026727 | U U | -3.210290 | -1.709041 | -1.304009 -2.027021 |
| <u>2</u> јп u | 1 028735 | 2.040379 | -1.020737 | 85 u | -2 523502 | -2.344129 | -2.02/921 |
| и Ц | 2 816957 | _0 121972 | 0 950226 | 05 II C | -2.525592 | -2.187279 | -2.249079 |
| C | 3 442586 | 2 563921 | 1 634778 | н | -3 771893 | -2 682447 | 1 433626 |
| н | 3 253681 | 3 418248 | 2 281354 | н | -4 987658 | -1 470803 | 1 049705 |
| 30 H | 3 304089 | 1 660044 | 2 225565 | Н | -4 857123 | -2 931891 | 0 064179 |
| Н | 4.476917 | 2.599685 | 1.303368 | 90 Li | 0.205956 | -0.761606 | -0.831201 |
| С | 2.777689 | 3.900231 | -0.363632 | / 21 | 0.200000 | 0.,01000 | 0.001201 |
| Н | 3.809931 | 3.920481 | -0.704917 | | | | |
| Н | 2.134468 | 3.993195 | -1.236718 | Li- | 328 | | |
| 35 н | 2.607767 | 4.758769 | 0.281144 | | | | |
| С | 2.108853 | -2.748555 | 0.393951 | 95 с | 3.204405 | 1.382307 | -0.827092 |
| Н | 2.020274 | -3.814395 | 0.533170 | С | 2.607836 | 0.351373 | 0.020004 |
| Н | 1.918291 | -2.136150 | 1.264773 | С | 2.613177 | 0.229474 | 1.394931 |
| С | 2.721906 | -3.108934 | -1.983024 | С | 1.466873 | -1.532200 | 0.558728 |
| 40 н | 2.039629 | -2.865297 | -2.796447 | С | 1.891258 | -0.951978 | 1.733921 |
| Н | 3.737273 | -2.955963 | -2.345154 | 100 н | 3.105514 | 0.896881 | 2.078059 |
| Н | 2.595777 | -4.155718 | -1.728154 | Н | 1.735921 | -1.345822 | 2.721528 |
| Н | -2.055729 | 2.248308 | -0.050674 | N | 1.882670 | -0.717418 | -0.461749 |
| Li | 0.375726 | 0.439446 | 0.465779 | С | 0.567027 | -2.713425 | 0.275272 |
| 45 | | | | 105 C | -0.654657 | -2.109951 | -0.367277 |
| | | | | 105 C | -2.265897 | -0.529207 | -0.509237 |
| Lı- | 261 | | | C | -2.185411 | -1.147637 | -1.722296 |
| ~ | 2 21 0 0 1 2 | 1 401114 | 0 000110 | С | -1.1633/5 | -2.149690 | -1.632276 |
| 50 c | -3.318913 | -1.491114 | -0.289113 | C | -2.965200 | 0./151/9 | -0.026687 |
| 500 | -2.492937 | -0.465513 | 0.339265 | 110 c | -1.849420 | 1.6/86/6 2.161262 | U.310443 1 512620 |
| C | -2.300010 | -0.099465 | 1.040012 | | -1.376103 | 2.101203 | 1 242204 |
| C | -1.009265 | 1.237002 | 1 722251 | C | -0.206944 | 2.952115 | 1.243294 -0.110064 |
| с ц | -1.440204 -2 012036 | 0.90UIZZ -0 551376 | 1.133231 2 167551 | U N | U.UUOJZU _1 318165 | 2.000402 -1 107/01 | -0.110904 0 300813 |
| 55 ¹¹ | _1 136419 | 1 477130 | 2.40/331 | IN N | -0 980195 | 2 109436 | -0 657827 |
| N | -1 598408 | 0 328310 | -0 396054 | 115 H | -2 767110 | -0 908844 | -2 594085 |
| C | 0 089359 | 2 160204 | -0 030696 | H LI | -1 839170 | 2 015197 | 2.354003 |
| C | 1.148091 | 1.214696 | -0.549160 | H | 0.382290 | 3.478369 | 1.956683 |
| C | 2.487774 | -0.619990 | -0.401027 | H | -1.355998 | -1.054944 | 1.314232 |
| - | - | | | | | | |

| Н | -0.838074 | -2.798761 | -2.424845 | 60 н | 0.839139 | 2.124244 | 1.384076 |
|---|---|--|---|--|---|---|---|
| Н | -1.080550 | 1,901869 | -1.636268 | C | 3.848421 | -2.208275 | 0.253328 |
| Н | 1.701216 | -0.907350 | -1.431938 | H | 3.990437 | -1.319093 | -0.358864 |
| С | -3.806252 | 0.435419 | 1.220983 | Н | 4.633812 | -2.241420 | 1.001590 |
| 5н | -3.213281 | 0.015682 | 2.032118 | Н | 3.945946 | -3.080037 | -0.392392 |
| Н | -4.264847 | 1.354840 | 1.578862 | 65 с | 2.354472 | -2.256786 | 2.230911 |
| Н | -4.591674 | -0.273691 | 0.973465 | Н | 1.391941 | -2.263440 | 2.721003 |
| С | -3.867213 | 1.283211 | -1.122879 | Н | 3.218046 | -2.323661 | 2.874064 |
| Н | -4.337605 | 2.199445 | -0.774977 | С | -3.042667 | -2.176512 | -1.760920 |
| 10 н | -3.316186 | 1.503309 | -2.034990 | Н | -2.758024 | -1.337882 | -2.394660 |
| Н | -4.644744 | 0.562573 | -1.365747 | 70 н | -2.827053 | -3.094416 | -2.303758 |
| С | 1.243888 | -3.699861 | -0.677764 | Н | -4.113217 | -2.120755 | -1.582295 |
| Н | 0.563907 | -4.519272 | -0.899499 | С | -2.753491 | -3.374788 | 0.406632 |
| Н | 1.527057 | -3.231183 | -1.618001 | Н | -2.556976 | -4.293370 | -0.140347 |
| 15 н | 2.138859 | -4.105676 | -0.213207 | H | -2.237362 | -3.428925 | 1.362868 |
| С | 0.220484 | -3.432472 | 1.580345 | 75 н | -3.821194 | -3.305009 | 0.601813 |
| Н | 1.123334 | -3.824997 | 2.043396 | С | -1.515976 | 3.587856 | 1.473537 |
| Н | -0.267408 | -2.774121 | 2.297535 | H | -2.503555 | 3.760541 | 1.894959 |
| H | -0.450020 | -4.260852 | 1.367489 | H | -0.895479 | 3.157548 | 2.257698 |
| 20 C | 3.118129 | 1.354978 | -2.155291 | H | -1.095135 | 4.545287 | 1.176108 |
| H | 3.577755 | 2.128654 | -2.750333 | 80 C | -2.572004 | 3.313065 | -0.768129 |
| H | 2.622356 | 0.563504 | -2.698562 | H | -2.170370 | 4.268419 | -1.099112 |
| С | 3.926962 | 2.474294 | -0.094673 | H | -2.717434 | 2.680823 | -1.642072 |
| 25 H | 3.2614/5 | 2.9/8256 | 0.606868 | Н | -3.543424 | 3.4///53 | -0.309506 |
| 23 н | 4./5/588 | 2.064/28 | 0.4/8406 | 95 | 3.444542 | 1.195849 | 1.3/986/ |
| н | 4.31/939 | 3.200800 | -0.793105 | 05 н | 4.442017 | 0.985570 | 1./3333U 2.110542 |
| п т÷ | 0.757654 | 0 689712 | -0.724303 | п | 2.0J7934 1 323810 | 1 165793 | _0 02/027 |
| ТПТ | 0.302700 | 0.000/12 | 0.004101 | ц | 4.525010 | 0 755512 | -1 726259 |
| 20 | | | | 11 | 4.110030 | 0.755512 | 1.720233 |
| 30 | | | | Н | 4 419908 | 2 450754 | -1 379160 |
| 30 T.i. | -368 | | | н 90 н | 4.419908 5.269305 | 2.450754 1 199400 | -1.379160 -0.463590 |
| 30 Li | -368 | | | н 90 н Li | 4.419908 5.269305 0.346162 | 2.450754 1.199400 -0.013630 | -1.379160 -0.463590 -0.716086 |
| 30 Li | -368 3.223093 | 1.460133 | 0.095328 | 90 н Li | 4.419908 5.269305 0.346162 | 2.450754 1.199400 -0.013630 | -1.379160 -0.463590 -0.716086 |
| 30 Li C C | -368 3.223093 1.891015 | 1.460133 1.777168 | 0.095328 -0.419012 | 90 H Li | 4.419908 5.269305 0.346162 | 2.450754 1.199400 -0.013630 | -1.379160 -0.463590 -0.716086 |
| 30 Li C 35 C | -368 3.223093 1.891015 1.458988 | 1.460133 1.777168 1.906286 | 0.095328 -0.419012 -1.722451 | Н 90 н Li Na- | 4.419908 5.269305 0.346162 | 2.450754 1.199400 -0.013630 | -1.379160 -0.463590 -0.716086 |
| 30 Li· 35 C C | -368 3.223093 1.891015 1.458988 -0.285049 | 1.460133 1.777168 1.906286 2.414199 | 0.095328 -0.419012 -1.722451 -0.372940 | 90 H Li 95 Na- | 4.419908 5.269305 0.346162 | 2.450754 1.199400 -0.013630 | -1.379160 -0.463590 -0.716086 |
| 30 Li 35 C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 | 1.460133 1.777168 1.906286 2.414199 2.303879 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 | 90 H Li 95 C | 4.419908 5.269305 0.346162 -170 -2.005645 | 2.450754 1.199400 -0.013630 -3.339793 | -1.379160 -0.463590 -0.716086 |
| 30 Li 35 C C C H | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 | 90 H Li 95 C C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 | -1.379160 -0.463590 -0.716086 -0.077750 -0.692323 |
| 30 Li C C C C C C C C C H H | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 | 90 H Li 95 C C C | 4.419908 5.269305 0.346162 •170 -2.005645 -0.709234 -0.335069 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 | -1.379160 -0.463590 -0.716086 -0.077750 -0.692323 -2.005860 |
| 30 Li 35 C C C C H H 40 N | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 | 90 ^H Li 95 ^{Na-} C C C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 | -1.379160 -0.463590 -0.716086 -0.077750 -0.692323 -2.005860 -2.030592 |
| 30 Li 35 C C C H H 40 N C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 | 90 H Li 95 C C 100 C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 | -1.379160 -0.463590 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 |
| 30 Li 35 C C C H 40 N C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 | 90 H Li 95 C C 100 C C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 | -1.379160 -0.463590 -0.716086 -0.077750 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 |
| 30 Li 35 C C C H 40 N C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 | 90 H Li 95 C C C 100 C C N | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 |
| 30 Li 35 C C C H 40 N C C C C 45 C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 | 90 H Li 95 C C C 100 C C N H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 |
| 30 Li 35 c c c H 40 N c c c 45 c | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 2.00221 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 | 90 H Li 95 C C C C C 100 C C N H H 105 H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 2.400255 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 |
| 30 Li 35 C C C H 40 N C C C 45 C C C C C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 0.00075 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 | 90 H Li 95 C C C 100 C C N H 105 H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 2.906240 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 2.121215 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 |
| 30 Li 35 c c c H H 40 N c c c 45 c c c c c | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 | 90 ^H Li 95 ^{Na-} 95 ^C C 100 ^C C 100 ^C C N H 105 ^H C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.95506 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 |
| 30 Li 35 C C C H H 40 N C C C 45 C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 | 90 H Li 95 C C C 100 C C N H 105 H C H H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 |
| $\begin{array}{c} 30 \\ \text{Li} \\ 35 \\ \text{c} $ | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 | 90 H Li 95 C C C 100 C C N H H 105 H C H H C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 |
| 30 Li 35 C C C H 40 N C C C C 45 C C C S0 C C C S0 C C C S0 C C C S S S S | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 | 90 H Li 95 C C C C 100 C C N H 105 H C H C H H C 110 H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 |
| 30 Li 35 C C C C H 40 N C C C C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 | 90 H Li 95 C C C 100 C C N H 105 H C H H H 105 H C H H H H 110 H H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 |
| 30 Li 35 C C C H 40 N C C C C C 45 C C C C C S 0 C C C S 0 C C C C S S C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 | 90 ^H Li 95 ^{Na-} 95 ^C C 100 ^C C 100 ^C C N H 105 ^H C H H 110 ^H H H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 |
| 30 Li 35 C C C H H 40 N C C C C C H H 40 N C C C C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 -3.132133 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 -1.323236 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 2.384747 | 90 ^H Li 95 ^{Na-} 95 ^C C 100 ^C C 100 ^C C N 105 ^H H C 110 ^H H H C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 -3.136657 | 2.450754 1.199400 -0.013630 -3.339793 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 -3.164061 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 -0.755348 |
| 30 Li 35 C C C H H A0 N C C C C H H A0 N C C C C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 -3.132133 -0.400288 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 -1.323236 -2.125394 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 2.384747 -2.804039 | 90 ^H Li 95 ^{Na-} C C C 100 ^C C N 105 ^H C H 110 ^H H H C H | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 -3.136657 -3.145217 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 -3.164061 -2.781273 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 -0.755348 -1.764886 |
| 30 Li 35 C C C H H H N C C C C H H H N C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 -3.132133 -0.400288 2.191511 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 -1.323236 -2.125394 -2.047507 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 2.384747 -2.804039 -2.022761 | 90 ^H Li 95 ^{Na-} 95 ^C C 100 ^C C 100 ^C C N 105 ^H H 105 ^H H C 110 ^H H H C 110 ^H H H C 115 ^H H | 4.419908 5.269305 0.346162 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 -3.136657 -3.145217 -4.088239 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 -3.164061 -2.781273 -3.418974 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 -0.755348 -1.764886 -0.315771 |
| 30 Li 35 C C C H 40 N C C C C C C C C C C C C C C C C C C | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 -3.132133 -0.400288 2.191511 -2.084123 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 -1.323236 -2.125394 -2.047507 0.438529 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 2.384747 -2.804039 -2.022761 -1.238337 | 90 H Li 95 C C C 100 C C C N H 105 H C H H 110 H H H C H Li | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 -3.136657 -3.145217 -4.088239 -1.984958 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 -3.164061 -2.781273 -3.418974 -3.871388 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 -0.755348 -1.764886 -0.315771 1.327587 |
| 30 Li: 35 C C C H 40 N C C C C C 45 C C C C C S0 C C C S0 C C C S0 C C S0 C C C S S S S S S S S S S S S S S S S S | -368 3.223093 1.891015 1.458988 -0.285049 0.091078 2.067806 -0.527026 0.802493 -1.633979 -2.146342 -2.528367 -2.812471 -2.570784 -2.303221 -0.809075 -0.036492 1.329480 1.359086 2.500824 -2.105524 0.047792 -3.132133 -0.400288 2.191511 -2.084123 -2.685975 | 1.460133 1.777168 1.906286 2.414199 2.303879 1.772947 2.523629 2.053375 2.668509 1.313361 -0.889198 -0.613663 0.782585 -2.171025 -2.203546 -2.113817 -2.068573 -2.124231 -2.189254 0.286160 -2.176736 -1.323236 -2.125394 -2.047507 0.438529 1.313400 | 0.095328 -0.419012 -1.722451 -0.372940 -1.692809 -2.597536 -2.544066 0.382913 0.258014 0.673372 0.336809 1.643210 1.856562 -0.422319 -0.654158 -1.793015 -1.381326 -0.001355 0.910291 -0.244042 0.411987 2.384747 -2.804039 -2.022761 -1.238337 2.783712 | 90 H Li 95 C C C 100 C C C 100 C C N H 105 H C H H 110 H H C H 110 H H C H C H C H C C C C C C C C C C C C | 4.419908 5.269305 0.346162 -170 -2.005645 -0.709234 -0.335069 1.068428 1.538762 2.887559 0.440947 -0.987251 1.677969 0.490825 3.896240 4.895506 3.759571 3.069042 2.492858 2.755108 4.112052 -3.136657 -3.145217 -4.088239 -1.984958 -1.382520 | 2.450754 1.199400 -0.013630 -0.013630 -3.038119 -2.805345 -2.599327 -2.708132 -2.621335 -2.959068 -2.856426 -2.465222 -3.181330 -2.131215 -2.099641 -1.767114 -3.129495 -2.543817 -4.170207 -3.065600 -3.164061 -2.781273 -3.418974 -3.871388 -4.777506 | -1.379160 -0.463590 -0.716086 -0.716086 -0.692323 -2.005860 -2.030592 -0.731936 -0.163955 0.057857 -2.858994 -2.905958 1.036922 -0.879190 -0.473991 -1.886425 1.238483 1.957195 1.319687 1.529067 -0.755348 -1.764886 -0.315771 1.327587 1.392782 |

| H | -2.991653 | -4.108495 | 1.654289 | 60 N | 0.497411 | -2.907494 | 0.128240 |
|--|---|---|---|--|--|---|---|
| Na | 0.000007 | -0.403309 | -0.923071 | п Н | -1.000930 | -1 529180 | -2.505059 |
| | | | | Н | 1.907729 | -1.059755 | 2.675640 |
| 5 Na- | -237 | | | H | 0.590335 | -3.355028 | 1.021902 |
| | | | | 65 с | 3.988763 | -2.153076 | -1.024592 |
| С | -1.832364 | -0.846027 | 1.408668 | Н | 3.764190 | -1.500319 | -1.865806 |
| С | -1.995939 | 0.056155 | 0.377126 | Н | 4.935907 | -1.846731 | -0.586049 |
| Ν | -2.712974 | -0.581567 | -0.597684 | Н | 4.097185 | -3.159449 | -1.420485 |
| 10 c | -3.021335 | -1.859191 | -0.212714 | С | 3.223510 | -3.178610 | 1.110490 |
| С | -2.478899 | -2.058601 | 1.032052 | 70 н | 2.522260 | -3.163100 | 1.942801 |
| Н | -2.586307 | -2.946262 | 1.628407 | Н | 3.224680 | -4.174606 | 0.673187 |
| Η | -3.036713 | -0.146926 | -1.442271 | Н | 4.210088 | -2.976116 | 1.519367 |
| C | 3.391423 | -0.266650 | 0.235482 | С | -3.079981 | -3.233644 | -0.688773 |
| 15 C | 2.116785 | 0.094076 | -0.392794 | 7, H | -3.138228 | -2.731979 | -1.642472 |
| С | 1.671443 | 0.022267 | -1.699617 | /5н | -3.994153 | -3.644217 | -0.289708 |
| C | 0.369183 | 0.588907 | -1.745561 | С | -1.850879 | -4.071729 | 1.293686 |
| C | 0.036134 | 0.987735 | -0.466//2 | H | -1.1//U28 | -4.92/428 | 1.23/143 |
| 20 1 | -1.304803 | 1.3/9409 | 0.11814/ | H | -1.494514 | -3.409446 | 2.084/92 |
| 20 N | 2 246029 | 0.0/1203 | U.332040 -2 520221 | 80 ^H | -2.829999 | -4.436495 | 1 142605 |
| п u | -0 237393 | -0.323773 | -2.559221 | оо с ц | 1 303268 | 3 838217 | 1 5/3321 |
| н Н | -0.237393 -1.330270 | -0 657146 | 2 340274 | н Н | 3 005867 | 3 861222 | 1 980929 |
| н | 1 167788 | 0.007140 | 1 307008 | н | 2 411931 | 4 906771 | 0 684883 |
| 25 C | -2 083566 | 2 238012 | -0 878257 | II C | 2 917547 | 3 118635 | -1 121392 |
| 20 С Н | -2.155690 | 1.777107 | -1.861540 | 85 H | 3.007794 | 4.138793 | -1.459412 |
| Н | -3.087619 | 2.425610 | -0.503758 | Н | 3.106975 | 2.351672 | -1.858684 |
| Н | -1.577130 | 3.190831 | -1.007785 | Na | 0.210690 | -0.136088 | -0.002303 |
| С | -1.145522 | 2.154198 | 1.426406 | | | | |
| 30 н | -0.673057 | 1.563070 | 2.208699 | | | | |
| Н | -0.552852 | 3.050650 | 1.257193 | 90 Na- | 344 | | |
| Η | -2.124529 | 2.449109 | 1.795081 | | | | |
| С | 4.329169 | -0.919662 | -0.443954 | С | 0.538901 | 2.226568 | -1.671521 |
| Н | 4.190445 | -1.212846 | -1.473350 | С | 0.132787 | 2.096290 | -0.375864 |
| 35 н | 5.271427 | -1.168697 | 0.017981 | N N | 1.063655 | 1.301507 | 0.268644 |
| С | 3.585450 | 0.147709 | 1.666861 | 95 C | 2.087324 | 0.976449 | -0.603322 |
| Н | 3.501098 | 1.229401 | 1.776088 | С | 1.774858 | 1.518640 | -1.815295 |
| Н | 2.848705 | -0.318857 | 2.323628 | Н | 2.354197 | 1.428714 | -2.715957 |
| 40 H | 4.569095 | -0.1494// | 2.013960 | С | 3.186357 | 0.046276 | -0.15/934 |
| 40 H | -3.6438// | -2.491816 | -0.81/968 | 100 c | 2.525183 | -1.269084 | U.18U336 1 277502 |
| Na | -0.120281 | -1./10935 | -0.462961 | 100 C | 2.323004 | -1.919448 | 1.3775U3 -0.226772 |
| | | | | C | I.ZJJUJJ | -3.110319 | -0.230773 |
| Na- | | | | C | 1 5/5882 | -3 086437 | 1 111055 |
| INCL | -277 | | | С н | 1.545882 2 720645 | -3.086437 -1 620742 | 1.111955 2 330142 |
| 45 | -277 | | | С Н Н | 1.545882 2.720645 1.251205 | -3.086437 -1.620742 -3.840433 | 1.111955 2.330142 1.818778 |
| 45 C | -277 | -0.400720 | 1.866348 | с н 105 N | 1.545882 2.720645 1.251205 1.879419 | -3.086437 -1.620742 -3.840433 -1.997047 | 1.111955 2.330142 1.818778 -0.783651 |
| 45 C | -277 2.164851 2.737583 | -0.400720 -0.771064 | 1.866348 0.668507 | с н 105 N н | 1.545882 2.720645 1.251205 1.879419 1.185006 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 | 1.111955 2.330142 1.818778 -0.783651 1.267269 |
| 45 с с N | -277 2.164851 2.737583 2.908598 | -0.400720 -0.771064 0.374932 | 1.866348 0.668507 -0.062563 | с Н 105 N Н С | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 |
| 45 C N C | -277 2.164851 2.737583 2.908598 2.484819 | -0.400720 -0.771064 0.374932 1.478231 | 1.866348 0.668507 -0.062563 0.642181 | С Н 105 N Н С С | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 |
| 45 C N 50 C | -277 2.164851 2.737583 2.908598 2.484819 2.005188 | -0.400720 -0.771064 0.374932 1.478231 1.013782 | 1.866348 0.668507 -0.062563 0.642181 1.849721 | С Н Н 105 N Н С С С | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 |
| 45 C N C 50 C H | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 | С Н 105 N Н С С С 110 С | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 |
| 45 C N C 50 C H C | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 | С Н 105 N Н С С С 110 С С | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 |
| 45 C N C 50 C H C H | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 | C H H 105 N H C C C 110 C C C | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 2.500756 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 |
| 45 C N 50 C H C H C | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 -1.933594 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 -3.360577 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 -0.027548 | C H H 105 N H C C C 110 C C N | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 -2.273231 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 2.500756 0.379611 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 -0.334643 |
| 45 c c N 50 c H c H c 55 c | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 -1.933594 -0.684625 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 -3.360577 -2.818383 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 -0.027548 -0.570207 | C H H 105 N H C C C 110 C C C N H | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 -2.273231 -3.145774 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 2.500756 0.379611 -1.369401 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 -0.334643 2.259977 |
| 45 c n 50 c H c H c c c h c c c c h c c c c c c c c c c c c c | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 -1.933594 -0.684625 -0.379918 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 -3.360577 -2.818383 -2.215611 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 -0.027548 -0.570207 -1.776591 | С Н 105 N Н С С С 110 С С С С П 110 С С С П Н 115 Н | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 -2.273231 -3.145774 -1.961046 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 2.500756 0.379611 -1.369401 0.989450 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 -0.334643 2.259977 2.837715 |
| 45 c N 50 c H c H c c H c c c h c c c c c c c c c c c c c | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 -1.933594 -0.684625 -0.379918 1.018278 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 -3.360577 -2.818383 -2.215611 -1.965296 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 -0.027548 -0.570207 -1.776591 -1.795603 | С Н 105 N Н С С С С П 110 С С С С П И Н 115 Н Н | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 -2.273231 -3.145774 -1.961046 0.020677 | -3.086437 -1.620742 -3.840433 -1.997047 1.311937 -1.817487 -0.770773 -0.663017 0.585262 1.218202 2.500756 0.379611 -1.369401 0.989450 2.764121 | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 -0.334643 2.259977 2.837715 -2.444697 |
| 45 c N 50 c H c H c c H c c c H c c c c c c c c c c c c c | -277 2.164851 2.737583 2.908598 2.484819 2.005188 1.631830 2.592112 3.404058 -1.933594 -0.684625 -0.379918 1.018278 1.543396 | -0.400720 -0.771064 0.374932 1.478231 1.013782 1.626833 2.848300 0.422206 -3.360577 -2.818383 -2.215611 -1.965296 -2.406607 | 1.866348 0.668507 -0.062563 0.642181 1.849721 2.649671 0.140495 -0.933745 -0.027548 -0.570207 -1.776591 -1.795603 -0.597997 | С H 105 N H C C C C C N H 110 C C C N H H H C C C N H H C C C N H H C C C N H H C C C N H H C C C C N H H C C C C N H H H C C C N H H H C C C N H H H C C C N H H H C C C N H H H C C C N H H H C C C N H H H H C C C N H H H H H H H C C C N H H H H H H H H H H H H H | 1.545882 2.720645 1.251205 1.879419 1.185006 -3.369850 -2.828506 -2.748070 -2.134226 -1.858552 -1.131047 -2.273231 -3.145774 -1.961046 0.020677 -2.203487 | $\begin{array}{c} -3.086437\\ -1.620742\\ -3.840433\\ -1.997047\\ 1.311937\\ -1.817487\\ -0.770773\\ -0.663017\\ 0.585262\\ 1.218202\\ 2.500756\\ 0.379611\\ -1.369401\\ 0.989450\\ 2.764121\\ 0.596266\end{array}$ | 1.111955 2.330142 1.818778 -0.783651 1.267269 -0.692749 0.179871 1.553986 1.856864 0.664856 0.339439 -0.334643 2.259977 2.837715 -2.444697 -1.313537 |

| С | -0.815225 | 3.260854 | 1.629669 | 60 н | 4.681694 | 0.920525 | -1.055201 |
|--|--|---|---|--------------|-----------|-----------|-----------|
| Н | -0.215895 | 2.670880 | 2.321649 | Н | 4.509935 | -0.643773 | -1.858318 |
| Н | -0.267197 | 4.168541 | 1.390568 | С | 4.202381 | -1.005825 | 0.811120 |
| H | -1.738109 | 3.532883 | 2.137129 | Н | 3.706383 | -1.427448 | 1.682878 |
| 5 c | -1.985069 | 3.392228 | -0.564776 | H | 4.740527 | -1.804540 | 0.306788 |
| Н | -2.252238 | 2.895492 | -1.495345 | 65 н | 4.917092 | -0.260574 | 1.152845 |
| Н | -2.901627 | 3.665172 | -0.047938 | С | -1.725155 | -3.911845 | -0.111655 |
| Н | -1.437650 | 4.299045 | -0.811546 | Н | -1.935058 | -3.712637 | -1.151941 |
| 10 u | -3.584301 | -3.046539 | -0.231503 | Н | -2.4556/1 | -4.480466 | 0.442/63 |
| 10 н | -3.3485UL | -3.321317 | 0.785855 | 70 H | -0.314517 | -3./341/8 | 1.924134 |
| н С | -4.020553 | -3.804864 -1.427004 | -0.862704 | /0 н | -0.256903 | -4.254/90 | 2.049229 |
| с ц | -3.000327 | -0.582150 | -2.110190 -2.138851 | п ц | -0.230803 | -1 333144 | 2.404547 |
| H | -2 777751 | -1 143432 | -2 654827 | C | -3 345626 | -0 864936 | 1 693756 |
| 15 н | -4.133602 | -2.258522 | -2.639628 | H | -3.979694 | -1.679764 | 2.027524 |
| C | 4.207152 | -0.138779 | -1.282970 | 75 н | -2.305972 | -1.173555 | 1.816951 |
| Н | 3.751756 | -0.526239 | -2.192088 | Н | -3.528992 | -0.013561 | 2.351042 |
| Н | 4.669773 | 0.816412 | -1.520134 | С | -4.626055 | -1.119692 | -0.413066 |
| Н | 4.980417 | -0.833159 | -0.964122 | Н | -4.866713 | -0.846284 | -1.428946 |
| 20 c | 3.905940 | 0.596879 | 1.075913 | Н | -5.223135 | -1.890581 | 0.048607 |
| Н | 3.232277 | 0.738389 | 1.919709 | 80 c | -0.909397 | 3.989170 | 1.299912 |
| Н | 4.690600 | -0.088906 | 1.387994 | Н | -1.280191 | 3.361882 | 2.108162 |
| Н | 4.355626 | 1.556362 | 0.834083 | Н | -0.156784 | 4.658214 | 1.711001 |
| н 25 н | 0.792199 | -3.837566 | -0.846737 | Н | -1.736981 | 4.583173 | 0.920457 |
| 23 Na | -0.193439 | -1.022578 | 0.700077 | C | 0.196635 | 4.115058 | -0.927188 |
| | | | | 6 5 н | 0.629821 | 3.583596 | -1.//3359 |
| No- | 381 | | | п u | -0.025510 | 4.722332 | -1.299730 |
| Na- | -204 | | | Na | -0 334993 | -0 288913 | -1 020222 |
| 30 c | 2.296540 | 1.055997 | 1.849660 | IVG | 0.001000 | 0.200910 | 1.020222 |
| С | 2.435793 | 0.728306 | 0.532834 | 90 | | | |
| Ν | 1.507799 | 1.470913 | -0.175410 | | | | |
| С | 0.818579 | 2.306021 | 0.686335 | | | | |
| C C | 1 273579 | | | | | | |
| 35 H | 1.2/00/0 | 2.053335 | 1.946971 | | | | |
| | 0.925196 | 2.053335 2.521007 | 1.946971 2.849513 | | | | |
| C | 0.925196 | 2.053335 2.521007 3.163166 | 1.946971 2.849513 0.161989 | | | | |
| C C | 0.925196 -0.304841 -1.335107 | 2.053335 2.521007 3.163166 2.222430 | 1.946971 2.849513 0.161989 -0.415230 | | | | |
| C C C | 0.925196 -0.304841 -1.335107 -1.754519 | 2.053335 2.521007 3.163166 2.222430 1.992996 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 | | | | |
| | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 | | | | |
| с с с 40 с н | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1 455733 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2 573992 | | | | |
| с с с 40 с н | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 | | | | |
| 40 c H H N | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 | | | | |
| 40 c H H H | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 | | | | |
| 40 c H H 45 c | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 | | | | |
| 40 c H H 45 c C | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 | | | | |
| 40 c H H 45 c C C | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 0.411932 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 -2.766863 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 -0.298744 | | | | |
| 40 c c c c c c c c c c c c c c c c c c c | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 0.411932 0.682327 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 -2.766863 -2.715144 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 -0.298744 -1.651497 | | | | |
| 40 c c c c c c c c c c c c c c c c c c c | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 0.411932 0.682327 1.788080 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 -2.766863 -2.715144 -1.837378 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 -0.298744 -1.651497 -1.840490 | | | | |
| 40 c c c c c c c c c c c c c c c c c c c | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 0.411932 0.682327 1.788080 2.175152 2.20667 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 -2.766863 -2.715144 -1.837378 -1.378064 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 -0.298744 -1.651497 -1.840490 -0.600721 | | | | |
| 40 c c c c c c c c c c c c c c c c c c c | 0.925196 -0.304841 -1.335107 -1.754519 -2.818188 -2.682199 -1.455733 -3.214350 -1.969135 1.608876 -3.648642 -0.605657 0.411932 0.682327 1.788080 2.175152 3.206627 1.202602 | 2.053335 2.521007 3.163166 2.222430 1.992996 0.508405 0.914716 2.553898 0.507235 1.301341 1.673265 -0.523236 -3.490692 -2.766863 -2.715144 -1.837378 -1.378064 -0.366406 | 1.946971 2.849513 0.161989 -0.415230 -1.707041 -0.365373 -1.678250 -2.573992 -2.518262 0.376470 -1.155719 0.262379 0.469987 -0.298744 -1.651497 -1.840490 -0.600721 -0.159828 | | | | |
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