

# Supporting Information

## Electrosynthesis of a $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ Methano Derivative from Trianionic $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$

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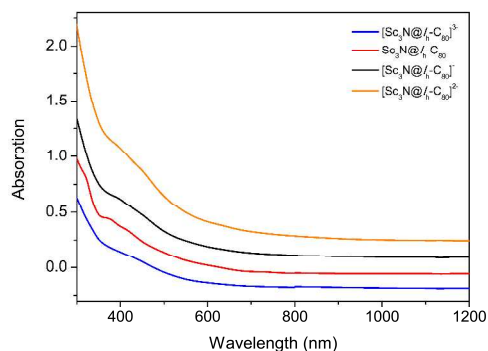
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**Table S1.** Relative energies ( $\text{kcal mol}^{-1}$ ) for different orientational isomers of  $[\text{M}_3\text{N}@I_h\text{-C}_{80}]^{n-}$  ( $\text{M} = \text{Sc}, \text{Lu}$ ;  $n = 2, 3$ ). S2

**Table S2.** Spin densities (in e) of the  $\text{M}_3\text{N}$  cluster for different orientational isomers of  $[\text{M}_3\text{N}@I_h\text{-C}_{80}]^{3-}$  ( $\text{M} = \text{Sc}, \text{Lu}$ ). S2

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**Table S1.** Relative energies ( $\text{kcal mol}^{-1}$ ) for different orientational isomers of  $[\text{M}_3\text{N}@I_h\text{-C}_{80}]^{n-}$  ( $\text{M} = \text{Sc}, \text{Lu}$ ;  $n = 2, 3$ ).

|          | Dianions |        | Trianions |        |
|----------|----------|--------|-----------|--------|
|          | M = Sc   | M = Lu | M = Sc    | M = Lu |
| isomer 1 | 6.6      | 5.9    | 4.1       | 2.0    |
| isomer 2 | 0.0      | 0.0    | 0.0       | 0.0    |
| isomer 3 | 6.9      | 5.6    | 4.4       | 1.9    |
| isomer 4 | 7.7      | 6.5    | 4.7       | 3.1    |

**Table S2.** Spin densities (in e) of the  $\text{M}_3\text{N}$  cluster for different orientational isomers of  $[\text{M}_3\text{N}@I_h\text{-C}_{80}]^{3-}$  ( $\text{M} = \text{Sc}, \text{Lu}$ ).

|      | $\text{Sc}_3\text{N}$ | $\text{Lu}_3\text{N}$ |
|------|-----------------------|-----------------------|
| Iso1 | 0.765                 | 0.676                 |
| Iso2 | 0.413                 | 0.091                 |
| Iso3 | 0.647                 | 0.796                 |
| Iso4 | 0.737                 | 0.555                 |

The xyz coordinates for the lowest energy structure of **1**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.572916 | -0.571415 | -3.113578 |
| C  | -2.450045 | 0.877840  | -3.143535 |
| C  | -1.524716 | -1.523325 | -3.529439 |
| C  | -3.282332 | -1.206386 | -2.022624 |
| Sc | -0.079871 | 0.049858  | -2.173389 |
| C  | -3.103055 | 1.615933  | -2.093728 |
| C  | -1.268327 | 1.509236  | -3.731486 |
| C  | -2.565779 | 2.840107  | -1.539088 |
| C  | -3.816951 | 0.958482  | -1.029853 |
| C  | 0.194465  | -0.456396 | 4.141024  |
| C  | 1.272397  | -1.326897 | 3.735774  |
| C  | -1.039883 | -1.118494 | 3.845598  |
| C  | 0.280772  | 0.961600  | 4.016241  |
| C  | -0.332350 | -1.280851 | -4.292985 |
| C  | -1.563815 | -2.641352 | -2.623062 |
| C  | 0.878367  | -1.742325 | -3.670310 |
| C  | 2.089237  | -0.960795 | -3.366856 |
| C  | 0.843077  | -2.855270 | -2.761712 |
| C  | -0.276542 | -0.276736 | -5.401582 |
| C  | -0.177121 | 0.869712  | -4.452436 |
| C  | 1.072296  | 1.327600  | -3.870538 |
| C  | -0.678141 | 2.623138  | -3.026394 |
| C  | -1.309818 | 3.334941  | -1.965672 |
| C  | 0.741171  | 2.513582  | -3.111753 |
| C  | -0.467640 | 4.009438  | -1.037896 |
| C  | -2.935066 | 2.928641  | -0.153409 |
| C  | 0.962345  | 3.882668  | -1.118833 |
| C  | -0.838160 | 4.105919  | 0.345597  |
| C  | 1.581626  | 3.100592  | -2.127791 |
| C  | 2.772399  | 2.389711  | -1.830768 |
| C  | 3.050294  | 1.101682  | -2.423015 |
| C  | 3.300088  | 2.409519  | -0.492237 |
| C  | 1.486723  | 3.891368  | 0.221433  |
| Sc | 1.556656  | 0.990853  | 0.791742  |
| C  | 2.181986  | 0.491252  | -3.404711 |
| C  | 2.808550  | -1.715905 | -2.348691 |
| C  | 3.760964  | 0.326195  | -1.443613 |
| C  | -3.753147 | -0.253665 | 1.528917  |
| C  | -3.641491 | 1.178312  | 1.456487  |
| C  | -3.870539 | -1.053084 | 0.345279  |
| C  | -3.115716 | -1.047437 | 2.550710  |
| C  | -3.714146 | 1.766183  | 0.162761  |
| C  | -2.849968 | 1.814366  | 2.454376  |
| C  | -2.055253 | 3.513195  | 0.814227  |
| C  | -3.869464 | -0.453830 | -0.965245 |
| C  | -3.317803 | -2.356474 | 0.626870  |
| C  | -2.667465 | -2.476869 | -1.739116 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.467707 | -3.808723 | -0.075092 |
| C  | -2.620104 | -3.045406 | -0.427548 |
| C  | -0.949473 | -3.775307 | 1.276519  |
| C  | -0.361760 | -3.982533 | -0.972741 |
| Sc | -1.294264 | -1.107435 | 0.964550  |
| C  | -2.864201 | -2.382841 | 2.012818  |
| C  | 2.947202  | -2.852320 | 0.271151  |
| C  | 3.717956  | -1.690432 | -0.073558 |
| C  | 2.602962  | -2.774854 | 1.667674  |
| C  | 2.059871  | -3.436070 | -0.676724 |
| C  | 3.626886  | -1.087520 | -1.365116 |
| C  | 3.853299  | -0.885355 | 1.115132  |
| C  | 3.920363  | 1.124486  | -0.252918 |
| C  | 1.337982  | -3.246126 | 2.134260  |
| C  | 3.155600  | -1.559044 | 2.189560  |
| C  | 0.704702  | -2.530054 | 3.195380  |
| C  | -0.733346 | -2.409381 | 3.262564  |
| C  | 0.486726  | -3.904003 | 1.195171  |
| C  | 0.846511  | -4.018133 | -0.190841 |
| C  | 2.614585  | 0.629247  | 3.133755  |
| C  | 2.482303  | -0.805483 | 3.190813  |
| C  | 3.413526  | 1.322675  | 2.147756  |
| C  | 1.520702  | 1.479732  | 3.519325  |
| C  | 3.961535  | 0.538684  | 1.054900  |
| C  | 2.770973  | 2.621487  | 1.902552  |
| C  | 2.670750  | 3.161369  | 0.562641  |
| C  | 0.364093  | 4.035473  | 1.125660  |
| C  | 1.592118  | 2.684509  | 2.745446  |
| C  | -1.607121 | -3.050422 | 2.326009  |
| C  | -0.387127 | -3.356866 | -2.250685 |
| C  | 2.042464  | -2.874169 | -1.993101 |
| C  | -2.208524 | -0.390173 | 3.460867  |
| C  | -2.136834 | 1.034442  | 3.438898  |
| C  | -0.895316 | 1.705494  | 3.721081  |
| C  | -0.846924 | 2.901610  | 2.917948  |
| C  | 0.382280  | 3.389215  | 2.392366  |
| C  | -2.055911 | 2.966068  | 2.134059  |
| N  | 0.031454  | -0.009961 | -0.113404 |
| H  | 0.682180  | -0.383775 | -5.927178 |
| C  | -1.407035 | -0.265102 | -6.416584 |
| C  | -1.984284 | -1.467302 | -6.847092 |
| C  | -1.818908 | 0.939046  | -7.001878 |
| C  | -2.965105 | -1.463910 | -7.842132 |
| H  | -1.668634 | -2.413587 | -6.403259 |
| C  | -2.799655 | 0.942365  | -7.997518 |
| H  | -1.373533 | 1.881509  | -6.677829 |
| C  | -3.377148 | -0.258727 | -8.418264 |
| H  | -3.409251 | -2.405959 | -8.164946 |
| H  | -3.113611 | 1.887210  | -8.442488 |

H -4.145715 -0.255735 -9.192468