Rotation of fullerene molecules in the crystal lattice of fullerene/porphyrin: C_{60} and Sc_{3}N@C_{80}

Yajuan Hao, Yaofeng Wang, Lukas Spree, and Fupin Liu

Electronic Supplementary Information

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1. Crystal data

Table S1. Crystal data Sc₃N@C₈₀.

| Crystal | Sc₃N@C₈₀NiOEP2(C₆H₆) | Sc₃N@C₈₀NiOEP2(C₆H₆) | Sc₃N@C₈₀NiOEP2(C₆H₆) |
|---------|----------------------|----------------------|----------------------|
| Formula | C₁₂₈H₅₆N₅NiSc₃      | C₁₂₈H₅₆N₅NiSc₃      | C₁₂₈H₅₆N₅NiSc₃      |
| Formula weight | 1857.36         | 1857.36             | 1857.36             |
| Color, habit | Black, block  | Black, block       | Black, block        |
| Crystal system | triclinic       | triclinic           | triclinic           |
| Space group | P1              | P1                  | P1                  |
| a, Å     | 14.720(3)        | 14.740(3)           | 14.750(3)           |
| b, Å     | 15.390(3)        | 15.410(3)           | 15.440(3)           |
| c, Å     | 17.670(4)        | 17.700(4)           | 17.730(4)           |
| α, deg   | 81.17(3)         | 81.20(3)            | 81.22(3)            |
| β, deg   | 74.54(3)         | 74.54(3)            | 74.56(3)            |
| γ, deg   | 86.24(3)         | 86.28(3)            | 86.31(3)            |
| Volume, Å³ | 3811.1(15)     | 3828.1(15)          | 3845.3(15)          |
| Z        | 2                 | 2                   | 2                   |
| T, K     | 100               | 130                 | 160                 |
| Radiation (λ, Å) | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) |
| Unique data (Rint) | 20749 (0.0289) | 20850 (0.0407) | 20938 (0.0559) |
| Parameters | 1333          | 1353                | 1363                |
| Restraints | 133           | 175                 | 240                 |
| Observed data (I > 2σ(I)) | 20586       | 20656               | 20585               |
| R₁<sup>a</sup> (observed data) | 0.0875 | 0.0922 | 0.0983 |
| wR₂<sup>b</sup> (all data) | 0.2417 | 0.2615 | 0.2841 |
| CCDC NO. | 2027144         | 2027145             | 2027146             |

\[
R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \quad \text{wR}_2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}}
\]

<sup>a</sup>For data with I > 2σ(I), <sup>b</sup>For all data.
Table S1. Crystal data Sc$_3$N@C$_{80}$-continued.

| Crystal          | Sc$_3$N@C$_{80}$NiOEP@2(C$_6$H$_6$) | Sc$_3$N@C$_{80}$NiOEP@2(C$_6$H$_6$) | Sc$_3$N@C$_{80}$NiOEP@2(C$_6$H$_6$) |
|------------------|------------------------------------|------------------------------------|------------------------------------|
| **Formula**      | C$_{128}$H$_{56}$N$_5$NiSc$_3$     | C$_{128}$H$_{56}$N$_5$NiSc$_3$     | C$_{128}$H$_{56}$N$_5$NiSc$_3$     |
| **Formula weight** | 1857.36                           | 1857.36                           | 1857.36                           |
| **Color, habit** | Black, block                       | Black, block                       | Black, block                       |
| **Crystal system** | triclinic                          | triclinic                          | triclinic                          |
| **Space group**  | P1                                 | P1                                 | P1                                 |
| **a**, Å         | 14.770(3)                          | 14.790(3)                          | 14.810(3)                          |
| **b**, Å         | 15.460(3)                          | 15.480(3)                          | 15.490(3)                          |
| **c**, Å         | 17.770(4)                          | 17.820(4)                          | 17.880(4)                          |
| **α**, deg       | 81.21(3)                           | 81.16(3)                           | 81.12(3)                           |
| **β**, deg       | 74.99(3)                           | 74.31(3)                           | 74.16(3)                           |
| **γ**, deg       | 86.28(3)                           | 86.17(3)                           | 86.10(3)                           |
| **Volume, Å$^3$** | 3871.8(15)                         | 3879.8(15)                         | 3897.3(15)                         |
| **Z**            | 2                                  | 2                                  | 2                                  |
| **T**, K         | 190                                | 220                                | 250                                |
| **Radiation (λ, Å)** | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) |
| **Unique data ($R_{int}$)** | 21056 (0.0447)                  | 21197 (0.0475)                    | 21172 (0.0217)                    |
| **Parameters**   | 1413                               | 1433                               | 1453                               |
| **Restraints**   | 1134                               | 1362                               | 1625                               |
| **Observed data (I > 2σ(I))** | 20690                             | 20521                             | 20467                             |
| **$R_1$** (observed data) | 0.0957                             | 0.0988                             | 0.1019                             |
| **w$R_2$** (all data) | 0.2893                             | 0.3019                             | 0.3140                             |
| **CCDC NO.**     | 2027147                            | 2027148                            | 2027149                            |

\[
R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \\
wR_2 = \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]}.
\]

*aFor data with I > 2σ(I), \(b\)For all data,
Table S1. Crystal data_ Sc$_3$N@C$_{80}$_continued.

| Crystal | Sc$_3$N@C$_{80}$NiOEP$_2$(C$_6$H$_6$) |
|---------|--------------------------------------|
| Formula | C$_{128}$H$_{56}$N$_5$NiSc$_3$       |
| Formula weight | 1857.36          |
| Color, habit | Black, block     |
| Crystal system | triclinic        |
| Space group | $P\bar{1}$        |
| $a$, Å    | 14.830(3)          |
| $b$, Å    | 15.500(3)          |
| $c$, Å    | 17.930(4)          |
| $\alpha$, deg | 81.08(3)    |
| $\beta$, deg | 74.03(3)    |
| $\gamma$, deg | 86.05(3)     |
| Volume, Å$^3$ | 3913.0(15) |
| Z        | 2                   |
| $T$, K   | 280                 |
| Radiation ($\lambda$, Å) | Synchrotron Radiation (0.7999) |
| Unique data ($R_{int}$) | 21315 (0.0234) |
| Parameters | 1451                |
| Restraints | 1655                |
| Observed data ($I > 2\sigma(I)$) | 20430          |
| $R_1$ $^a$ (observed data) | 0.1060 |
| $wR_2$ $^b$ (all data) | 0.3292 |
| CCDC NO. | 2027150             |

\[
R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \quad \text{for data with } I > 2\sigma(I), \quad wR_2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}} \quad \text{for all data},
\]

$^a$For data with $I > 2\sigma(I)$, $^b$For all data,
### Table S2. Crystal data $\text{C}_{60}$.

| Crystal | $\text{C}_{60}\text{NiOEP} \cdot 2(\text{C}_6\text{H}_6)$ | $\text{C}_{60}\text{NiOEP} \cdot 2(\text{C}_6\text{H}_6)$ | $\text{C}_{60}\text{NiOEP} \cdot 2(\text{C}_6\text{H}_6)$ |
|---------|-------------------|-------------------|-------------------|
| **Formula** | $\text{C}_{108}\text{H}_{56}\text{N}_4\text{Ni}$ | $\text{C}_{108}\text{H}_{56}\text{N}_4\text{Ni}$ | $\text{C}_{108}\text{H}_{56}\text{N}_4\text{Ni}$ |
| **Formula weight** | 1468.27 | 1468.27 | 1468.27 |
| **Color, habit** | Black, block | Black, block | Black, block |
| **Crystal system** | Triclinic | Triclinic | Triclinic |
| **Space group** | $P\bar{1}$ | $P\bar{1}$ | $P\bar{1}$ |
| $a$, Å | 14.130(3) | 14.130(3) | 14.130(3) |
| $b$, Å | 14.380(3) | 14.410(3) | 14.440(3) |
| $c$, Å | 17.200(3) | 17.290(4) | 17.410(4) |
| $\alpha$, deg | 87.54(3) | 87.72(3) | 87.96(4) |
| $\beta$, deg | 75.78(3) | 75.78(3) | 75.78(3) |
| $\gamma$, deg | 75.61(3) | 75.74(3) | 75.92(3) |
| Volume, Å$^3$ | 3280.9(13) | 3306.7(13) | 3338.9(13) |
| $Z$ | 2 | 2 | 2 |
| $T$, K | 100 | 160 | 220 |
| **Radiation (λ, Å)** | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) | Synchrotron Radiation (0.7999) |
| Unique data ($R_{\text{int}}$) | 17754 (0.0225) | 17893 (0.0506) | 18160 (0.0363) |
| Parameters | 1026 | 1026 | 1027 |
| Restraints | 0 | 0 | 0 |
| Observed data ($I > 2\sigma(I)$) | 17546 | 17811 | 18041 |
| $R_1$ | 0.0383 | 0.0486 | 0.0589 |
| $wR_2$ | 0.1015 | 0.1308 | 0.1679 |
| **CCDC NO.** | 2027151 | 2027152 | 2027153 |

\[
R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \quad \text{and} \quad wR_2 = \sqrt{\frac{\sum [w(F_o^2 - F_c^2)]^2}{\sum [w(F_o^2)]}}.
\]

$^a$For data with $I > 2\sigma(I)$, $^b$For all data.
Table S2. Crystal data _C_60_ continued.

| Crystal | C_{60}NiOEP_{32}(C_6H_6) |
|---------|--------------------------|
| Formula | C_{200}H_{56}N_{4}Ni |
| Formula weight | 1468.27 |
| Color, habit | Black, block |
| Crystal system | triclinic |
| Space group | P̅1 |
| a, Å | 14.150(3) |
| b, Å | 14.470(3) |
| c, Å | 17.520(4) |
| α, deg | 88.18(3) |
| β, deg | 75.80(3) |
| γ, deg | 76.08(3) |
| Volume, Å³ | 3374.1(13) |
| Z | 2 |
| T, K | 280 |
| Radiation (λ, Å) | Synchrotron Radiation (0.7999) |
| Unique data (R_int) | 18384 (0.0500) |
| Parameters | 1015 |
| Restraints | 24 |
| Observed data (I > 2σ(I)) | 18188 |
| R_1 a (observed data) | 0.0688 |
| wR_2 b (all data) | 0.2005 |
| CCDC NO. | 2027154 |

\[
R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \quad \text{a For data with I > 2σ(I),}
\]

\[
wR_2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}} \quad \text{b For all data,}
\]
2. Structure parameters

Table S3. Nearest cage carbon-Ni contact distances as a function of temperature

| Temperature (K) | 100   | 130   | 160   | 190   | 220   | 250   | 280   |
|-----------------|-------|-------|-------|-------|-------|-------|-------|
| Ho$_2$LuN@C$_{80}$ (Å) | 2.810(6) | 2.812(7) | 2.795(8) | 2.81(1) | -     | 2.85(2) | 2.86(2) |
| Lu$_2$N@C$_{80}$ (Å) | 2.79(2) | -     | 2.83(1) | -     | 2.83(3) | -     | 2.83(2) |
| Sc$_3$N@C$_{80}$ (Å) | 2.766(3) | 2.774(4) | 2.787(4) | 2.809(4) | 2.821(5) | 2.835(6) | 2.846(6) |
| C$_{60}$ (Å)     | 3.006(2) | -     | 3.025(2) | -     | 3.054(3) | -     | 3.089(4) |

Table S4. Metal site occupancy in Sc$_3$N@C$_{80}$ as a function of temperatures

| Temperature (K) | 100   | 130   | 160   | 190   | 220   | 250   | 280   |
|-----------------|-------|-------|-------|-------|-------|-------|-------|
| Sc1             | 0.231(3) | 0.246(3) | 0.276(3) | 0.223(6) | 0.213(5) | 0.199(5) | 0.190(5) |
| Sc2             | 0.478(3) | 0.395(3) | 0.334(3) | 0.206(6) | 0.179(6) | 0.168(6) | 0.152(6) |
| Sc3             | 0.290(3) | 0.239(3) | 0.198(3) | 0.120(5) | 0.105(5) | 0.096(5) | 0.086(5) |
| Sc4             | 0.183(3) | 0.175(3) | 0.107(3) | 0.081(4) | 0.084(4) | 0.089(4) | 0.101(4) |
| Sc5             | 0.202(3) | 0.197(3) | 0.108(3) | 0.076(4) | 0.076(4) | 0.081(4) | 0.083(4) |
| Sc6             | 0.170(3) | 0.196(3) | 0.197(3) | 0.150(5) | 0.141(5) | 0.154(7) | 0.149(7) |
| Sc7             | 0.213(3) | 0.205(3) | 0.198(3) | 0.132(4) | 0.132(5) | 0.126(5) | 0.117(5) |
| Sc8             | 0.225(3) | 0.226(3) | 0.219(3) | 0.102(5) | 0.090(4) | 0.069(4) | 0.070(4) |
| Sc9             | 0.464(3) | 0.378(3) | 0.352(3) | 0.235(7) | 0.220(6) | 0.200(6) | 0.184(5) |
| Sc10            | 0.136(3) | 0.153(3) | 0.154(3) | 0.148(5) | 0.168(6) | 0.078(6) | 0.095(6) |
| Sc11            | 0.070(3) | 0.095(3) | 0.231(3) | 0.110(5) | 0.109(5) | 0.089(5) | 0.085(5) |
| Sc12            | 0.232(3) | 0.233(3) | 0.222(3) | 0.164(5) | 0.158(5) | 0.157(5) | 0.144(5) |
| Sc13            | 0.107(3) | 0.107(3) | 0.133(3) | 0.126(6) | 0.099(5) | 0.095(5) | 0.090(4) |
| Sc14            | 0.080(3) | 0.102(3) | 0.076(4) | 0.101(5) | 0.108(5) | 0.110(5) | 0.110(5) |
| Sc15            | 0.075(3) | 0.102(3) | 0.070(3) | 0.083(4) | 0.099(4) | 0.094(4) | 0.094(4) |
| Sc16            | 0.068(3) | 0.055(4) | 0.079(4) | 0.087(5) | 0.102(5) | 0.091(4) | 0.091(4) |
| Sc17            | 0.052(3) | 0.081(4) | 0.088(4) | 0.091(4) | 0.100(4) | 0.080(5) | 0.080(5) |
| Sc18            | 0.074(3) | 0.087(4) | 0.091(4) | 0.100(4) | 0.106(5) | 0.094(5) | 0.094(5) |
| Sc19            | 0.093(5) | 0.104(5) | 0.073(5) | 0.080(5) | 0.117(5) | 0.120(6) | 0.047(4) |
| Sc20            | 0.101(5) | 0.100(5) | 0.081(4) | 0.081(4) | 0.051(4) | 0.051(4) | 0.051(4) |
3. Ellipsoids comparison on variable temperatures

Figure S1. Ellipsoids of C1P of NiOEP and C61 of C80 fullerene cage at 100 and 280 K highlighted at 80% probability level. The N1 of the Sc3N cluster is drawn to show the orientation of the C61 as well as its ellipsoid changes on temperature. (a) shows the ellipsoids viewed from the lateral direction of C61 to highlight the increment of the radial direction; (b) is shown in Figure 1 in the manuscript to view both the radial and lateral directions properly; (c) shows the ellipsoids viewed from the radial direction of C61 to highlight the increment of the lateral direction.
4. Reported pristine $\text{Sc}_3\text{N}@\text{C}_{80}$ structure

**Figure S2.** $\text{Sc}_3\text{N}@\text{C}_{80}/\text{NiOEP}/\text{benzene}, 100\text{K}$. The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, red for nickel, and pink for scandium.

**Figure S3.** $\text{Sc}_3\text{N}@\text{C}_{80}/\text{CoOEP}/\text{benzene}/\text{chloroform}, 130\text{K}$. Drawn with the data from ref. ² The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color
code: grey for carbon, blue for nitrogen, green for chlorine, white for hydrogen, cyan for cobalt, and pink for scandium.

**Figure S4.** $\text{Sc}_3\text{N}@\text{C}_{80}/\text{o-xylene}$, 90K. Drawn with the data from ref. 3 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, and pink for scandium.

**Figure S5.** $\text{Sc}_3\text{N}@\text{C}_{80}/\text{p-xylene}$, two orientations of the $\text{C}_{80}$ cage, 100K. Drawn with the data from ref. 4 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, and pink for scandium. The two orientations of the fullerene cage are differentiated by colors (grey and red).
Figure S6. Sc$_3$N@C$_{80}$/o-DCB, 100K. Drawn with the data from ref. 5 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, green for chlorine, and pink for scandium.

Figure S7. Sc$_3$N@C$_{80}$/decapyrrylcorannulene/dichloromethane, 100K. Drawn with the data from ref. 6 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, green for chlorine, and pink for scandium. The fullerene cage is highlighted with red color from the co-crystallized decapyrrylcorannulene.
Figure S8. Sc$_3$N@C$_{80}$/triptycene/o-DCB, 100K. Drawn with the data from ref. 5 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, green for chlorine, and pink for scandium.

Figure S9. Sc$_3$N@C$_{80}$/Zn$_2$BisPy/p-xylene-1, two orientations of the C$_{80}$ cage, 100K. Drawn with the data from ref. 4 The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, red for oxygen, cyan for zinc, and pink for scandium. The two orientations of the fullerene cage are differentiated by colors (grey and red).
Figure S10. Sc$_3$N@C$_{80}$/Zn$_2$BisPy/p-xylene-2, three orientations of the C$_{80}$ cage, 100K. Drawn with the data from ref. The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). The displacement parameters are shown at the 30% probability level. Color code: grey for carbon, blue for nitrogen, white for hydrogen, red for oxygen, cyan for zinc, and pink for scandium. The three orientations of the fullerene cage are differentiated by colors (grey, red, and green).
5. Temperature driven dynamics of Sc$_3$N and Ho$_2$LuN clusters in C$_{80}$.

Figure S11. Molecular structure of Sc$_3$N@C$_{80}$NiOEP·2(C$_6$H$_6$) measured with single-crystal X-ray diffraction at variable temperatures from 100 to 280 K. The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). Color code: grey for carbon, pink for Sc, and blue for N. As comparison, the molecular structure of Ho$_2$LuN@C$_{80}$NiOEP·2(C$_6$H$_6$) measured with single-crystal X-ray diffraction at variable temperatures from 100 to 280 K was shown. The metal sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). Color code: grey for carbon, brown for Lu, cyan for Ho, and blue for N.
Figure S12. Molecular structures of $\text{Sc}_3\text{N}@\text{C}_{80}/\text{NiOEP}$ and $\text{Ho}_2\text{LuN}@\text{C}_{80}/\text{NiOEP}$ measured at variable temperatures. To highlight the relative position of the $\text{M}_3\text{N}$ cluster to the NiOEP, C$_{80}$ cage and the solvent molecules are omitted for clarity. The displacement parameters are shown at the 30% probability level except for the $\text{M}_3$. The $\text{M}_3$ sites are shown as spheres whose radii are scaling proportional to the site occupancy (the bigger the sphere, the higher the occupancy). Color code: grey for carbon, blue for nitrogen, white for hydrogen, red for nickel, pink for scandium, brown for Lu, and cyan for Ho.

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