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# 5-Halo substituted porphyrin

## Bond lengths and angles

### **Table S1:** Bond distances, angles, and atom displacement of compounds **1**-**3**.

| **Bond Distances, Bond Angles, Atom Displacements** | **1** | **2** | **2A** | **3** |
| --- | --- | --- | --- | --- |
| CCDC code | MS563 | NESHUO | MS546 | UDERUR |
| N–Ca (Å) | 1.373(4) | 1.384(11) | 1.381(3) | 1.370(5) |
| Ca–Cb (Å) | 1.437(9) | 1.430(17) | 1.433(6) | 1.441(14) |
| Ca–Cm (Å) | 1.392(5) | 1.377(18) | 1.382(7) | 1.399(8) |
| Cb–Cb (Å) | 1.347(2) | 1.326(18) | 1.346(3) | 1.357(9) |
| ∠CaCbCb (°) | 107.6(5) | 107.6(9) | 107.0(3) | 107.3(7) |
| ∠NCaCb (°) | 108.6(9) | 110.0(12) | 110.8(4) | 108.9(19) |
| ∠NCaCm (°) | 125.2(10) | 125.2(13) | 125.7(2) | 125.8(7) |
| ∠CaNCa (°) | 107.6(9) | 104.7(8) | 104.4(15) | 107(2) |
| ∠CmCaCb (°) | 126.2(10) | 124.7(18) | 123.4(4) | 125.3(19) |
| ∠CaCmCa (°) | 127.0(2) | 123(2) | 122.8(8) | 125(2) |
| Δ24 (Å) | 0.0287 | 0.1769 | 0.0396 | 0.0781 |
| ΔN (Å) | 0.023(15) | 0.015(12) | 0.020(3) | 0.030(2) |
| ΔCa (Å) | 0.022(13) | 0.200(2) | 0.040(17) | 0.050(3) |
| ΔCb (Å) | 0.033(18) | 0.140(4) | 0.030(2) | 0.150(5) |
| ΔCm (Å) | 0.040(2) | 0.360(3) | 0.070(2) | 0.050(3) |
| ∠ pyrrole tilt (°) | 1.8(4) | 11.2(11) | 2.4(8) | 4.0(2) |
| N···N dist (adj) (Å) | 2.910(4) | 2.748(15) | 2.770(2) | 2.920(7) |
| N···N dist (opp) (Å) | 4.118(15) | 3.886(12) | 3.917(9) | 4.120(7) |

# 5-Halo-15-phenyl substituted porphyrin

## Bond lengths and angles

### **Table S2:** Bond distances, angles, and atom displacement of compounds **4**-**8**

| **Bond Distances, Bond Angles, Atom Displacements** | **4** | **5** | **6** | **7** | **8\_1** | **8\_2** |
| --- | --- | --- | --- | --- | --- | --- |
| CCDC code | DGIB005a | MS567 | KJF150xp | DGIB007b | TCD662 | TCD662 |
| N–Ca (Å) | 1.367(2) | 1.371(4) | 1.371(6) | 1.382(4) | 1.370(4) | 1.373(4) |
| Ca–Cb (Å) | 1.444(4) | 1.441(5) | 1.441(7) | 1.435(5) | 1.439(9) | 1.436(12) |
| Ca–Cm (Å) | 1.402(7) | 1.400(5) | 1.399(13) | 1.385(6) | 1.402(6) | 1.401(7) |
| Cb–Cb (Å) | 1.352(4) | 1.350(5) | 1.3414(8) | 1.335(4) | 1.344(6) | 1.349(8) |
| ∠CaCbCb (°) | 107.3(3) | 107.4(2) | 107.8(5) | 107.2(10) | 107.8(3) | 107.6(6) |
| ∠NCaCb (°) | 108.7(5) | 108.7(5) | 108.1(9) | 110.6(3) | 108.1(9) | 108.4(8) |
| ∠NCaCm (°) | 126.0(8) | 125.8(10) | 126.1(12) | 125.9(11) | 126.3(15) | 126.0(15) |
| ∠CaNCa (°) | 107.9(5) | 107.7(6) | 108.3(10) | 104.3(15) | 108.3(13) | 107.9(11) |
| ∠CmCaCb (°) | 125.2(7) | 125.4(12) | 125.8(8) | 123.4(9) | 125.6(15) | 125.6(14) |
| ∠CaCmCa (°) | 125.9(18) | 126.0(13) | 125.8(14) | 122.2(20) | 125.6(18) | 125.7(17) |
| Δ24 (Å) | 0.0564 | 0.0688 | 0.0573 | 0.0591 | 0.0553 | 0.0612 |
| ΔN (Å) | 0.070(5) | 0.060(6) | 0.030(3) | 0.020(14) | 0.030(3) | 0.030(3) |
| ΔCa (Å) | 0.036(18) | 0.060(4) | 0.040(3) | 0.050(3) | 0.040(4) | 0.050(3) |
| ΔCb (Å) | 0.070(3) | 0.060(5) | 0.080(6) | 0.080(6) | 0.080(5) | 0.080(6) |
| ΔCm (Å) | 0.050(3) | 0.110(4) | 0.070(3) | 0.070(3) | 0.070(4) | 0.080(2) |
| ∠ pyrrole tilt (°) | 4.2(18) | 4.7(15) | 3.8(13) | 3.2(14) | 3.8(12) | 4.0(10) |
| N···N dist (adj) (Å) | 2.930(3) | 2.918(11) | 2.926(9) | 2.766(16) | 2.930(2) | 2.920(3) |
| N···N dist (opp) (Å) | 4.141(7) | 4.130(4) | 4.140(2) | 3.912(4) | 4.140(3) | 4.130(3) |

# 5,15-Dihalo substituted porphyrin

## **Table S3:** List of hydrogen···halogen and halogen···halogen interactions seen in compounds **9-15**.

|  |  |  |  |
| --- | --- | --- | --- |
|  | D···H–A | Distance (Å) | Angle (°) |
| **9** | Br1···H18–C18 | 3.071(3) | 148.1(1) |
|  | Br1···H204–C204 | 3.126(3) | 125.4(1) |
|  | Br1···H205–C205 | 3.200(3) | 149.3(1) |
| **10** | Br1···H10C–C107 | 3.156(5) | 141.7(1) |
| **11** | Br2···Br2–C10 | 3.433(13) | 152.4(11) |
|  | Br1···H20E–C203 | 3.153(8) | 155.4(2) |
|  | Br1···H20F–C204 | 3.270(5) | 127.9(2) |
| **12** | Br1···H48–C46 | 3.207(18) | 130.7(8) |
| **13** | Br2···H10I–C105 | 3.079(3) | 125.2(13) |
|  | Br2···H2–C2 | 3.323(4) | 139.7(9) |
|  | Br2···H20A–C207 | 3.174(4) | 139.7(9) |
|  | Br1···H12–C12 | 3.210(4) | 149.5(8) |
| **13A** | Br2···H6–C8 | 3.214(4) | 149.6(8) |
|  | Br1···H10–C18 | 3.328(4) | 139.7(8) |
|  | Br1···H31–C34 | 3.181(4) | 130.2(11) |
|  | Br1···H20–C25 | 3.070(4) | 125.3(13) |
| **14** | Br1···H28–C33 | 3.065(5) | 144.1(15) |
|  | Br1···H10–C18 | 3.453(5) | 150.3(17) |
|  | Br2···H6–C8 | 3.306(5) | 157.8(17) |
|  | Br2···H14–C22 | 3.323(6) | 123.6(15) |
|  | Br2···H27–C33 | 3.129(6) | 132.0(13) |
| **15** | Br1···H23–C35 | 2.979(3) | 158.1(16) |
|  | Br2···H11–C26 | 2.856(3) | 161.5(15) |
|  | Br2···H12–C27 | 3.064(4) | 132.3(15) |

# Bond lengths and angles

## **Table S4:** Bond distances, angles, and atom displacement of compounds **9**-**12**.

| **Bond Distances, Bond Angles, Atom Displacements** | **9** | **10** | **11** | **12** |
| --- | --- | --- | --- | --- |
| CCDC code | MS545 | HE006 | HE015 | NOGWEN |
| N–Ca (Å) | 1.375(2) | 1.371(9) | 1.384(5) | 1.360(4) |
| Ca–Cb (Å) | 1.441(9) | 1.439(7) | 1.433(8) | 1.420(3) |
| Ca–Cm (Å) | 1.396(3) | 1.399(6) | 1.384(7) | 1.430(3) |
| Cb–Cb (Å) | 1.352(7) | 1.352(3) | 1.344(5) | 1.320(3) |
| ∠CaCbCb (°) | 107.5(6) | 107.4(6) | 107.4(5) | 107.1(19) |
| ∠NCaCb (°) | 108.8(10) | 108.9(13) | 109.8(6) | 110.5(14) |
| ∠NCaCm (°) | 125.1(14) | 125.2(9) | 124.3(11) | 124.0(3) |
| ∠CaNCa (°) | 107.5(12) | 107.5(15) | 105.5(3) | 104.0(2) |
| ∠CmCaCb (°) | 126.1(11) | 125.9(9) | 125.5(8) | 125.1(19) |
| ∠CaCmCa (°) | 127.2(16) | 126.9(19) | 122.0(3) | 125.9(20) |
| Δ24 (Å) | 0.0174 | 0.0459 | 0.3228 | 0.034 |
| ΔN (Å) | 0.029(19) | 0.043(14) | 0.050(4) | 0.022(12) |
| ΔCa (Å) | 0.012(10) | 0.031(15) | 0.370(8) | 0.026(15) |
| ΔCb (Å) | 0.016(13) | 0.059(18) | 0.250(19) | 0.040(3) |
| ΔCm (Å) | 0.019(17) | 0.052(8) | 0.650(4) | 0.041(10) |
| ∠ pyrrole tilt (°) | 1.2(4) | 3.2(4) | 20.8(12) | 2.3(8) |
| N···N dist (adj) (Å) | 2.918(7) | 2.920(18) | 2.700(3) | 2.890(2) |
| N···N dist (opp) (Å) | 4.127(13) | 4.13(3) | 3.822(13) | 4.090(2) |

## **Table S5:** Bond distances, angles, and atom displacement of compounds **13**-**15**.

| **Bond Distances, Bond Angles, Atom Displacements** | **13** | **13A** | **14** | **15** |
| --- | --- | --- | --- | --- |
| CCDC code | MS556 | HUMWES | HUMWAO | LASMOK |
| N–Ca (Å) | 1.372(3) | 1.371(3) | 1.37(5) | 1.377(4) |
| Ca–Cb (Å) | 1.440(4) | 1.442(6) | 1.438(6) | 1.445(4) |
| Ca–Cm (Å) | 1.398(5) | 1.400(4) | 1.398(7) | 1.398(4) |
| Cb–Cb (Å) | 1.351(17) | 1.356(16) | 1.347(5) | 1.351(3) |
| ∠CaCbCb (°) | 107.4(3) | 107.2(3) | 107.48(16) | 107.1(3) |
| ∠NCaCb (°) | 108.8(5) | 109.1(6) | 108.7(6) | 109.8(4) |
| ∠NCaCm (°) | 125.0(9) | 125.1(9) | 125.4(13) | 124.5(12) |
| ∠CaNCa (°) | 107.5(5) | 107.4(7) | 107.7(7) | 106.16(9) |
| ∠CmCaCb (°) | 126.1(9) | 125.8(9) | 125.9(12) | 125.7(8) |
| ∠CaCmCa (°) | 126.0(2) | 126.0(2) | 126.0(2) | 127.3(15) |
| Δ24 (Å) | 0.155 | 0.154 | 0.0582 | 0.048 |
| ΔN (Å) | 0.050(2) | 0.050(2) | 0.040(3) | 0.070(4) |
| ΔCa (Å) | 0.120(5) | 0.120(5) | 0.040(3) | 0.028(9) |
| ΔCb (Å) | 0.280(4) | 0.280(4) | 0.080(6) | 0.070(4) |
| ΔCm (Å) | 0.090(2) | 0.090(2) | 0.080(3) | 0.020(14) |
| ∠ pyrrole tilt (°) | 6.8(12) | 6.8(12) | 3.7(19) | 3.7(19) |
| N···N dist (adj) (Å) | 2.910(2) | 2.910(2) | 2.918(8) | 2.895(2) |
| N···N dist (opp) (Å) | 4.110(2) | 4.110(2) | 4.130(4) | 4.094(4) |

# 5,10-Dihalo substituted porphyrin

## **Table S6:** Bond distances, angles, and atom displacement of compounds **16**-**19**.

| **Bond Distances, Bond Angles, Atom Displacements** | **16** | **16A** | **17** | **18** | **19** |
| --- | --- | --- | --- | --- | --- |
| CCDC code | RAKGAN | MS529 | ZOXQUA | ZOXCAS | BASDOR |
| N–Ca (Å) | 1.375(12) | 1.366(6) | 1.377(11) | 1.374(2) | 1.369(2) |
| Ca–Cb (Å) | 1.438(13) | 1.438(12) | 1.432(14) | 1.439(5) | 1.442(6) |
| Ca–Cm (Å) | 1.406(10) | 1.400(12) | 1.388(18) | 1.402(7) | 1.400(5) |
| Cb–Cb (Å) | 1.341(7) | 1.347(11) | 1.341(15) | 1.341(7) | 1.351(7) |
| ∠CaCbCb (°) | 107.8(13) | 107.4(7) | 107.5(10) | 107.4(2) | 107.3(3) |
| ∠NCaCb (°) | 108.4(14) | 108.6(16) | 109.5(5) | 109.4(3) | 108.9(9) |
| ∠NCaCm (°) | 125.1(9) | 125.9(3) | 124.8(16) | 124.4(9) | 125.3(12) |
| ∠CaNCa (°) | 107.6(12) | 107.9(19) | 106.1(4) | 106.4(4) | 107.5(13) |
| ∠CmCaCb (°) | 126.3(15) | 125.4(14) | 125.6(18) | 126.1(12) | 125.7(13) |
| ∠CaCmCa (°) | 126.5(11) | 125.6(10) | 125.0(2) | 127.0(18) | 126.8(18) |
| Δ24 (Å) | 0.159 | 0.113 | 0.125 | 0.106 | 0.043 |
| ΔN (Å) | 0.050(3) | 0.040(4) | 0.030(18) | 0.011(11) | 0.003(3) |
| ΔCa (Å) | 0.140(8) | 0.080(5) | 0.140(4) | 0.110(4) | 0.050(7) |
| ΔCb (Å) | 0.190(9) | 0.200(6) | 0.090(7) | 0.100(8) | 0.034(5) |
| ΔCm (Å) | 0.242(12) | 0.080(5) | 0.250(3) | 0.200(4) | 0.090(2) |
| ∠ pyrrole tilt (°) | 9.0(14) | 5(3) | 7.6(5) | 6.5(16) | 2.7(3) |
| N···N dist (adj) (Å) | 2.920(2) | 2.915(16) | 2.841(6) | 2.890(12) | 2.919(2) |
| N···N dist (opp) (Å) | 4.130(4) | 4.120(4) | 4.017(6) | 4.090(2) | 4.130(4) |

# Honourable mentions

## **Table S7:** Bond distances, angles, and atom displacement of compounds **20**-**24**.

| **Bond Distances, Bond Angles, Atom Displacements** | **20** | **21** | **22** | **23** | **24** |
| --- | --- | --- | --- | --- | --- |
| CCDC code | YISZAD | QUGMEM | QUGMIQ | MORBEC | HE014 |
| N–Ca (Å) | 1.368(10) | 1.381(4) | 1.380(8) | 1.390(20) | 1.369(5) |
| Ca–Cb (Å) | 1.452(9) | 1.440(9) | 1.436(7) | 1.440(2) | 1.438(6) |
| Ca–Cm (Å) | 1.390(5) | 1.387(5) | 1.388(6) | 1.376(17) | 1.404(4) |
| Cb–Cb (Å) | 1.366(6) | 1.333(9) | 1.344(5) | 1.340(2) | 1.350(4) |
| ∠CaCbCb (°) | 106.8(6) | 107.5(4) | 107.3(11) | 107.0(11) | 107.5(4) |
| ∠NCaCb (°) | 109.3(17) | 109.5(3) | 109.7(4) | 111.0(8) | 108.6(8) |
| ∠NCaCm (°) | 124.4(3) | 124.7(15) | 125.0(14) | 124.6(18) | 126.4(4) |
| ∠CaNCa (°) | 107.0(2) | 105.8(3) | 105.8(3) | 104.0(11) | 107.9(8) |
| ∠CmCaCb (°) | 126.3(16) | 125.3(18) | 124.9(18) | 124.3(14) | 125.0(5) |
| ∠CaCmCa (°) | 128.8(14) | 121.5(12) | 121.3(12) | 123.4(19) | 124.9(8) |
| Δ24 (Å) | 0.023 | 0.327 | 0.303 | 0.166 | 0.047 |
| ΔN (Å) | 0.030(14) | 0.032(19) | 0.021(18) | 0.031(16) | 0.023(20) |
| ΔCa (Å) | 0.014(16) | 0.380(5) | 0.350(3) | 0.190(4) | 0.040(3) |
| ΔCb (Å) | 0.029(16) | 0.250(12) | 0.240(6) | 0.130(7) | 0.050(3) |
| ΔCm (Å) | 0.020(14) | 0.660(3) | 0.620(7) | 0.340(4) | 0.070(6) |
| ∠ pyrrole tilt (°) | 1.8(6) | 20.9(8) | 19.3(11) | 10.2(7) | 2.8(12) |
| N···N dist (adj) (Å) | 2.926(6) | 2.704(18) | 2.716(15) | 2.737(15) | 2.910(2) |
| N···N dist (opp) (Å) | 4.140(7) | 3.824(8) | 3.840(20) | 3.869(12) | 4.118(13) |

# DFT Tables

## **Table S8:** Molecular orbital energies (HOMO, LUMO) and singlet state properties (S1, f1) together with the porphyrin-phenyl dihedral.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Series 1** | **HOMO (eV)** | **LUMO (eV)** | **S1 (nm)** | **f1** | **Dihedral (°)** |
| **1:1** | -6.68 | -1.08 | 592 | 0.0023 | 69.2 |
| **1:2** | -6.75 | -0.90 | 520 | 0.0012 | 82.6 |
| **1:3** | -6.68 | -1.18 | 585 | 0.0202 | 69.1 |
| **1:4** | -6.85 | -1.00 | 522 | 0.0050 | 81.9 |
| **1:5** | -6.64 | -1.32 | 612 | 0.0465 | 68.9 |
| **1:6** | -6.82 | -1.14 | 532 | 0.0304 | 81.6 |
| **1:7** | -6.76 | -1.24 | 603 | 0.0023 | 72.8 |
| **1:8** | -6.91 | -1.08 | 529 | 0.0003 | 81.6 |
| **1:9** | -6.83 | -1.40 | 614 | 0.0059 | 78.0 |
| **1:10** | -6.96 | -1.24 | 539 | 0.0033 | 81.4 |
| **1D** | -6.77 | -1.24 | 603 | 0.0018 | 74.1 |
| **2D** | -6.90 | -1.09 | 530 | 0.0009 | 82.8 |
| **1:11** | -6.84 | -1.08 | 614 | 0.0071 | 81.4 |
| **1:12** | -6.96 | -1.27 | 541 | 0.0061 | 81.5 |
| **3D** | -6.77 | -1.24 | 602 | 0.0020 | 75.8 |
| **1:13** | -6.89 | -1.09 | 532 | 0.0004 | 80.2 |
| **1:14** | -6.83 | -1.18 | 614 | 0.0116 | 87.6 |
| **1:15** | -6.94 | -1.28 | 545 | 0.0115 | 81.5 |

S1=first singlet state; f1=oscillator strength

## **Table S9:** Molecular orbital energies (HOMO, LUMO).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Series 2** | **HOMO (eV)** | **LUMO (eV)** | **S1 (nm)** | **f1** | **Dihedral (°)** |
| **2:1** | -6.76 | -1.08 | 585 | 0.0006 | 71.4 |
| **2:2** | -6.84 | -1.25 | 595 | 0.0007 | 78.3 |
| **1D** | -6.77 | -1.24 | 603 | 0.0018 | 74.1 |
| **1:11** | -6.84 | -1.08 | 614 | 0.0071 | 81.4 |
| **2:3** | -6.90 | -1.41 | 607 | 0.0024 | 73.9 |
| **2:4** | -6.97 | -1.57 | 620 | 0.0065 | 80.1 |
| **2:5** | -6.77 | -1.35 | 601 | 0.0037 | 79.3 |
| **2:6** | -6.83 | -1.38 | 612 | 0.0051 | 75.6 |

## **Table S10:** Molecular orbital energies (HOMO, LUMO).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Series 3** | **HOMO (eV)** | **LUMO (eV)** | **S1 (nm)** | **f1** | **Dihedral (°)** |
| **3:1** | -6.82 | -1.37 | 566 | 0.0171 | 74.2 |
| **3:2** | -6.69 | -1.17 | 614 | 0.0060 | 75.4 |
| **2:6** | -6.83 | -1.38 | 612 | 0.0051 | 75.6 |
| **3:3** | -6.83 | -1.37 | 608 | 0.0048 | 75.8 |

# Series 1

## **Table S11:** Bond distances, angles, and atom displacement of compounds **1:1**-**1:6**.

| **Bond Distances, Bond Angles, Atom Displacements** | **1:1** | **1:2** | **1:3** | **1:4** | **1:5** | **1:6** |
| --- | --- | --- | --- | --- | --- | --- |
| CCDC code | Base | Base-Ni | F-Mono | F-Mono-Ni | F-Di | F-Di-Ni |
| N–Ca (Å) | 1.363(4) | 1.374(13) | 1.363(7) | 1.374(4) | 1.363(4) | 1.374(14) |
| Ca–Cb (Å) | 1.446(13) | 1.44(2) | 1.445(15) | 1.438(5) | 1.443(13) | 1.436(4) |
| Ca–Cm (Å) | 1.398(6) | 1.384(5) | 1.399(11) | 1.384(7) | 1.398(6) | 1.383(5) |
| Cb–Cb (Å) | 1.361(8) | 1.355 | 1.361(8) | 1.356(3) | 1.362(8) | 1.3566(2) |
| ∠CaCbCb (°) | 107.0(9) | 106.556(17) | 106.9(9) | 106.5(3) | 106.8(9) | 106.4(5) |
| ∠NCaCb (°) | 109(2) | 111.07(15) | 109(2) | 111.2(4) | 109(2) | 111.4(5) |
| ∠NCaCm (°) | 126.0(8) | 125.72(12) | 125.7(8) | 125.3(7) | 125.3(4) | 125.0(8) |
| ∠CaNCa (°) | 107(3) | 104.7417(11) | 107(3) | 104.5(3) | 107(3) | 104.267(14) |
| ∠CmCaCb (°) | 124(2) | 123.16(7) | 125(2) | 123.4(4) | 125(2) | 123.6(2) |
| ∠CaCmCa (°) | 126(2) | 122.9(10) | 126(3) | 123.4(17) | 126(3) | 123.9(20) |
| Δ24 (Å) | 0.0185 | 0.1003 | 0.0194 | 0.1084 | 0.02 | 0.1049 |
| ΔN (Å) | 0.033(5) | 0.007(2) | 0.034(6) | 0.008(3) | 0.035(6) | 0.007(3) |
| ΔCa (Å) | 0.013(4) | 0.116(4) | 0.013(4) | 0.125(4) | 0.014(4) | 0.122(4) |
| ΔCb (Å) | 0.022(4) | 0.081(6) | 0.023(5) | 0.087(8) | 0.024(5) | 0.084(7) |
| ΔCm (Å) | 0.009(6) | 0.202(3) | 0.01(6) | 0.217(5) | 0.01(7) | 0.211(4) |
| ∠ pyrrole tilt (°) | 1.46(18) | 6.33(6) | 1.5(2) | 6.84(13) | 1.6(2) | 6.64(8) |
| N···N dist (adj) (Å) | 2.92(12) | 2.77(2) | 2.92(11) | 2.77(2) | 2.92(11) | 2.77(2) |
| N···N dist (opp) (Å) | 4.13(8) | 3.92 | 4.13(8) | 3.92 | 4.13(7) | 3.9216(4) |

## **Table S12:** Bond distances, angles, and atom displacement of compounds **1:7**-**1:10, 1D, 2D**.

| **Bond Distances, Bond Angles, Atom Displacements** | **1:7** | **1:8** | **1:9** | **1:10** | **1D** | **2D** |
| --- | --- | --- | --- | --- | --- | --- |
| CCDC code | Cl-Mono | Cl-Mono-Ni | Cl-Di | Cl-Di-Ni | Br-Mono | Br-Mono-Ni |
| N–Ca (Å) | 1.364(4) | 1.3739(15) | 1.364(4) | 1.3741(3) | 1.364(4) | 1.374(2) |
| Ca–Cb (Å) | 1.446(14) | 1.439(2) | 1.445(14) | 1.4384(7) | 1.446(13) | 1.4395(16) |
| Ca–Cm (Å) | 1.399(5) | 1.387(4) | 1.401(3) | 1.3887(9) | 1.4(5) | 1.387(4) |
| Cb–Cb (Å) | 1.36(8) | 1.3549(3) | 1.359(8) | 1.35509(16) | 1.359(8) | 1.3544(10) |
| ∠CaCbCb (°) | 107.0(9) | 106.58(15) | 107.0(9) | 106.6(2) | 107.0(9) | 106.62(12) |
| ∠NCaCb (°) | 109(2) | 111.01(14) | 109(2) | 110.9(17) | 109(2) | 110.89(12) |
| ∠NCaCm (°) | 125.7(6) | 125.2(7) | 125.5(11) | 124.8(9) | 125.8(7) | 125.2(7) |
| ∠CaNCa (°) | 107(3) | 104.78(6) | 107(3) | 104.897(12) | 107(3) | 104.93(3) |
| ∠CmCaCb (°) | 125(2) | 123.6(6) | 125(2) | 124.1(7) | 125(2) | 123.7(7) |
| ∠CaCmCa (°) | 126.3(17) | 122.9(11) | 126.6(9) | 123.0(12) | 126.3(15) | 122.8(11) |
| Δ24 (Å) | 0.0175 | 0.1744 | 0.0137 | 0.2249 | 0.0167 | 0.1914 |
| ΔN (Å) | 0.03(6) | 0.01(3) | 0.023(4) | 0.008(6) | 0.028(5) | 0.004(4) |
| ΔCa (Å) | 0.011(4) | 0.202(5) | 0.009(4) | 0.261(5) | 0.011(4) | 0.223(6) |
| ΔCb (Å) | 0.021(5) | 0.141(6) | 0.017(4) | 0.181(11) | 0.02(5) | 0.155(13) |
| ΔCm (Å) | 0.01(6) | 0.3518(18) | 0.007(7) | 0.457(7) | 0.01(6) | 0.389(14) |
| ∠ pyrrole tilt (°) | 1.4(2) | 11.05(2) | 1.09(18) | 14.33(13) | 1.3(2) | 12.2(3) |
| N···N dist (adj) (Å) | 2.92(5) | 2.763(9) | 2.92(20) | 2.752(2) | 2.92(3) | 2.76(6) |
| N···N dist (opp) (Å) | 4.13(8) | 3.91(1) | 4.13(7) | 3.89(1) | 4.13(8) | 3.90(1) |

## **Table S13:** Bond distances, angles, and atom displacement of compounds **1:11**-**1:15, 3D**.

| **Bond Distances, Bond Angles, Atom Displacements** | **1:11** | **1:12** | **3D** | **1:13** | **1:14** | **1:15** |
| --- | --- | --- | --- | --- | --- | --- |
| CCDC code | Br-Di | Br-Di-Ni | I-Mono | I-Mono-Ni | I-Di | I-Di-Ni |
| N–Ca (Å) | 1.365(4) | 1.3737(11) | 1.365(5) | 1.374(2) | 1.366(4) | 1.3742(19) |
| Ca–Cb (Å) | 1.446(13) | 1.4388(2) | 1.446(14) | 1.4398(18) | 1.446(13) | 1.4398(13) |
| Ca–Cm (Å) | 1.401(3) | 1.39(3) | 1.4(6) | 1.388(4) | 1.402(3) | 1.3914(8) |
| Cb–Cb (Å) | 1.358(8) | 1.3552(5) | 1.359(8) | 1.3549(14) | 1.357(8) | 1.3544(7) |
| ∠CaCbCb (°) | 107.0(9) | 106.66(9) | 107.0(9) | 106.66(13) | 107.1(9) | 106.75(5) |
| ∠NCaCb (°) | 109(2) | 110.75(5) | 109(2) | 110.75(20) | 109(2) | 110.51(15) |
| ∠NCaCm (°) | 125.6(14) | 124.8(9) | 125.8(9) | 125.2(7) | 125.7(18) | 124.8(9) |
| ∠CaNCa (°) | 107(3) | 105.0935(18) | 107(3) | 105.12(7) | 107(3) | 105.36(2) |
| ∠CmCaCb (°) | 125(2) | 124.2(9) | 125(2) | 123.8(9) | 125(3) | 124.4(11) |
| ∠CaCmCa (°) | 126.6(5) | 122.8(10) | 126.2(10) | 122.6(8) | 126.4(3) | 122.4(7) |
| Δ24 (Å) | 0.0102 | 0.2476 | 0.0155 | 0.2226 | 0.0032 | 0.2724 |
| ΔN (Å) | 0.017(3) | 0.008(7) | 0.026(5) | 0.012(8) | 0.0051(10) | 0.009(8) |
| ΔCa (Å) | 0.006(3) | 0.287(5) | 0.01(4) | 0.258(9) | 0.0019(10) | 0.316(5) |
| ΔCb (Å) | 0.013(3) | 0.199(13) | 0.019(5) | 0.179(9) | 0.0041(8) | 0.219(16) |
| ΔCm (Å) | 0.006(5) | 0.504(9) | 0.009(6) | 0.45(11) | 0.002(17) | 0.556(14) |
| ∠ pyrrole tilt (°) | 0.8(12) | 15.8(13) | 1.21(19) | 14.1(3) | 0.25(3) | 17.41(14) |
| N···N dist (adj) (Å) | 2.92(5) | 2.747(7) | 2.921(8) | 2.753(6) | 2.93(9) | 2.74(12) |
| N···N dist (opp) (Å) | 4.13(7) | 3.89(1) | 4.13(8) | 3.89(1) | 4.14(7) | 3.875(3) |

## **Table S14:** Comparative tables between crystal structure and calculated structure of compounds **1**-**3** where D signifies the calculated structure.

| **Bond Distances, Bond Angles, Atom Displacements** | **1** | **1D** | **2** | **2D** | **3** | **3D** |
| --- | --- | --- | --- | --- | --- | --- |
|  | MS563 | Br-Mono | NESHUO | Br-Mono-Ni | UDERUR | I-Mono |
| N–Ca (Å) | 1.373(4) | 1.364(4) | 1.384(11) | 1.374(2) | 1.370(5) | 1.365(5) |
| Ca–Cb (Å) | 1.437(9) | 1.446(13) | 1.430(17) | 1.4395(16) | 1.441(14) | 1.446(14) |
| Ca–Cm (Å) | 1.392(5) | 1.4(5) | 1.377(18) | 1.387(4) | 1.399(8) | 1.4(6) |
| Cb–Cb (Å) | 1.347(2) | 1.359(8) | 1.326(18) | 1.3544(10) | 1.357(9) | 1.359(8) |
| ∠CaCbCb (°) | 107.6(5) | 107.0(9) | 107.6(9) | 106.62(12) | 107.3(7) | 107.0(9) |
| ∠NCaCb (°) | 108.6(9) | 109(2) | 110.0(12) | 110.89(12) | 108.9(19) | 109(2) |
| ∠NCaCm (°) | 125.2(10) | 125.8(7) | 125.2(13) | 125.2(7) | 125.8(7) | 125.8(9) |
| ∠CaNCa (°) | 107.6(9) | 107(3) | 104.7(8) | 104.93(3) | 107(2) | 107(3) |
| ∠CmCaCb (°) | 126.2(10) | 125(2) | 124.7(18) | 123.7(7) | 125.3(19) | 125(2) |
| ∠CaCmCa (°) | 127.0(2) | 126.3(15) | 123(2) | 122.8(11) | 125(2) | 126.2(10) |
| Δ24 (Å) | 0.0287 | 0.0167 | 0.1769 | 0.1914 | 0.0781 | 0.0155 |
| ΔN (Å) | 0.023(15) | 0.028(5) | 0.015(12) | 0.004(4) | 0.030(2) | 0.026(5) |
| ΔCa (Å) | 0.022(13) | 0.011(4) | 0.200(2) | 0.223(6) | 0.050(3) | 0.01(4) |
| ΔCb (Å) | 0.033(18) | 0.02(5) | 0.140(4) | 0.155(13) | 0.150(5) | 0.019(5) |
| ΔCm (Å) | 0.040(2) | 0.01(6) | 0.360(3) | 0.389(14) | 0.050(3) | 0.009(6) |
| ∠ pyrrole tilt (°) | 1.8(4) | 1.3(2) | 11.2(11) | 12.2(3) | 4.0(2) | 1.21(19) |
| N···N dist (adj) (Å) | 2.910(4) | 2.92(3) | 2.748(15) | 2.76(6) | 2.920(7) | 2.921(8) |
| N···N dist (opp) (Å) | 4.118(15) | 4.13(8) | 3.886(12) | 3.90(1) | 4.120(7) | 4.13(8) |

# Series 2

## **Table S15:** Bond distances, angles, and atom displacement of compounds **2:1**-**2:6, 1D,** and **1:11**.

| **Bond Distances, Bond Angles, Atom Displacements** | **2:1** | **2:2** | **2:3** | **2:4** | **2:5** | **2:6** | **1D** | **1:11** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |  |
| N–Ca (Å) | 1.362(4) | 1.364(4) | 1.364(5) | 1.365(4) | 1.364(5) | 1.365(5) | 1.364(4) | 1.365(4) |
| Ca–Cb (Å) | 1.447(13) | 1.446(14) | 1.445(13) | 1.445(14) | 1.446(13) | 1.445(13) | 1.446(13) | 1.446(13) |
| Ca–Cm (Å) | 1.396(5) | 1.397(6) | 1.399(5) | 1.401(3) | 1.4(6) | 1.401(4) | 1.4(5) | 1.401(3) |
| Cb–Cb (Å) | 1.361(8) | 1.36(8) | 1.359(8) | 1.357(8) | 1.359(8) | 1.358(8) | 1.359(8) | 1.358(8) |
| ∠CaCbCb (°) | 106.9(9) | 107.0(9) | 107.0(9) | 107.0(9) | 107.0(9) | 107.0(9) | 107.0(9) | 107.0(9) |
| ∠NCaCb (°) | 109(2) | 109(2) | 109(2) | 109(2) | 109(2) | 109(2) | 109(2) | 109(2) |
| ∠NCaCm (°) | 125.8(6) | 125.6(9) | 125.4(11) | 125.2(10) | 125.8(13) | 125.6(10) | 125.8(7) | 125.6(14) |
| ∠CaNCa (°) | 108(3) | 107(3) | 107(3) | 107(3) | 107(3) | 107(3) | 107(3) | 107(3) |
| ∠CmCaCb (°) | 125(2) | 125(2) | 125(2) | 125(2) | 125(2) | 125(2) | 125(2) | 125(2) |
| ∠CaCmCa (°) | 126.4(15) | 126.7(6) | 126.9(14) | 127.2(8) | 126.3(14) | 126.5(12) | 126.3(15) | 126.6(5) |
| Δ24 (Å) | 0.0125 | 0.0108 | 0.0148 | 0.012 | 0.0227 | 0.0282 | 0.0167 | 0.0102 |
| ΔN (Å) | 0.016(5) | 0.012(2) | 0.014(3) | 0.01(2) | 0.02(13) | 0.018(13) | 0.028(5) | 0.017(3) |
| ΔCa (Å) | 0.006(4) | 0.005(4) | 0.008(5) | 0.007(4) | 0.01(8) | 0.016(8) | 0.011(4) | 0.006(3) |
| ΔCb (Å) | 0.02(12) | 0.019(9) | 0.026(11) | 0.023(8) | 0.044(16) | 0.056(16) | 0.02(5) | 0.013(3) |
| ΔCm (Å) | 0.006(3) | 0.004(3) | 0.007(3) | 0.004(3) | 0.007(15) | 0.007(3) | 0.01(6) | 0.006(5) |
| ∠ pyrrole tilt (°) | 0.8(6) | 0.6(5) | 0.8(6) | 0.7(4) | 1.4(9) | 1.6(10) | 1.3(2) | 0.8(12) |
| N···N dist (adj) (Å) | 2.92(6) | 2.92(3) | 2.92(5) | 2.93(3) | 2.92(8) | 2.92(2) | 2.92(3) | 2.92(5) |
| N···N dist (opp) (Å) | 4.13(9) | 4.13(8) | 4.13(7) | 4.14(7) | 4.13(8) | 4.13(7) | 4.13(8) | 4.13(7) |

# Series 3

## **Table S16:** Bond distances, angles, and atom displacement of compounds **3:1**-**3:3, 2:4**.

| **Bond Distances, Bond Angles, Atom Displacements** | **3:1** | **3:2** | **2:6** | **3:3** |
| --- | --- | --- | --- | --- |
| CCDC code | F | Cl | Br | I |
| N–Ca (Å) | 1.363(10) | 1.364(4) | 1.365(5) | 1.366(6) |
| Ca–Cb (Å) | 1.444(17) | 1.445(13) | 1.445(13) | 1.446(14) |
| Ca–Cm (Å) | 1.398(16) | 1.401(3) | 1.401(4) | 1.402(6) |
| Cb–Cb (Å) | 1.362(12) | 1.359(8) | 1.358(8) | 1.357(8) |
| ∠CaCbCb (°) | 106.8(10) | 107.0(9) | 107.0(9) | 107.1(9) |
| ∠NCaCb (°) | 109(2) | 109(2) | 109(2) | 108(2) |
| ∠NCaCm (°) | 125.3(12) | 125.5(9) | 125.6(10) | 125.7(10) |
| ∠CaNCa (°) | 107(3) | 107(3) | 107(3) | 107(3) |
| ∠CmCaCb (°) | 125(2) | 125(2) | 125(2) | 125(2) |
| ∠CaCmCa (°) | 126(2) | 126.6(13) | 126.5(12) | 126.4(9) |
| Δ24 (Å) | 0.0213 | 0.0255 | 0.0282 | 0.0324 |
| ΔN (Å) | 0.022(13) | 0.019(13) | 0.018(13) | 0.016(12) |
| ΔCa (Å) | 0.01(8) | 0.013(8) | 0.016(8) | 0.019(7) |
| ΔCb (Å) | 0.04(17) | 0.05(16) | 0.056(16) | 0.066(15) |
| ΔCm (Å) | 0.006(3) | 0.007(2) | 0.007(3) | 0.007(3) |
| ∠ pyrrole tilt (°) | 1.5(7) | 1.5(10) | 1.6(10) | 1.8(9) |
| N···N dist (adj) (Å) | 2.916(10) | 2.921(8) | 2.923(2) | 2.926(5) |
| N···N dist (opp) (Å) | 4.12(8) | 4.13(7) | 4.13(7) | 4.14(7) |

# Crystal data and refinement

## **Table S17:** Details of XRD data refinement.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***Compound*** | **1** | **2A** | **4** | **5** |
| ***Identification code*** | MS563 | MS546 | DGIB005A | MS567 |
| *CCDC deposition #* | 2069451 | 2069452 | 2069454 | 2069455 |
| *Empirical formula* | C32H21BrN4 | C34H20N4Ni | C40H29ClN4 | C38H25BrN4 |
| *Formula weight* | 541.44 | 543.25 | 601.12 | 617.53 |
| *Temperature/K* | 100(2) | 100(2) | 100(2) | 100(2) |
| *Crystal system* | monoclinic | monoclinic | monoclinic | triclinic |
| *Space group* | C2/c | C2/c | P21/c | P |
| *a/Å* | 35.1971(15) | 35.0351(14) | 20.4292(7) | 6.3629(3) |
| *b/Å* | 6.2785(3) | 6.3588(2) | 10.0496(4) | 12.5190(5) |
| *c/Å* | 27.1730(13) | 26.5311(10) | 14.7840(5) | 18.7822(8) |
| *α/°* | 90 | 90 | 90 | 101.002(2) |
| *β/°* | 125.029(2) | 125.756(3) | 95.238(2) | 92.447(2) |
| *γ/°* | 90 | 90 | 90 | 101.742(2) |
| *Volume/Å3* | 4917.1(4) | 4796.5(3) | 3022.56(19) | 1432.72(11) |
| *Z* | 8 | 8 | 4 | 2 |
| *Dcalc g/cm3* | 1.463 | 1.505 | 1.321 | 1.431 |
| *μ/mm‑1* | 2.503 | 1.421 | 1.396 | 2.223 |
| *F(000)* | 2208.0 | 2240.0 | 1256.0 | 632.0 |
| *Crystal size/mm3* | 0.09×0.05×0.03 | 0.50×0.30×0.20 | 0.16×0.12×0.03 | 0.30×0.20×0.10 |
| *Radiation* | CuK*α* | CuK*α* | CuK*α* | CuK*α* |
| *Wavelength/Å* | *λ* = 1.54178 | *λ* = 1.54178 | *λ* = 1.54178 | *λ* = 1.54178 |
| *2θ/°* | 6.694-130.928 | 6.812-130.986 | 4.344-136.752 | 4.810-131.982 |
| *Reflections collected* | 11234 | 13351 | 23715 | 12765 |
| *Independent reflections* | 4045 | 4000 | 5526 | 4822 |
| *Rint* | 0.0384 | 0.0399 | 0.0782 | 0.0277 |
| *Rsigma* | 0.0452 | 0.0421 | 0.0766 | 0.0357 |
| *Restraints* | 30 | 0 | 0 | 0 |
| *Parameters* | 344 | 352 | 408 | 388 |
| *GooF* | 1.171 | 1.033 | 1.039 | 1.053 |
| *R1 [I> 2σ (I)]* | 0.0509 | 0.0349 | 0.0694 | 0.0308 |
| *wR2 [I> 2σ (I)]* | 0.1147 | 0.0896 | 0.1892 | 0.0775 |
| *R1 [all data]* | 0.0557 | 0.0405 | 0.0968 | 0.0320 |
| *wR2 [all data]* | 0.1167 | 0.0935 | 0.2143 | 0.0785 |
| *Largest peak/e Å-3* | 0.69 | 0.29 | 0.65 | 0.46 |
| *Deepest hole/e Å-3* | -0.73 | -0.33 | -0.33 | -0.38 |

## **Table S18:** Details of XRD data refinement.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***Compound*** | **6** | **7** | **8** | **9** |
| ***Identification code*** | KJF150xp | dgib007b | tcd662 | MS545 |
| *CCDC deposition #* | 2069460 | 2069457 | 2069453 | 2069456 |
| *Empirical formula* | C38H41BrN4 | C38H39BrN4Ni | C38H41IN4 | C16H10BrN2 |
| *Formula weight* | 633.66 | 690.35 | 680.65 | 310.17 |
| *Temperature/K* | 100(2) | 100(2) | 100(2) | 112(2) |
| *Crystal system* | triclinic | triclinic | triclinic | monoclinic |
| *Space group* | P | P | P | P21/n |
| *a/Å* | 4.8845(6) | 4.8416(2) | 4.8665(3) | 11.2118(7) |
| *b/Å* | 12.1267(12) | 13.9112(6) | 24.1992(13) | 6.2678(4) |
| *c/Å* | 26.324(3) | 23.8431(10) | 27.2069(14) | 17.6195(11) |
| *α/°* | 100.441(3) | 106.2510(10) | 74.9098(18) | 90 |
| *β/°* | 91.101(3) | 92.6350(10) | 89.9892(19) | 100.350(2) |
| *γ/°* | 90.923(3) | 91.003(2) | 89.030(2) | 90 |
| *Volume/Å3* | 1532.8(3) | 1539.33(11) | 3093.1(3) | 1218.03(13) |
| *Z* | 2 | 2 | 4 | 4 |
| *Dcalc g/cm3* | 1.373 | 1.489 | 1.462 | 1.691 |
| *μ/mm‑1* | 1.375 | 1.963 | 1.070 | 4.463 |
| *F(000)* | 664.0 | 716.0 | 1400.0 | 620.0 |
| *Crystal size/mm3* | 0.45×0.30×0.12 | 0.28×0.08×0.04 | 1.00×0.08×0.04 | 0.30×0.30×0.30 |
| *Radiation* | MoK*α* | MoK*α* | MoK*α* | CuK*α* |
| *Wavelength/Å* | *λ* = 0.71073 | *λ* = 0.71073 | *λ* = 0.71073 | *λ* = 1.54178 |
| *2θ/°* | 3.148-51.252 | 5.304-52.880 | 5.342-50.500 | 8.694-133.954 |
| *Reflections collected* | 37076 | 25173 | 25863 | 9061 |
| *Independent reflections* | 5709 | 6288 | 11142 | 2105 |
| *Rint* | 0.0972 | 0.0603 | 0.0637 | 0.0279 |
| *Rsigma* | 0.0765 | 0.0529 | 0.0893 | 0.0207 |
| *Restraints* | 73 | 1 | 39 | 0 |
| *Parameters* | 454 | 399 | 746 | 172 |
| *GooF* | 1.043 | 1.058 | 1.058 | 1.131 |
| *R1 [I> 2σ (I)]* | 0.0652 | 0.0460 | 0.0625 | 0.0261 |
| *wR2 [I> 2σ (I)]* | 0.1525 | 0.1066 | 0.1225 | 0.0682 |
| *R1 [all data]* | 0.0949 | 0.0713 | 0.1005 | 0.0265 |
| *wR2 [all data]* | 0.1646 | 0.1215 | 0.1373 | 0.0684 |
| *Largest peak/e Å-3* | 0.85 | 1.16 | 1.44 | 0.32 |
| *Deepest hole/e Å-3* | -0.95 | -0.78 | -1.76 | -0.34 |

## **Table S19:** Details of XRD data refinement.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***Compound*** | **10** | **11** | **13** | **16A** |
| ***Identification code*** | HE006 | HE015 | MS556 | MS529 |
| *CCDC deposition #* | 2069458 | 2069462 | 2069461 | 2069463 |
| *Empirical formula* | C34H24Br2N4 | C30H30Br2N4Ni | C35H34Br2N4O3 | C44H42N4Si2 |
| *Formula weight* | 648.39 | 665.11 | 718.48 | 682.99 |
| *Temperature/K* | 100(2) | 100(2) | 100(2) | 123(2) |
| *Crystal system* | orthorhombic | monoclinic | triclinic | triclinic |
| *Space group* | Pbcn | C2/c | P | P |
| *a/Å* | 16.6909(12) | 44.0507(16) | 7.9893(7) | 10.955(3) |
| *b/Å* | 6.2095(4) | 10.2192(4) | 11.6397(10) | 12.739(3) |
| *c/Å* | 25.1966(17) | 11.8461(4) | 17.1706(15) | 15.334(4) |
| *α/°* | 90 | 90 | 90.536(3) | 82.457(5) |
| *β/°* | 90 | 91.771(3) | 97.989(3) | 74.585(5) |
| *γ/°* | 90 | 90 | 107.786(3) | 66.493(4) |
| *Volume/Å3* | 2611.4(3) | 5330.1(3) | 1503.4(2) | 1891.0(8) |
| *Z* | 4 | 8 | 2 | 2 |
| *Dcalc g/cm3* | 1.649 | 1.658 | 1.587 | 1.200 |
| *μ/mm‑1* | 4.191 | 4.768 | 3.774 | 0.130 |
| *F(000)* | 1304.0 | 2688.0 | 732.0 | 724.0 |
| *Crystal size/mm3* | 0.40×0.35×0.30 | 0.35×0.10×0.05 | 0.50×0.46×0.10 | 0.5 × 0.3 × 0.3 |
| *Radiation* | CuK*α* | CuK*α* | CuK*α* | MoK*α* |
| *Wavelength/Å* | *λ* = 1.54178 | *λ* = 1.54178 | *λ* = 1.54178 | *λ* = 0.71073 |
| *2θ/°* | 7.016-134.196 | 4.014-133.988 | 7.988-131.99 | 3.188-54.998 |
| *Reflections collected* | 12171 | 18037 | 17701 | 17504 |
| *Independent reflections* | 2265 | 4611 | 5093 | 8581 |
| *Rint* | 0.0295 | 0.0810 | 0.0269 | 0.0626 |
| *Rsigma* | 0.0262 | 0.0474 | 0.0299 | 0.0940 |
| *Restraints* | 0 | 18 | 0 | 0 |
| *Parameters* | 182 | 348 | 401 | 459 |
| *GooF* | 1.058 | 1.032 | 1.054 | 1.251 |
| *R1 [I> 2σ (I)]* | 0.0282 | 0.0443 | 0.0253 | 0.1176 |
| *wR2 [I> 2σ (I)]* | 0.0757 | 0.1181 | 0.0655 | 0.2190 |
| *R1 [all data]* | 0.0295 | 0.0476 | 0.0255 | 0.1507 |
| *wR2 [all data]* | 0.0772 | 0.1209 | 0.0657 | 0.2316 |
| *Largest peak/e Å-3* | 0.54 | 1.17 | 0.37 | 0.38 |
| *Deepest hole/e Å-3* | -0.32 | -1.53 | -0.32 | -0.44 |

## **Table S20:** Details of XRD data refinement.

|  |  |
| --- | --- |
| ***Compound*** | **24** |
| ***Identification code*** | HE014 |
| *CCDC deposition #* | 2069459 |
| *Empirical formula* | C43H58N4Si |
| *Formula weight* | 659.02 |
| *Temperature/K* | 100(2) |
| *Crystal system* | triclinic |
| *Space group* | P |
| *a/Å* | 10.2392(4) |
| *b/Å* | 11.2462(5) |
| *c/Å* | 17.1716(7) |
| *α/°* | 96.815(2) |
| *β/°* | 97.845(2) |
| *γ/°* | 90.696(2) |
| *Volume/Å3* | 1944.19(14) |
| *Z* | 2 |
| *Dcalc g/cm3* | 1.126 |
| *μ/mm‑1* | 0.778 |
| *F(000)* | 716.0 |
| *Crystal size/mm3* | 0.48 × 0.06 × 0.04 |
| *Radiation* | CuK*α* |
| *Wavelength/Å* | *λ* = 1.54178 |
| *2θ/°* | 10.478-115.286 |
| *Reflections collected* | 15036 |
| *Independent reflections* | 5308 |
| *Rint* | 0.0325 |
| *Rsigma* | 0.0403 |
| *Restraints* | 33 |
| *Parameters* | 470 |
| *GooF* | 1.037 |
| *R1 [I> 2σ (I)]* | 0.0428 |
| *wR2 [I> 2σ (I)]* | 0.1113 |
| *R1 [all data]* | 0.0474 |
| *wR2 [all data]* | 0.1154 |
| *Largest peak/e Å-3* | 0.43 |
| *Deepest hole/e Å-3* | -0.42 |

# Complete NSD tables

## **Table S21:** NSD out-put of compounds **1**-**23**.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CCDC | com | Dip | B2g | B1g | Eu(x) | Eu(y) | A1g | A2g |  | Doop | B2u | B1u | A2u | Eg(x) | Eg(y) | A1u |
| MS563 | **1** | 0.24 | -0.12 | 0.02 | 0.03 | -0.03 | 0.20 | 0.00 |  | 0.15 | -0.08 | 0.10 | 0.05 | -0.01 | 0.06 | 0.02 |
| NESHUO | **2** | 0.25 | -0.06 | 0.02 | -0.02 | 0.01 | -0.24 | -0.01 |  | 1.01 | 0.10 | 1.00 | -0.06 | 0.03 | 0.06 | 0.00 |
| MS546 | **2A** | 0.13 | -0.06 | 0.02 | 0.02 | -0.02 | -0.11 | -0.01 |  | 0.22 | -0.06 | 0.20 | 0.04 | 0.01 | 0.07 | 0.01 |
| UDERUR | **3** | 0.29 | -0.20 | -0.03 | -0.05 | 0.02 | 0.20 | 0.00 |  | 0.47 | 0.42 | 0.13 | -0.06 | -0.15 | 0.09 | -0.02 |
| DGIB005 | **4** | 0.25 | -0.10 | -0.03 | 0.00 | 0.00 | 0.23 | 0.01 |  | 0.31 | 0.05 | 0.02 | -0.05 | 0.11 | 0.28 | -0.01 |
| ms567 | **5** | 0.21 | 0.01 | 0.04 | -0.01 | -0.01 | 0.21 | -0.01 |  | 0.39 | 0.10 | 0.31 | -0.10 | -0.05 | 0.20 | -0.01 |
| KJF150 | **6** | 0.22 | 0.00 | 0.01 | 0.00 | 0.00 | 0.22 | 0.00 |  | 0.36 | -0.22 | -0.08 | -0.02 | -0.27 | -0.06 | -0.01 |
| DGIB007 | **7** | 0.14 | 0.05 | -0.01 | 0.02 | 0.02 | -0.12 | 0.00 |  | 0.36 | 0.26 | 0.08 | -0.01 | 0.24 | 0.00 | 0.01 |
| tcd662\_1 | **8\_1** | 0.23 | -0.04 | 0.00 | -0.01 | 0.02 | 0.23 | 0.00 |  | 0.34 | -0.16 | 0.10 | 0.05 | -0.07 | -0.27 | 0.00 |
| tcd662\_2 | **8\_2** | 0.22 | -0.06 | -0.01 | -0.01 | -0.01 | 0.21 | -0.01 |  | 0.37 | 0.20 | -0.05 | -0.02 | -0.06 | -0.30 | 0.00 |
| MS545 | **9** | 0.25 | 0.00 | -0.06 | 0.00 | 0.00 | 0.24 | -0.01 |  | 0.08 | 0.00 | 0.00 | 0.00 | -0.01 | 0.08 | 0.00 |
| HE006 | **10** | 0.24 | -0.06 | -0.02 | 0.00 | 0.00 | 0.23 | -0.01 |  | 0.24 | 0.00 | 0.00 | 0.00 | 0.03 | 0.23 | 0.00 |
| HE015 | **11** | 0.49 | -0.14 | 0.01 | 0.03 | 0.02 | -0.47 | -0.01 |  | 1.90 | 0.55 | 1.81 | -0.19 | 0.07 | -0.05 | 0.00 |
| NOGWEN | **12** | 0.19 | 0.02 | -0.02 | -0.01 | -0.01 | 0.18 | -0.01 |  | 0.17 | 0.08 | -0.02 | -0.02 | -0.15 | -0.01 | 0.00 |
| MS556 | **13** | 0.19 | 0.08 | 0.02 | -0.01 | -0.02 | 0.17 | 0.00 |  | 0.90 | 0.86 | -0.24 | -0.03 | 0.02 | -0.10 | 0.00 |
| HUMWES | **13A** | 0.19 | -0.08 | -0.02 | -0.02 | 0.01 | 0.17 | 0.00 |  | 0.89 | 0.85 | -0.24 | 0.03 | 0.10 | 0.02 | 0.00 |
| HUMWAO | **14** | 0.22 | -0.05 | -0.04 | 0.01 | 0.01 | 0.21 | 0.00 |  | 0.36 | 0.22 | 0.01 | -0.06 | 0.26 | 0.11 | -0.02 |
| LASMOK | **15** | 0.21 | -0.02 | -0.01 | 0.00 | 0.01 | 0.21 | 0.00 |  | 0.28 | 0.08 | -0.01 | -0.25 | 0.10 | 0.02 | -0.01 |
| RAKGAN | **16** | 0.21 | 0.07 | -0.01 | 0.00 | 0.00 | 0.20 | -0.01 |  | 0.89 | 0.57 | -0.67 | -0.16 | -0.01 | -0.07 | 0.00 |
| MS529 | **16A** | 0.17 | 0.04 | 0.01 | 0.00 | 0.00 | 0.16 | -0.01 |  | 0.67 | 0.60 | -0.21 | -0.10 | -0.14 | 0.11 | 0.01 |
| ZOXQUA | **17** | 0.03 | -0.01 | 0.00 | 0.01 | 0.02 | 0.01 | 0.01 |  | 0.73 | 0.23 | -0.69 | 0.02 | -0.03 | 0.05 | -0.01 |
| ZOXCAS | **18** | 0.18 | 0.01 | 0.04 | -0.01 | 0.04 | 0.17 | -0.01 |  | 0.64 | 0.27 | -0.56 | -0.01 | 0.11 | 0.05 | 0.00 |
| BASDOR | **19** | 0.23 | 0.00 | -0.02 | 0.02 | 0.00 | 0.23 | 0.00 |  | 0.25 | 0.00 | -0.25 | 0.00 | 0.00 | 0.00 | 0.00 |
| YISZAD | **20** | 0.26 | -0.01 | 0.06 | 0.00 | 0.00 | 0.26 | 0.00 |  | 0.12 | 0.00 | 0.00 | 0.00 | 0.08 | 0.09 | 0.00 |
| QUGMEM | **21** | 0.47 | 0.02 | -0.01 | 0.00 | -0.03 | -0.46 | 0.04 |  | 1.89 | 0.34 | -1.85 | -0.09 | 0.09 | 0.00 | -0.01 |
| QUGMIQ | **22** | 0.42 | -0.04 | 0.00 | -0.01 | -0.01 | -0.41 | 0.00 |  | 1.74 | 0.00 | 1.72 | -0.09 | 0.14 | -0.14 | 0.00 |
| MORBEC | **23** | 0.23 | -0.05 | 0.01 | -0.01 | 0.02 | -0.22 | 0.00 |  | 0.96 | 0.23 | 0.93 | -0.02 | 0.07 | -0.01 | -0.02 |
| HE014 | **24** | 0.21 | -0.07 | 0.01 | 0.00 | 0.00 | 0.20 | 0.00 |  | 0.29 | -0.10 | -0.16 | -0.01 | 0.01 | 0.21 | 0.00 |

## **Table S22:** NSD out-put series 1.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **CCDC** | **COM** | **Dip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |  | **Doop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
|  | **1:1** | 0.38 | -0.32 | -0.05 | 0.00 | 0.00 | 0.21 | 0.00 |  | 0.08 | 0.00 | 0.00 | 0.00 | 0.06 | 0.06 | 0.00 |
|  | **1:2** | 0.14 | -0.06 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |  | 0.57 | 0.00 | 0.57 | 0.01 | -0.01 | -0.01 | 0.00 |
|  | **1:3** | 0.37 | -0.31 | -0.04 | 0.00 | 0.00 | 0.21 | -0.01 |  | 0.09 | 0.00 | -0.01 | 0.00 | -0.06 | -0.06 | 0.00 |
|  | **1:4** | 0.14 | -0.07 | 0.00 | 0.00 | 0.00 | -0.13 | 0.00 |  | 0.61 | 0.00 | 0.61 | 0.01 | -0.02 | -0.02 | 0.00 |
|  | **1:5** | 0.37 | 0.31 | 0.03 | 0.00 | 0.00 | 0.21 | -0.01 |  | 0.09 | 0.00 | 0.00 | 0.00 | -0.06 | 0.07 | 0.00 |
|  | **1:6** | 0.15 | -0.08 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |  | 0.59 | 0.00 | 0.59 | 0.01 | -0.02 | -0.02 | 0.00 |
|  | **1:7** | 0.26 | -0.13 | -0.04 | -0.02 | 0.02 | 0.22 | 0.00 |  | 0.08 | 0.00 | -0.01 | 0.00 | 0.06 | 0.05 | 0.00 |
|  | **1:8** | 0.19 | 0.04 | 0.00 | 0.02 | 0.02 | -0.18 | 0.00 |  | 0.99 | 0.00 | -0.99 | 0.01 | -0.01 | 0.01 | 0.00 |
|  | **1:9** | 0.23 | -0.03 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |  | 0.07 | 0.00 | 0.00 | 0.00 | -0.04 | 0.05 | 0.00 |
|  | **1:10** | 0.24 | -0.01 | 0.00 | 0.00 | 0.00 | -0.24 | 0.00 |  | 1.28 | 0.00 | 1.28 | 0.02 | -0.02 | -0.02 | 0.00 |
|  | **1D** | 0.24 | 0.09 | 0.04 | -0.02 | -0.03 | 0.22 | 0.00 |  | 0.08 | 0.00 | 0.01 | 0.00 | -0.05 | 0.06 | 0.00 |
|  | **2D** | 0.20 | -0.03 | 0.00 | 0.02 | -0.02 | -0.20 | 0.00 |  | 1.09 | 0.00 | -1.09 | -0.02 | 0.03 | 0.03 | 0.00 |
|  | **1:11** | 0.26 | -0.11 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |  | 0.05 | 0.00 | 0.00 | 0.00 | -0.03 | 0.04 | 0.00 |
|  | **1:12** | 0.27 | 0.00 | 0.00 | 0.01 | 0.00 | -0.27 | 0.00 |  | 1.41 | 0.00 | -1.41 | 0.03 | -0.02 | 0.02 | 0.00 |
|  | **3D** | 0.23 | -0.02 | -0.04 | 0.03 | -0.03 | 0.23 | 0.00 |  | 0.07 | 0.00 | -0.01 | 0.00 | -0.06 | -0.05 | 0.00 |
|  | **1:13** | 0.24 | -0.02 | 0.00 | -0.02 | 0.02 | -0.24 | 0.00 |  | 1.26 | 0.00 | 1.26 | 0.03 | 0.00 | 0.00 | 0.00 |
|  | **1:14** | 0.33 | -0.22 | 0.02 | 0.00 | 0.00 | 0.24 | 0.00 |  | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 |
|  | **1:15** | 0.31 | -0.02 | 0.00 | 0.01 | 0.01 | -0.31 | 0.00 |  | 1.56 | 0.00 | -1.55 | 0.04 | -0.02 | 0.02 | 0.00 |

## **Table S23:** NSD out-put series 2.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Series 2** |  | **Dip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |  | **Doop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
|  | **2:1** | 0.28 | -0.18 | 0.06 | 0.00 | -0.01 | 0.21 | 0.00 |  | 0.07 | -0.06 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  | **2:2** | 0.24 | 0.06 | 0.04 | 0.02 | -0.03 | 0.22 | 0.00 |  | 0.06 | -0.05 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
|  | **2:3** | 0.28 | -0.14 | 0.03 | 0.04 | -0.01 | 0.23 | 0.00 |  | 0.08 | -0.07 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  | **2:4** | 0.26 | 0.06 | 0.02 | 0.02 | 0.02 | 0.25 | 0.00 |  | 0.07 | -0.07 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
|  | **2:5** | 0.30 | 0.20 | 0.03 | 0.01 | -0.02 | 0.22 | 0.00 |  | 0.14 | -0.12 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  | **2:6** | 0.24 | 0.00 | 0.02 | 0.03 | 0.00 | 0.24 | 0.00 |  | 0.17 | -0.16 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  | **1D** | 0.24 | 0.09 | 0.04 | -0.02 | -0.03 | 0.22 | 0.00 |  | 0.08 | 0.00 | 0.01 | 0.00 | -0.05 | 0.06 | 0.00 |
|  | **1:11** | 0.26 | -0.11 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |  | 0.05 | 0.00 | 0.00 | 0.00 | -0.03 | 0.04 | 0.00 |

## **Table S24:** NSD out-put series 3.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Series 3** |  | **Dip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |  | **Doop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
|  | **3:1** | 0.21 | 0.00 | 0.03 | -0.01 | 0.00 | 0.21 | 0.00 |  | 0.13 | -0.11 | 0.00 | 0.02 | 0.00 | -0.06 | 0.00 |
|  | **3:2** | 0.23 | 0.00 | 0.02 | 0.02 | 0.00 | 0.23 | 0.00 |  | 0.15 | -0.14 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  | **2:6** | 0.24 | 0.00 | 0.02 | 0.03 | 0.00 | 0.24 | 0.00 |  | 0.17 | -0.16 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  | **3:3** | 0.25 | 0.00 | 0.02 | 0.05 | 0.00 | 0.25 | 0.00 |  | 0.20 | -0.19 | 0.00 | 0.01 | 0.00 | -0.05 | 0.00 |

## NSD tables and plots for crystal structures

### NSD result generated from **1** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | -0.12 | 0.02 | 0.03 | -0.03 | 0.20 | 0.00 |
| ext. | 0.24 | 0.00 | -0.12 | 0.02 | 0.03 | -0.03 | 0.20 | 0.00 |
|  |  |  | 0.00 | -0.02 | -0.01 | 0.02 | 0.00 | 0.00 |
| total | 0.25 | 0.00 | -0.12 | 0.02 | 0.03 | -0.03 | 0.20 | 0.00 |
|  |  |  | 0.00 | -0.02 | -0.01 | 0.02 | 0.00 | 0.00 |
|  |  |  | -0.02 | -0.03 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | 0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.02 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.25 | 0.00 | 0.13 | 0.04 | 0.03 | 0.03 | 0.21 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.15 | 0.00 | -0.08 | 0.10 | 0.05 | -0.01 | 0.06 | 0.02 |
| ext. | 0.17 | 0.00 | -0.07 | 0.10 | 0.06 | -0.02 | 0.06 | 0.02 |
|  |  |  | 0.03 | 0.01 | 0.03 | -0.02 | -0.03 | 0.01 |
| total | 0.17 | 0.00 | -0.07 | 0.10 | 0.06 | -0.02 | 0.06 | 0.02 |
|  |  |  | 0.03 | 0.01 | 0.03 | -0.02 | -0.03 | 0.01 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | -0.01 | 0.00 |  |
| comp. | 0.17 | 0.00 | 0.08 | 0.10 | 0.07 | 0.03 | 0.07 | 0.02 |

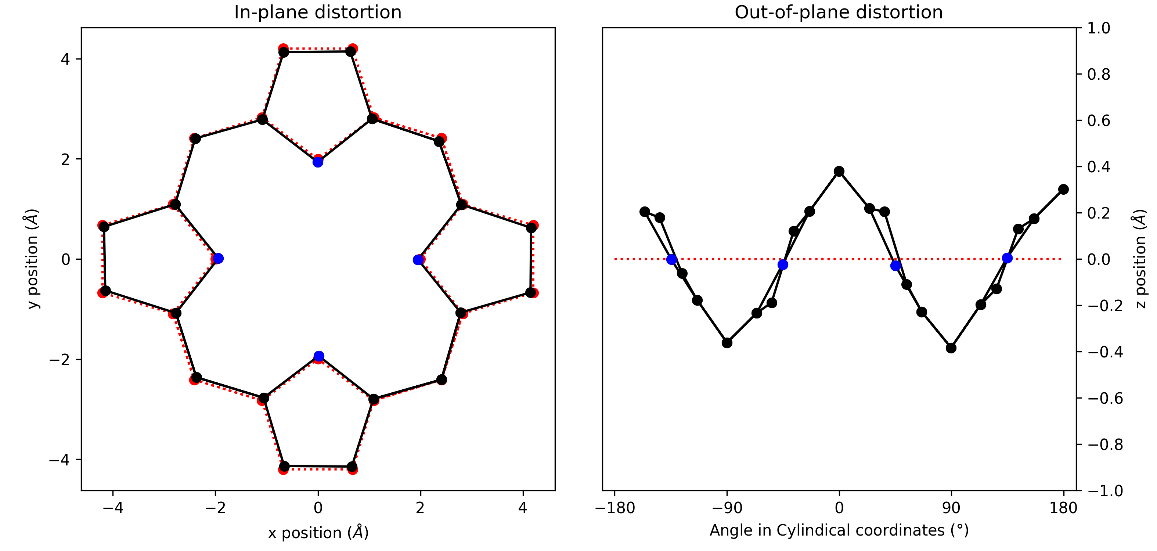


**Figure S87:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.25 | 0.00 | -0.06 | 0.02 | -0.02 | 0.01 | -0.24 | -0.01 |
| ext. | 0.25 | 0.00 | -0.06 | 0.02 | -0.02 | 0.01 | -0.24 | -0.01 |
|  |  |  | 0.03 | 0.01 | 0.02 | -0.01 | 0.02 | 0.00 |
| total | 0.27 | 0.00 | -0.06 | 0.02 | -0.02 | 0.01 | -0.24 | -0.01 |
|  |  |  | 0.03 | 0.01 | 0.02 | -0.01 | 0.02 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.01 | -0.02 | -0.01 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.01 | -0.02 | -0.06 | 0.01 |
|  |  |  | 0.00 | 0.02 | -0.01 | 0.01 | -0.03 | 0.02 |
|  |  |  | -0.02 | 0.03 | -0.01 | 0.01 | 0.04 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.02 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
| comp. | 0.27 | 0.00 | 0.07 | 0.04 | 0.04 | 0.04 | 0.25 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.01 | 0.00 | 0.10 | 1.00 | -0.06 | 0.03 | 0.06 | 0.00 |
| ext. | 1.01 | 0.00 | 0.10 | 1.00 | -0.06 | 0.03 | 0.06 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.03 | -0.05 | -0.05 | -0.01 |
| total | 1.01 | 0.00 | 0.10 | 1.00 | -0.06 | 0.03 | 0.06 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.03 | -0.05 | -0.05 | -0.01 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.01 | 0.00 | 0.10 | 1.00 | 0.06 | 0.06 | 0.08 | 0.01 |

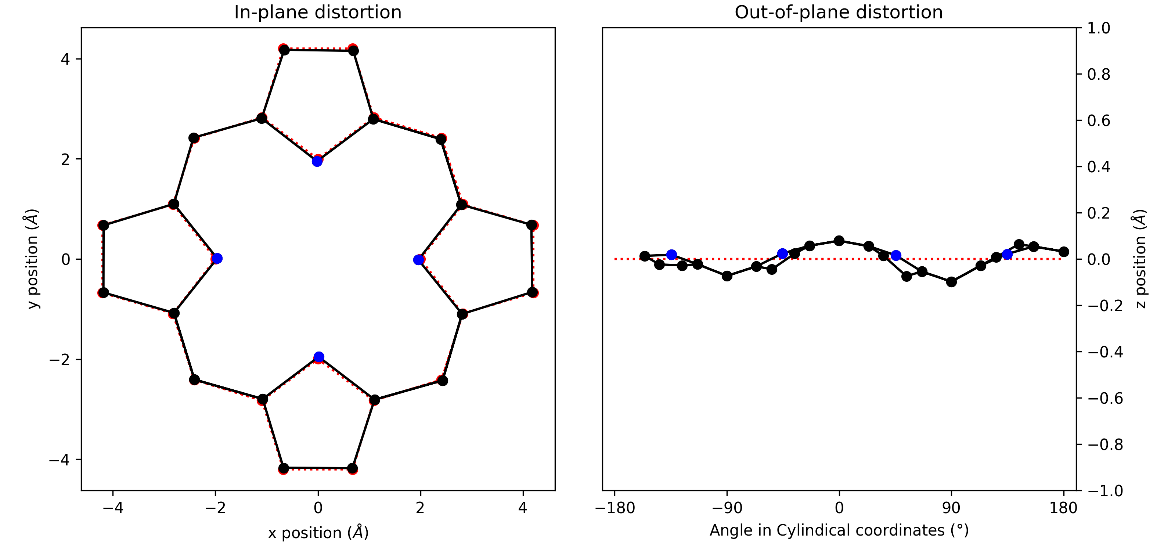


**Figure 88:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2A** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.13 | 0.00 | -0.06 | 0.02 | 0.02 | -0.02 | -0.11 | -0.01 |
| ext. | 0.14 | 0.00 | -0.06 | 0.02 | 0.02 | -0.02 | -0.12 | -0.01 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.01 | -0.04 | 0.00 |
| total | 0.15 | 0.00 | -0.06 | 0.02 | 0.02 | -0.02 | -0.12 | -0.01 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.01 | -0.04 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.15 | 0.00 | 0.06 | 0.02 | 0.02 | 0.02 | 0.13 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.22 | 0.00 | -0.06 | 0.20 | 0.04 | 0.01 | 0.07 | 0.01 |
| ext. | 0.23 | 0.00 | -0.06 | 0.20 | 0.05 | 0.01 | 0.07 | 0.01 |
|  |  |  | 0.01 | 0.00 | 0.03 | -0.01 | -0.03 | 0.00 |
| total | 0.23 | 0.00 | -0.06 | 0.20 | 0.05 | 0.01 | 0.07 | 0.01 |
|  |  |  | 0.01 | 0.00 | 0.03 | -0.01 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  |  | -0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.23 | 0.00 | 0.06 | 0.20 | 0.06 | 0.01 | 0.08 | 0.01 |

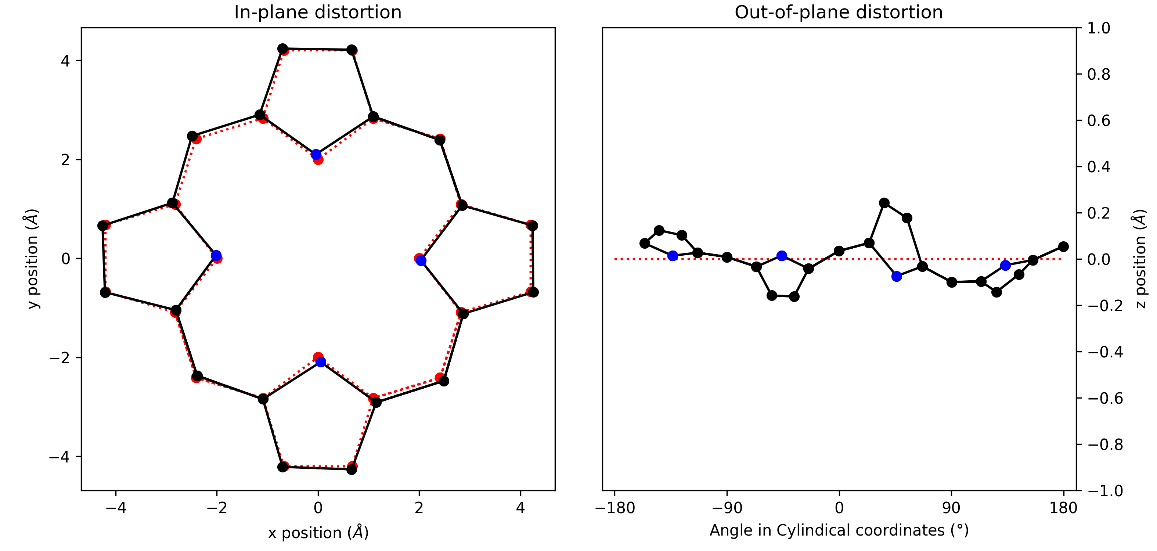


**Figure 89:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **3** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.29 | 0.00 | -0.20 | -0.03 | -0.05 | 0.02 | 0.20 | 0.00 |
| ext. | 0.30 | 0.00 | -0.20 | -0.04 | -0.05 | 0.02 | 0.20 | 0.00 |
|  |  |  | -0.04 | -0.07 | 0.02 | -0.04 | -0.02 | 0.01 |
| total | 0.32 | 0.00 | -0.20 | -0.04 | -0.05 | 0.02 | 0.20 | 0.00 |
|  |  |  | -0.04 | -0.07 | 0.02 | -0.04 | -0.02 | 0.01 |
|  |  |  | -0.01 | -0.06 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.01 | 0.01 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
| comp. | 0.32 | 0.00 | 0.20 | 0.10 | 0.05 | 0.05 | 0.21 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.47 | 0.00 | 0.42 | 0.13 | -0.06 | -0.15 | 0.09 | -0.02 |
| ext. | 0.48 | 0.00 | 0.41 | 0.13 | -0.06 | -0.15 | 0.09 | -0.02 |
|  |  |  | -0.11 | -0.01 | 0.00 | -0.01 | 0.00 | -0.01 |
| total | 0.48 | 0.00 | 0.41 | 0.13 | -0.06 | -0.15 | 0.09 | -0.02 |
|  |  |  | -0.11 | -0.01 | 0.00 | -0.01 | 0.00 | -0.01 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | -0.01 | 0.00 |  |
| comp. | 0.48 | 0.00 | 0.43 | 0.13 | 0.06 | 0.15 | 0.09 | 0.02 |

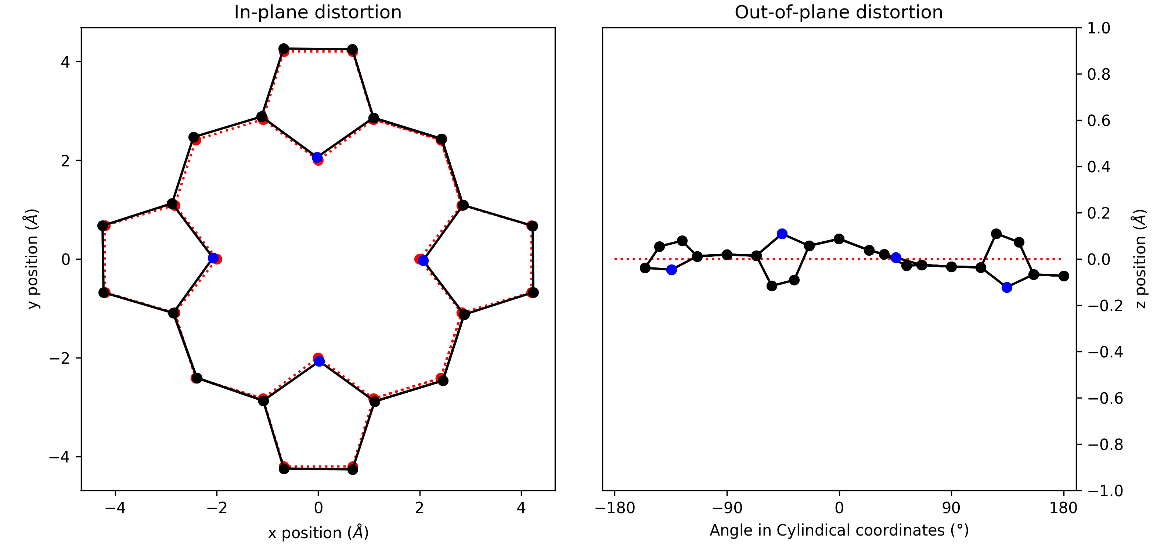


**Figure 90:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **4** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.25 | 0.00 | -0.10 | -0.03 | 0.00 | 0.00 | 0.23 | 0.01 |
| ext. | 0.25 | 0.00 | -0.10 | -0.03 | 0.00 | 0.00 | 0.23 | 0.01 |
|  |  |  | -0.02 | 0.01 | 0.01 | -0.02 | -0.02 | 0.00 |
| total | 0.27 | 0.00 | -0.10 | -0.02 | 0.00 | 0.00 | 0.23 | 0.01 |
|  |  |  | -0.02 | 0.01 | 0.01 | -0.01 | -0.02 | 0.00 |
|  |  |  | -0.01 | 0.01 | 0.00 | 0.01 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | 0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.02 | 0.00 |
|  |  |  | -0.01 | 0.00 | -0.01 | 0.01 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.01 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.27 | 0.00 | 0.10 | 0.03 | 0.03 | 0.03 | 0.24 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.31 | 0.00 | 0.05 | 0.02 | -0.05 | 0.11 | 0.28 | -0.01 |
| ext. | 0.33 | 0.00 | 0.05 | 0.02 | -0.05 | 0.11 | 0.28 | -0.01 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.00 | 0.10 | 0.01 |
| total | 0.33 | 0.00 | 0.05 | 0.02 | -0.05 | 0.11 | 0.28 | -0.01 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.00 | 0.10 | 0.01 |
|  |  |  | 0.00 | 0.00 | 0.01 | -0.01 | -0.02 |  |
|  |  |  |  |  |  | -0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.01 |  |
| comp. | 0.33 | 0.00 | 0.05 | 0.02 | 0.05 | 0.11 | 0.30 | 0.01 |

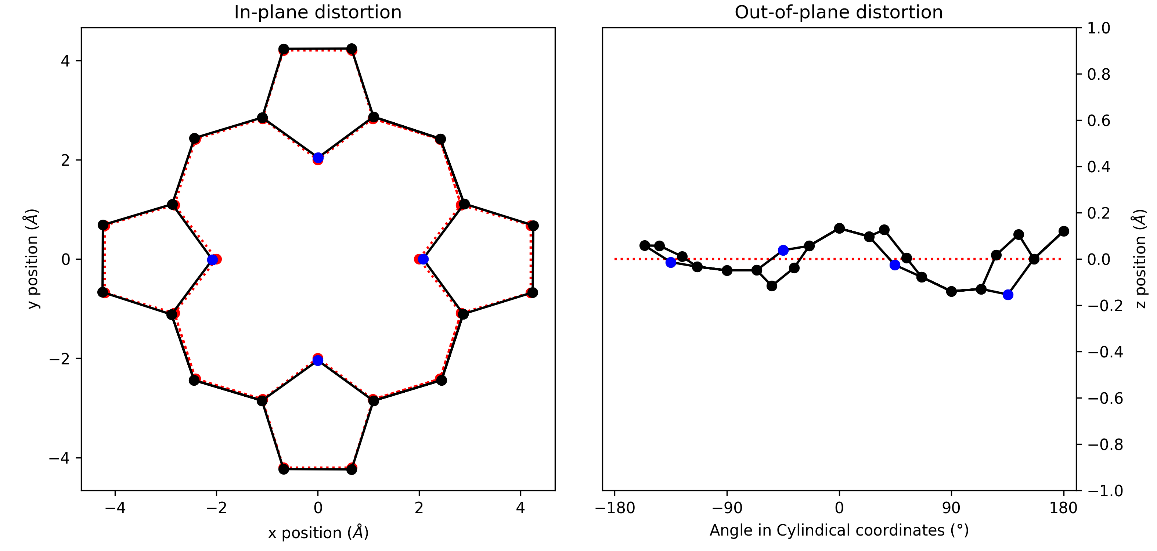


**Figure 91:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **5** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.21 | 0.00 | 0.01 | 0.04 | -0.01 | -0.01 | 0.21 | -0.01 |
| ext. | 0.22 | 0.00 | 0.01 | 0.04 | -0.01 | -0.01 | 0.21 | -0.01 |
|  |  |  | 0.01 | 0.03 | 0.01 | 0.01 | -0.02 | 0.00 |
| total | 0.23 | 0.00 | 0.01 | 0.04 | -0.01 | -0.01 | 0.21 | -0.01 |
|  |  |  | 0.01 | 0.03 | 0.01 | 0.01 | -0.02 | 0.00 |
|  |  |  | -0.01 | 0.02 | 0.01 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.01 | -0.02 | -0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.23 | 0.00 | 0.03 | 0.06 | 0.02 | 0.02 | 0.22 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.39 | 0.00 | 0.10 | 0.31 | -0.10 | -0.05 | 0.20 | -0.01 |
| ext. | 0.41 | 0.00 | 0.10 | 0.31 | -0.10 | -0.05 | 0.20 | -0.01 |
|  |  |  | 0.03 | 0.00 | -0.04 | 0.01 | 0.09 | -0.01 |
| total | 0.41 | 0.00 | 0.10 | 0.31 | -0.10 | -0.05 | 0.20 | -0.01 |
|  |  |  | 0.03 | 0.00 | -0.04 | 0.01 | 0.09 | -0.01 |
|  |  |  | 0.00 | 0.00 | 0.01 | 0.02 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | -0.01 |  |
|  |  |  |  |  |  | -0.01 | 0.01 |  |
| comp. | 0.41 | 0.00 | 0.11 | 0.31 | 0.11 | 0.05 | 0.22 | 0.01 |

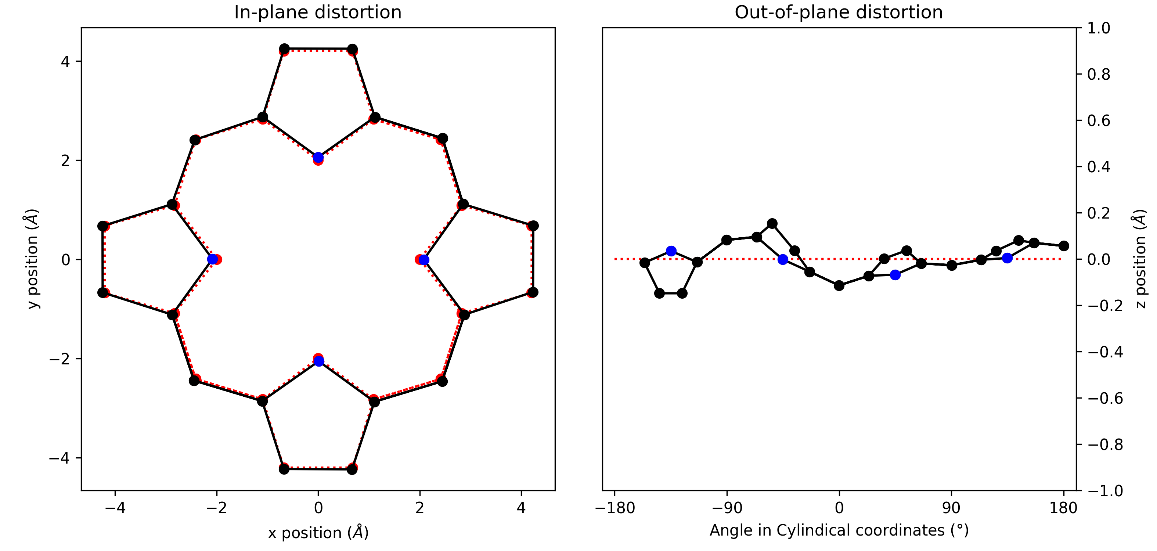


**Figure 92:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **6** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.22 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.22 | 0.00 |
| ext. | 0.23 | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 | 0.22 | 0.00 |
|  |  |  | -0.01 | 0.01 | 0.03 | 0.02 | -0.03 | 0.00 |
| total | 0.25 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.23 | 0.00 |
|  |  |  | -0.01 | 0.01 | 0.03 | 0.02 | -0.03 | 0.00 |
|  |  |  | 0.01 | 0.02 | -0.01 | 0.01 | 0.06 | 0.00 |
|  |  |  | -0.01 | 0.00 | -0.01 | -0.02 | -0.02 | -0.01 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | -0.02 | 0.03 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | -0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | -0.01 |  |  |
| comp. | 0.25 | 0.00 | 0.03 | 0.03 | 0.03 | 0.04 | 0.24 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.36 | 0.00 | -0.22 | -0.08 | -0.02 | -0.27 | -0.06 | -0.01 |
| ext. | 0.36 | 0.00 | -0.22 | -0.08 | -0.02 | -0.27 | -0.06 | -0.01 |
|  |  |  | 0.01 | 0.01 | 0.00 | 0.03 | 0.01 | 0.00 |
| total | 0.36 | 0.00 | -0.22 | -0.08 | -0.02 | -0.27 | -0.06 | -0.01 |
|  |  |  | 0.02 | 0.01 | 0.00 | 0.03 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | -0.01 | 0.01 |  |
| comp. | 0.36 | 0.00 | 0.22 | 0.08 | 0.02 | 0.27 | 0.06 | 0.01 |

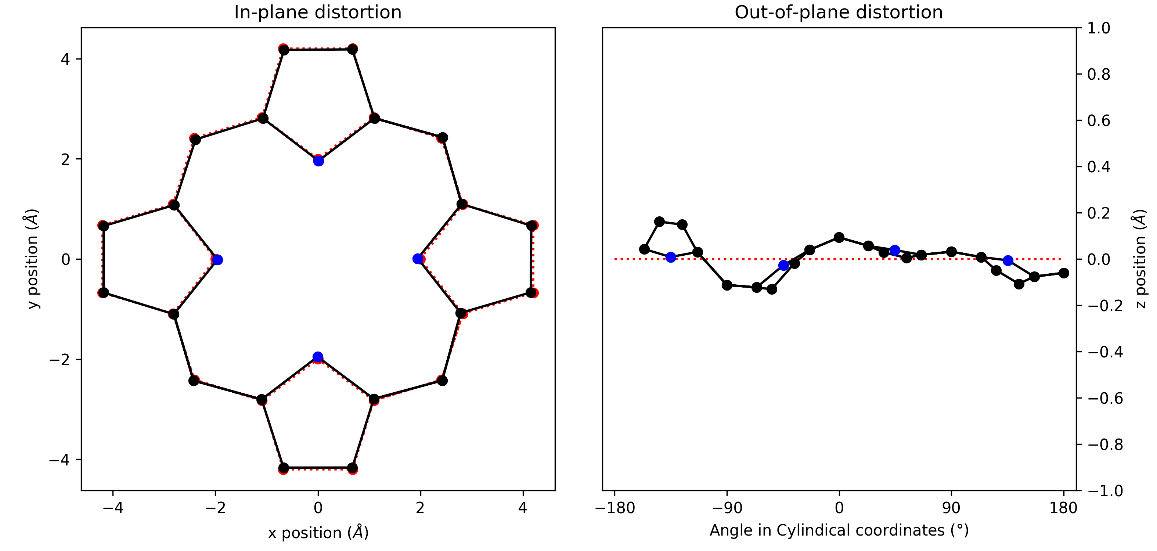


**Figure 93:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **7** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.14 | 0.00 | 0.05 | -0.01 | 0.02 | 0.02 | -0.12 | 0.00 |
| ext. | 0.15 | 0.00 | 0.05 | -0.01 | 0.02 | 0.02 | -0.12 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.03 | 0.01 | -0.05 | 0.00 |
| total | 0.16 | 0.00 | 0.05 | -0.01 | 0.02 | 0.02 | -0.13 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.03 | 0.01 | -0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | -0.01 | -0.04 | 0.00 |
|  |  |  | -0.01 | 0.00 | -0.02 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
| comp. | 0.16 | 0.00 | 0.05 | 0.01 | 0.04 | 0.03 | 0.14 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.36 | 0.00 | 0.26 | 0.08 | -0.01 | 0.24 | 0.00 | 0.01 |
| ext. | 0.37 | 0.00 | 0.26 | 0.08 | 0.00 | 0.23 | 0.00 | 0.01 |
|  |  |  | 0.00 | 0.00 | 0.03 | -0.09 | -0.02 | 0.00 |
| total | 0.37 | 0.00 | 0.26 | 0.08 | 0.00 | 0.23 | 0.00 | 0.01 |
|  |  |  | 0.00 | 0.00 | 0.03 | -0.09 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.01 | 0.00 |  |
| comp. | 0.37 | 0.00 | 0.26 | 0.08 | 0.03 | 0.25 | 0.02 | 0.01 |

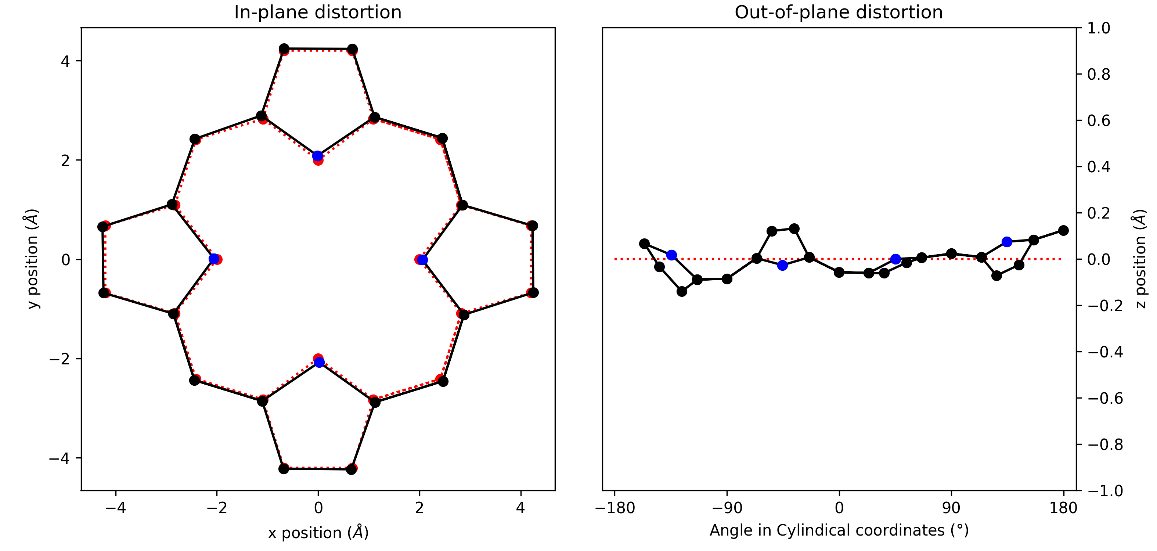


**Figure 94:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **8\_1** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | -0.04 | 0.00 | -0.01 | 0.02 | 0.23 | 0.00 |
| ext. | 0.24 | 0.00 | -0.04 | 0.00 | -0.01 | 0.02 | 0.23 | 0.00 |
|  |  |  | -0.03 | -0.03 | 0.02 | 0.01 | -0.04 | -0.01 |
| total | 0.26 | 0.00 | -0.04 | 0.00 | -0.01 | 0.02 | 0.23 | 0.00 |
|  |  |  | -0.03 | -0.03 | 0.02 | 0.01 | -0.04 | -0.01 |
|  |  |  | 0.02 | -0.02 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | -0.02 | 0.00 | -0.02 | -0.01 | -0.02 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | -0.01 | 0.02 |  |
|  |  |  |  |  | -0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | -0.01 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.06 | 0.04 | 0.03 | 0.03 | 0.24 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.34 | 0.00 | -0.16 | 0.10 | 0.05 | -0.07 | -0.27 | 0.00 |
| ext. | 0.34 | 0.00 | -0.16 | 0.10 | 0.05 | -0.07 | -0.27 | 0.00 |
|  |  |  | 0.01 | -0.01 | 0.00 | 0.01 | 0.03 | 0.00 |
| total | 0.34 | 0.00 | -0.16 | 0.10 | 0.05 | -0.07 | -0.27 | 0.00 |
|  |  |  | 0.01 | -0.01 | 0.00 | 0.01 | 0.03 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.01 | 0.02 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.01 | 0.00 |  |
| comp. | 0.34 | 0.00 | 0.16 | 0.10 | 0.05 | 0.07 | 0.28 | 0.00 |

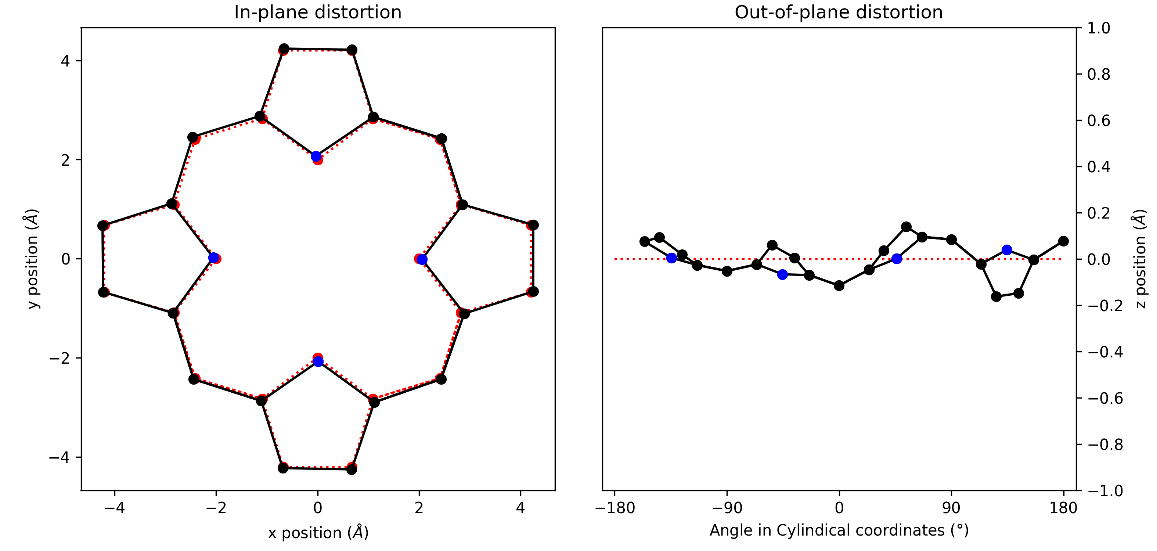


**Figure 95:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **8\_2** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.22 | 0.00 | -0.06 | -0.01 | -0.01 | -0.01 | 0.21 | -0.01 |
| ext. | 0.23 | 0.00 | -0.06 | -0.01 | -0.01 | -0.01 | 0.21 | -0.01 |
|  |  |  | -0.03 | -0.02 | -0.03 | -0.02 | -0.04 | 0.00 |
| total | 0.25 | 0.00 | -0.06 | -0.01 | -0.01 | -0.01 | 0.22 | -0.01 |
|  |  |  | -0.03 | -0.02 | -0.03 | -0.02 | -0.04 | 0.00 |
|  |  |  | 0.01 | -0.02 | 0.00 | 0.01 | 0.06 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.02 | 0.01 | -0.01 | -0.01 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
| comp. | 0.25 | 0.00 | 0.07 | 0.03 | 0.04 | 0.03 | 0.23 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.37 | 0.00 | 0.20 | -0.05 | -0.02 | -0.06 | -0.30 | 0.00 |
| ext. | 0.37 | 0.00 | 0.20 | -0.05 | -0.02 | -0.06 | -0.30 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.03 | 0.04 | 0.01 |
| total | 0.37 | 0.00 | 0.20 | -0.05 | -0.02 | -0.06 | -0.30 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.03 | 0.04 | 0.01 |
|  |  |  | 0.00 | -0.01 | 0.00 | -0.01 | 0.02 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | -0.01 |  |
| comp. | 0.37 | 0.00 | 0.20 | 0.05 | 0.02 | 0.06 | 0.30 | 0.01 |

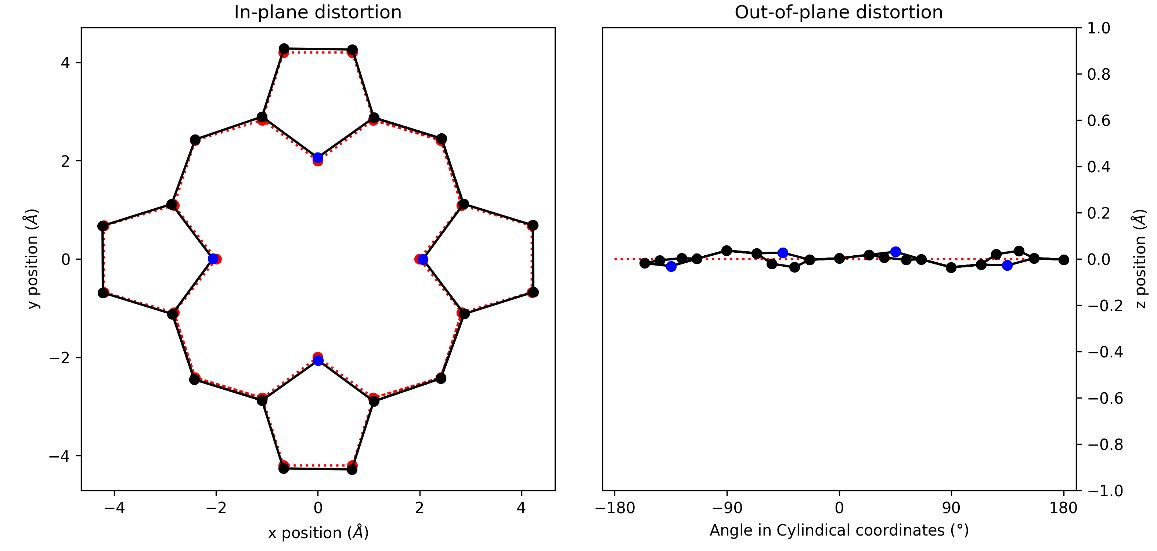


**Figure 96:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **9** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.25 | 0.00 | 0.00 | -0.06 | 0.00 | 0.00 | 0.24 | -0.01 |
| ext. | 0.25 | 0.00 | 0.00 | -0.06 | 0.00 | 0.00 | 0.24 | -0.01 |
|  |  |  | -0.02 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 |
| total | 0.26 | 0.00 | 0.00 | -0.06 | 0.00 | 0.00 | 0.24 | -0.01 |
|  |  |  | -0.02 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.03 | 0.03 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.04 | 0.08 | 0.00 | 0.00 | 0.25 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.08 | 0.00 |
| ext. | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.08 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.06 | 0.02 | 0.00 |
| total | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.08 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.06 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.01 | 0.00 |  |
| comp. | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.07 | 0.08 | 0.00 |

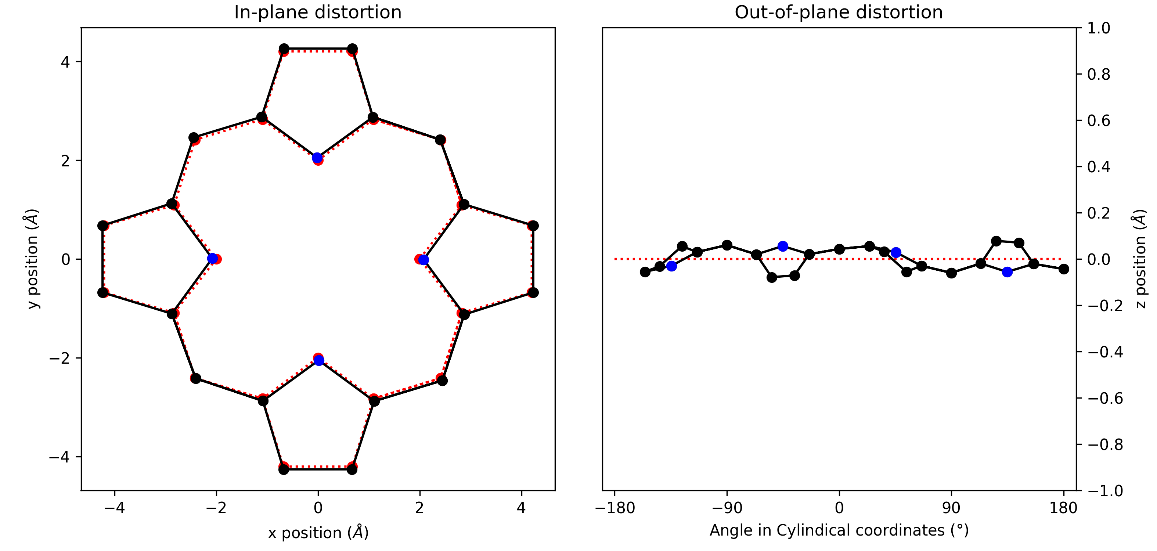


**Figure 97:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **10** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | -0.06 | -0.02 | 0.00 | 0.00 | 0.23 | -0.01 |
| ext. | 0.24 | 0.00 | -0.06 | -0.02 | 0.00 | 0.00 | 0.23 | -0.01 |
|  |  |  | -0.01 | 0.04 | 0.00 | 0.00 | 0.00 | -0.01 |
| total | 0.26 | 0.00 | -0.06 | -0.02 | 0.00 | 0.00 | 0.23 | -0.01 |
|  |  |  | -0.01 | 0.04 | 0.00 | 0.00 | 0.00 | -0.01 |
|  |  |  | -0.03 | 0.04 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.07 | 0.06 | 0.00 | 0.00 | 0.24 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.23 | 0.00 |
| ext. | 0.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.23 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.04 | 0.00 | 0.00 |
| total | 0.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.23 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.04 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.02 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | -0.02 |  |
|  |  |  |  |  |  | -0.01 | 0.01 |  |
| comp. | 0.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.24 | 0.00 |

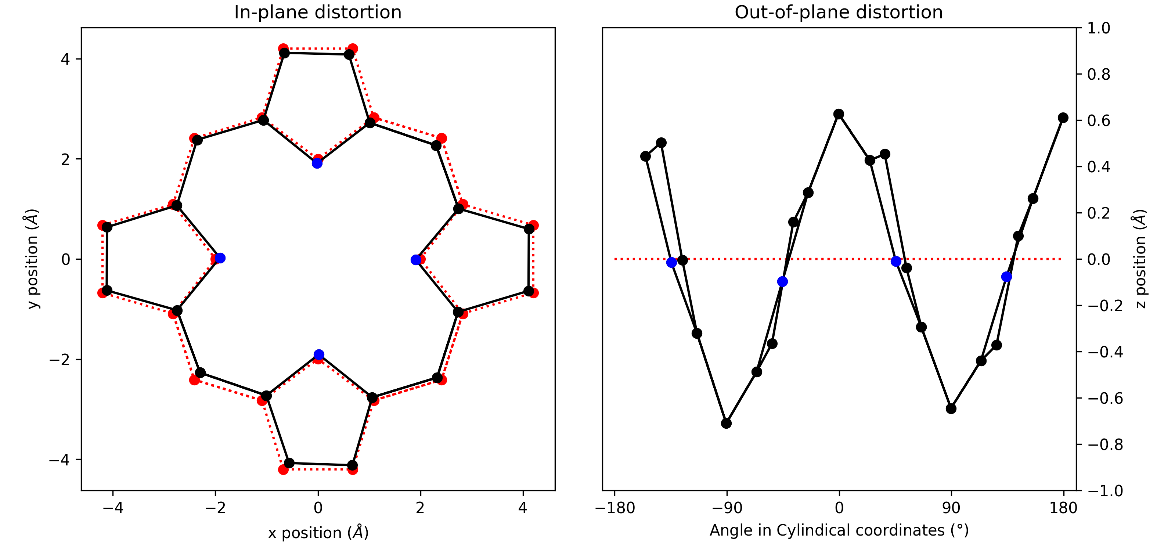


**Figure 98:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **11** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.49 | 0.01 | -0.14 | 0.01 | 0.03 | 0.02 | -0.47 | -0.01 |
| ext. | 0.53 | 0.01 | -0.14 | 0.01 | 0.03 | 0.02 | -0.47 | -0.01 |
|  |  |  | 0.05 | 0.01 | -0.01 | -0.01 | 0.16 | 0.07 |
| total | 0.54 | 0.00 | -0.14 | 0.01 | 0.03 | 0.02 | -0.47 | -0.01 |
|  |  |  | 0.05 | 0.01 | -0.01 | -0.01 | 0.16 | 0.07 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.01 | 0.02 | -0.01 |
|  |  |  | 0.04 | 0.01 | 0.02 | 0.01 | -0.11 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.03 | 0.02 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.07 |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.02 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.54 | 0.00 | 0.15 | 0.02 | 0.04 | 0.03 | 0.51 | 0.08 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.90 | 0.00 | 0.55 | 1.81 | -0.19 | 0.07 | -0.05 | 0.00 |
| ext. | 1.90 | 0.00 | 0.55 | 1.81 | -0.19 | 0.07 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.06 | -0.03 | 0.00 | 0.00 |
| total | 1.90 | 0.00 | 0.54 | 1.81 | -0.19 | 0.07 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.06 | -0.03 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.02 | -0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.90 | 0.00 | 0.55 | 1.81 | 0.20 | 0.07 | 0.05 | 0.00 |

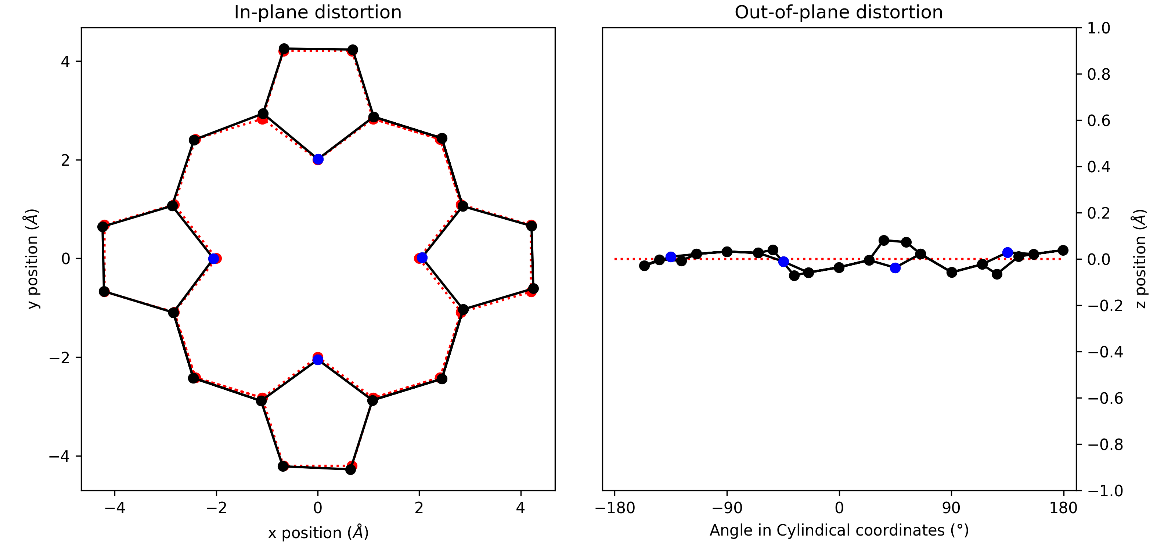


**Figure 99:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from 12 (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.19 | 0.01 | 0.02 | -0.02 | -0.01 | -0.01 | 0.18 | -0.01 |
| ext. | 0.21 | 0.01 | 0.02 | -0.02 | -0.01 | -0.01 | 0.18 | -0.01 |
|  |  |  | -0.07 | -0.05 | -0.01 | 0.00 | 0.01 | 0.01 |
| total | 0.26 | 0.00 | 0.02 | -0.02 | -0.01 | -0.01 | 0.18 | -0.01 |
|  |  |  | -0.07 | -0.05 | -0.01 | 0.00 | 0.01 | 0.01 |
|  |  |  | 0.05 | 0.03 | 0.01 | -0.01 | 0.03 | 0.00 |
|  |  |  | 0.02 | 0.02 | -0.01 | -0.01 | -0.09 | 0.00 |
|  |  |  | 0.00 | 0.05 | 0.01 | -0.01 | 0.01 | -0.01 |
|  |  |  | -0.02 | 0.02 | -0.01 | -0.01 | -0.02 |  |
|  |  |  |  |  | 0.02 | -0.01 |  |  |
|  |  |  |  |  | 0.02 | -0.02 |  |  |
|  |  |  |  |  | -0.05 | -0.03 |  |  |
|  |  |  |  |  | 0.02 | -0.01 |  |  |
|  |  |  |  |  | 0.02 | -0.01 |  |  |
| comp. | 0.26 | 0.00 | 0.09 | 0.08 | 0.07 | 0.05 | 0.21 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.17 | 0.00 | 0.08 | -0.02 | -0.02 | -0.15 | -0.01 | 0.00 |
| ext. | 0.19 | 0.00 | 0.08 | -0.02 | -0.02 | -0.15 | -0.01 | 0.00 |
|  |  |  | -0.04 | 0.02 | 0.01 | 0.05 | -0.03 | 0.02 |
| total | 0.20 | 0.00 | 0.08 | -0.02 | -0.02 | -0.15 | -0.01 | 0.00 |
|  |  |  | -0.04 | 0.02 | 0.01 | 0.05 | -0.03 | 0.02 |
|  |  |  | -0.01 | 0.04 | 0.00 | -0.03 | 0.00 |  |
|  |  |  |  |  |  | 0.02 | 0.01 |  |
|  |  |  |  |  |  | -0.03 | 0.00 |  |
| comp. | 0.20 | 0.00 | 0.09 | 0.04 | 0.03 | 0.17 | 0.04 | 0.02 |

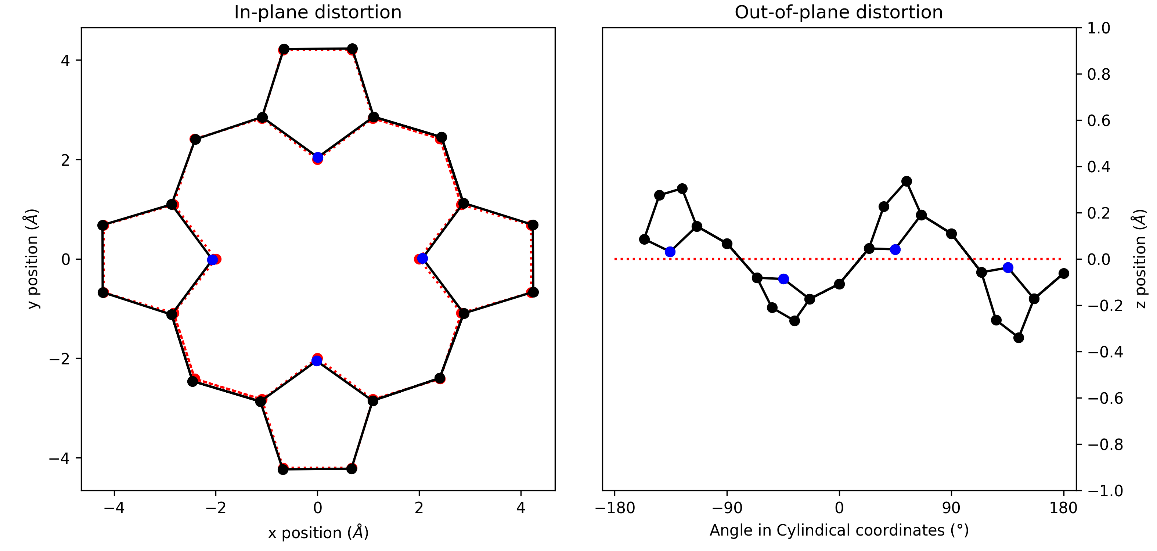


**Figure 100:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **13** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.19 | 0.00 | 0.08 | 0.02 | -0.01 | -0.02 | 0.17 | 0.00 |
| ext. | 0.20 | 0.00 | 0.08 | 0.02 | -0.01 | -0.02 | 0.17 | 0.00 |
|  |  |  | -0.01 | 0.02 | -0.02 | 0.01 | -0.01 | -0.02 |
| total | 0.21 | 0.00 | 0.08 | 0.02 | -0.01 | -0.02 | 0.18 | 0.00 |
|  |  |  | -0.01 | 0.02 | -0.02 | 0.01 | -0.01 | -0.02 |
|  |  |  | 0.03 | 0.01 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.01 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.21 | 0.00 | 0.09 | 0.03 | 0.02 | 0.02 | 0.19 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.90 | 0.00 | 0.86 | -0.24 | -0.03 | 0.02 | -0.10 | 0.00 |
| ext. | 0.90 | 0.00 | 0.86 | -0.24 | -0.03 | 0.02 | -0.10 | 0.00 |
|  |  |  | -0.03 | 0.00 | -0.01 | 0.00 | 0.01 | 0.00 |
| total | 0.90 | 0.00 | 0.86 | -0.24 | -0.03 | 0.02 | -0.10 | 0.00 |
|  |  |  | -0.03 | 0.00 | -0.01 | 0.00 | 0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.90 | 0.00 | 0.86 | 0.24 | 0.03 | 0.02 | 0.10 | 0.00 |

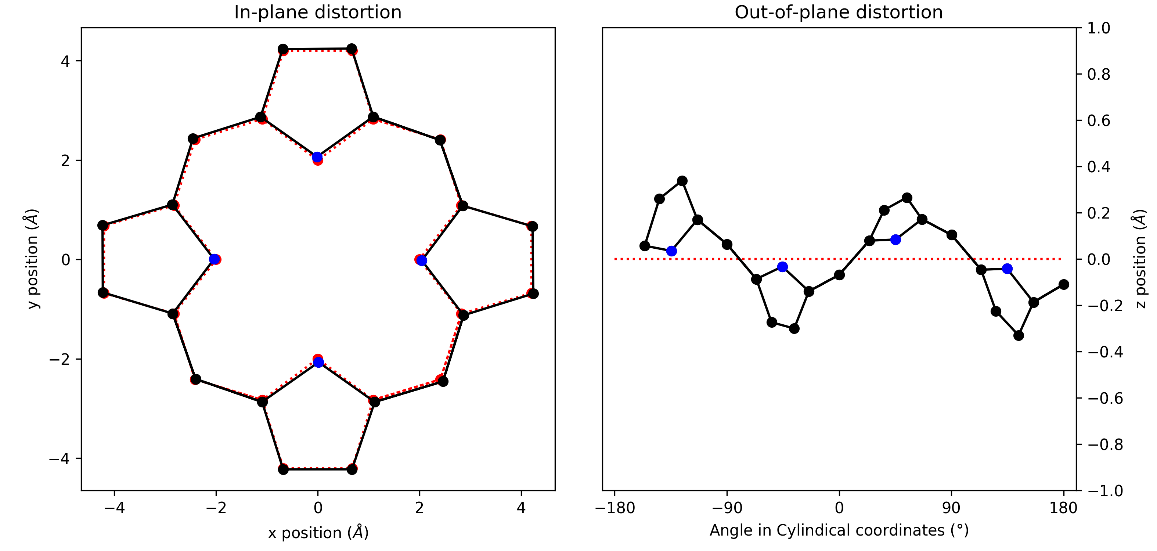


**Figure 101:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **13A** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.19 | 0.00 | -0.08 | -0.02 | -0.02 | 0.01 | 0.17 | 0.00 |
| ext. | 0.20 | 0.00 | -0.08 | -0.02 | -0.02 | 0.01 | 0.17 | 0.00 |
|  |  |  | 0.01 | -0.02 | 0.01 | 0.02 | -0.01 | -0.02 |
| total | 0.21 | 0.00 | -0.08 | -0.02 | -0.02 | 0.01 | 0.18 | 0.00 |
|  |  |  | 0.01 | -0.02 | 0.01 | 0.02 | -0.01 | -0.02 |
|  |  |  | -0.03 | -0.02 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.21 | 0.00 | 0.09 | 0.03 | 0.02 | 0.02 | 0.19 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.89 | 0.00 | 0.85 | -0.24 | 0.03 | 0.10 | 0.02 | 0.00 |
| ext. | 0.89 | 0.00 | 0.85 | -0.24 | 0.03 | 0.10 | 0.02 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| total | 0.89 | 0.00 | 0.85 | -0.24 | 0.03 | 0.10 | 0.02 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.01 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.89 | 0.00 | 0.85 | 0.24 | 0.03 | 0.10 | 0.02 | 0.00 |

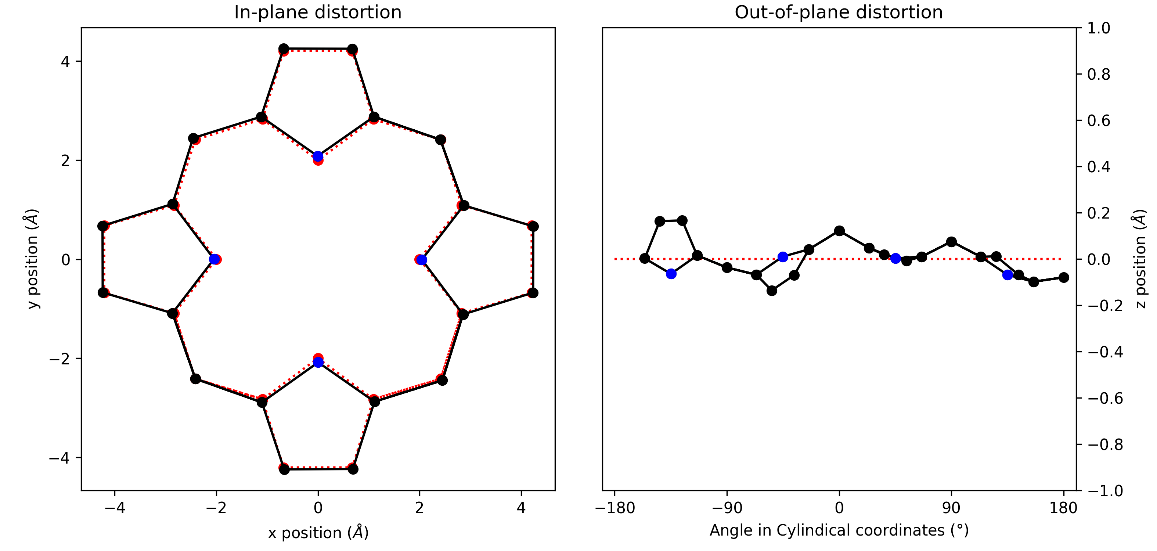


**Figure 102:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **14** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.22 | 0.00 | -0.05 | -0.04 | 0.01 | 0.01 | 0.21 | 0.00 |
| ext. | 0.22 | 0.00 | -0.05 | -0.04 | 0.01 | 0.01 | 0.21 | 0.00 |
|  |  |  | 0.01 | -0.02 | -0.01 | 0.00 | -0.01 | 0.00 |
| total | 0.23 | 0.00 | -0.05 | -0.04 | 0.01 | 0.01 | 0.21 | 0.00 |
|  |  |  | 0.01 | -0.02 | -0.01 | 0.00 | -0.01 | 0.00 |
|  |  |  | -0.03 | -0.02 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | 0.02 | -0.01 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.02 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.23 | 0.00 | 0.06 | 0.05 | 0.01 | 0.02 | 0.22 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.36 | 0.00 | 0.22 | 0.01 | -0.06 | 0.26 | 0.11 | -0.02 |
| ext. | 0.37 | 0.00 | 0.22 | 0.01 | -0.06 | 0.25 | 0.11 | -0.02 |
|  |  |  | -0.04 | 0.00 | -0.05 | -0.05 | 0.03 | 0.00 |
| total | 0.37 | 0.00 | 0.22 | 0.01 | -0.06 | 0.25 | 0.11 | -0.02 |
|  |  |  | -0.04 | 0.00 | -0.05 | -0.05 | 0.03 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | -0.03 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.01 | 0.00 |  |
| comp. | 0.37 | 0.00 | 0.22 | 0.01 | 0.08 | 0.26 | 0.11 | 0.02 |

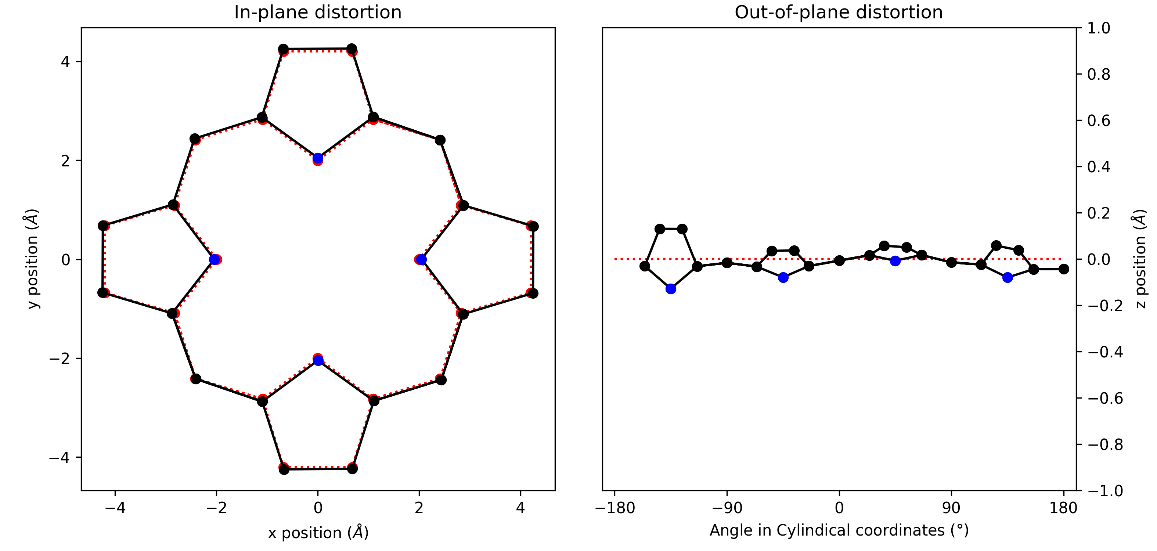


**Figure 103:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **15** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.21 | 0.00 | -0.02 | -0.01 | 0.00 | 0.01 | 0.21 | 0.00 |
| ext. | 0.21 | 0.00 | -0.02 | -0.01 | 0.00 | 0.01 | 0.21 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.01 | 0.02 | 0.00 |
| total | 0.22 | 0.00 | -0.02 | -0.01 | 0.00 | 0.01 | 0.21 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.01 | 0.02 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | -0.01 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.22 | 0.00 | 0.04 | 0.01 | 0.01 | 0.01 | 0.21 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.28 | 0.00 | 0.08 | -0.01 | -0.25 | 0.10 | 0.02 | -0.01 |
| ext. | 0.29 | 0.00 | 0.08 | -0.01 | -0.25 | 0.11 | 0.02 | -0.01 |
|  |  |  | 0.00 | 0.00 | 0.03 | 0.07 | 0.00 | 0.00 |
| total | 0.29 | 0.00 | 0.08 | -0.01 | -0.25 | 0.11 | 0.02 | -0.01 |
|  |  |  | 0.00 | 0.00 | 0.03 | 0.07 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.29 | 0.00 | 0.08 | 0.01 | 0.25 | 0.13 | 0.02 | 0.01 |

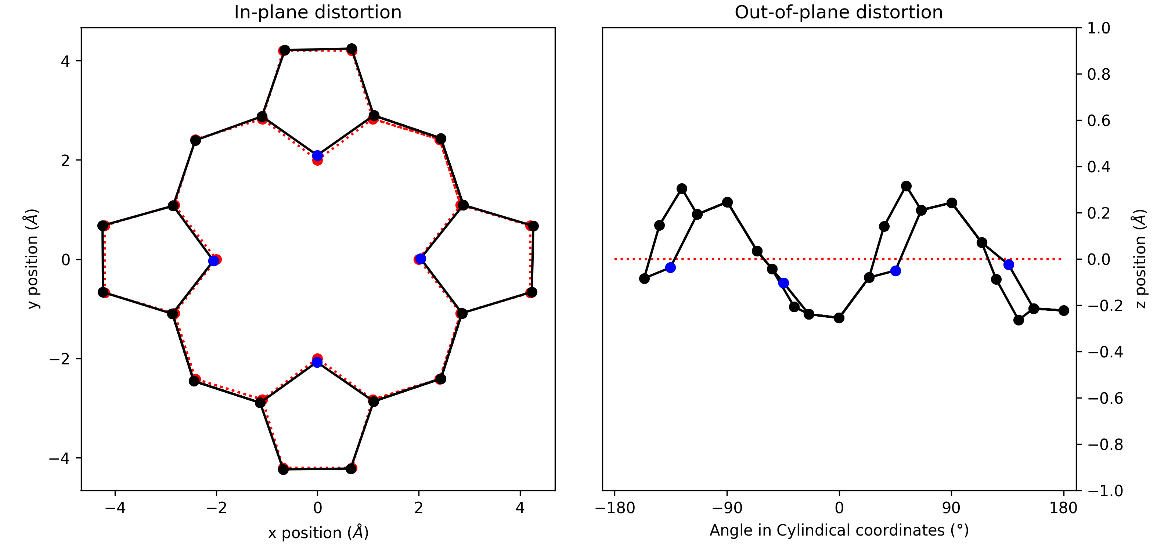


**Figure 104** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **16** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.21 | 0.00 | 0.07 | -0.01 | 0.00 | 0.00 | 0.20 | -0.01 |
| ext. | 0.22 | 0.00 | 0.07 | -0.01 | 0.00 | 0.00 | 0.20 | -0.01 |
|  |  |  | 0.00 | -0.04 | -0.01 | 0.02 | 0.00 | -0.03 |
| total | 0.25 | 0.00 | 0.07 | -0.01 | 0.00 | 0.00 | 0.20 | -0.02 |
|  |  |  | 0.00 | -0.04 | -0.01 | 0.02 | 0.00 | -0.03 |
|  |  |  | -0.01 | -0.04 | 0.00 | 0.00 | 0.07 | -0.01 |
|  |  |  | -0.01 | 0.02 | 0.00 | -0.03 | -0.04 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.02 | 0.02 | 0.00 | -0.02 |
|  |  |  | 0.01 | -0.01 | -0.01 | 0.02 | 0.02 |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.25 | 0.00 | 0.07 | 0.07 | 0.03 | 0.04 | 0.22 | 0.04 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.89 | 0.00 | 0.57 | -0.67 | -0.16 | -0.01 | -0.07 | 0.00 |
| ext. | 0.90 | 0.00 | 0.57 | -0.67 | -0.16 | -0.01 | -0.07 | 0.00 |
|  |  |  | -0.07 | -0.02 | -0.01 | 0.00 | -0.05 | 0.00 |
| total | 0.90 | 0.00 | 0.57 | -0.67 | -0.16 | -0.01 | -0.07 | 0.00 |
|  |  |  | -0.07 | -0.02 | -0.01 | 0.00 | -0.05 | 0.00 |
|  |  |  | -0.02 | 0.01 | 0.00 | 0.01 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | -0.02 | 0.00 |  |
| comp. | 0.90 | 0.00 | 0.57 | 0.67 | 0.16 | 0.02 | 0.08 | 0.00 |

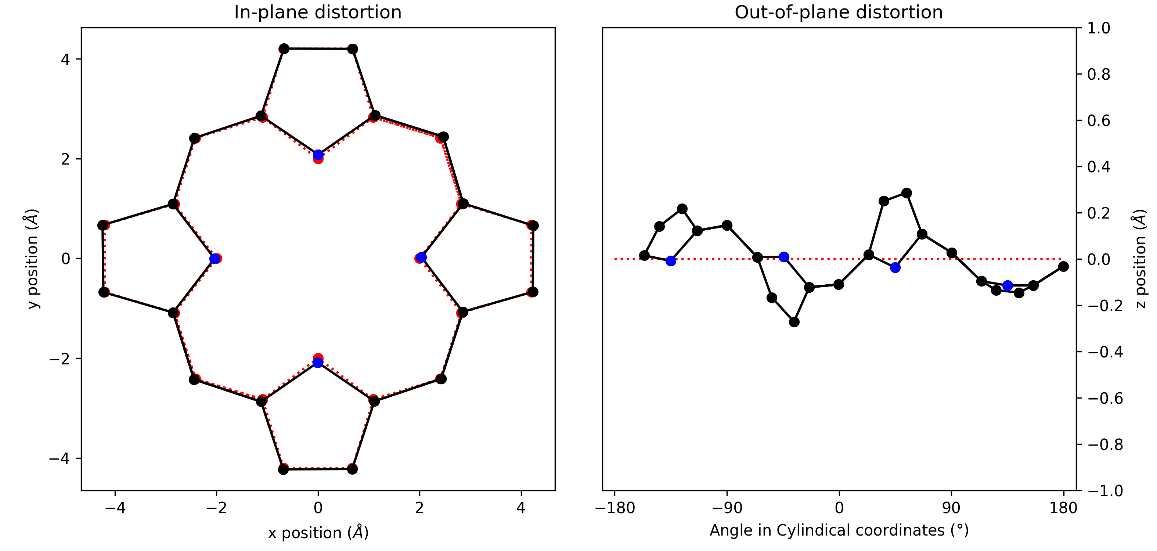


**Figure 105:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **16A** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.17 | 0.00 | 0.04 | 0.01 | 0.00 | 0.00 | 0.16 | -0.01 |
| ext. | 0.19 | 0.00 | 0.04 | 0.00 | 0.00 | 0.00 | 0.16 | -0.01 |
|  |  |  | 0.00 | -0.06 | 0.00 | -0.04 | -0.03 | -0.01 |
| total | 0.21 | 0.00 | 0.04 | 0.00 | 0.00 | 0.00 | 0.17 | -0.01 |
|  |  |  | 0.00 | -0.06 | 0.00 | -0.04 | -0.03 | -0.01 |
|  |  |  | 0.01 | -0.05 | 0.00 | 0.00 | 0.07 | -0.01 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.01 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.01 | 0.00 | 0.01 | 0.01 | 0.01 |
|  |  |  | 0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
| comp. | 0.21 | 0.00 | 0.04 | 0.08 | 0.02 | 0.04 | 0.19 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.67 | 0.00 | 0.60 | -0.21 | -0.10 | -0.14 | 0.11 | 0.01 |
| ext. | 0.68 | 0.00 | 0.60 | -0.21 | -0.10 | -0.14 | 0.11 | 0.01 |
|  |  |  | -0.07 | -0.01 | -0.02 | 0.04 | 0.07 | 0.01 |
| total | 0.68 | 0.00 | 0.60 | -0.21 | -0.10 | -0.14 | 0.11 | 0.01 |
|  |  |  | -0.07 | -0.01 | -0.02 | 0.04 | 0.07 | 0.01 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.02 | 0.01 |  |
|  |  |  |  |  |  | 0.01 | -0.01 |  |
|  |  |  |  |  |  | -0.02 | 0.00 |  |
| comp. | 0.68 | 0.00 | 0.61 | 0.21 | 0.10 | 0.15 | 0.13 | 0.02 |

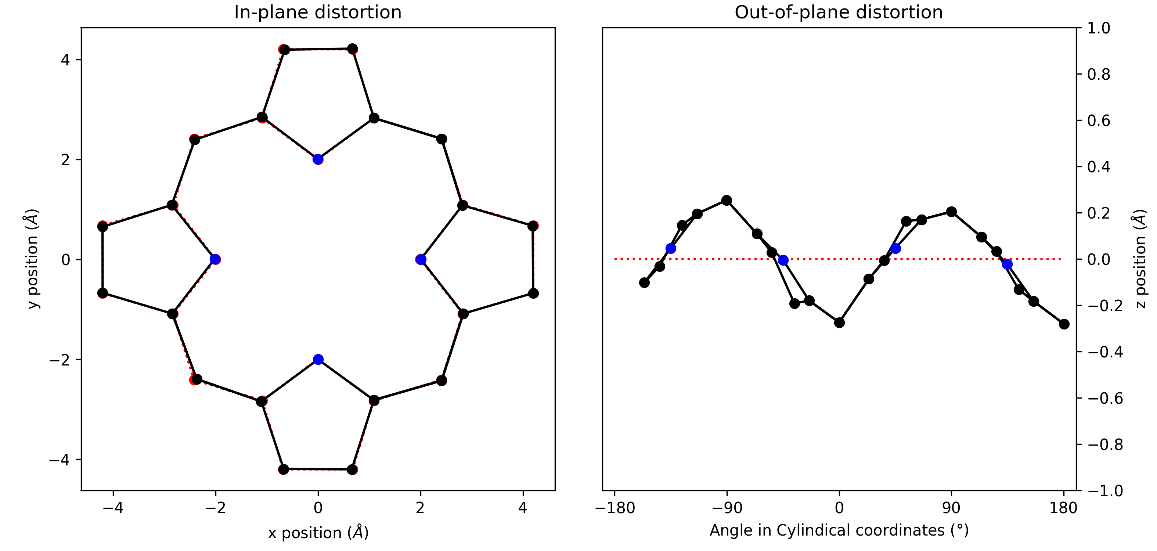


**Figure 106:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **17** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.03 | 0.00 | -0.01 | 0.00 | 0.01 | 0.02 | 0.01 | 0.01 |
| ext. | 0.05 | 0.00 | -0.01 | 0.00 | 0.01 | 0.02 | 0.01 | 0.01 |
|  |  |  | -0.02 | 0.00 | 0.01 | 0.00 | 0.02 | -0.01 |
| total | 0.09 | 0.00 | -0.01 | 0.00 | 0.01 | 0.02 | 0.01 | 0.01 |
|  |  |  | -0.02 | 0.00 | 0.01 | 0.00 | 0.02 | -0.01 |
|  |  |  | -0.01 | 0.01 | -0.01 | 0.00 | 0.03 | 0.00 |
|  |  |  | 0.00 | 0.01 | -0.02 | 0.01 | -0.03 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.01 | 0.00 | -0.02 | -0.01 |
|  |  |  | -0.01 | -0.02 | -0.02 | -0.01 | 0.02 |  |
|  |  |  |  |  | -0.02 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.03 | 0.01 |  |  |
|  |  |  |  |  | 0.03 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
| comp. | 0.09 | 0.00 | 0.03 | 0.02 | 0.06 | 0.03 | 0.06 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.73 | 0.00 | 0.23 | -0.69 | 0.02 | -0.03 | 0.05 | -0.01 |
| ext. | 0.74 | 0.00 | 0.23 | -0.69 | 0.02 | -0.03 | 0.05 | -0.01 |
|  |  |  | 0.04 | -0.02 | 0.06 | 0.01 | 0.00 | 0.01 |
| total | 0.74 | 0.00 | 0.23 | -0.69 | 0.02 | -0.03 | 0.05 | -0.01 |
|  |  |  | 0.04 | -0.02 | 0.06 | 0.01 | 0.00 | 0.01 |
|  |  |  | -0.01 | -0.01 | -0.01 | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.02 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.74 | 0.00 | 0.23 | 0.69 | 0.06 | 0.04 | 0.05 | 0.01 |

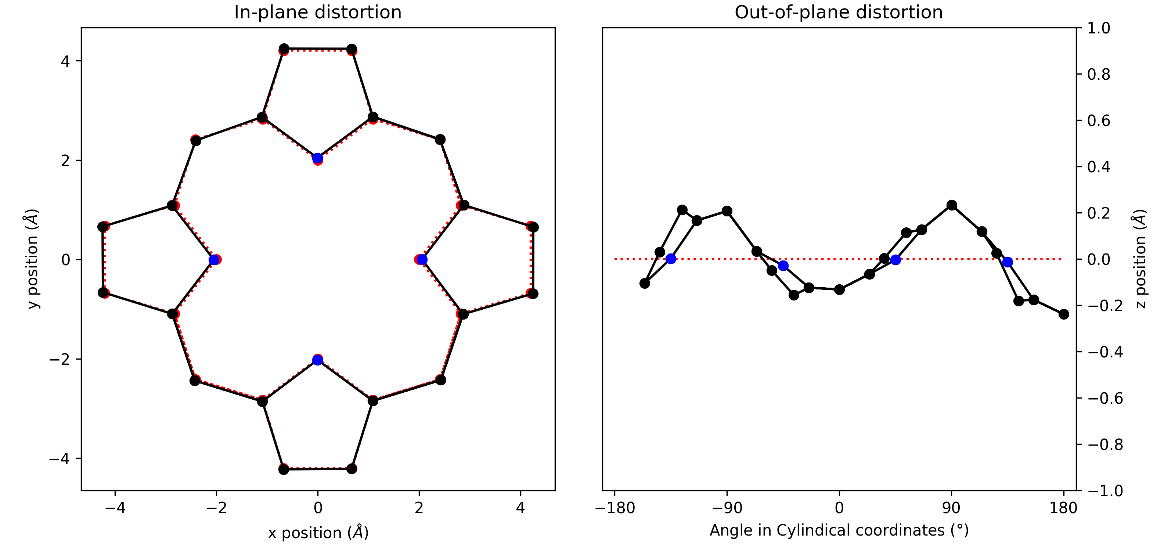


**Figure 107:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **18** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.18 | 0.00 | 0.01 | 0.04 | -0.01 | 0.04 | 0.17 | -0.01 |
| ext. | 0.18 | 0.00 | 0.01 | 0.04 | -0.01 | 0.04 | 0.17 | -0.01 |
|  |  |  | 0.01 | 0.01 | -0.01 | 0.02 | 0.03 | -0.02 |
| total | 0.19 | 0.00 | 0.01 | 0.04 | -0.01 | 0.04 | 0.17 | -0.01 |
|  |  |  | 0.01 | 0.01 | -0.01 | 0.02 | 0.03 | -0.02 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | 0.03 | 0.00 |
|  |  |  | -0.01 | 0.00 | -0.01 | -0.02 | -0.04 | 0.00 |
|  |  |  | 0.01 | 0.01 | 0.01 | 0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.19 | 0.00 | 0.02 | 0.04 | 0.02 | 0.05 | 0.18 | 0.02 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.64 | 0.00 | 0.27 | -0.56 | -0.01 | 0.11 | 0.05 | 0.00 |
| ext. | 0.64 | 0.00 | 0.27 | -0.56 | -0.02 | 0.11 | 0.05 | 0.00 |
|  |  |  | -0.03 | -0.01 | -0.04 | -0.06 | -0.05 | 0.01 |
| total | 0.64 | 0.00 | 0.27 | -0.56 | -0.02 | 0.11 | 0.05 | 0.00 |
|  |  |  | -0.03 | -0.01 | -0.04 | -0.06 | -0.05 | 0.01 |
|  |  |  | 0.00 | -0.01 | 0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.01 |  |
| comp. | 0.64 | 0.00 | 0.27 | 0.56 | 0.04 | 0.12 | 0.07 | 0.01 |

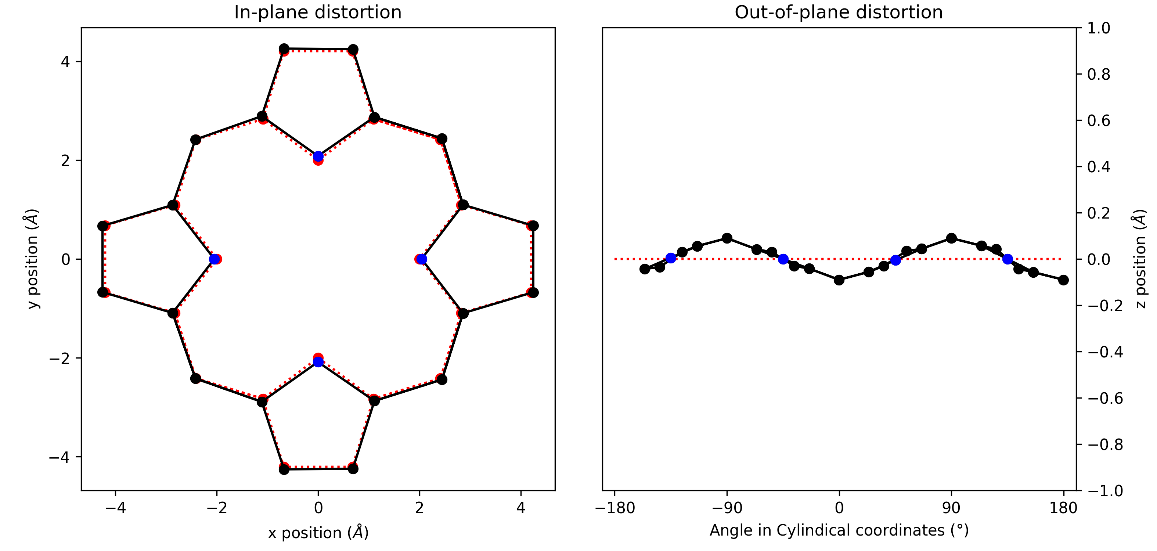


**Figure 108:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **19** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | 0.00 | -0.02 | 0.02 | 0.00 | 0.23 | 0.00 |
| ext. | 0.23 | 0.00 | 0.00 | -0.02 | 0.02 | 0.00 | 0.23 | 0.00 |
|  |  |  | 0.00 | -0.04 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.25 | 0.00 | 0.00 | -0.02 | 0.02 | 0.00 | 0.23 | 0.00 |
|  |  |  | 0.00 | -0.04 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.03 | -0.02 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.03 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.01 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.25 | 0.00 | 0.00 | 0.05 | 0.04 | 0.00 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.25 | 0.00 | 0.00 | -0.25 | 0.00 | 0.00 | 0.00 | 0.00 |
| ext. | 0.25 | 0.00 | 0.00 | -0.25 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 |
| total | 0.25 | 0.00 | 0.00 | -0.25 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.01 | 0.00 |  |
|  |  |  |  |  |  | 0.01 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.25 | 0.00 | 0.00 | 0.25 | 0.00 | 0.02 | 0.00 | 0.01 |

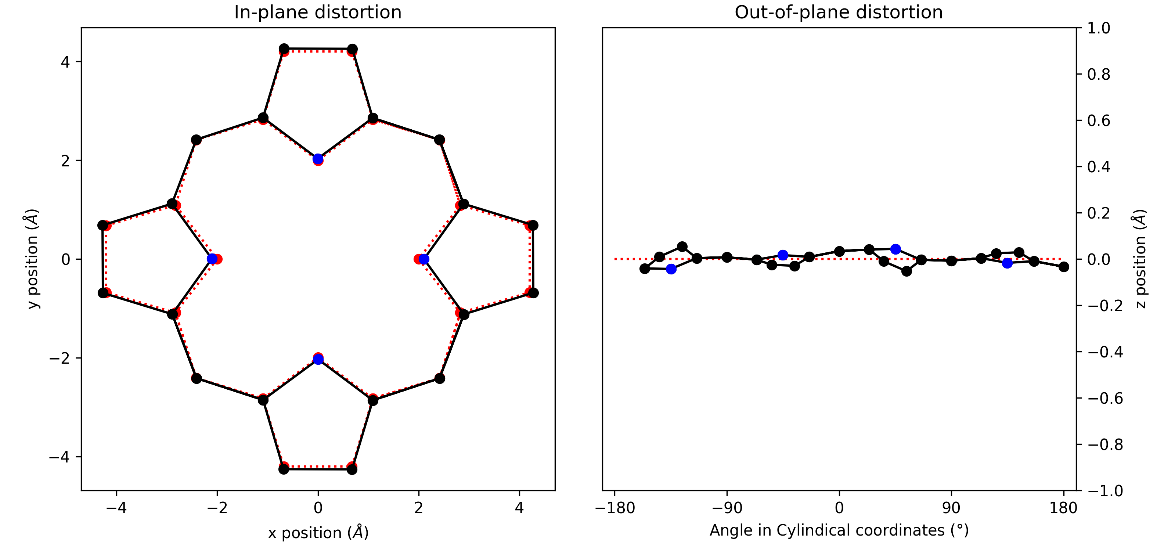


**Figure 109:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **20** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.26 | 0.00 | -0.01 | 0.06 | 0.00 | 0.00 | 0.26 | 0.00 |
| ext. | 0.28 | 0.00 | -0.01 | 0.06 | 0.00 | 0.00 | 0.26 | 0.00 |
|  |  |  | -0.01 | 0.06 | 0.00 | 0.00 | 0.06 | 0.00 |
| total | 0.29 | 0.00 | -0.01 | 0.07 | 0.00 | 0.00 | 0.26 | 0.00 |
|  |  |  | -0.01 | 0.06 | 0.00 | 0.00 | 0.06 | 0.00 |
|  |  |  | 0.01 | 0.05 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.29 | 0.00 | 0.02 | 0.10 | 0.00 | 0.00 | 0.27 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.12 | 0.00 | 0.00 | 0.00 | 0.00 | 0.08 | 0.09 | 0.00 |
| ext. | 0.14 | 0.00 | 0.00 | 0.00 | 0.00 | 0.09 | 0.09 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.05 | -0.02 | 0.00 |
| total | 0.14 | 0.00 | 0.00 | 0.00 | 0.00 | 0.09 | 0.09 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.05 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.14 | 0.00 | 0.00 | 0.00 | 0.00 | 0.10 | 0.09 | 0.00 |

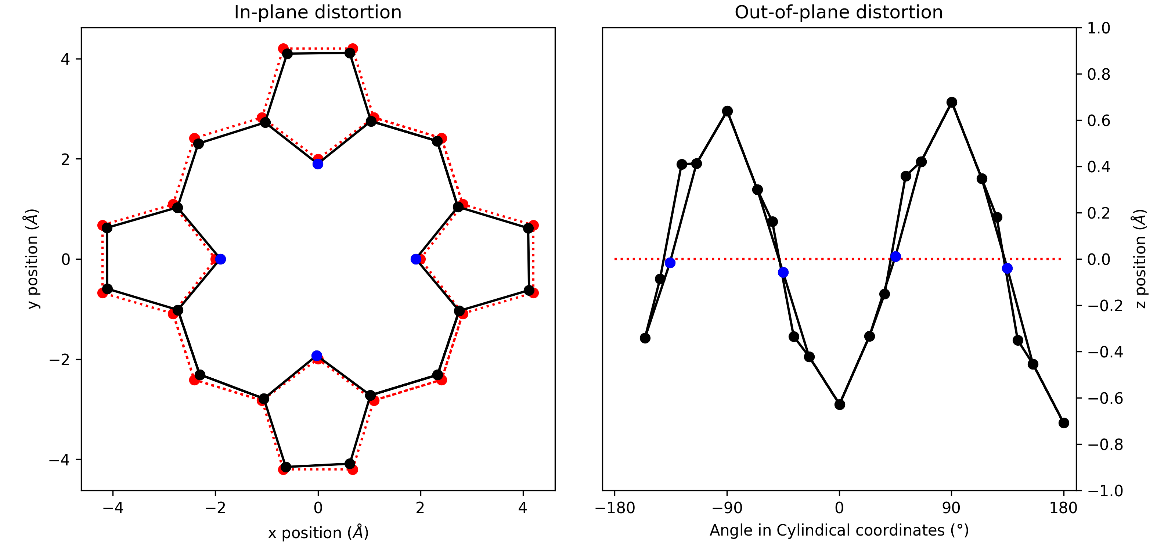


**Figure 110:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from 21 (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.47 | 0.01 | 0.02 | -0.01 | 0.00 | -0.03 | -0.46 | 0.04 |
| ext. | 0.50 | 0.01 | 0.02 | -0.01 | 0.00 | -0.03 | -0.46 | 0.04 |
|  |  |  | 0.01 | -0.01 | -0.02 | -0.01 | 0.17 | -0.06 |
| total | 0.52 | 0.00 | 0.02 | -0.01 | 0.00 | -0.03 | -0.46 | 0.03 |
|  |  |  | 0.01 | -0.01 | -0.02 | -0.01 | 0.17 | -0.06 |
|  |  |  | -0.02 | 0.00 | -0.03 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.04 | 0.02 | -0.13 | -0.01 |
|  |  |  | 0.00 | 0.00 | 0.01 | -0.01 | -0.01 | -0.02 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.08 |  |
|  |  |  |  |  | 0.00 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.52 | 0.00 | 0.03 | 0.02 | 0.05 | 0.04 | 0.51 | 0.07 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.89 | 0.00 | 0.34 | -1.85 | -0.09 | 0.09 | 0.00 | -0.01 |
| ext. | 1.89 | 0.00 | 0.34 | -1.85 | -0.09 | 0.09 | 0.00 | -0.01 |
|  |  |  | 0.00 | -0.02 | 0.01 | -0.02 | -0.02 | 0.00 |
| total | 1.89 | 0.00 | 0.34 | -1.85 | -0.09 | 0.09 | 0.00 | -0.01 |
|  |  |  | 0.00 | -0.02 | 0.01 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | -0.02 | 0.00 | -0.02 | -0.02 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.01 |  |
| comp. | 1.89 | 0.00 | 0.34 | 1.85 | 0.09 | 0.10 | 0.03 | 0.01 |

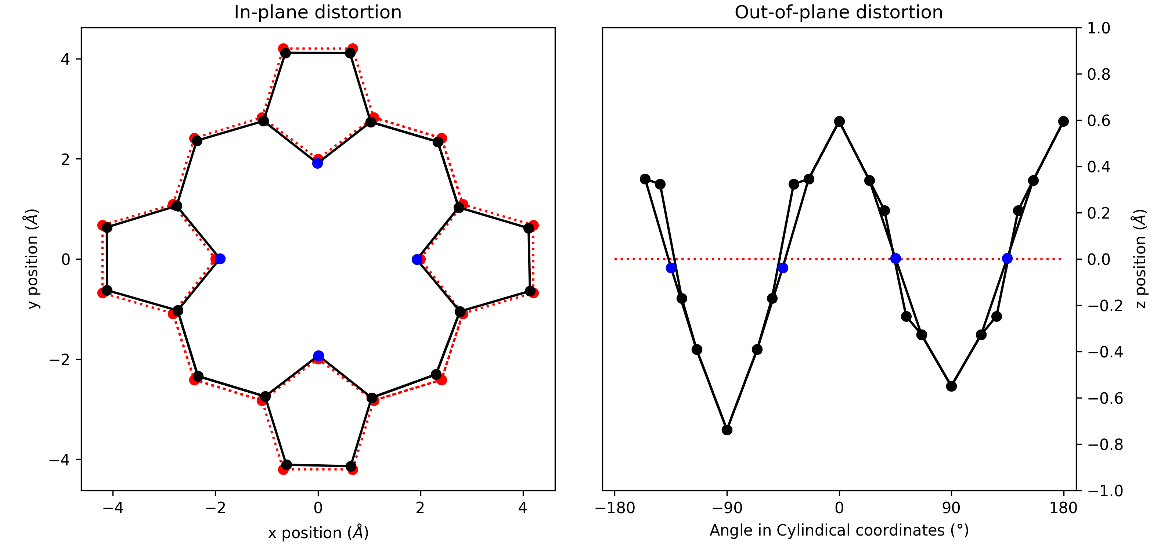


**Figure 111:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **22** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.42 | 0.01 | -0.04 | 0.00 | -0.01 | -0.01 | -0.41 | 0.00 |
| ext. | 0.44 | 0.00 | -0.04 | 0.00 | -0.01 | -0.01 | -0.41 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.02 | -0.02 | 0.13 | 0.00 |
| total | 0.46 | 0.00 | -0.04 | 0.00 | -0.01 | -0.01 | -0.41 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.02 | -0.02 | 0.13 | 0.00 |
|  |  |  | 0.03 | 0.00 | 0.01 | 0.01 | 0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.03 | 0.03 | -0.10 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | -0.02 | -0.01 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.01 | 0.01 | 0.06 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.46 | 0.00 | 0.06 | 0.00 | 0.05 | 0.05 | 0.45 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.74 | 0.00 | 0.00 | 1.72 | -0.09 | 0.14 | -0.14 | 0.00 |
| ext. | 1.74 | 0.00 | 0.00 | 1.72 | -0.09 | 0.14 | -0.14 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.05 | -0.01 | 0.01 | 0.00 |
| total | 1.74 | 0.00 | 0.00 | 1.72 | -0.09 | 0.14 | -0.14 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.05 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.03 | 0.00 | -0.05 | 0.05 |  |
|  |  |  |  |  |  | -0.01 | 0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.74 | 0.00 | 0.00 | 1.72 | 0.10 | 0.15 | 0.15 | 0.00 |

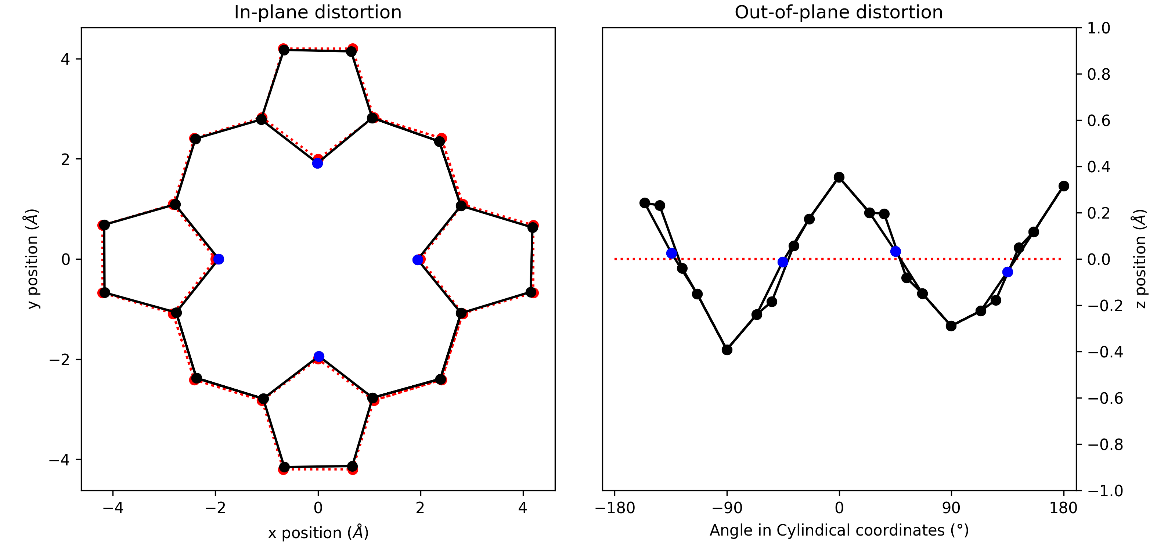


**Figure 112:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **23** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | -0.05 | 0.01 | -0.01 | 0.02 | -0.22 | 0.00 |
| ext. | 0.23 | 0.00 | -0.05 | 0.01 | -0.01 | 0.02 | -0.22 | 0.00 |
|  |  |  | 0.03 | 0.01 | -0.02 | 0.00 | 0.04 | -0.01 |
| total | 0.26 | 0.00 | -0.05 | 0.01 | -0.01 | 0.02 | -0.22 | 0.00 |
|  |  |  | 0.03 | 0.01 | -0.02 | 0.00 | 0.04 | -0.01 |
|  |  |  | -0.02 | -0.01 | 0.01 | 0.00 | -0.04 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.00 | -0.02 | -0.03 | -0.03 |
|  |  |  | 0.01 | 0.01 | -0.01 | -0.02 | -0.03 | 0.01 |
|  |  |  | 0.00 | 0.01 | 0.01 | 0.01 | 0.02 |  |
|  |  |  |  |  | 0.04 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | -0.03 |  |  |
|  |  |  |  |  | 0.01 | -0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
|  |  |  |  |  | -0.02 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.06 | 0.03 | 0.05 | 0.05 | 0.24 | 0.03 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.96 | 0.00 | 0.23 | 0.93 | -0.02 | 0.07 | -0.01 | -0.02 |
| ext. | 0.97 | 0.00 | 0.23 | 0.93 | -0.02 | 0.07 | -0.01 | -0.02 |
|  |  |  | 0.04 | 0.02 | 0.01 | -0.04 | 0.05 | 0.02 |
| total | 0.97 | 0.00 | 0.23 | 0.93 | -0.02 | 0.07 | -0.01 | -0.02 |
|  |  |  | 0.04 | 0.02 | 0.01 | -0.04 | 0.05 | 0.02 |
|  |  |  | 0.00 | 0.02 | 0.01 | -0.03 | 0.02 |  |
|  |  |  |  |  |  | 0.01 | -0.01 |  |
|  |  |  |  |  |  | 0.03 | 0.00 |  |
| comp. | 0.97 | 0.00 | 0.24 | 0.93 | 0.02 | 0.09 | 0.05 | 0.03 |

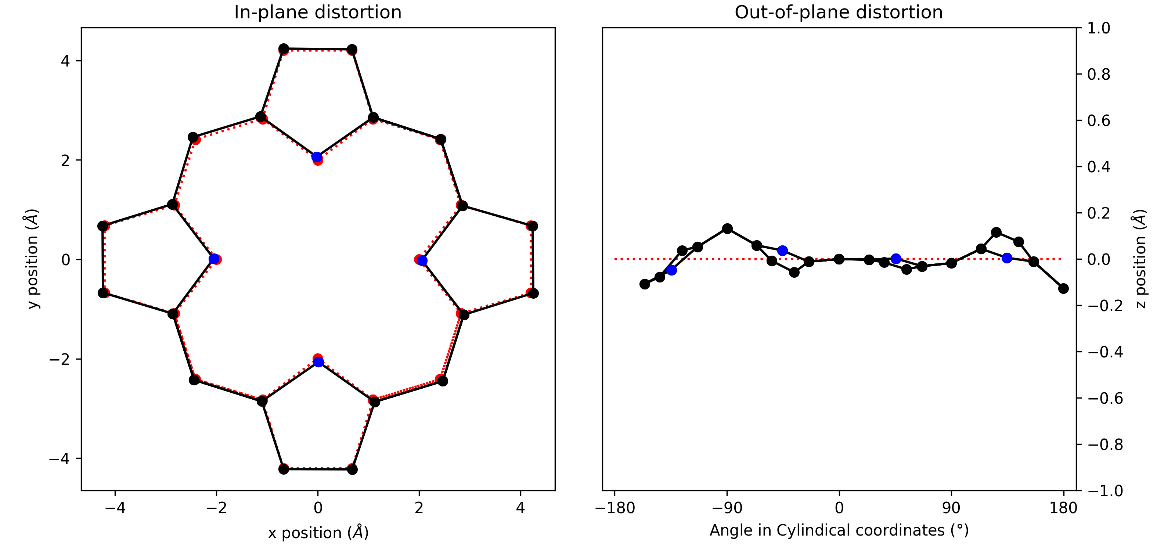


**Figure 113:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **24** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.21 | 0.00 | -0.07 | 0.01 | 0.00 | 0.00 | 0.20 | 0.00 |
| ext. | 0.22 | 0.00 | -0.07 | 0.01 | 0.00 | 0.00 | 0.20 | 0.00 |
|  |  |  | -0.01 | -0.02 | -0.02 | 0.01 | -0.04 | 0.00 |
| total | 0.23 | 0.00 | -0.07 | 0.01 | 0.00 | 0.00 | 0.20 | 0.00 |
|  |  |  | -0.01 | -0.02 | -0.02 | 0.01 | -0.04 | 0.00 |
|  |  |  | -0.01 | -0.02 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
| comp. | 0.23 | 0.00 | 0.07 | 0.03 | 0.02 | 0.02 | 0.21 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.29 | 0.00 | -0.10 | -0.16 | -0.01 | 0.01 | 0.21 | 0.00 |
| ext. | 0.30 | 0.00 | -0.10 | -0.16 | -0.01 | 0.01 | 0.21 | 0.00 |
|  |  |  | -0.04 | -0.01 | 0.01 | 0.04 | -0.07 | 0.00 |
| total | 0.30 | 0.00 | -0.10 | -0.16 | -0.01 | 0.01 | 0.21 | 0.00 |
|  |  |  | -0.04 | -0.01 | 0.01 | 0.04 | -0.07 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.01 | -0.02 |  |
|  |  |  |  |  |  | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.01 | 0.01 |  |
| comp. | 0.30 | 0.00 | 0.11 | 0.16 | 0.01 | 0.04 | 0.22 | 0.00 |



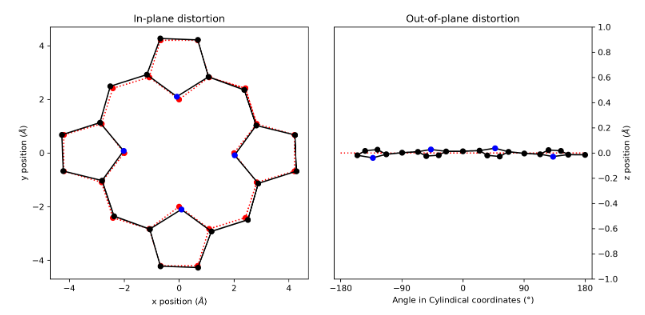
**Figure 114:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

## NSD tables and plots for DFT structures series 1

### NSD result generated from **1:1** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.38 | 0.00 | -0.32 | -0.05 | 0.00 | 0.00 | 0.21 | 0.00 |
| ext. | 0.40 | 0.00 | -0.32 | -0.05 | 0.00 | 0.00 | 0.21 | 0.00 |
|  |  |  | -0.05 | -0.09 | 0.00 | 0.00 | 0.00 | 0.00 |
| total | 0.41 | 0.00 | -0.32 | -0.05 | 0.00 | 0.00 | 0.21 | 0.00 |
|  |  |  | -0.05 | -0.09 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.06 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.41 | 0.00 | 0.32 | 0.12 | 0.00 | 0.00 | 0.22 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.06 | 0.00 |
| ext. | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.05 | 0.03 | 0.00 |
| total | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.05 | 0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 0.08 | 0.07 | 0.00 |

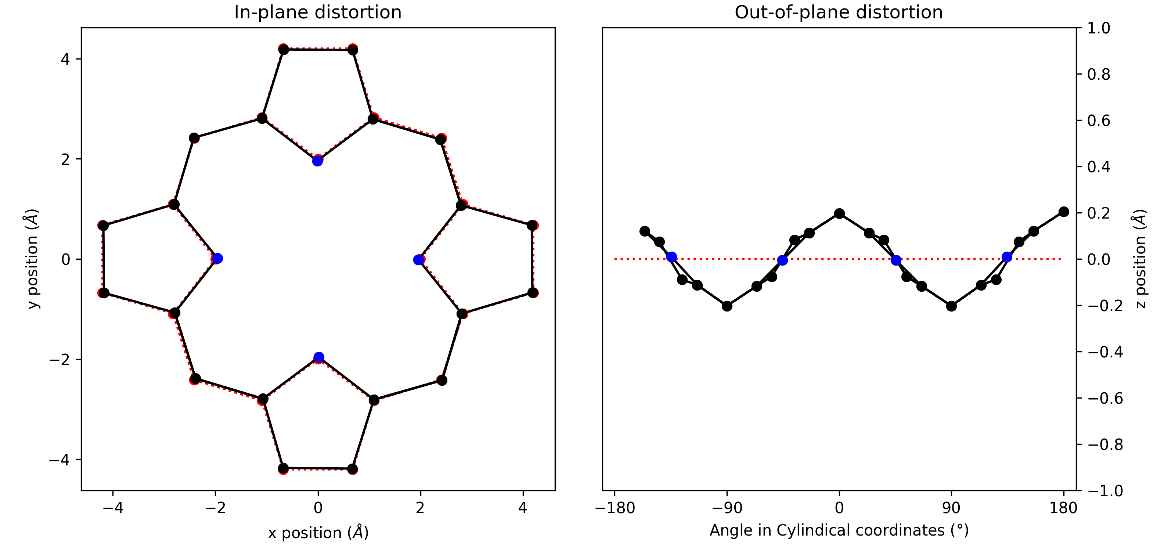


**Figure 115:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:2** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.14 | 0.00 | -0.06 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |
| ext. | 0.14 | 0.00 | -0.07 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| total | 0.15 | 0.00 | -0.06 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.15 | 0.00 | 0.07 | 0.00 | 0.00 | 0.00 | 0.13 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.57 | 0.00 | 0.00 | 0.57 | 0.01 | -0.01 | -0.01 | 0.00 |
| ext. | 0.57 | 0.00 | 0.00 | 0.57 | 0.01 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
| total | 0.57 | 0.00 | 0.00 | 0.57 | 0.01 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.57 | 0.00 | 0.00 | 0.57 | 0.01 | 0.02 | 0.02 | 0.00 |

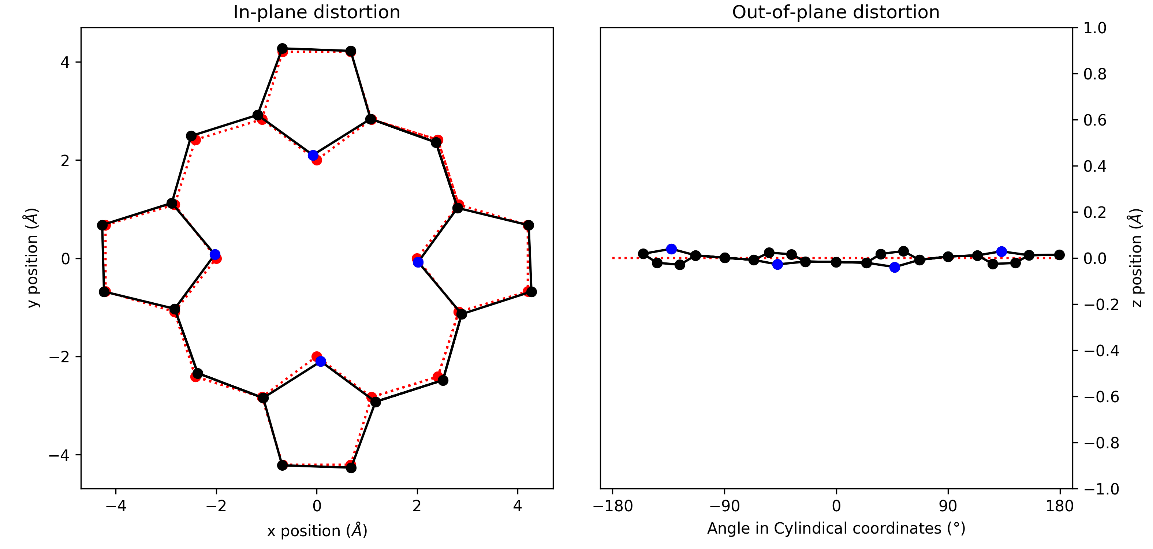


**Figure 116:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:3** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.37 | 0.00 | -0.31 | -0.04 | 0.00 | 0.00 | 0.21 | -0.01 |
| ext. | 0.39 | 0.00 | -0.31 | -0.04 | 0.00 | 0.00 | 0.21 | -0.01 |
|  |  |  | -0.05 | -0.09 | 0.01 | 0.01 | 0.01 | 0.00 |
| total | 0.40 | 0.00 | -0.31 | -0.04 | 0.00 | 0.00 | 0.21 | -0.01 |
|  |  |  | -0.05 | -0.09 | 0.01 | 0.01 | 0.01 | 0.00 |
|  |  |  | -0.01 | -0.06 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.02 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | -0.01 | 0.02 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.01 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.02 |  |  |
| comp. | 0.40 | 0.00 | 0.31 | 0.11 | 0.02 | 0.03 | 0.22 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.09 | 0.00 | 0.00 | -0.01 | 0.00 | -0.06 | -0.06 | 0.00 |
| ext. | 0.11 | 0.00 | 0.00 | -0.01 | 0.00 | -0.07 | -0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.05 | -0.03 | 0.00 |
| total | 0.11 | 0.00 | 0.00 | -0.01 | 0.00 | -0.07 | -0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.05 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.11 | 0.00 | 0.00 | 0.01 | 0.00 | 0.08 | 0.07 | 0.00 |

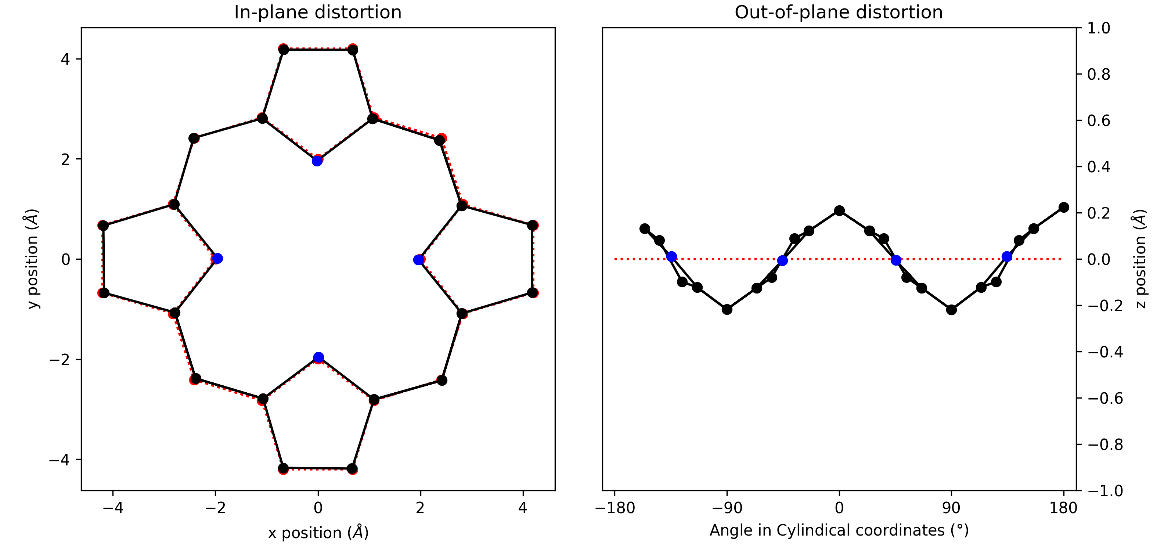


**Figure 117:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:4** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.14 | 0.00 | -0.07 | 0.00 | 0.00 | 0.00 | -0.13 | 0.00 |
| ext. | 0.15 | 0.00 | -0.07 | 0.00 | 0.00 | 0.00 | -0.13 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.15 | 0.00 | -0.07 | 0.00 | 0.00 | 0.00 | -0.13 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.01 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | -0.01 |  |  |
| comp. | 0.15 | 0.00 | 0.08 | 0.00 | 0.02 | 0.02 | 0.13 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.61 | 0.00 | 0.00 | 0.61 | 0.01 | -0.02 | -0.02 | 0.00 |
| ext. | 0.61 | 0.00 | 0.00 | 0.61 | 0.01 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
| total | 0.61 | 0.00 | 0.00 | 0.61 | 0.01 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.61 | 0.00 | 0.00 | 0.61 | 0.01 | 0.02 | 0.02 | 0.00 |

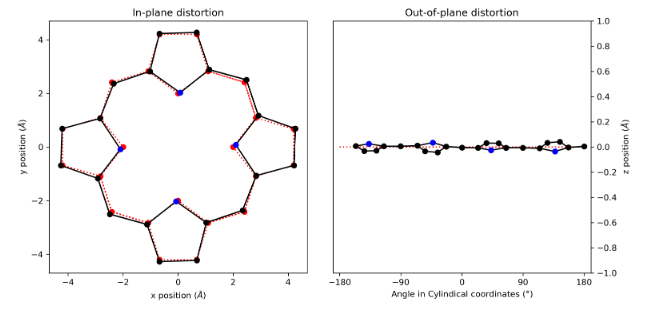


**Figure 118:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:5** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.37 | 0.00 | 0.31 | 0.03 | 0.00 | 0.00 | 0.21 | -0.01 |
| ext. | 0.39 | 0.00 | 0.31 | 0.03 | 0.00 | 0.00 | 0.21 | -0.01 |
|  |  |  | 0.05 | 0.08 | 0.00 | 0.00 | 0.02 | 0.01 |
| total | 0.40 | 0.00 | 0.31 | 0.03 | 0.00 | 0.00 | 0.21 | -0.01 |
|  |  |  | 0.05 | 0.09 | 0.00 | 0.00 | 0.02 | 0.01 |
|  |  |  | 0.03 | 0.06 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.01 | 0.01 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.40 | 0.00 | 0.32 | 0.11 | 0.00 | 0.00 | 0.22 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.09 | 0.00 | 0.00 | 0.00 | 0.00 | -0.06 | 0.07 | 0.00 |
| ext. | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | -0.06 | 0.07 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.03 | 0.05 | 0.00 |
| total | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | -0.06 | 0.07 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.03 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.07 | 0.09 | 0.00 |

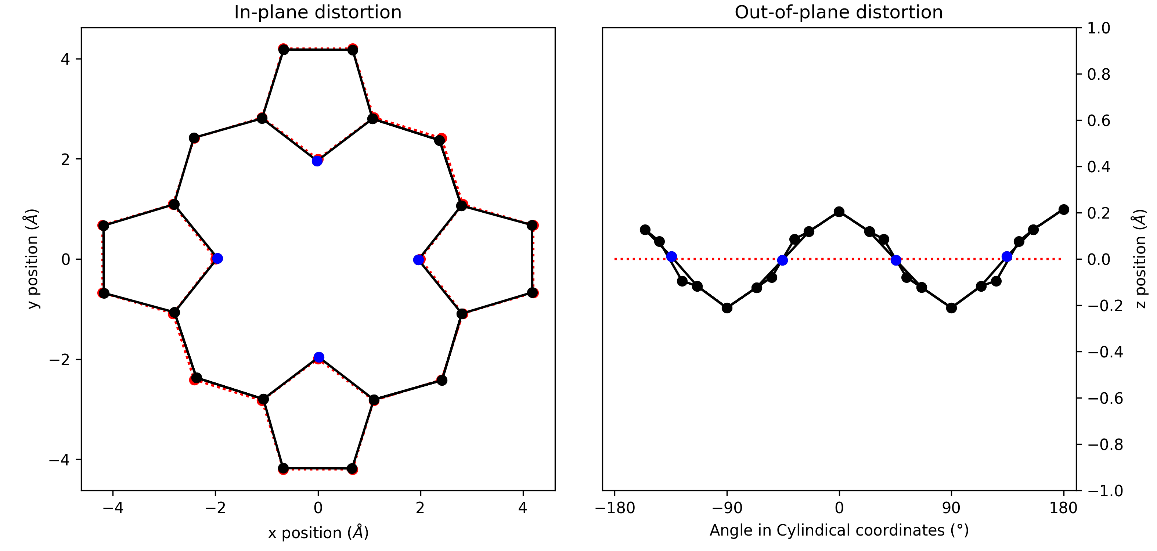


**Figure 119:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:6** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.15 | 0.00 | -0.08 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |
| ext. | 0.15 | 0.00 | -0.08 | 0.00 | 0.00 | 0.00 | -0.12 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 |
| total | 0.16 | 0.00 | -0.08 | 0.00 | 0.00 | 0.00 | -0.13 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | -0.03 | 0.00 | 0.00 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.16 | 0.00 | 0.09 | 0.00 | 0.00 | 0.00 | 0.13 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.59 | 0.00 | 0.00 | 0.59 | 0.01 | -0.02 | -0.02 | 0.00 |
| ext. | 0.59 | 0.00 | 0.00 | 0.59 | 0.01 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
| total | 0.59 | 0.00 | 0.00 | 0.59 | 0.01 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.59 | 0.00 | 0.00 | 0.59 | 0.01 | 0.02 | 0.02 | 0.00 |

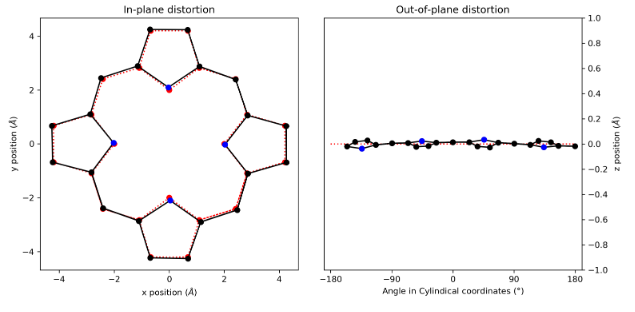


**Figure 120:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:7** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.26 | 0.00 | -0.13 | -0.04 | -0.02 | 0.02 | 0.22 | 0.00 |
| ext. | 0.28 | 0.00 | -0.13 | -0.04 | -0.02 | 0.02 | 0.22 | 0.00 |
|  |  |  | -0.01 | -0.09 | 0.01 | -0.02 | 0.00 | 0.00 |
| total | 0.29 | 0.00 | -0.13 | -0.04 | -0.02 | 0.02 | 0.22 | 0.00 |
|  |  |  | -0.01 | -0.09 | 0.01 | -0.02 | 0.00 | 0.00 |
|  |  |  | -0.01 | -0.06 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.29 | 0.00 | 0.14 | 0.12 | 0.02 | 0.03 | 0.23 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.08 | 0.00 | 0.00 | -0.01 | 0.00 | 0.06 | 0.05 | 0.00 |
| ext. | 0.10 | 0.00 | 0.00 | -0.01 | 0.00 | 0.06 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.04 | 0.02 | 0.00 |
| total | 0.10 | 0.00 | 0.00 | -0.01 | 0.00 | 0.06 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.04 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.10 | 0.00 | 0.00 | 0.01 | 0.00 | 0.08 | 0.06 | 0.00 |

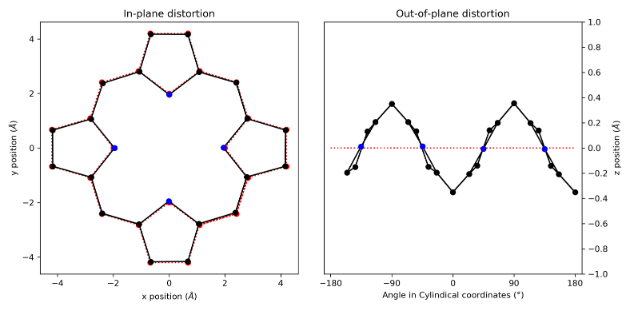


**Figure 121:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:8** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.19 | 0.00 | 0.04 | 0.00 | 0.02 | 0.02 | -0.18 | 0.00 |
| ext. | 0.19 | 0.00 | 0.04 | 0.00 | 0.02 | 0.02 | -0.18 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | 0.04 | 0.00 |
| total | 0.20 | 0.00 | 0.04 | 0.00 | 0.02 | 0.02 | -0.18 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | 0.04 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | 0.00 | -0.02 | 0.00 |
|  |  |  | -0.01 | 0.00 | -0.01 | -0.01 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.20 | 0.00 | 0.04 | 0.00 | 0.03 | 0.03 | 0.19 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.99 | 0.00 | 0.00 | -0.99 | 0.01 | -0.01 | 0.01 | 0.00 |
| ext. | 0.99 | 0.00 | 0.00 | -0.99 | 0.01 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.02 | 0.00 |
| total | 0.99 | 0.00 | 0.00 | -0.99 | 0.01 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.99 | 0.00 | 0.00 | 0.99 | 0.01 | 0.02 | 0.02 | 0.00 |

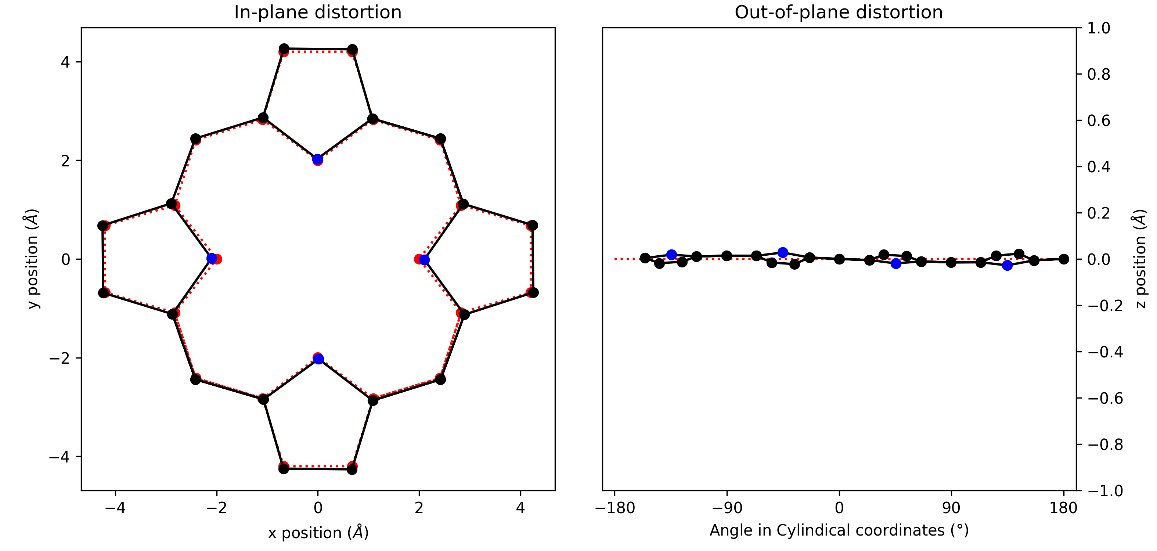


**Figure 122:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:9** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | -0.03 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |
| ext. | 0.25 | 0.00 | -0.03 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |
|  |  |  | -0.02 | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.26 | 0.00 | -0.04 | 0.03 | 0.00 | 0.00 | 0.23 | 0.00 |
|  |  |  | -0.02 | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.02 | 0.06 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.05 | 0.11 | 0.00 | 0.00 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.07 | 0.00 | 0.00 | 0.00 | 0.00 | -0.04 | 0.05 | 0.00 |
| ext. | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | -0.04 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.03 | 0.00 |
| total | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | -0.04 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 | 0.06 | 0.00 |

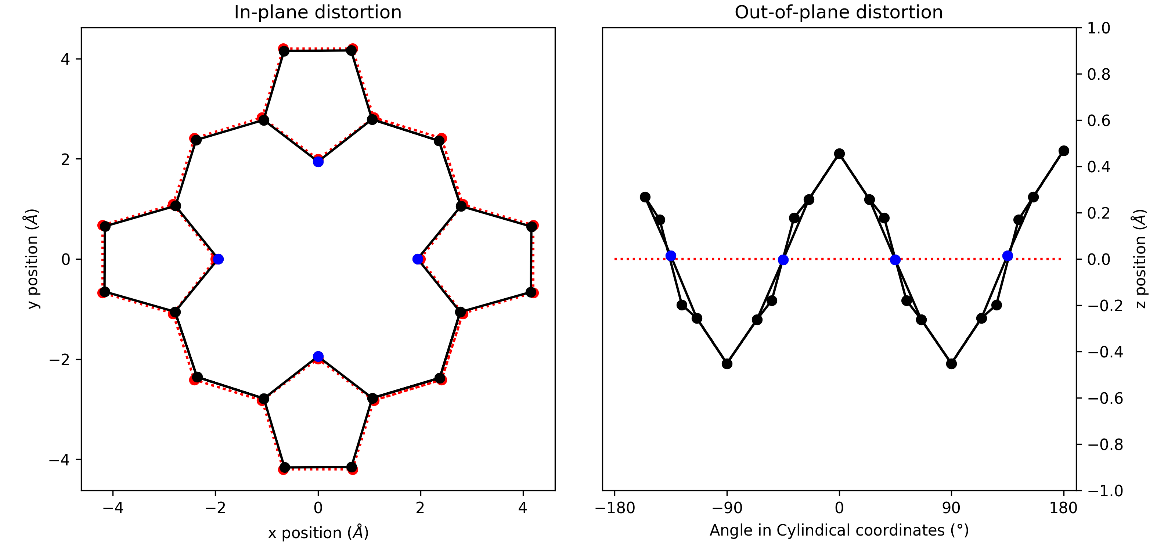


**Figure 123:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:10** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.24 | 0.00 |
| ext. | 0.26 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.24 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.09 | 0.00 |
| total | 0.27 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.24 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.09 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | -0.02 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.27 | 0.00 | 0.03 | 0.00 | 0.01 | 0.01 | 0.26 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.28 | 0.00 | 0.00 | 1.28 | 0.02 | -0.02 | -0.02 | 0.00 |
| ext. | 1.28 | 0.00 | 0.00 | 1.28 | 0.02 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | -0.01 | 0.00 |
| total | 1.28 | 0.00 | 0.00 | 1.28 | 0.02 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.28 | 0.00 | 0.00 | 1.28 | 0.03 | 0.02 | 0.02 | 0.00 |

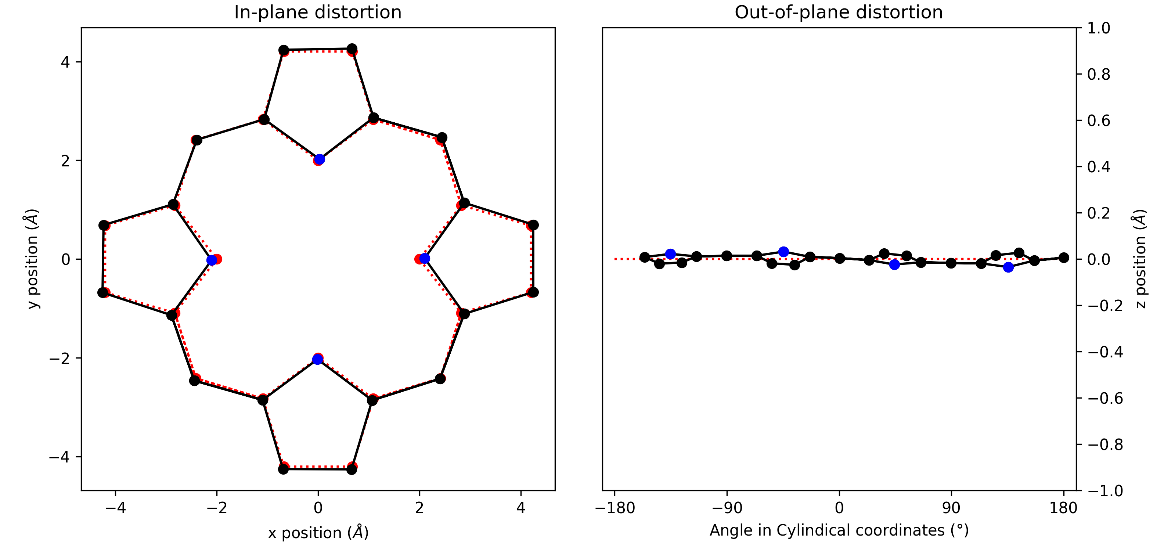


**Figure 124:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1D** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | 0.09 | 0.04 | -0.02 | -0.03 | 0.22 | 0.00 |
| ext. | 0.26 | 0.00 | 0.09 | 0.04 | -0.02 | -0.03 | 0.22 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.03 | 0.01 | 0.00 | 0.00 |
| total | 0.28 | 0.00 | 0.09 | 0.04 | -0.02 | -0.03 | 0.23 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.03 | 0.01 | 0.00 | 0.00 |
|  |  |  | 0.01 | 0.06 | 0.01 | 0.00 | 0.04 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.01 | 0.01 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.01 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.28 | 0.00 | 0.09 | 0.11 | 0.04 | 0.03 | 0.23 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.08 | 0.00 | 0.00 | 0.01 | 0.00 | -0.05 | 0.06 | 0.00 |
| ext. | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 | -0.05 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.04 | 0.00 |
| total | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 | -0.05 | 0.06 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.02 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 | 0.06 | 0.07 | 0.00 |

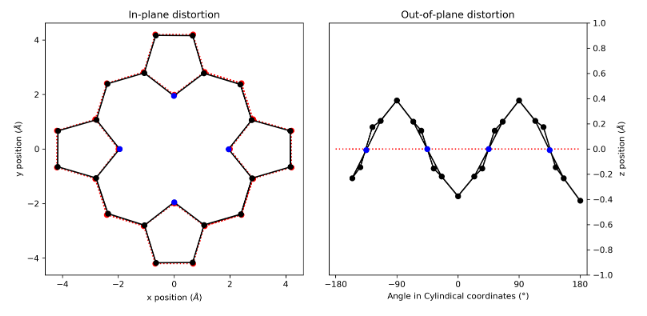


**Figure 125:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2D** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.20 | 0.00 | -0.03 | 0.00 | 0.02 | -0.02 | -0.20 | 0.00 |
| ext. | 0.21 | 0.00 | -0.03 | 0.00 | 0.02 | -0.02 | -0.20 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.01 | 0.06 | 0.00 |
| total | 0.22 | 0.00 | -0.03 | 0.00 | 0.02 | -0.02 | -0.20 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.01 | 0.06 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | -0.02 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | 0.01 | -0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.02 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.22 | 0.00 | 0.03 | 0.00 | 0.02 | 0.02 | 0.21 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.09 | 0.00 | 0.00 | -1.09 | -0.02 | 0.03 | 0.03 | 0.00 |
| ext. | 1.09 | 0.00 | 0.00 | -1.09 | -0.02 | 0.03 | 0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |
| total | 1.09 | 0.00 | 0.00 | -1.09 | -0.02 | 0.03 | 0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.09 | 0.00 | 0.00 | 1.09 | 0.02 | 0.03 | 0.03 | 0.00 |

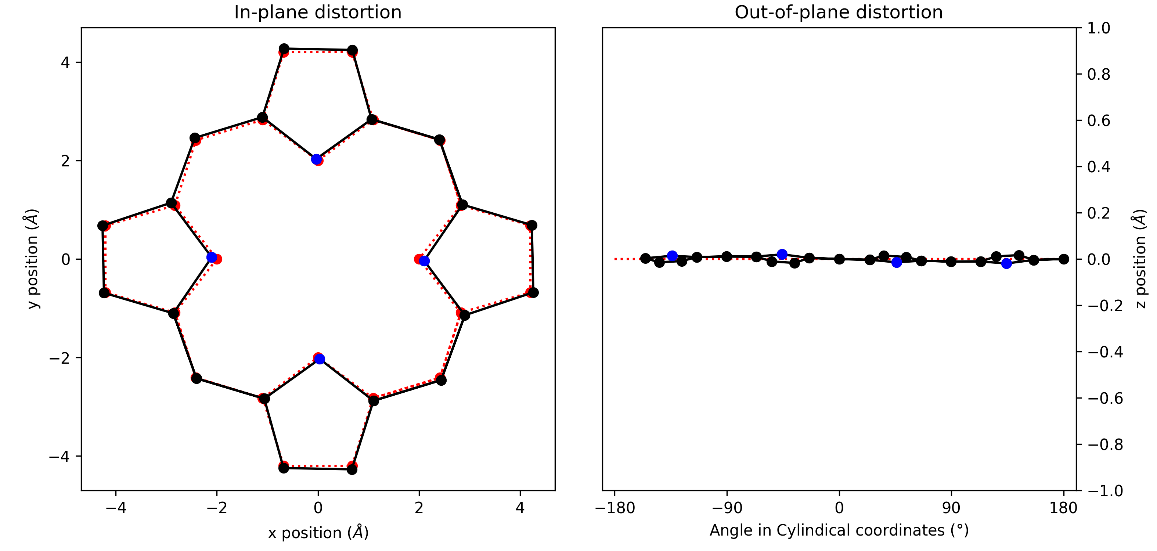


**Figure 126:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:11** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.26 | 0.00 | -0.11 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |
| ext. | 0.28 | 0.00 | -0.11 | 0.02 | 0.00 | 0.00 | 0.23 | 0.00 |
|  |  |  | -0.04 | 0.08 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.29 | 0.00 | -0.11 | 0.03 | 0.00 | 0.00 | 0.24 | 0.00 |
|  |  |  | -0.04 | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.02 | 0.06 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.29 | 0.00 | 0.13 | 0.11 | 0.00 | 0.00 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.05 | 0.00 | 0.00 | 0.00 | 0.00 | -0.03 | 0.04 | 0.00 |
| ext. | 0.06 | 0.00 | 0.00 | 0.00 | 0.00 | -0.03 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.02 | 0.00 |
| total | 0.06 | 0.00 | 0.00 | 0.00 | 0.00 | -0.03 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.01 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.06 | 0.00 | 0.00 | 0.00 | 0.00 | 0.04 | 0.04 | 0.00 |

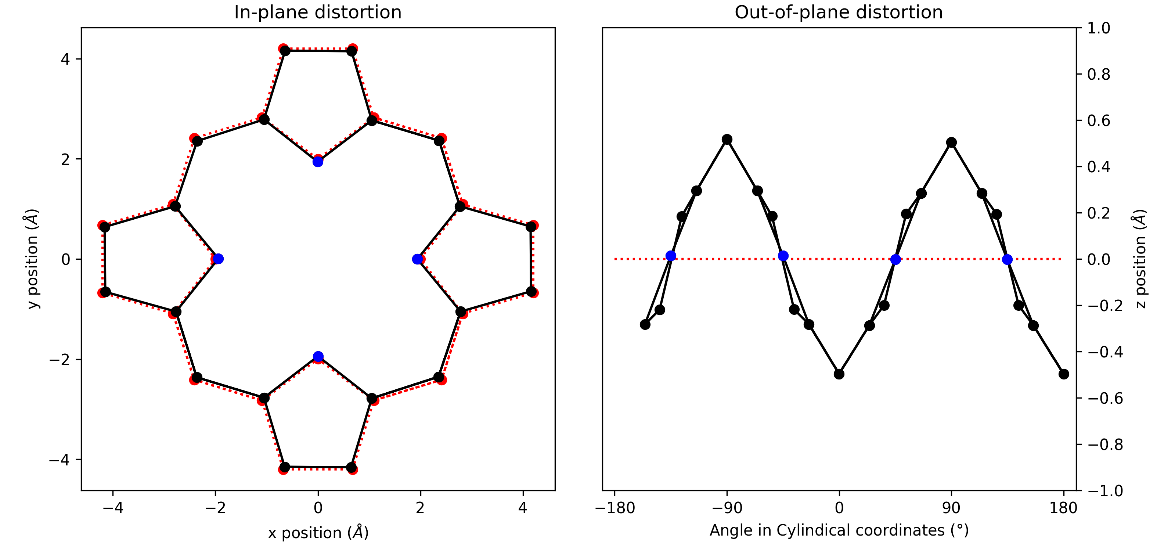


**Figure 127:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:12** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.27 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | -0.27 | 0.00 |
| ext. | 0.29 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | -0.27 | 0.00 |
|  |  |  | -0.02 | 0.00 | -0.01 | -0.01 | 0.11 | 0.00 |
| total | 0.30 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | -0.27 | 0.00 |
|  |  |  | -0.02 | 0.00 | -0.01 | -0.01 | 0.11 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | -0.07 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.03 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.30 | 0.00 | 0.04 | 0.00 | 0.01 | 0.01 | 0.30 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.41 | 0.00 | 0.00 | -1.41 | 0.03 | -0.02 | 0.02 | 0.00 |
| ext. | 1.41 | 0.00 | 0.00 | -1.41 | 0.03 | -0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | -0.01 | 0.01 | 0.00 |
| total | 1.41 | 0.00 | 0.00 | -1.41 | 0.03 | -0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.41 | 0.00 | 0.00 | 1.41 | 0.03 | 0.02 | 0.02 | 0.00 |

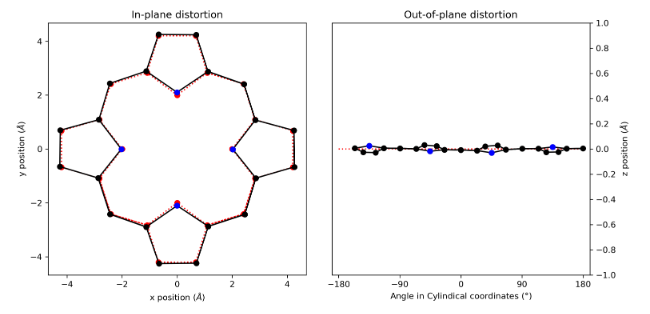


**Figure 128:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **3D** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | -0.02 | -0.04 | 0.03 | -0.03 | 0.23 | 0.00 |
| ext. | 0.25 | 0.00 | -0.02 | -0.04 | 0.03 | -0.03 | 0.23 | 0.00 |
|  |  |  | 0.01 | -0.09 | -0.02 | 0.03 | 0.00 | 0.00 |
| total | 0.27 | 0.00 | -0.02 | -0.04 | 0.03 | -0.03 | 0.23 | 0.00 |
|  |  |  | 0.01 | -0.09 | -0.02 | 0.03 | 0.00 | 0.00 |
|  |  |  | -0.01 | -0.06 | 0.00 | 0.01 | 0.04 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.27 | 0.00 | 0.03 | 0.12 | 0.04 | 0.04 | 0.23 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.07 | 0.00 | 0.00 | -0.01 | 0.00 | -0.06 | -0.05 | 0.00 |
| ext. | 0.09 | 0.00 | 0.00 | -0.01 | 0.00 | -0.06 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.04 | -0.02 | 0.00 |
| total | 0.09 | 0.00 | 0.00 | -0.01 | 0.00 | -0.06 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | -0.04 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 | 0.07 | 0.05 | 0.00 |

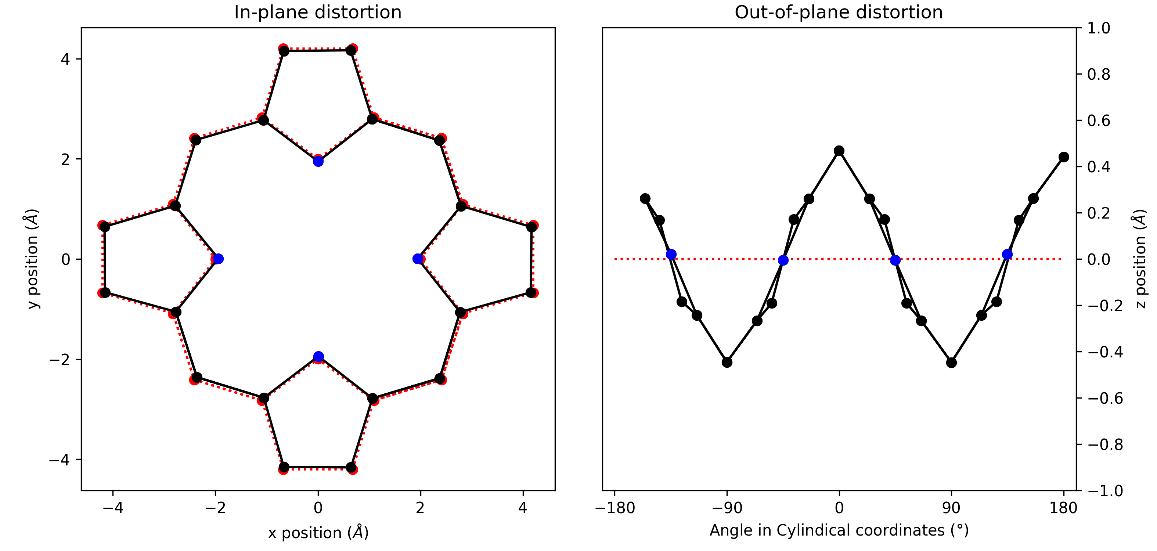


**Figure 129:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:13** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | -0.02 | 0.00 | -0.02 | 0.02 | -0.24 | 0.00 |
| ext. | 0.26 | 0.00 | -0.02 | 0.00 | -0.02 | 0.02 | -0.24 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.02 | -0.02 | 0.08 | 0.00 |
| total | 0.26 | 0.00 | -0.02 | 0.00 | -0.02 | 0.02 | -0.24 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.02 | -0.02 | 0.08 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.01 | -0.01 | -0.02 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.01 | -0.01 | -0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | 0.02 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.02 | 0.00 | 0.04 | 0.03 | 0.26 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.26 | 0.00 | 0.00 | 1.26 | 0.03 | 0.00 | 0.00 | 0.00 |
| ext. | 1.27 | 0.00 | 0.00 | 1.26 | 0.03 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.03 | -0.03 | 0.00 |
| total | 1.27 | 0.00 | 0.00 | 1.26 | 0.03 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | -0.03 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.02 | 0.00 | 0.00 | -0.01 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.27 | 0.00 | 0.00 | 1.26 | 0.03 | 0.03 | 0.03 | 0.00 |

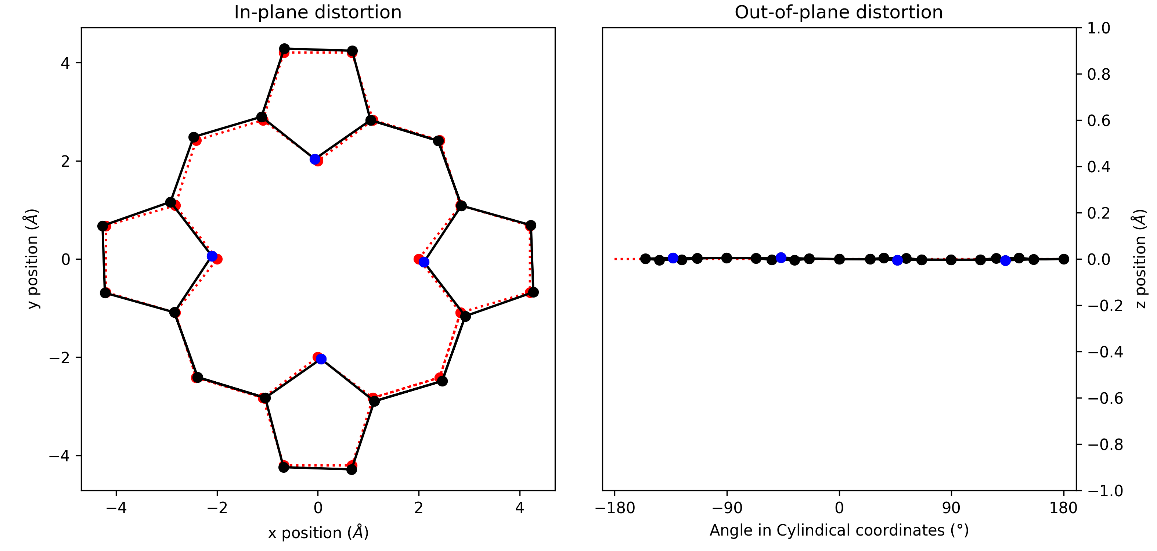


**Figure 130:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:14** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.33 | 0.00 | -0.22 | 0.02 | 0.00 | 0.00 | 0.24 | 0.00 |
| ext. | 0.35 | 0.00 | -0.22 | 0.02 | 0.00 | 0.00 | 0.24 | 0.00 |
|  |  |  | -0.07 | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 |
| total | 0.36 | 0.00 | -0.22 | 0.02 | 0.00 | 0.00 | 0.25 | 0.00 |
|  |  |  | -0.07 | 0.09 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.02 | 0.06 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | -0.01 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.36 | 0.00 | 0.24 | 0.11 | 0.00 | 0.00 | 0.25 | 0.01 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 |
| ext. | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 |



**Figure 131:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **1:15** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.31 | 0.01 | -0.02 | 0.00 | 0.01 | 0.01 | -0.31 | 0.00 |
| ext. | 0.34 | 0.00 | -0.02 | 0.00 | 0.01 | 0.01 | -0.31 | 0.00 |
|  |  |  | -0.03 | 0.00 | -0.01 | -0.01 | 0.13 | 0.00 |
| total | 0.35 | 0.00 | -0.02 | 0.00 | 0.01 | 0.01 | -0.31 | 0.00 |
|  |  |  | -0.03 | 0.00 | -0.01 | -0.01 | 0.13 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 |
|  |  |  | -0.01 | 0.00 | 0.00 | 0.00 | -0.08 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.04 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.35 | 0.00 | 0.05 | 0.00 | 0.01 | 0.01 | 0.35 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 1.56 | 0.00 | 0.00 | -1.55 | 0.04 | -0.02 | 0.02 | 0.00 |
| ext. | 1.56 | 0.00 | 0.00 | -1.55 | 0.04 | -0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.03 | -0.01 | 0.01 | 0.00 |
| total | 1.56 | 0.00 | 0.00 | -1.55 | 0.04 | -0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.03 | -0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.03 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 1.56 | 0.00 | 0.00 | 1.56 | 0.05 | 0.02 | 0.02 | 0.00 |



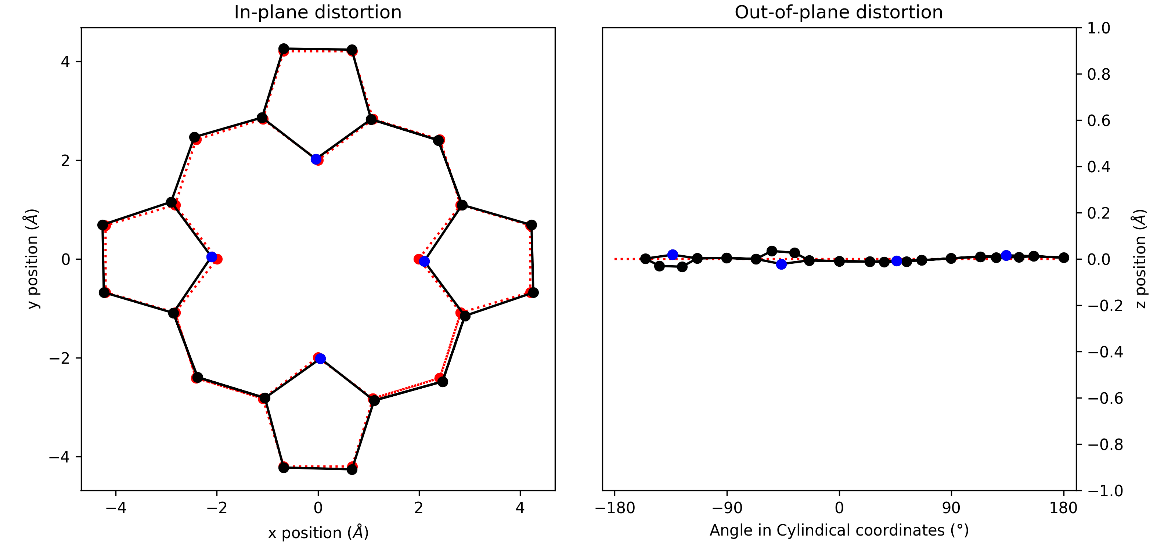
**Figure 132:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core.  
Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

## NSD tables and plots for DFT structures series 2

### NSD result generated from **2:1** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.28 | 0.00 | -0.18 | 0.06 | 0.00 | -0.01 | 0.21 | 0.00 |
| ext. | 0.30 | 0.00 | -0.18 | 0.06 | 0.00 | -0.01 | 0.21 | 0.00 |
|  |  |  | -0.03 | 0.09 | 0.02 | 0.01 | 0.01 | 0.00 |
| total | 0.31 | 0.00 | -0.18 | 0.06 | 0.00 | -0.01 | 0.21 | 0.00 |
|  |  |  | -0.03 | 0.09 | 0.02 | 0.01 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.06 | 0.00 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.31 | 0.00 | 0.18 | 0.13 | 0.02 | 0.02 | 0.22 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.07 | 0.00 | -0.06 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
| ext. | 0.08 | 0.00 | -0.05 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
| total | 0.08 | 0.00 | -0.05 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.08 | 0.00 | 0.06 | 0.01 | 0.00 | 0.03 | 0.04 | 0.00 |



**Figure 133:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2:2** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | 0.06 | 0.04 | 0.02 | -0.03 | 0.22 | 0.00 |
| ext. | 0.25 | 0.00 | 0.07 | 0.04 | 0.02 | -0.03 | 0.22 | 0.00 |
|  |  |  | 0.02 | 0.09 | 0.00 | 0.03 | 0.01 | 0.00 |
| total | 0.27 | 0.00 | 0.07 | 0.05 | 0.01 | -0.03 | 0.22 | 0.00 |
|  |  |  | 0.02 | 0.09 | 0.00 | 0.03 | 0.01 | 0.00 |
|  |  |  | -0.01 | 0.06 | -0.01 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.27 | 0.00 | 0.07 | 0.12 | 0.02 | 0.04 | 0.23 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.06 | 0.00 | -0.05 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
| ext. | 0.07 | 0.00 | -0.05 | 0.00 | 0.00 | -0.03 | -0.02 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
| total | 0.07 | 0.00 | -0.05 | 0.00 | 0.00 | -0.03 | -0.02 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.07 | 0.00 | 0.06 | 0.00 | 0.00 | 0.03 | 0.03 | 0.00 |

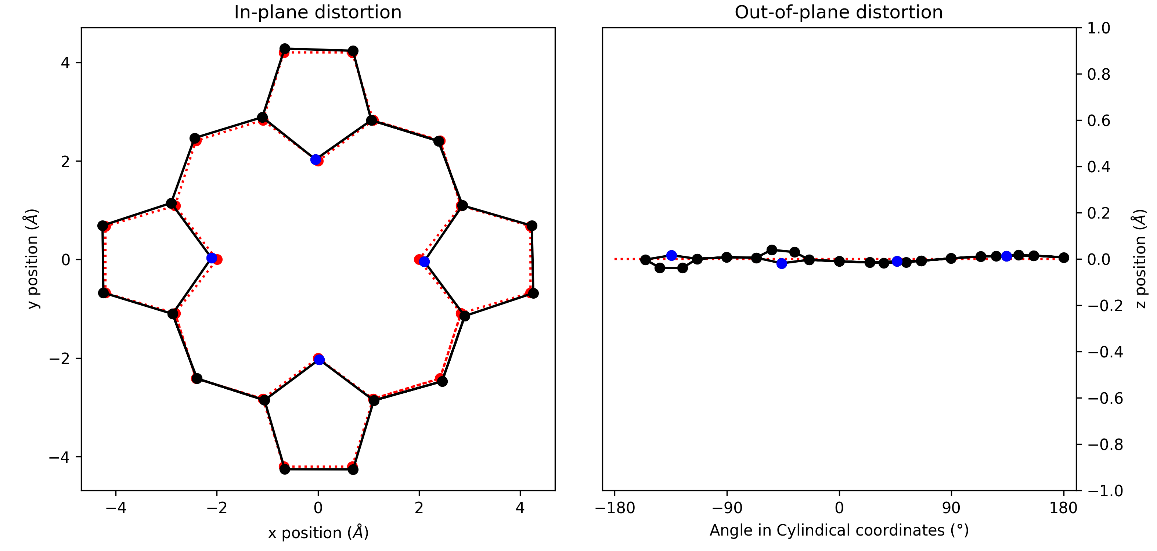


**Figure 134:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2:3** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.28 | 0.00 | -0.14 | 0.03 | 0.04 | -0.01 | 0.23 | 0.00 |
| ext. | 0.29 | 0.00 | -0.14 | 0.03 | 0.04 | -0.01 | 0.23 | 0.00 |
|  |  |  | -0.02 | 0.09 | -0.03 | 0.02 | 0.02 | 0.00 |
| total | 0.31 | 0.00 | -0.14 | 0.04 | 0.04 | -0.01 | 0.24 | 0.00 |
|  |  |  | -0.02 | 0.09 | -0.03 | 0.02 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.06 | -0.01 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.31 | 0.00 | 0.14 | 0.11 | 0.05 | 0.02 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.08 | 0.00 | -0.07 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
| ext. | 0.09 | 0.00 | -0.07 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
| total | 0.09 | 0.00 | -0.07 | -0.01 | 0.00 | -0.03 | -0.03 | 0.00 |
|  |  |  | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.09 | 0.00 | 0.08 | 0.01 | 0.00 | 0.03 | 0.03 | 0.00 |

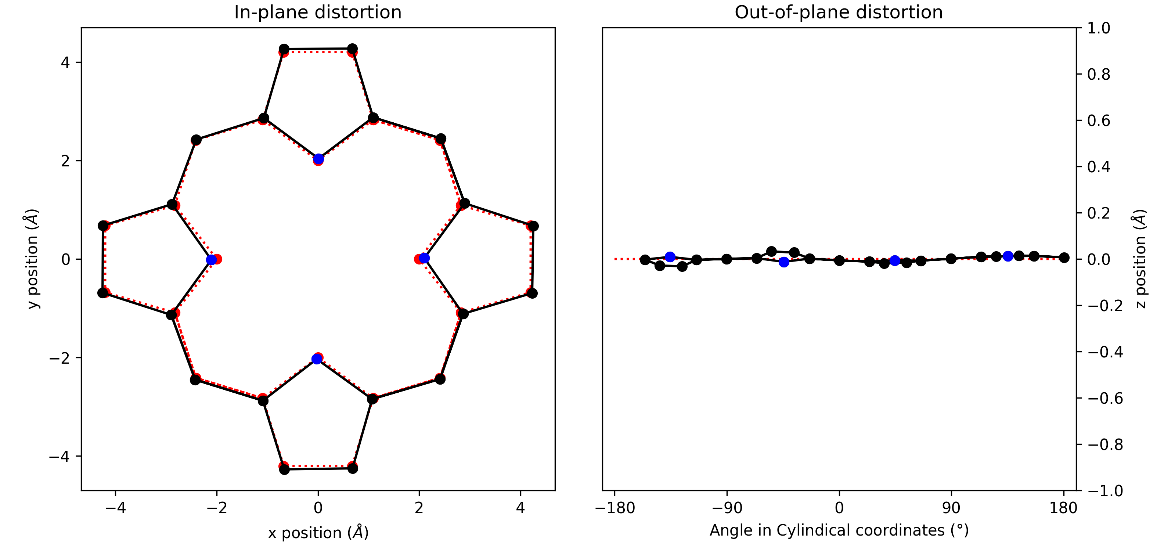


**Figure 135:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2:4** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.26 | 0.00 | 0.06 | 0.02 | 0.02 | 0.02 | 0.25 | 0.00 |
| ext. | 0.27 | 0.00 | 0.06 | 0.02 | 0.02 | 0.02 | 0.25 | 0.00 |
|  |  |  | 0.02 | 0.09 | 0.00 | 0.00 | 0.02 | 0.00 |
| total | 0.29 | 0.00 | 0.06 | 0.02 | 0.02 | 0.02 | 0.25 | 0.00 |
|  |  |  | 0.02 | 0.09 | -0.01 | 0.00 | 0.02 | 0.00 |
|  |  |  | -0.01 | 0.06 | -0.01 | 0.00 | 0.05 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | -0.01 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.29 | 0.00 | 0.07 | 0.11 | 0.02 | 0.02 | 0.26 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.07 | 0.00 | -0.07 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
| ext. | 0.07 | 0.00 | -0.06 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
| total | 0.07 | 0.00 | -0.06 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 |
|  |  |  | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.07 | 0.00 | 0.07 | 0.00 | 0.00 | 0.02 | 0.03 | 0.00 |

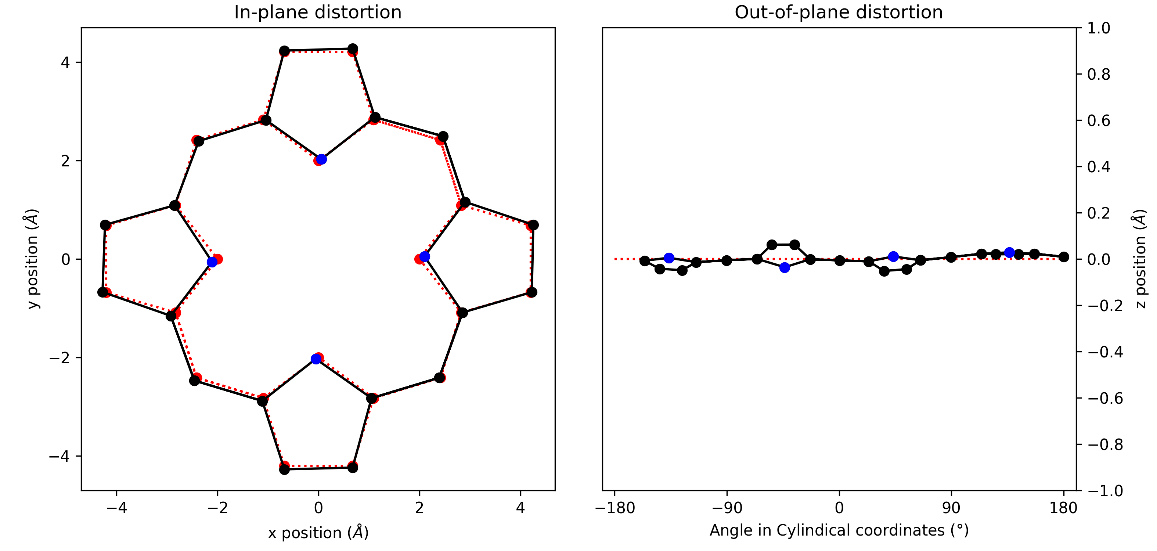


**Figure 136:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2:5** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.30 | 0.00 | 0.20 | 0.03 | 0.01 | -0.02 | 0.22 | 0.00 |
| ext. | 0.32 | 0.00 | 0.20 | 0.03 | 0.01 | -0.02 | 0.22 | 0.00 |
|  |  |  | 0.04 | 0.09 | 0.02 | 0.01 | 0.00 | 0.00 |
| total | 0.33 | 0.00 | 0.21 | 0.04 | 0.01 | -0.02 | 0.22 | 0.00 |
|  |  |  | 0.04 | 0.09 | 0.02 | 0.01 | 0.00 | 0.00 |
|  |  |  | -0.01 | 0.06 | -0.01 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.01 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.33 | 0.00 | 0.21 | 0.11 | 0.03 | 0.03 | 0.23 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.14 | 0.00 | -0.12 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
| ext. | 0.15 | 0.00 | -0.12 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | 0.00 | 0.00 | -0.04 | 0.00 |
| total | 0.15 | 0.00 | -0.12 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | 0.00 | 0.00 | -0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.15 | 0.00 | 0.13 | 0.00 | 0.01 | 0.01 | 0.07 | 0.00 |

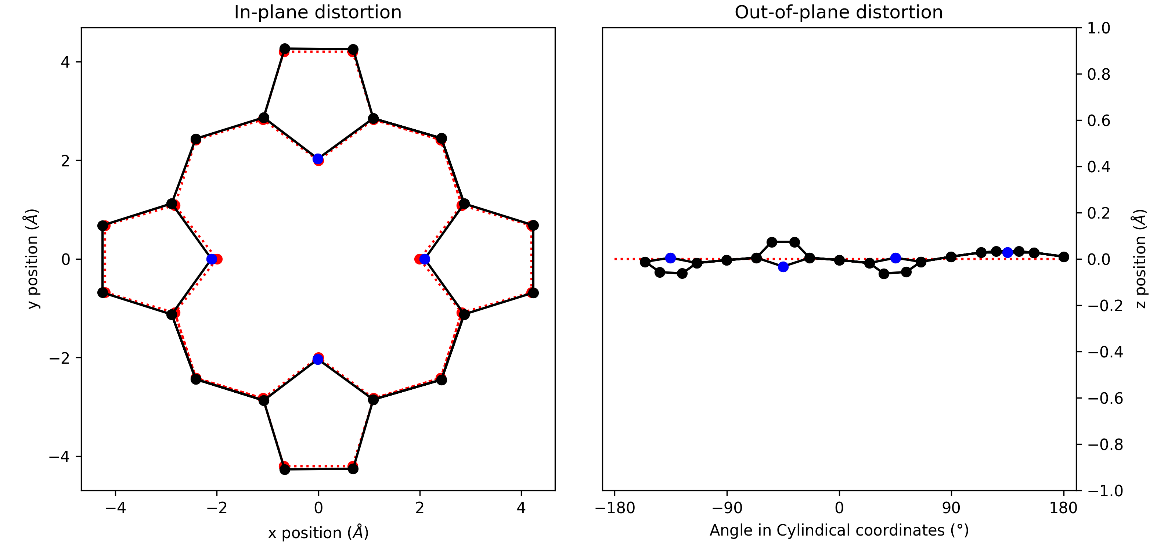


**Figure 137:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **2:6** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.24 | 0.00 | 0.00 | 0.02 | 0.03 | 0.00 | 0.24 | 0.00 |
| ext. | 0.25 | 0.00 | 0.00 | 0.02 | 0.03 | 0.00 | 0.24 | 0.00 |
|  |  |  | 0.00 | 0.08 | -0.01 | 0.00 | 0.01 | 0.00 |
| total | 0.27 | 0.00 | 0.00 | 0.02 | 0.03 | 0.00 | 0.24 | 0.00 |
|  |  |  | 0.00 | 0.09 | -0.01 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.06 | -0.01 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
| comp. | 0.27 | 0.00 | 0.00 | 0.11 | 0.04 | 0.00 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.17 | 0.00 | -0.16 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
| ext. | 0.18 | 0.00 | -0.16 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.03 | 0.00 |
| total | 0.18 | 0.00 | -0.16 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.18 | 0.00 | 0.17 | 0.00 | 0.01 | 0.00 | 0.07 | 0.00 |



**Figure 138:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

## NSD tables and plots for DFT structures series 3

### NSD result generated from **3:1** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.21 | 0.00 | 0.00 | 0.03 | -0.01 | 0.00 | 0.21 | 0.00 |
| ext. | 0.23 | 0.00 | 0.00 | 0.04 | -0.01 | 0.00 | 0.21 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.03 | 0.00 | 0.02 | 0.00 |
| total | 0.26 | 0.00 | 0.00 | 0.04 | -0.01 | 0.00 | 0.21 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.03 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.06 | 0.00 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.04 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.02 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.02 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
|  |  |  |  |  | -0.03 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.00 | 0.11 | 0.06 | 0.00 | 0.22 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.13 | 0.00 | -0.11 | 0.00 | 0.02 | 0.00 | -0.06 | 0.00 |
| ext. | 0.14 | 0.00 | -0.11 | 0.00 | 0.02 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.04 | 0.00 |
| total | 0.14 | 0.00 | -0.11 | 0.00 | 0.02 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.14 | 0.00 | 0.11 | 0.00 | 0.02 | 0.00 | 0.07 | 0.00 |

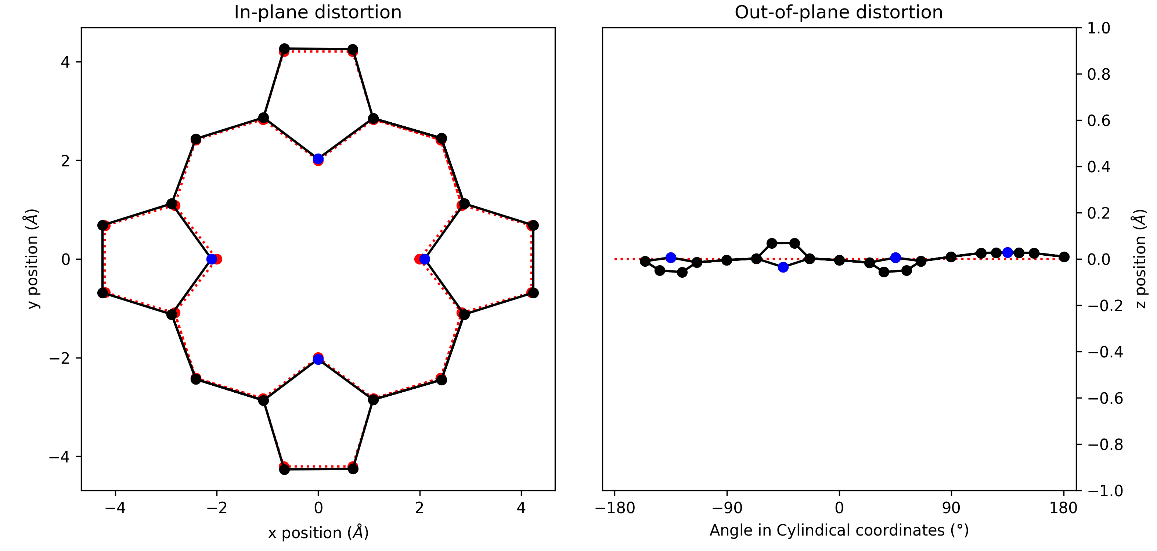


**Figure 139:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **3:2** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.23 | 0.00 | 0.00 | 0.02 | 0.02 | 0.00 | 0.23 | 0.00 |
| ext. | 0.25 | 0.00 | 0.00 | 0.02 | 0.02 | 0.00 | 0.23 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 |
| total | 0.26 | 0.00 | 0.00 | 0.03 | 0.02 | 0.00 | 0.23 | 0.00 |
|  |  |  | 0.00 | 0.09 | 0.00 | 0.00 | 0.01 | 0.00 |
|  |  |  | 0.00 | 0.06 | -0.01 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.01 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | -0.01 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
| comp. | 0.26 | 0.00 | 0.00 | 0.11 | 0.03 | 0.00 | 0.24 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.15 | 0.00 | -0.14 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
| ext. | 0.16 | 0.00 | -0.14 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.04 | 0.00 |
| total | 0.16 | 0.00 | -0.14 | 0.00 | 0.01 | 0.00 | -0.06 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.16 | 0.00 | 0.15 | 0.00 | 0.01 | 0.00 | 0.07 | 0.00 |

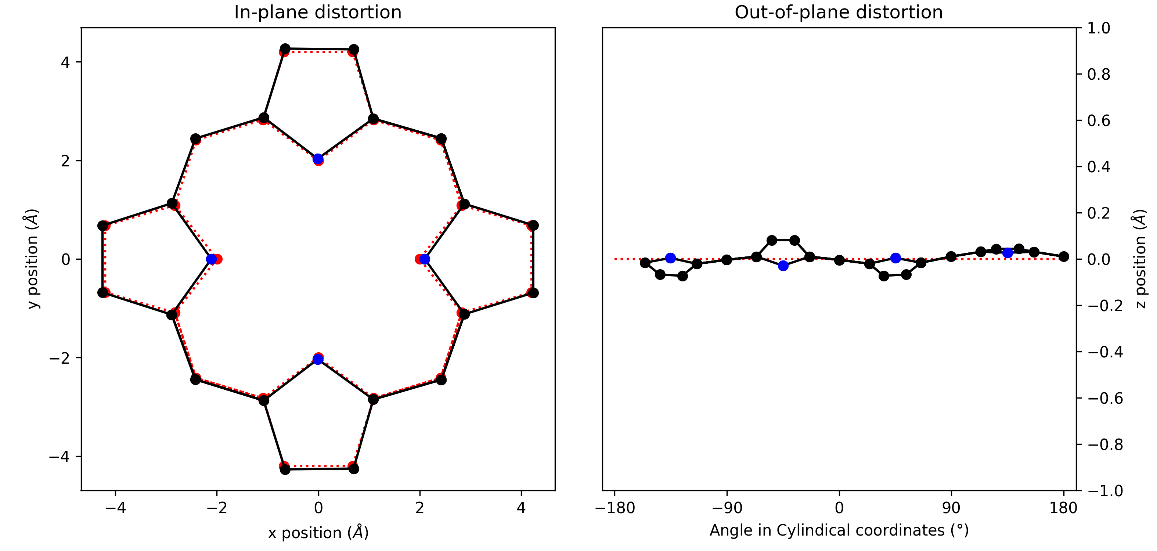


**Figure 140:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

### NSD result generated from **3:3** (in Å)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δip** | **δip** | **B2g** | **B1g** | **Eu(x)** | **Eu(y)** | **A1g** | **A2g** |
| min. | 0.25 | 0.00 | 0.00 | 0.02 | 0.05 | 0.00 | 0.25 | 0.00 |
| ext. | 0.27 | 0.00 | 0.00 | 0.02 | 0.05 | 0.00 | 0.25 | 0.00 |
|  |  |  | 0.00 | 0.09 | -0.02 | 0.00 | 0.00 | 0.00 |
| total | 0.28 | 0.00 | 0.00 | 0.02 | 0.05 | 0.00 | 0.25 | 0.00 |
|  |  |  | 0.00 | 0.09 | -0.02 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | 0.06 | -0.02 | 0.00 | 0.04 | 0.00 |
|  |  |  | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 |
|  |  |  | 0.00 | -0.01 | 0.00 | 0.00 | 0.02 | 0.00 |
|  |  |  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | -0.01 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.00 | 0.00 |  |  |
|  |  |  |  |  | 0.01 | 0.00 |  |  |
| comp. | 0.28 | 0.00 | 0.00 | 0.11 | 0.06 | 0.00 | 0.25 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **basis** | **Δoop** | **δoop** | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| min. | 0.20 | 0.00 | -0.19 | 0.00 | 0.01 | 0.00 | -0.05 | 0.00 |
| ext. | 0.20 | 0.00 | -0.19 | 0.00 | 0.01 | 0.00 | -0.05 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.03 | 0.00 |
| total | 0.20 | 0.00 | -0.19 | 0.00 | 0.01 | 0.00 | -0.05 | 0.00 |
|  |  |  | 0.04 | 0.00 | -0.01 | 0.00 | -0.03 | 0.00 |
|  |  |  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
|  |  |  |  |  |  | 0.00 | 0.00 |  |
| comp. | 0.20 | 0.00 | 0.19 | 0.00 | 0.01 | 0.00 | 0.06 | 0.00 |



**Figure 141:** (a) in-plane and (b) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.