Supporting Information

Crystallographic and DFT studies on host-guest complexes
consisting of zinc bisporphyrinates and 1-phenylethylamine

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Bond lengths [Å] and angles [°] for [ZnNi-AmBis]·(1-PEA) (Table S1) ...................S2
Bond lengths [Å] and angles [°] for [Zn2-AmBis]·(R-1-PEA)2 (Table S2) .................S12

IR spectra (Figure S1-S4) ..........................................................................................S32
NMR spectra (Figure S5-S8) .......................................................................................S34
UV-Vis spectra (Figure S9-S10) ..................................................................................S38

TGA diagrams for [Zn2-AmBis]·(R-1-PEA)2 and [ZnNi-AmBis]·(R-1-PEA) (Figure S11-S12)
.................................................................................................................................S39

Relative energies of DFT-optimized conformer A·R-1-PEA and conformer B·R-1-PEA
(Figure S13) .............................................................................................................S40

Relative energies of DFT-optimized conformer A·(R-1-PEA)2 and conformer B·(R-1-PEA)2
(Figure S14) ............................................................................................................S41

Cartesian coordinates for Geometry Optimized Conformers ......................................S42
Table S1. Bond lengths [Å] and angles [°] for [ZnNi-AmBis]·(1-PEA).

| Bond                  | Length [Å] | Bond                  | Length [Å] |
|-----------------------|------------|-----------------------|------------|
| Zn(1)-N(11)           | 2.044(3)   | Zn(1)-N(13)           | 2.057(2)   |
| Zn(1)-N(12)           | 2.063(2)   | Zn(1)-N(14)           | 2.070(2)   |
| Zn(1)-N(1A)           | 2.21(3)    | Zn(1)-N(1B)           | 2.24(3)    |
| N(1A)-C(7A)           | 1.475(10)  | N(1A)-H(1A)           | 0.8600     |
| N(1A)-H(1B)           | 0.8600     | C(7A)-C(8A)           | 1.491(9)   |
| C(7A)-C(1A)           | 1.525(9)   | C(7A)-H(7A)           | 0.9800     |
| C(8A)-H(8A)           | 0.9600     | C(8A)-H(8B)           | 0.9600     |
| C(8A)-H(8C)           | 0.9600     | C(1A)-C(2A)           | 1.3900     |
| C(1A)-C(6A)           | 1.3900     | C(2A)-C(3A)           | 1.3900     |
| C(2A)-H(2A)           | 0.9300     | C(3A)-C(4A)           | 1.3900     |
| C(3A)-H(3A)           | 0.9300     | C(4A)-C(5A)           | 1.3900     |
| C(4A)-H(4A)           | 0.9300     | C(5A)-C(6A)           | 1.3900     |
| C(5A)-H(5A)           | 0.9300     | C(6A)-H(6A)           | 0.9300     |
| N(1B)-C(7B)           | 1.477(10)  | N(1B)-H(1A1)          | 0.8600     |
| N(1B)-H(1A2)          | 0.8600     | C(7B)-C(8B)           | 1.515(10)  |
| C(7B)-C(1B)           | 1.528(9)   | C(7B)-H(7AA)          | 0.9800     |
| C(8B)-H(8A1)          | 0.9600     | C(8B)-H(8A2)          | 0.9600     |
| C(8B)-H(8A3)          | 0.9600     | C(1B)-C(2B)           | 1.3900     |
| C(1B)-C(6B)           | 1.3900     | C(2B)-C(3B)           | 1.3900     |
| C(2B)-H(2AA)          | 0.9300     | C(3B)-C(4B)           | 1.3900     |
| C(3B)-H(3AA)          | 0.9300     | C(4B)-C(5B)           | 1.3900     |
| C(4B)-H(4AA)          | 0.9300     | C(5B)-C(6B)           | 1.3900     |
| C(5B)-H(5AA)          | 0.9300     | C(6B)-H(6AA)          | 0.9300     |
| N(11)-C(1A2)          | 1.373(4)   | N(11)-C(1A1)          | 1.383(4)   |
| N(12)-C(1A3)          | 1.369(4)   | N(12)-C(1A4)          | 1.372(4)   |
| N(13)-C(1A5)          | 1.378(4)   | N(13)-C(1A6)          | 1.383(3)   |
| N(14)-C(1A8)          | 1.375(4)   | N(14)-C(1A7)          | 1.380(4)   |
| C(1A1)-C(1M1)         | 1.400(4)   | C(1A1)-C(1B1)         | 1.440(5)   |
| C(1A2)-C(1M2)         | 1.399(5)   | C(1A2)-C(1B2)         | 1.439(5)   |
| C(1A3)-C(1M2)         | 1.394(5)   | C(1A3)-C(1B3)         | 1.453(5)   |
| C(1A4)-C(1M3)         | 1.410(4)   | C(1A4)-C(1B4)         | 1.449(4)   |
| C(1A5)-C(1M3)         | 1.400(4)   | C(1A5)-C(1B5)         | 1.440(4)   |
| C(1A6)-C(1M4)         | 1.402(4)   | C(1A6)-C(1B6)         | 1.439(4)   |
|     |          |          |          |          |
|-----|----------|----------|----------|----------|
| C(1A7)-C(1M4) | 1.396(4) | C(1A7)-C(1B7) | 1.448(4) |
| C(1A8)-C(1M1) | 1.399(4) | C(1A8)-C(1B8) | 1.445(4) |
| C(1B1)-C(1B2) | 1.331(5) | C(1B1)-H(1BF) | 0.9300   |
| C(1B2)-H(1BH) | 0.9300   | C(1B3)-C(1B4) | 1.330(5) |
| C(1B3)-H(1BB) | 0.9300   | C(1B4)-H(1BG) | 0.9300   |
| C(1B5)-C(1B6) | 1.354(4) | C(1B5)-H(1BA) | 0.9300   |
| C(1B6)-H(1BC) | 0.9300   | C(1B7)-C(1B8) | 1.341(5) |
| C(1B7)-H(1BE) | 0.9300   | C(1B8)-H(1BD) | 0.9300   |
| C(1M1)-C(111) | 1.511(4) | C(1M2)-C(121) | 1.506(4) |
| C(1M3)-C(131) | 1.500(4) | C(1M4)-C(141) | 1.503(4) |
| C(111)-C(116) | 1.384(5) | C(111)-C(112) | 1.396(5) |
| C(112)-C(113) | 1.387(4) | C(112)-N(011) | 1.414(4) |
| C(113)-C(114) | 1.387(5) | C(113)-H(11A) | 0.9300   |
| C(114)-C(115) | 1.373(6) | C(114)-H(11B) | 0.9300   |
| C(115)-C(116) | 1.376(5) | C(115)-H(11C) | 0.9300   |
| C(116)-H(11D) | 0.9300   | C(121)-C(122) | 1.363(6) |
| C(121)-C(126) | 1.370(6) | C(122)-C(123) | 1.401(7) |
| C(122)-H(12A) | 0.9300   | C(123)-C(124) | 1.336(8) |
| C(123)-H(12B) | 0.9300   | C(124)-C(125) | 1.338(8) |
| C(124)-H(12C) | 0.9300   | C(125)-C(126) | 1.397(6) |
| C(125)-H(12D) | 0.9300   | C(126)-H(12E) | 0.9300   |
| C(131)-C(132) | 1.376(5) | C(131)-C(136) | 1.379(5) |
| C(132)-C(133) | 1.381(5) | C(132)-H(13A) | 0.9300   |
| C(133)-C(134) | 1.377(5) | C(133)-H(13B) | 0.9300   |
| C(134)-C(135) | 1.354(5) | C(134)-H(13C) | 0.9300   |
| C(135)-C(136) | 1.389(5) | C(135)-H(13D) | 0.9300   |
| C(136)-H(13E) | 0.9300   | C(141)-C(146) | 1.389(5) |
| C(141)-C(142) | 1.391(4) | C(142)-C(143) | 1.402(5) |
| C(142)-H(14A) | 0.9300   | C(143)-C(144) | 1.371(6) |
| C(143)-H(14B) | 0.9300   | C(144)-C(145) | 1.363(6) |
| C(144)-H(14C) | 0.9300   | C(145)-C(146) | 1.391(5) |
| C(145)-H(14D) | 0.9300   | C(146)-H(14E) | 0.9300   |
| Ni(1)-N(22)   | 1.972(2) | Ni(1)-N(24)  | 1.977(2) |
| Ni(1)-N(23)   | 1.977(3) | Ni(1)-N(21)  | 1.981(2) |
| N(21)-C(2A2)  | 1.380(4) | N(21)-C(2A1) | 1.381(3) |
| Bond                     | Distance  | Bond                     | Distance  |
|--------------------------|-----------|--------------------------|-----------|
| N(22)-C(2A4)             | 1.381(4)  | N(22)-C(2A3)             | 1.383(4)  |
| N(23)-C(2A5)             | 1.375(4)  | N(23)-C(2A6)             | 1.377(4)  |
| N(24)-C(2A8)             | 1.379(4)  | N(24)-C(2A7)             | 1.386(4)  |
| C(2A1)-C(2M1)            | 1.394(4)  | C(2A1)-C(2B1)            | 1.428(4)  |
| C(2A2)-C(2M2)            | 1.396(4)  | C(2A2)-C(2B2)            | 1.432(4)  |
| C(2A3)-C(2M2)            | 1.381(4)  | C(2A3)-C(2B3)            | 1.443(4)  |
| C(2A4)-C(2M3)            | 1.385(5)  | C(2A4)-C(2B4)            | 1.428(4)  |
| C(2A5)-C(2M3)            | 1.390(5)  | C(2A5)-C(2B5)            | 1.427(5)  |
| C(2A6)-C(2M4)            | 1.393(4)  | C(2A6)-C(2B6)            | 1.438(5)  |
| C(2A7)-C(2M4)            | 1.383(4)  | C(2A7)-C(2B7)            | 1.440(4)  |
| C(2A8)-C(2M1)            | 1.387(4)  | C(2A8)-C(2B8)            | 1.447(4)  |
| C(2B1)-C(2B2)            | 1.337(4)  | C(2B1)-H(2BC)            | 0.9300    |
| C(2B2)-H(2BD)            | 0.9300    | C(2B3)-C(2B4)            | 1.327(5)  |
| C(2B3)-H(2BG)            | 0.9300    | C(2B4)-H(2BH)            | 0.9300    |
| C(2B5)-C(2B6)            | 1.340(5)  | C(2B5)-H(2BF)            | 0.9300    |
| C(2B6)-H(2BB)            | 0.9300    | C(2B7)-C(2B8)            | 1.333(5)  |
| C(2B7)-H(2BG)            | 0.9300    | C(2B8)-H(2BE)            | 0.9300    |
| C(2M1)-C(211)            | 1.504(4)  | C(2M2)-C(221)            | 1.504(4)  |
| C(2M3)-C(231)            | 1.504(5)  | C(2M4)-C(241)            | 1.497(4)  |
| C(211)-C(212)            | 1.391(4)  | C(211)-C(216)            | 1.409(4)  |
| C(212)-C(213)            | 1.384(4)  | C(212)-H(21A)            | 0.9300    |
| C(213)-C(214)            | 1.377(4)  | C(213)-H(21B)            | 0.9300    |
| C(214)-C(215)            | 1.381(4)  | C(214)-H(21C)            | 0.9300    |
| C(215)-C(216)            | 1.397(4)  | C(215)-H(21D)            | 0.9300    |
| C(216)-N(013)            | 1.416(4)  | C(221)-C(226)            | 1.379(6)  |
| C(221)-C(222)            | 1.381(5)  | C(222)-C(223)            | 1.405(5)  |
| C(222)-H(22A)            | 0.9300    | C(223)-C(224)            | 1.354(7)  |
| C(223)-H(22B)            | 0.9300    | C(224)-C(225)            | 1.365(7)  |
| C(224)-H(22C)            | 0.9300    | C(225)-C(226)            | 1.391(6)  |
| C(225)-H(22D)            | 0.9300    | C(226)-H(22E)            | 0.9300    |
| C(231)-C(236)            | 1.330(7)  | C(231)-C(232)            | 1.387(7)  |
| C(232)-C(233)            | 1.370(6)  | C(232)-H(23A)            | 0.9300    |
| C(233)-C(234)            | 1.361(8)  | C(233)-H(23B)            | 0.9300    |
| C(234)-C(235)            | 1.362(10) | C(234)-H(23D)            | 0.9300    |
| C(235)-C(236)            | 1.447(7)  | C(235)-H(23C)            | 0.9300    |
| Bond          | Length  | Bond          | Length  |
|---------------|---------|---------------|---------|
| C(236)-H(23E) | 0.9300  | C(241)-C(246) | 1.375(5) |
| C(241)-C(242) | 1.382(5) | C(242)-C(243) | 1.388(6) |
| C(242)-H(24A) | 0.9300  | C(243)-C(244) | 1.351(7) |
| C(243)-H(24B) | 0.9300  | C(244)-C(245) | 1.369(7) |
| C(244)-H(24C) | 0.9300  | C(245)-C(246) | 1.391(6) |
| C(245)-H(24D) | 0.9300  | C(246)-H(24E) | 0.9300  |
| C(011)-C(016) | 1.388(5) | C(011)-C(012) | 1.403(5) |
| C(011)-C(017) | 1.506(5) | C(012)-C(013) | 1.385(5) |
| C(012)-H(01F) | 0.9300  | C(013)-C(014) | 1.382(5) |
| C(013)-C(018) | 1.504(5) | C(014)-C(015) | 1.397(5) |
| C(014)-H(01E) | 0.9300  | C(015)-C(016) | 1.379(6) |
| C(015)-N(012) | 1.400(5) | C(016)-H(01G) | 0.9300  |
| C(017)-O(011) | 1.216(4) | C(017)-N(011) | 1.337(5) |
| C(018)-O(012) | 1.215(4) | C(018)-N(013) | 1.344(4) |
| N(011)-H(01B) | 0.8600  | N(012)-H(01C) | 0.8600  |
| N(012)-H(01D) | 0.8600  | N(013)-H(01A) | 0.8600  |
| N(11)-Zn(1)-N(13) | 160.55(11) | N(11)-Zn(1)-N(12) | 88.43(10) |
| N(13)-Zn(1)-N(12) | 88.38(10) | N(11)-Zn(1)-N(14) | 88.98(10) |
| N(13)-Zn(1)-N(14) | 88.04(9) | N(12)-Zn(1)-N(14) | 161.67(11) |
| N(11)-Zn(1)-N(1A) | 106.8(7) | N(13)-Zn(1)-N(1A) | 92.6(7) |
| N(12)-Zn(1)-N(1A) | 94.3(6) | N(14)-Zn(1)-N(1A) | 103.9(6) |
| N(11)-Zn(1)-N(1B) | 102.3(9) | N(13)-Zn(1)-N(1B) | 97.1(8) |
| N(12)-Zn(1)-N(1B) | 102.2(6) | N(14)-Zn(1)-N(1B) | 96.1(6) |
| C(2A)-C(1A)-C(6A) | 120.0 | C(2A)-C(1A)-C(7A) | 120.0 |
| C(2A)-C(1A)-C(6A) | 120.0 | C(2A)-C(1A)-C(7A) | 120.0 |
| C(2A)-C(1A)-C(6A) | 120.0 | C(2A)-C(1A)-C(7A) | 120.0 |
| C(2A)-C(1A)-C(6A) | 120.0 | C(2A)-C(1A)-C(7A) | 120.0 |
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|-----------------------------|-----------|-----------------------------|-----------|
| C(1A)-C(2A)-H(2A)          | 120.0     | C(3A)-C(2A)-H(2A)          | 120.0     |
| C(4A)-C(3A)-C(2A)          | 120.0     | C(4A)-C(3A)-H(3A)          | 120.0     |
| C(2A)-C(3A)-H(3A)          | 120.0     | C(3A)-C(4A)-C(5A)          | 120.0     |
| C(3A)-C(4A)-H(4A)          | 120.0     | C(5A)-C(4A)-H(4A)          | 120.0     |
| C(6A)-C(5A)-C(4A)          | 120.0     | C(6A)-C(5A)-H(5A)          | 120.0     |
| C(4A)-C(5A)-H(5A)          | 120.0     | C(5A)-C(6A)-C(1A)          | 120.0     |
| C(5A)-C(6A)-H(6A)          | 120.0     | C(1A)-C(6A)-H(6A)          | 120.0     |
| C(7B)-N(1B)-Zn(1)          | 125(2)    | C(7B)-N(1B)-H(1A1)         | 120.0     |
| Zn(1)-N(1B)-H(1A1)         | 69.9      | C(7B)-N(1B)-H(1A2)         | 120.0     |
| Zn(1)-N(1B)-H(1A2)         | 77.1      | H(1A1)-N(1B)-H(1A2)        | 120.0     |
| N(1B)-C(7B)-C(8B)          | 96.8(16)  | N(1B)-C(7B)-C(1B)          | 120(2)    |
| C(8B)-C(7B)-C(1B)          | 108.5(11) | N(1B)-C(7B)-H(7AA)         | 110.2     |
| C(8B)-C(7B)-H(7AA)         | 110.2     | C(1B)-C(7B)-H(7AA)         | 110.2     |
| C(7B)-C(8B)-H(8A1)         | 109.5     | C(7B)-C(8B)-H(8A2)         | 109.5     |
| H(8A1)-C(8B)-H(8A2)        | 109.5     | C(7B)-C(8B)-H(8A3)         | 109.5     |
| H(8A1)-C(8B)-H(8A3)        | 109.5     | H(8A2)-C(8B)-H(8A3)        | 109.5     |
| C(2B)-C(1B)-C(6B)          | 120.0     | C(2B)-C(1B)-C(7B)          | 122.2(11) |
| C(6B)-C(1B)-C(7B)          | 117.7(11) | C(1B)-C(2B)-C(3B)          | 120.0     |
| C(1B)-C(2B)-H(2AA)         | 120.0     | C(3B)-C(2B)-H(2AA)         | 120.0     |
| C(4B)-C(3B)-C(2B)          | 120.0     | C(4B)-C(3B)-H(3AA)         | 120.0     |
| C(2B)-C(3B)-H(3AA)         | 120.0     | C(3B)-C(4B)-C(5B)          | 120.0     |
| C(3B)-C(4B)-H(4AA)         | 120.0     | C(5B)-C(4B)-H(4AA)         | 120.0     |
| C(4B)-C(5B)-C(6B)          | 120.0     | C(4B)-C(5B)-H(5AA)         | 120.0     |
| C(6B)-C(5B)-H(5AA)         | 120.0     | C(5B)-C(6B)-C(1B)          | 120.0     |
| C(5B)-C(6B)-H(6AA)         | 120.0     | C(1B)-C(6B)-H(6AA)         | 120.0     |
| C(1A2)-N(11)-C(1A1)        | 106.0(3)  | C(1A2)-N(11)-Zn(1)         | 127.0(2)  |
| C(1A1)-N(11)-Zn(1)         | 125.6(2)  | C(1A3)-N(12)-C(1A4)        | 106.7(3)  |
| C(1A3)-N(12)-Zn(1)         | 127.0(2)  | C(1A4)-N(12)-Zn(1)         | 126.1(2)  |
| C(1A5)-N(13)-C(1A6)        | 106.2(2)  | C(1A5)-N(13)-Zn(1)         | 125.35(19)|
| C(1A6)-N(13)-Zn(1)         | 127.50(19)| C(1A8)-N(14)-C(1A7)        | 106.6(2)  |
| C(1A8)-N(14)-Zn(1)         | 125.57(19)| C(1A7)-N(14)-Zn(1)         | 127.9(2)  |
| N(11)-C(1A1)-C(1M1)        | 125.1(3)  | N(11)-C(1A1)-C(1B1)        | 109.4(3)  |
| C(1M1)-C(1A1)-C(1B1)       | 125.5(3)  | N(11)-C(1A2)-C(1M2)        | 125.4(3)  |
| N(11)-C(1A2)-C(1B2)        | 109.4(3)  | C(1M2)-C(1A2)-C(1B2)       | 125.1(3)  |
| N(12)-C(1A3)-C(1M2)        | 125.7(3)  | N(12)-C(1A3)-C(1B3)        | 109.0(3)  |
| Bond                                | Angle (°) |
|-------------------------------------|-----------|
| C(1M2)-C(1A3)-C(1B3)               | 125.3(3)  |
| N(12)-C(1A4)-C(1B4)                | 109.4(3)  |
| N(13)-C(1A5)-C(1M3)                | 125.5(3)  |
| C(1M3)-C(1A5)-C(1B5)               | 124.3(3)  |
| N(13)-C(1A6)-C(1B6)                | 109.3(2)  |
| N(14)-C(1A7)-C(1M4)                | 125.4(3)  |
| C(1M4)-C(1A7)-C(1B7)               | 125.4(3)  |
| N(14)-C(1A8)-C(1B8)                | 109.4(3)  |
| C(1B2)-C(1B1)-C(1A1)               | 107.3(3)  |
| C(1B1)-C(1B2)-H(1BF)               | 126.4     |
| C(1B4)-C(1B3)-C(1A3)               | 107.7(3)  |
| C(1A3)-C(1B3)-H(1BB)               | 126.2     |
| C(1B3)-C(1B4)-H(1BG)               | 126.4     |
| C(1B6)-C(1B5)-C(1A5)               | 106.8(3)  |
| C(1A5)-C(1B5)-H(1BA)               | 126.6     |
| C(1B5)-C(1B6)-H(1BC)               | 126.2     |
| C(1B8)-C(1B7)-C(1A7)               | 107.4(3)  |
| C(1A7)-C(1B7)-H(1BE)               | 126.3     |
| C(1B7)-C(1B8)-H(1BD)               | 126.3     |
| C(1A8)-C(1M1)-C(1A1)               | 125.4(3)  |
| C(1A1)-C(1M1)-C(111)               | 115.7(3)  |
| C(1A3)-C(1M2)-C(121)               | 118.1(3)  |
| C(1A5)-C(1M3)-C(1A4)               | 124.5(3)  |
| C(1A4)-C(1M3)-C(131)               | 117.2(3)  |
| C(1A7)-C(1M4)-C(141)               | 117.9(2)  |
| C(116)-C(111)-C(112)               | 118.8(3)  |
| C(112)-C(111)-C(1M1)               | 121.0(3)  |
| C(113)-C(112)-N(011)               | 123.4(3)  |
| C(112)-C(113)-C(114)               | 119.9(4)  |
| C(114)-C(113)-H(11A)               | 120.0     |
| C(115)-C(114)-H(11B)               | 119.7     |
| C(114)-C(115)-C(116)               | 119.2(4)  |
| C(116)-C(115)-H(11C)               | 120.4     |
| C(115)-C(116)-H(11D)               | 119.2     |
| Bond                       | Angle (deg) | Bond                       | Angle (deg) |
|---------------------------|-------------|---------------------------|-------------|
| C(122)-C(121)-C(126)     | 118.3(4)    | C(122)-C(121)-C(1M2)     | 120.6(4)    |
| C(126)-C(121)-C(1M2)     | 121.1(3)    | C(121)-C(122)-C(123)     | 120.7(5)    |
| C(121)-C(122)-H(12A)     | 119.7       | C(123)-C(122)-H(12A)     | 119.7       |
| C(124)-C(123)-C(122)     | 119.8(5)    | C(124)-C(123)-H(12B)     | 120.1       |
| C(122)-C(123)-H(12B)     | 120.1       | C(123)-C(124)-C(125)     | 120.7(4)    |
| C(123)-C(124)-H(12C)     | 119.7       | C(125)-C(124)-H(12C)     | 119.7       |
| C(124)-C(125)-C(126)     | 120.5(5)    | C(124)-C(125)-H(12D)     | 119.8       |
| C(126)-C(125)-H(12D)     | 119.8       | C(121)-C(126)-C(125)     | 120.0(5)    |
| C(121)-C(126)-H(12E)     | 120.0       | C(125)-C(126)-H(12E)     | 120.0       |
| C(132)-C(131)-C(136)     | 117.6(3)    | C(132)-C(131)-C(1M3)     | 120.9(3)    |
| C(136)-C(131)-C(1M3)     | 121.5(3)    | C(131)-C(132)-C(133)     | 121.5(3)    |
| C(131)-C(132)-H(13A)     | 119.2       | C(133)-C(132)-H(13A)     | 119.2       |
| C(134)-C(133)-C(132)     | 120.0(3)    | C(134)-C(133)-H(13B)     | 120.0       |
| C(132)-C(133)-H(13B)     | 120.0       | C(135)-C(134)-C(133)     | 119.2(3)    |
| C(135)-C(134)-H(13C)     | 120.4       | C(133)-C(134)-H(13C)     | 120.4       |
| C(134)-C(135)-C(136)     | 120.8(4)    | C(134)-C(135)-H(13D)     | 119.6       |
| C(136)-C(135)-H(13D)     | 119.6       | C(131)-C(136)-C(135)     | 120.9(3)    |
| C(131)-C(136)-H(13E)     | 119.5       | C(135)-C(136)-H(13E)     | 119.5       |
| C(146)-C(141)-C(142)     | 118.5(3)    | C(146)-C(141)-C(1M4)     | 119.8(3)    |
| C(142)-C(141)-C(1M4)     | 121.7(3)    | C(141)-C(142)-C(143)     | 119.6(4)    |
| C(141)-C(142)-H(14A)     | 120.2       | C(143)-C(142)-H(14A)     | 120.2       |
| C(144)-C(143)-C(142)     | 120.4(3)    | C(144)-C(143)-H(14B)     | 119.8       |
| C(142)-C(143)-H(14B)     | 119.8       | C(145)-C(144)-C(143)     | 120.7(3)    |
| C(145)-C(144)-H(14C)     | 119.7       | C(143)-C(144)-H(14C)     | 119.7       |
| C(144)-C(145)-C(146)     | 119.4(4)    | C(144)-C(145)-H(14D)     | 120.3       |
| C(146)-C(145)-H(14D)     | 120.3       | C(141)-C(146)-C(145)     | 121.3(3)    |
| C(141)-C(146)-H(14E)     | 119.3       | C(145)-C(146)-H(14E)     | 119.3       |
| N(22)-Ni(1)-N(24)        | 171.93(12)  | N(22)-Ni(1)-N(23)        | 90.35(10)   |
| N(24)-Ni(1)-N(23)        | 89.60(10)   | N(22)-Ni(1)-N(21)        | 89.91(10)   |
| N(24)-Ni(1)-N(21)        | 90.04(9)    | N(23)-Ni(1)-N(21)        | 179.26(12)  |
| C(2A2)-N(21)-C(2A1)      | 105.1(2)    | C(2A2)-N(21)-Ni(1)       | 127.38(19)  |
| C(2A1)-N(21)-Ni(1)       | 127.16(19)  | C(2A4)-N(22)-C(2A3)      | 105.2(2)    |
| C(2A4)-N(22)-Ni(1)       | 127.0(2)    | C(2A3)-N(22)-Ni(1)       | 127.8(2)    |
| C(2A5)-N(23)-C(2A6)      | 105.1(3)    | C(2A5)-N(23)-Ni(1)       | 126.9(2)    |
| C(2A6)-N(23)-Ni(1)       | 127.9(2)    | C(2A8)-N(24)-C(2A7)      | 105.2(2)    |
| Bond | Distance (Å) | Bond | Distance (Å) |
|------|-------------|------|-------------|
| C(2A8)-N(24)-Ni(1) | 127.17(19) | C(2A7)-N(24)-Ni(1) | 127.58(19) |
| N(21)-C(2A1)-C(2M1) | 125.7(3) | N(21)-C(2A1)-C(2B1) | 110.1(2) |
| C(2M1)-C(2A1)-C(2B1) | 124.3(3) | N(21)-C(2A2)-C(2M2) | 125.6(3) |
| N(21)-C(2A2)-C(2B2) | 110.0(3) | C(2M2)-C(2A2)-C(2B2) | 124.4(3) |
| C(2M2)-C(2A3)-N(22) | 125.7(3) | C(2B2)-C(2B1)-C(2A1) | 107.5(3) |
| N(22)-C(2A3)-C(2B3) | 109.3(3) | C(2A1)-C(2B1)-H(2BC) | 126.2 |
| N(22)-C(2A4)-C(2B4) | 110.3(3) | C(2B1)-C(2B2)-H(2BD) | 107.2(3) |
| N(23)-C(2A5)-C(2M3) | 125.3(3) | C(2B4)-C(2B3)-C(2A3) | 107.5(3) |
| N(23)-C(2A6)-C(2B6) | 110.2(3) | C(2A3)-C(2B3)-H(2BG) | 107.8(3) |
| C(2M4)-C(2A7)-N(24) | 126.1(3) | C(2B5)-C(2B6)-H(2BB) | 106.6 |
| N(24)-C(2A7)-C(2B7) | 110.0(3) | C(2A4)-C(2B4)-H(2BH) | 126.3 |
| N(24)-C(2A8)-C(2B8) | 109.9(2) | C(2B6)-C(2B5)-H(2BF) | 107.5(3) |
| C(2B2)-C(2B1)-C(2A1) | 107.5(3) | C(2A5)-C(2B5)-H(2BF) | 107.8(3) |
| C(2B1)-C(2B2)-H(2BD) | 126.4 | C(2B5)-C(2B6)-H(2BB) | 126.6 |
| C(2B4)-C(2B3)-C(2A3) | 107.5(3) | C(2A6)-C(2B6)-H(2BB) | 118.2(2) |
| C(2B4)-C(2B3)-C(2A3) | 107.8(3) | C(2A1)-C(2B1)-H(2BC) | 119.0(2) |
| C(2B5)-C(2B6)-H(2BB) | 126.6 | C(2A3)-C(2B3)-H(2BG) | 123.1(3) |
| C(2B5)-C(2B6)-H(2BB) | 126.6 | C(2A4)-C(2B4)-C(2A2) | 124.4(3) |
| C(2B8)-C(2B7)-C(2A7) | 107.5(3) | C(2A2)-C(2B2)-H(2BD) | 123.9(3) |
| C(2A7)-C(2B7)-H(2BA) | 126.3 | C(2A3)-C(2B3)-C(2A5) | 126.2 |
| C(2B7)-C(2B8)-H(2BE) | 126.3 | C(2A5)-C(2B5)-H(2BF) | 125.6(3) |
| C(2B7)-C(2B8)-H(2BE) | 126.3 | C(2A2)-C(2B2)-C(2A1) | 119.3 |
| C(2A8)-C(2M1)-C(2A1) | 122.7(2) | C(2A8)-C(2M1)-C(2A1) | 127.58(19) |
| C(2A1)-C(2M1)-C(211) | 119.0(2) | C(2A3)-C(2M2)-C(2A2) | 118.0(3) |
| C(2A3)-C(2M2)-C(221) | 118.0(3) | C(2A2)-C(2M2)-C(221) | 118.7(3) |
| C(2A4)-C(2M3)-C(2A5) | 123.5(3) | C(2A4)-C(2M3)-C(231) | 121.4(3) |
| C(2A5)-C(2M3)-C(231) | 118.0(3) | C(2A7)-C(2M4)-C(2A6) | 119.8(3) |
| C(2A7)-C(2M4)-C(241) | 117.8(3) | C(2A6)-C(2M4)-C(241) | 120.8(3) |
| C(212)-C(211)-C(216) | 118.7(2) | C(213)-C(212)-C(211) | 121.4(3) |
| C(216)-C(211)-C(2M1) | 120.5(3) | C(211)-C(212)-H(21A) | 119.3 |
| C(213)-C(212)-H(21A) | 119.3 | C(214)-C(213)-H(21B) | 120.4 |
| Bond                  | Angle (°) | Bond                  | Angle (°) |
|----------------------|-----------|----------------------|-----------|
| C(212)-C(213)-H(21B) | 120.4     | C(213)-C(214)-C(215) | 121.0(3)  |
| C(213)-C(214)-H(21C) | 119.5     | C(215)-C(214)-H(21C) | 119.5     |
| C(214)-C(215)-C(216) | 120.0(3)  | C(214)-C(215)-H(21D) | 120.0     |
| C(216)-C(215)-H(21D) | 120.0     | C(215)-C(216)-C(211) | 119.5(3)  |
| C(215)-C(216)-N(013) | 122.4(3)  | C(211)-C(216)-N(013) | 118.1(2)  |
| C(226)-C(221)-C(222) | 117.8(3)  | C(226)-C(221)-C(2M2) | 120.9(3)  |
| C(222)-C(221)-C(2M2) | 121.2(3)  | C(221)-C(222)-C(223) | 120.3(4)  |
| C(221)-C(222)-H(22A) | 119.9     | C(223)-C(222)-H(22A) | 119.9     |
| C(224)-C(223)-C(222) | 120.8(4)  | C(224)-C(223)-H(22B) | 119.6     |
| C(222)-C(223)-H(22B) | 119.6     | C(223)-C(224)-C(225) | 119.6(4)  |
| C(223)-C(224)-H(22C) | 120.2     | C(225)-C(224)-H(22C) | 120.2     |
| C(224)-C(225)-C(226) | 120.1(5)  | C(224)-C(225)-H(22D) | 119.9     |
| C(226)-C(225)-H(22D) | 119.9     | C(221)-C(226)-C(225) | 121.3(4)  |
| C(221)-C(226)-H(22E) | 119.3     | C(225)-C(226)-H(22E) | 119.3     |
| C(236)-C(231)-C(232) | 118.9(4)  | C(236)-C(231)-C(2M3) | 120.5(4)  |
| C(232)-C(231)-C(2M3) | 120.6(4)  | C(233)-C(232)-C(231) | 122.7(6)  |
| C(233)-C(232)-H(23A) | 118.6     | C(231)-C(232)-H(23A) | 118.6     |
| C(234)-C(233)-C(232) | 117.5(6)  | C(234)-C(233)-H(23B) | 121.2     |
| C(232)-C(233)-H(23B) | 121.2     | C(233)-C(234)-C(235) | 122.6(5)  |
| C(233)-C(234)-H(23D) | 118.7     | C(235)-C(234)-H(23D) | 118.7     |
| C(234)-C(235)-C(236) | 117.6(7)  | C(234)-C(235)-H(23C) | 121.2     |
| C(236)-C(235)-H(23C) | 121.2     | C(231)-C(236)-C(235) | 120.4(6)  |
| C(231)-C(236)-H(23E) | 119.8     | C(235)-C(236)-H(23E) | 119.8     |
| C(246)-C(241)-C(242) | 117.9(3)  | C(246)-C(241)-C(2M4) | 121.8(3)  |
| C(242)-C(241)-C(2M4) | 120.2(3)  | C(241)-C(242)-C(243) | 121.0(4)  |
| C(241)-C(242)-H(24A) | 119.5     | C(243)-C(242)-H(24A) | 119.5     |
| C(244)-C(243)-C(242) | 120.3(5)  | C(244)-C(243)-H(24B) | 119.8     |
| C(242)-C(243)-H(24B) | 119.8     | C(243)-C(244)-C(245) | 119.7(4)  |
| C(243)-C(244)-H(24C) | 120.1     | C(245)-C(244)-H(24C) | 120.1     |
| C(244)-C(245)-C(246) | 120.4(5)  | C(244)-C(245)-H(24D) | 119.8     |
| C(246)-C(245)-H(24D) | 119.8     | C(241)-C(246)-C(245) | 120.6(4)  |
| C(241)-C(246)-H(24E) | 119.7     | C(245)-C(246)-H(24E) | 119.7     |
| C(016)-C(011)-C(012) | 118.8(3)  | C(016)-C(011)-C(017) | 118.4(3)  |
| C(012)-C(011)-C(017) | 122.8(3)  | C(013)-C(012)-C(011) | 119.7(3)  |
| C(013)-C(012)-H(01F) | 120.1     | C(011)-C(012)-H(01F) | 120.1     |
| Bond          | Angle (°) | Bond          | Angle (°) |
|--------------|-----------|--------------|-----------|
| C(014)-C(013)-C(012) | 120.6(3) | C(014)-C(013)-C(018) | 122.0(3) |
| C(012)-C(013)-C(018) | 117.3(3) | C(013)-C(014)-C(015) | 120.2(4) |
| C(013)-C(014)-H(01E) | 119.9    | C(015)-C(014)-H(01E) | 119.9    |
| C(016)-C(015)-C(014) | 119.0(4) | C(016)-C(015)-N(012) | 121.4(4) |
| C(014)-C(015)-N(012) | 119.6(4) | C(015)-C(016)-C(011) | 121.7(3) |
| C(015)-C(016)-H(01G) | 119.1    | C(011)-C(016)-H(01G) | 119.1    |
| O(011)-C(017)-N(011) | 122.3(4) | O(011)-C(017)-C(011) | 121.6(4) |
| N(011)-C(017)-C(011) | 116.0(3) | O(012)-C(018)-N(013) | 123.2(3) |
| O(012)-C(018)-C(013) | 120.7(3) | N(013)-C(018)-C(013) | 116.1(3) |
| C(017)-N(011)-C(112) | 131.5(3) | C(017)-N(011)-H(01B) | 114.2    |
| C(112)-N(011)-H(01B) | 114.2    | C(015)-N(012)-H(01C) | 120.0    |
| C(015)-N(012)-H(01D) | 120.0    | H(01C)-N(012)-H(01D) | 120.0    |
| C(018)-N(013)-C(216) | 129.4(3) | C(018)-N(013)-H(01A) | 115.3    |
| C(216)-N(013)-H(01A) | 115.3    |
Table S2. Bond lengths [Å] and angles [°] for [Zn₂-AmBis]·(R-1-PEA)₂.

| Bond                        | Length/Angle |
|-----------------------------|--------------|
| Zn(1)-N(11)                 | 2.062(8)     |
| Zn(1)-N(13)                 | 2.081(7)     |
| Zn(1)-N(1B)                 | 2.12(3)      |
| N(11)-C(1A2)                | 1.388(11)    |
| N(12)-C(1A3)                | 1.362(12)    |
| N(13)-C(1A5)                | 1.372(11)    |
| N(14)-C(1A7)                | 1.353(11)    |
| C(1M1)-C(1A2)               | 1.381(14)    |
| C(1M1)-C(111)               | 1.530(10)    |
| C(1M2)-C(1A5)               | 1.405(12)    |
| C(1M3)-C(1A7)               | 1.387(11)    |
| C(1M4)-C(1A8)               | 1.436(12)    |
| C(1A1)-C(1B1)               | 1.443(13)    |
| C(1A3)-C(1B3)               | 1.417(15)    |
| C(1A5)-C(1B5)               | 1.448(12)    |
| C(1A7)-C(1B7)               | 1.475(11)    |
| C(1B1)-C(1B2)               | 1.342(14)    |
| C(1B2)-H(1B2)               | 0.9400       |
| C(1B3)-H(1B3)               | 0.9400       |
| C(1B5)-C(1B6)               | 1.377(14)    |
| C(1B6)-H(1B6)               | 0.9400       |
| C(1B7)-H(1B7)               | 0.9400       |
| C(111)-C(112)               | 1.3900       |
| C(112)-C(113)               | 1.3900       |
| C(113)-C(114)               | 1.3900       |
| C(114)-C(115)               | 1.3900       |
| C(115)-C(116)               | 1.3900       |
| C(116)-H(116)               | 0.9400       |
| C(121)-C(126)               | 1.3905       |
| C(122)-H(122)               | 0.9400       |
| C(123)-H(123)               | 0.9400       |
| C(124)-H(124)               | 0.9400       |
| Bond                  | Length (Å) | Bond                  | Length (Å) |
|-----------------------|------------|-----------------------|------------|
| C(125)-H(125)         | 0.9400     | C(126)-N(011)         | 1.382(4)   |
| C(131)-C(136)         | 1.3898     | C(131)-C(132)         | 1.3901     |
| C(132)-C(133)         | 1.3900     | C(132)-H(132)         | 0.9400     |
| C(133)-C(134)         | 1.3905     | C(133)-H(133)         | 0.9400     |
| C(134)-C(135)         | 1.3899     | C(134)-H(134)         | 0.9400     |
| C(135)-C(136)         | 1.3899     | C(135)-H(135)         | 0.9400     |
| C(136)-H(136)         | 0.9400     | C(141)-C(142)         | 1.3900     |
| C(141)-C(146)         | 1.3900     | C(142)-C(143)         | 1.3900     |
| C(142)-H(14C)         | 0.9400     | C(143)-C(144)         | 1.3900     |
| C(143)-H(14D)         | 0.9400     | C(144)-C(145)         | 1.3900     |
| C(144)-H(14E)         | 0.9400     | C(145)-C(146)         | 1.3900     |
| C(145)-H(14F)         | 0.9400     | C(146)-H(14G)         | 0.9400     |
| N(1A)-C(12A)          | 1.55(2)    | N(1A)-H(1A1)          | 0.9000     |
| N(1A)-H(1A2)          | 0.9000     | C(11A)-C(12A)         | 1.44(3)    |
| C(11A)-H(11A)         | 0.9700     | C(11A)-H(11B)         | 0.9700     |
| C(11A)-H(11C)         | 0.9700     | C(12A)-C(13A)         | 1.65(2)    |
| C(12A)-H(12A)         | 0.9900     | C(13A)-C(14A)         | 1.3900     |
| C(13A)-C(18A)         | 1.3900     | C(14A)-C(15A)         | 1.3900     |
| C(14A)-H(14A)         | 0.9400     | C(15A)-C(16A)         | 1.3900     |
| C(15A)-H(15A)         | 0.9400     | C(16A)-C(17A)         | 1.3900     |
| C(16A)-H(16A)         | 0.9400     | C(17A)-C(18A)         | 1.3900     |
| C(17A)-H(17A)         | 0.9400     | C(18A)-H(18A)         | 0.9400     |
| N(1B)-C(12B)          | 1.26(4)    | N(1B)-H(1B9)          | 0.9000     |
| N(1B)-H(1BX)          | 0.9000     | C(11B)-C(12B)         | 1.53(4)    |
| C(11B)-H(11D)         | 0.9700     | C(11B)-H(11E)         | 0.9700     |
| C(11B)-H(11F)         | 0.9700     | C(12B)-C(13B)         | 1.39(3)    |
| C(12B)-H(12B)         | 0.9900     | C(13B)-C(14B)         | 1.3900     |
| C(13B)-C(18B)         | 1.3900     | C(14B)-C(15B)         | 1.3900     |
| C(14B)-H(14B)         | 0.9400     | C(15B)-C(16B)         | 1.3900     |
| C(15B)-H(15B)         | 0.9400     | C(16B)-C(17B)         | 1.3900     |
| C(16B)-H(16B)         | 0.9400     | C(17B)-C(18B)         | 1.3900     |
| C(17B)-H(17B)         | 0.9400     | C(18B)-H(18B)         | 0.9400     |
| Zn(2)-N(22)           | 2.062(8)   | Zn(2)-N(24)           | 2.071(8)   |
| Zn(2)-N(23)           | 2.072(7)   | Zn(2)-N(21)           | 2.076(7)   |
| Zn(2)-N(2)            | 2.178(8)   | N(21)-C(2A1)          | 1.366(11)  |
| Bond                      | Distance   | Bond                      | Distance   |
|--------------------------|------------|--------------------------|------------|
| N(21)-C(2A2)             | 1.382(12)  | N(22)-C(2A3)             | 1.367(12)  |
| N(22)-C(2A4)             | 1.368(12)  | N(23)-C(2B6)             | 1.360(11)  |
| N(23)-C(2A5)             | 1.375(11)  | N(24)-C(2A8)             | 1.348(12)  |
| N(24)-C(2A7)             | 1.367(11)  | C(2M1)-C(2A3)            | 1.378(13)  |
| C(2M1)-C(2A2)            | 1.383(13)  | C(2M1)-C(2A4)            | 1.397(13)  |
| C(2M2)-C(2A4)            | 1.397(13)  | C(2M2)-C(2A5)            | 1.403(12)  |
| C(2M2)-C(2A7)            | 1.408(12)  | C(2M3)-C(2A5)            | 1.409(12)  |
| C(2M4)-C(2A1)            | 1.392(12)  | C(2M3)-C(2A7)            | 1.398(12)  |
| C(2M4)-C(2A4)            | 1.497(11)  | C(2M4)-C(2A8)            | 1.490(10)  |
| C(2A1)-C(2A2)            | 1.470(13)  | C(2B1)-H(2B1)            | 0.9400     |
| C(2A2)-C(2A3)            | 1.464(13)  | C(2A3)-C(2B3)            | 1.474(12)  |
| C(2A4)-C(2B4)            | 1.456(13)  | C(2A5)-C(2B3)            | 1.439(13)  |
| C(2A6)-C(2B5)            | 1.333(12)  | C(2A6)-C(2B6)            | 1.446(12)  |
| C(2A6)-H(2A6)            | 0.9400     | C(2A7)-C(2B7)            | 1.421(12)  |
| C(2A8)-C(2B8)            | 1.487(12)  | C(2A8)-H(2B1)            | 0.9400     |
| C(2B3)-C(2B4)            | 1.331(15)  | C(2B3)-H(2B4)            | 0.9400     |
| C(2B4)-H(2B5)            | 0.9400     | C(2B5)-H(2B6)            | 0.9400     |
| C(2B7)-C(2B8)            | 1.387(13)  | C(2B7)-H(2B7)            | 0.9400     |
| C(2B8)-H(2B8)            | 0.9400     | C(2B8)-H(2B7)            | 0.9400     |
| C(2B8)-H(2B8)            | 0.9400     | C(211)-C(212)            | 1.3900     |
| C(211)-C(212)            | 1.3900     | C(211)-C(213)            | 1.3900     |
| C(212)-H(212)            | 0.9400     | C(212)-H(216)            | 0.9400     |
| C(213)-H(213)            | 0.9400     | C(213)-C(214)            | 1.3900     |
| C(214)-H(214)            | 0.9400     | C(214)-C(215)            | 1.3900     |
| C(215)-H(215)            | 0.9400     | C(215)-C(216)            | 1.3900     |
| C(215)-H(215)            | 0.9400     | C(216)-H(216)            | 0.9400     |
| C(216)-H(216)            | 0.9400     | C(216)-C(217)            | 1.386(9)   |
| C(217)-C(218)            | 1.398(9)   | C(221)-C(222)            | 1.392(9)   |
| C(221)-C(222)            | 1.386(9)   | C(222)-C(223)            | 0.9400     |
| C(222)-C(223)            | 1.386(9)   | C(223)-C(224)            | 0.9400     |
| C(223)-C(224)            | 1.362(10)  | C(223)-C(225)            | 0.9400     |
| C(224)-C(225)            | 1.342(10)  | C(224)-C(226)            | 0.9400     |
| C(225)-C(226)            | 1.390(9)   | C(225)-H(225)            | 0.9400     |
| C(226)-H(226)            | 0.9400     | C(231)-C(232)            | 1.388(7)   |
| C(231)-C(232)            | 1.409(7)   | C(232)-C(233)            | 1.383(8)   |
| C(232)-H(232)            | 0.9400     | C(233)-C(234)            | 1.372(8)   |
| C(233)-H(233)            | 0.9400     | C(234)-C(235)            | 1.373(8)   |
| C(234)-H(234)            | 0.9400     | C(235)-C(236)            | 1.397(7)   |
| Bond                     | Length  | Bond                     | Length  |
|-------------------------|---------|-------------------------|---------|
| C(235)-H(235)           | 0.9400  | C(236)-N(013)           | 1.450(9) |
| C(241)-C(246)           | 1.356(9) | C(241)-C(242)           | 1.385(9) |
| C(242)-C(243)           | 1.367(10) | C(242)-H(242)           | 0.9400  |
| C(243)-C(244)           | 1.352(12) | C(243)-H(243)           | 0.9400  |
| C(244)-C(245)           | 1.332(12) | C(244)-H(244)           | 0.9400  |
| C(245)-C(246)           | 1.391(10) | C(245)-H(245)           | 0.9400  |
| C(246)-H(246)           | 0.9400  | N(2)-C(022)             | 1.527(11)|
| N(2)-H(2A)              | 0.9000  | N(2)-H(2B)              | 0.9000  |
| C(021)-C(022)           | 1.521(15)| C(021)-H(02A)           | 0.9700  |
| C(021)-H(02B)           | 0.9700  | C(021)-H(02C)           | 0.9700  |
| C(022)-C(023)           | 1.501(9) | C(022)-H(022)           | 0.9900  |
| C(023)-C(024)           | 1.3900  | C(023)-C(028)           | 1.3900  |
| C(024)-C(025)           | 1.3900  | C(024)-H(024)           | 0.9400  |
| C(025)-C(026)           | 1.3900  | C(025)-H(025)           | 0.9400  |
| C(026)-C(027)           | 1.3900  | C(026)-H(026)           | 0.9400  |
| C(027)-C(028)           | 1.3900  | C(027)-H(027)           | 0.9400  |
| C(028)-H(028)           | 0.9400  | Zn(3)-N(33)             | 2.063(8) |
| Zn(3)-N(31)             | 2.070(7) | Zn(3)-N(32)             | 2.072(7) |
| Zn(3)-N(34)             | 2.082(8) | Zn(3)-N(3)              | 2.189(9) |
| N(31)-C(3A2)            | 1.373(12) | N(31)-C(3A1)           | 1.386(11)|
| N(32)-C(3A4)            | 1.372(11) | N(32)-C(3A3)           | 1.383(11)|
| N(33)-C(3A5)            | 1.365(11) | N(33)-C(3A6)           | 1.392(12)|
| N(34)-C(3A7)            | 1.358(11) | N(34)-C(3A8)           | 1.371(11)|
| C(3M1)-C(3A2)           | 1.397(12) | C(3M1)-C(3A3)           | 1.412(12)|
| C(3M1)-C(311)           | 1.518(9)  | C(3M2)-C(3A5)           | 1.421(13)|
| C(3M2)-C(3A4)           | 1.425(12) | C(3M2)-C(321)           | 1.485(10)|
| C(3M3)-C(3A7)           | 1.410(13) | C(3M3)-C(3A6)           | 1.422(13)|
| C(3M3)-C(31A)           | 1.506(11) | C(3M3)-C(31B)           | 1.515(11)|
| C(3M4)-C(3A1)           | 1.402(13) | C(3M4)-C(3A8)           | 1.413(12)|
| C(3M4)-C(341)           | 1.503(9)  | C(3A1)-C(3B1)           | 1.406(13)|
| C(3A2)-C(3B2)           | 1.451(12) | C(3A3)-C(3B3)           | 1.423(13)|
| C(3A4)-C(3B4)           | 1.440(12) | C(3A5)-C(3B5)           | 1.435(13)|
| C(3A6)-C(3B6)           | 1.380(13) | C(3A7)-C(3B7)           | 1.425(13)|
| C(3A8)-C(3B8)           | 1.416(13) | C(3B1)-C(3B2)           | 1.306(13)|
| C(3B1)-H(3B1)           | 0.9400  | C(3B2)-H(3B2)           | 0.9400  |
| Bond                  | Distance   | Bond                  | Distance   |
|-----------------------|------------|-----------------------|------------|
| C(3B3)-C(3B4)         | 1.354(13)  | C(3B3)-H(3B3)         | 0.9400     |
| C(3B4)-H(3B4)         | 0.9400     | C(3B5)-C(3B6)         | 1.355(14)  |
| C(3B5)-H(3B5)         | 0.9400     | C(3B6)-H(3B6)         | 0.9400     |
| C(3B7)-C(3B8)         | 1.307(13)  | C(3B7)-H(3B7)         | 0.9400     |
| C(3B8)-H(3B8)         | 0.9400     | C(311)-C(312)         | 1.3900     |
| C(311)-C(316)         | 1.3900     | C(312)-C(313)         | 1.3900     |
| C(312)-H(312)         | 0.9400     | C(313)-C(314)         | 1.3900     |
| C(313)-H(313)         | 0.9400     | C(314)-C(315)         | 1.3900     |
| C(314)-H(314)         | 0.9400     | C(315)-C(316)         | 1.3900     |
| C(315)-H(315)         | 0.9400     | C(316)-N(021)         | 1.390(8)   |
| C(321)-C(322)         | 1.3900     | C(321)-C(326)         | 1.3900     |
| C(322)-C(323)         | 1.3900     | C(322)-H(32C)         | 0.9400     |
| C(323)-C(324)         | 1.3900     | C(323)-H(32D)         | 0.9400     |
| C(324)-C(325)         | 1.3900     | C(324)-H(32E)         | 0.9400     |
| C(325)-C(326)         | 1.3900     | C(325)-H(32F)         | 0.9400     |
| C(326)-H(32G)         | 0.9400     | C(31A)-C(32A)         | 1.3900     |
| C(31A)-C(36A)         | 1.3900     | C(32A)-C(33A)         | 1.3900     |
| C(32A)-H(32A)         | 0.9400     | C(33A)-C(34A)         | 1.3900     |
| C(33A)-H(33A)         | 0.9400     | C(34A)-C(35A)         | 1.3900     |
| C(34A)-H(34A)         | 0.9400     | C(35A)-C(36A)         | 1.3900     |
| C(35A)-H(35A)         | 0.9400     | C(36A)-H(36A)         | 0.9400     |
| C(31B)-C(32B)         | 1.3900     | C(31B)-C(36B)         | 1.3900     |
| C(32B)-C(33B)         | 1.3900     | C(32B)-H(32B)         | 0.9400     |
| C(33B)-C(34B)         | 1.3900     | C(33B)-H(33B)         | 0.9400     |
| C(34B)-C(35B)         | 1.3900     | C(34B)-H(34B)         | 0.9400     |
| C(35B)-C(36B)         | 1.3900     | C(35B)-H(35B)         | 0.9400     |
| C(36B)-H(36B)         | 0.9400     | C(341)-C(342)         | 1.3900     |
| C(341)-C(346)         | 1.3900     | C(342)-C(343)         | 1.3900     |
| C(342)-H(34C)         | 0.9400     | C(343)-C(344)         | 1.3900     |
| C(343)-H(34D)         | 0.9400     | C(344)-C(345)         | 1.3900     |
| C(344)-H(34E)         | 0.9400     | C(345)-C(346)         | 1.3900     |
| C(345)-H(34F)         | 0.9400     | C(346)-H(34G)         | 0.9400     |
| N(3)-C(037)           | 1.438(15)  | N(3)-H(3A)            | 0.9000     |
| N(3)-H(3B)            | 0.9000     | C(031)-C(032)         | 1.3900     |
| C(031)-C(036)         | 1.3900     | C(031)-C(037)         | 1.692(17)  |
| Bond                  | Length   | Bond                  | Length   |
|----------------------|----------|----------------------|----------|
| C(032)-C(033)        | 1.3900   | C(032)-H(032)        | 0.9400   |
| C(033)-C(034)        | 1.3900   | C(033)-H(033)        | 0.9400   |
| C(034)-C(035)        | 1.3900   | C(034)-H(034)        | 0.9400   |
| C(035)-C(036)        | 1.3900   | C(035)-H(035)        | 0.9400   |
| C(036)-H(036)        | 0.9400   | C(037)-C(038)        | 1.431(18) |
| C(037)-H(037)        | 0.9900   | C(038)-H(03A)        | 0.9700   |
| C(038)-H(03B)        | 0.9700   | C(038)-H(03C)        | 0.9700   |
| Zn(4)-N(41)          | 2.049(7) | Zn(4)-N(43)          | 2.068(7) |
| Zn(4)-N(42)          | 2.089(7) | Zn(4)-N(44)          | 2.103(7) |
| Zn(4)-N(4)           | 2.143(7) | N(41)-C(4A2)         | 1.369(12) |
| N(41)-C(4A1)         | 1.371(11)| N(42)-C(4A4)         | 1.342(11) |
| N(42)-C(4A3)         | 1.344(13)| N(43)-C(4A5)         | 1.367(10) |
| N(43)-C(4A6)         | 1.384(11)| N(44)-C(4A8)         | 1.358(10) |
| N(44)-C(4A7)         | 1.366(11)| C(4M1)-C(4A2)        | 1.405(13) |
| C(4M1)-C(4A3)        | 1.430(14)| C(4M1)-C(411)        | 1.468(10) |
| C(4M2)-C(4A5)        | 1.382(13)| C(4M2)-C(4A4)        | 1.406(13) |
| C(4M2)-C(421)        | 1.490(11)| C(4M3)-C(4A7)        | 1.397(12) |
| C(4M3)-C(4A6)        | 1.428(11)| C(4M3)-C(431)        | 1.500(9)  |
| C(4M4)-C(4A8)        | 1.409(13)| C(4M4)-C(4A1)        | 1.423(12) |
| C(4M4)-C(441)        | 1.495(9) | C(4A1)-C(4B1)        | 1.462(12) |
| C(4A2)-C(4B2)        | 1.466(12)| C(4A3)-C(4B3)        | 1.458(14) |
| C(4A4)-C(4B4)        | 1.449(13)| C(4A5)-C(4B5)        | 1.469(12) |
| C(4A6)-C(4B6)        | 1.411(12)| C(4A7)-C(4B7)        | 1.409(12) |
| C(4A8)-C(4B8)        | 1.436(13)| C(4B1)-C(4B2)        | 1.318(14) |
| C(4B1)-H(4B1)        | 0.9400   | C(4B2)-H(4B2)        | 0.9400   |
| C(4B3)-C(4B4)        | 1.340(15)| C(4B3)-H(4B3)        | 0.9400   |
| C(4B4)-H(4B4)        | 0.9400   | C(4B5)-C(4B6)        | 1.339(12) |
| C(4B5)-H(4B5)        | 0.9400   | C(4B6)-H(4B6)        | 0.9400   |
| C(4B7)-C(4B8)        | 1.320(13)| C(4B7)-H(4B7)        | 0.9400   |
| C(4B8)-H(4B8)        | 0.9400   | C(411)-C(412)        | 1.3900   |
| C(411)-C(416)        | 1.3900   | C(412)-C(413)        | 1.3900   |
| C(412)-H(412)        | 0.9400   | C(413)-C(414)        | 1.3900   |
| C(413)-H(413)        | 0.9400   | C(414)-C(415)        | 1.3900   |
| C(414)-H(414)        | 0.9400   | C(415)-C(416)        | 1.3900   |
| C(415)-H(415)        | 0.9400   | C(416)-H(416)        | 0.9400   |
| Bond          | Length   | Bond          | Length   |
|--------------|----------|--------------|----------|
| C(421)-C(422) | 1.379(8) | C(421)-C(426) | 1.389(8) |
| C(422)-C(423) | 1.368(8) | C(422)-H(422) | 0.9400   |
| C(423)-C(424) | 1.357(9)  | C(423)-H(423) | 0.9400   |
| C(424)-C(425) | 1.348(9)  | C(424)-H(424) | 0.9400   |
| C(425)-C(426) | 1.389(9)  | C(425)-H(425) | 0.9400   |
| C(426)-H(426) | 0.9400   | C(431)-C(432) | 1.3900   |
| C(431)-C(436) | 1.3900   | C(432)-C(433) | 1.3900   |
| C(432)-H(432) | 0.9400   | C(433)-C(434) | 1.3900   |
| C(433)-H(433) | 0.9400   | C(434)-C(435) | 1.3900   |
| C(434)-H(434) | 0.9400   | C(435)-C(436) | 1.3900   |
| C(435)-H(435) | 0.9400   | C(436)-H(436) | 0.9400   |
| C(441)-C(446) | 1.3899   | C(441)-C(442) | 1.3903   |
| C(442)-N(023) | 1.387(4)  | C(442)-C(443) | 1.3903   |
| C(443)-C(444) | 1.3906   | C(443)-H(443) | 0.9400   |
| C(444)-C(445) | 1.3899   | C(444)-H(444) | 0.9400   |
| C(445)-C(446) | 1.3897   | C(445)-H(445) | 0.9400   |
| C(446)-H(446) | 0.9400   | N(4)-C(047)   | 1.465(10) |
| N(4)-H(41)    | 0.9000   | N(4)-H(42)    | 0.9000   |
| C(047)-C(048) | 1.483(15) | C(047)-C(041) | 1.524(8) |
| C(047)-H(47A) | 0.9900   | C(048)-H(48A) | 0.9700   |
| C(048)-H(48B) | 0.9700   | C(048)-H(48C) | 0.9700   |
| C(041)-C(042) | 1.3900   | C(041)-C(046) | 1.3900   |
| C(042)-C(043) | 1.3900   | C(042)-H(042) | 0.9400   |
| C(043)-C(044) | 1.3900   | C(043)-H(043) | 0.9400   |
| C(044)-C(045) | 1.3900   | C(044)-H(044) | 0.9400   |
| C(045)-C(046) | 1.3900   | C(045)-H(045) | 0.9400   |
| C(046)-H(046) | 0.9400   | N(011)-C(18)  | 1.337(12) |
| N(011)-H(011) | 0.8700   | N(012)-C(15)  | 1.401(10) |
| N(012)-H(01D) | 0.8700   | N(012)-H(01E) | 0.8700   |
| N(013)-C(17)  | 1.360(11) | N(013)-H(013) | 0.8700   |
| O(011)-C(18)  | 1.215(12) | O(012)-C(17)  | 1.177(11) |
| C(11)-C(12)   | 1.3900   | C(11)-C(16)   | 1.3900   |
| C(11)-C(17)   | 1.521(10) | C(12)-C(13)   | 1.3900   |
| C(12)-H(12)   | 0.9400   | C(13)-C(14)   | 1.3900   |
| C(13)-C(18)   | 1.501(10) | C(14)-C(15)   | 1.3900   |
| Bond                  | Distance | Bond                  | Distance |
|----------------------|----------|----------------------|----------|
| C(14)-H(14)          | 0.9400   | C(15)-C(16)          | 1.3900   |
| C(16)-H(16)          | 0.9400   | N(021)-C(27)         | 1.336(12) |
| N(021)-H(021)        | 0.8700   | N(022)-C(21)         | 1.381(10) |
| N(022)-H(02D)        | 0.8700   | N(022)-H(02E)        | 0.8700   |
| N(023)-C(28)         | 1.378(11)| N(023)-H(023)        | 0.8700   |
| O(021)-C(27)         | 1.267(11)| O(022)-C(28)         | 1.220(11) |
| C(21)-C(22)          | 1.3900   | C(21)-C(26)          | 1.3900   |
| C(22)-C(23)          | 1.3900   | C(22)-H(22)          | 0.9400   |
| C(23)-C(24)          | 1.3900   | C(23)-C(27)          | 1.467(10) |
| C(24)-C(25)          | 1.3900   | C(24)-H(24A)         | 0.9400   |
| C(25)-C(26)          | 1.3900   | C(25)-C(28)          | 1.521(10) |
| C(26)-H(26)          | 0.9400   |                       |          |
| N(11)-Zn(1)-N(14)   | 88.7(3)  | N(11)-Zn(1)-N(13)   | 158.5(3) |
| N(14)-Zn(1)-N(13)   | 88.1(3)  | N(11)-Zn(1)-N(12)   | 87.8(3)  |
| N(14)-Zn(1)-N(12)   | 159.6(3) | N(13)-Zn(1)-N(12)   | 87.8(3)  |
| N(11)-Zn(1)-N(1B)   | 102.2(8) | N(14)-Zn(1)-N(1B)   | 96.9(8)  |
| N(13)-Zn(1)-N(1B)   | 99.3(8)  | N(12)-Zn(1)-N(1B)   | 103.5(8) |
| N(11)-Zn(1)-N(1A)   | 110.2(4) | N(14)-Zn(1)-N(1A)   | 106.3(4) |
| N(13)-Zn(1)-N(1A)   | 91.1(4)  | N(12)-Zn(1)-N(1A)   | 93.8(4)  |
| C(1A2)-N(11)-C(1A1) | 105.2(8) | C(1A2)-N(11)-Zn(1)  | 128.5(6) |
| C(1A1)-N(11)-Zn(1)  | 125.8(6) | C(1A3)-N(12)-C(1A4) | 107.4(8) |
| C(1A3)-N(12)-Zn(1)  | 125.9(6) | C(1A4)-N(12)-Zn(1)  | 124.7(6) |
| C(1A5)-N(13)-C(1A6) | 106.5(7) | C(1A5)-N(13)-Zn(1)  | 126.5(6) |
| C(1A6)-N(13)-Zn(1)  | 126.9(5) | C(1A7)-N(14)-C(1A8) | 106.9(7) |
| C(1A7)-N(14)-Zn(1)  | 126.6(6) | C(1A8)-N(14)-Zn(1)  | 126.0(6) |
| C(1A2)-C(1M1)-C(1A3)| 128.2(9) | C(1A2)-C(1M1)-C(111)| 116.1(8) |
| C(1A3)-C(1M1)-C(111)| 115.6(8) | C(1A4)-C(1M2)-C(1A5)| 125.7(8) |
| C(1A4)-C(1M2)-C(121)| 117.0(7) | C(1A5)-C(1M2)-C(121)| 117.1(7) |
| C(1A7)-C(1M3)-C(1A6)| 123.2(8) | C(1A7)-C(1M3)-C(131)| 119.7(7) |
| C(1A6)-C(1M3)-C(131)| 117.0(7) | C(1A1)-C(1M4)-C(1A8)| 126.6(8) |
| C(1A1)-C(1M4)-C(141)| 117.7(7) | C(1A8)-C(1M4)-C(141)| 115.5(8) |
| C(1M4)-C(1A1)-N(11) | 124.9(8) | C(1M4)-C(1A1)-C(1B1)| 125.4(9) |
| N(11)-C(1A1)-C(1B1) | 109.7(8) | C(1M1)-C(1A2)-N(11) | 122.5(9) |
| C(1M1)-C(1A2)-C(1B2) | 127.7(9) | N(11)-C(1A2)-C(1B2) | 109.8(8) |
| N(12)-C(1A3)-C(1M1) | 124.8(9) | N(12)-C(1A3)-C(1B3) | 109.3(8) |
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|-----------------------------|-----------|-----------------------------|-----------|
| (1M1)-C(1A3)-C(1B3)        | 125.9(9)  | (12)-C(1A4)-C(1M2)         | 125.9(8)  |
| (12)-C(1A4)-C(1B4)         | 108.9(9)  | (1M2)-C(1A4)-C(1B4)        | 125.1(8)  |
| (13)-C(1A5)-C(1M2)         | 124.8(8)  | (13)-C(1A5)-C(1B5)         | 110.9(7)  |
| (1M2)-C(1A5)-C(1B5)        | 124.2(8)  | (13)-C(1A6)-C(1M3)         | 126.1(8)  |
| (13)-C(1A6)-C(1B6)         | 109.5(8)  | (1M3)-C(1A6)-C(1B6)        | 124.4(9)  |
| (14)-C(1A7)-C(1M3)         | 128.4(7)  | (14)-C(1A7)-C(1B7)         | 109.3(7)  |
| (1M3)-C(1A7)-C(1B7)        | 122.3(8)  | (14)-C(1A8)-C(1B8)         | 110.0(8)  |
| (14)-C(1A8)-C(1M4)         | 123.3(8)  | C(1B8)-C(1A8)-C(1M4)       | 126.6(8)  |
| (1B2)-C(1B1)-C(1A1)        | 107.0(8)  | (1B2)-C(1B1)-H(1B1)        | 126.5     |
| (1A1)-C(1B1)-H(1B1)        | 126.5     | (1A2)-C(1B2)-H(1B2)        | 125.9     |
| (1B1)-C(1B2)-H(1B2)        | 125.9     | (1B4)-C(1B3)-H(1B3)        | 126.4     |
| (1B4)-C(1B3)-C(1A3)        | 107.2(9)  | (1B3)-C(1B4)-C(1A4)        | 107.1(9)  |
| (1A3)-C(1B3)-H(1B3)        | 126.4     | (1B4)-C(1B4)-H(1B4)        | 126.5     |
| (1B4)-C(1B5)-C(1A5)        | 106.5(8)  | (1B6)-C(1B5)-H(1B5)        | 126.7     |
| (1B5)-C(1B6)-H(1B6)        | 126.7     | (1B5)-C(1B6)-C(1A6)        | 106.6(8)  |
| (1B5)-C(1B6)-H(1B6)        | 126.7     | (1A6)-C(1B6)-H(1B6)        | 126.7     |
| (1B8)-C(1B7)-C(1A7)        | 105.1(8)  | (1B8)-C(1B7)-H(1B7)        | 127.5     |
| (1A7)-C(1B7)-H(1B7)        | 127.5     | (1B7)-C(1B8)-C(1A8)        | 108.5(7)  |
| (1B7)-C(1B8)-H(1B8)        | 125.8     | (1A8)-C(1B8)-H(1B8)        | 125.8     |
| (112)-C(111)-C(116)        | 120.0     | (112)-C(111)-C(1M1)        | 120.7(4)  |
| (116)-C(111)-C(1M1)        | 119.2(4)  | (111)-C(112)-C(113)        | 120.0     |
| (111)-C(112)-H(112)        | 120.0     | (113)-C(112)-H(112)        | 120.0     |
| (114)-C(113)-C(112)        | 120.0     | (114)-C(113)-H(113)        | 120.0     |
| (112)-C(113)-H(113)        | 120.0     | (113)-C(114)-C(115)        | 120.0     |
| (113)-C(114)-H(114)        | 120.0     | (115)-C(114)-H(114)        | 120.0     |
| (116)-C(115)-C(114)        | 120.0     | (116)-C(115)-H(115)        | 120.0     |
| (114)-C(115)-H(115)        | 120.0     | (115)-C(116)-C(111)        | 120.0     |
| (115)-C(116)-H(116)        | 120.0     | (111)-C(116)-H(116)        | 120.0     |
| (122)-C(121)-C(126)        | 120.0     | (122)-C(121)-C(1M2)        | 119.3(3)  |
| (126)-C(121)-C(1M2)        | 120.2(3)  | (121)-C(122)-C(123)        | 120.0     |
| (121)-C(122)-H(122)        | 120.0     | (123)-C(122)-H(122)        | 120.0     |
| (124)-C(123)-C(122)        | 119.9     | (124)-C(123)-H(123)        | 120.0     |
| (122)-C(123)-H(123)        | 120.0     | (123)-C(124)-H(125)        | 120.1     |
| (123)-C(124)-H(124)        | 120.0     | (125)-C(124)-H(124)        | 120.0     |
| Bond/Distance | Value  | Bond/Distance | Value |
|---------------|--------|---------------|-------|
| C(124)-C(125)-C(126) | 120.0  | C(124)-C(125)-H(125) | 120.0 |
| C(126)-C(125)-H(125) | 120.0  | N(011)-C(126)-C(125) | 121.7(3) |
| N(011)-C(126)-C(121) | 118.2(3) | C(125)-C(126)-C(121) | 120.0 |
| C(136)-C(131)-C(132) | 120.0  | C(136)-C(131)-C(1M3) | 117.7(4) |
| C(132)-C(131)-C(1M3) | 122.3(4) | C(133)-C(132)-C(131) | 120.0 |
| C(133)-C(132)-H(132) | 120.0  | C(131)-C(132)-H(132) | 120.0 |
| C(132)-C(133)-C(134) | 120.0  | C(132)-C(133)-H(133) | 120.0 |
| C(134)-C(133)-H(133) | 120.0  | C(135)-C(134)-C(133) | 120.0 |
| C(135)-C(134)-H(134) | 120.0  | C(133)-C(134)-H(134) | 120.0 |
| C(134)-C(135)-C(136) | 120.0  | C(134)-C(135)-H(135) | 120.0 |
| C(136)-C(135)-H(135) | 120.0  | C(131)-C(136)-C(135) | 120.0 |
| C(131)-C(136)-H(136) | 120.0  | C(135)-C(136)-H(136) | 120.0 |
| C(142)-C(141)-C(146) | 120.0  | C(142)-C(141)-C(1M4) | 120.6(5) |
| C(146)-C(141)-C(1M4) | 119.3(5) | C(143)-C(142)-C(141) | 120.0 |
| C(143)-C(142)-H(14C) | 120.0  | C(141)-C(142)-H(14C) | 120.0 |
| C(144)-C(143)-C(142) | 120.0  | C(144)-C(143)-H(14D) | 120.0 |
| C(142)-C(143)-H(14D) | 120.0  | C(143)-C(144)-C(145) | 120.0 |
| C(143)-C(144)-H(14E) | 120.0  | C(145)-C(144)-H(14E) | 120.0 |
| C(146)-C(145)-C(144) | 120.0  | C(146)-C(145)-H(14F) | 120.0 |
| C(144)-C(145)-H(14F) | 120.0  | C(145)-C(146)-C(141) | 120.0 |
| C(145)-C(146)-H(14G) | 120.0  | C(141)-C(146)-H(14G) | 120.0 |
| C(12A)-N(1A)-Zn(1) | 122.6(11) | C(12A)-N(1A)-H(1A1) | 106.7 |
| Zn(1)-N(1A)-H(1A1) | 106.7  | C(12A)-N(1A)-H(1A2) | 106.7 |
| Zn(1)-N(1A)-H(1A2) | 106.7  | H(1A1)-N(1A)-H(1A2) | 106.6 |
| C(12A)-C(11A)-H(11A) | 109.5  | C(12A)-C(11A)-H(11B) | 109.5 |
| H(11A)-C(11A)-H(11B) | 109.5  | C(12A)-C(11A)-H(11C) | 109.5 |
| H(11A)-C(11A)-H(11C) | 109.5  | H(11B)-C(11A)-H(11C) | 109.5 |
| C(11A)-C(12A)-N(1A) | 113.7(17) | C(11A)-C(12A)-C(13A) | 118.7(15) |
| N(1A)-C(12A)-C(13A) | 106.4(14) | C(11A)-C(12A)-H(12A) | 105.7 |
| N(1A)-C(12A)-H(12A) | 105.7  | C(13A)-C(12A)-H(12A) | 105.7 |
| C(14A)-C(13A)-C(18A) | 120.0  | C(14A)-C(13A)-C(12A) | 112.5(11) |
| C(18A)-C(13A)-C(12A) | 126.7(11) | C(15A)-C(14A)-C(13A) | 120.0 |
| C(15A)-C(14A)-H(14A) | 120.0  | C(13A)-C(14A)-H(14A) | 120.0 |
| C(16A)-C(15A)-C(14A) | 120.0  | C(16A)-C(15A)-H(15A) | 120.0 |
| C(14A)-C(15A)-H(15A) | 120.0  | C(15A)-C(16A)-C(17A) | 120.0 |
| Bond/Angle/Angle | Value | Bond/Angle/Angle | Value |
|------------------|-------|------------------|-------|
| C(15A)-C(16A)-H(16A) | 120.0 | C(17A)-C(16A)-H(16A) | 120.0 |
| C(18A)-C(17A)-C(16A) | 120.0 | C(18A)-C(17A)-H(17A) | 120.0 |
| C(16A)-C(17A)-H(17A) | 120.0 | C(17A)-C(18A)-C(13A) | 120.0 |
| C(17A)-C(18A)-H(18A) | 120.0 | C(13A)-C(18A)-H(18A) | 120.0 |
| C(12B)-N(1B)-Zn(1) | 147(2) | C(12B)-N(1B)-H(1B9) | 100.1 |
| Zn(1)-N(1B)-H(1B9) | 100.1 | C(12B)-N(1B)-H(1BX) | 100.1 |
| H(1B9)-N(1B)-H(1BX) | 104.2 | N(1B)-C(12B)-C(13B) | 128(3) |
| N(1B)-C(12B)-C(11B) | 105(2) | N(1B)-C(12B)-H(12B) | 103.7 |
| C(12B)-C(11B)-H(11D) | 109.5 | C(12B)-C(11B)-H(11E) | 109.5 |
| H(11D)-C(11B)-H(11E) | 109.5 | C(12B)-C(11B)-H(11F) | 109.5 |
| C(12B)-C(11B)-H(11F) | 109.5 | H(11D)-C(11B)-H(11F) | 109.5 |
| N(1B)-C(12B)-C(13B) | 128(3) | N(1B)-C(12B)-C(11B) | 111(3) |
| C(13B)-C(12B)-C(11B) | 111(3) | C(13B)-C(12B)-H(12B) | 103.7 |
| C(13B)-C(12B)-H(12B) | 103.7 | C(13B)-C(12B)-H(12B) | 103.7 |
| C(14B)-C(13B)-C(18B) | 120.0 | C(14B)-C(13B)-C(12B) | 138(2) |
| C(14B)-C(13B)-C(12B) | 138(2) | C(14B)-C(13B)-C(12B) | 138(2) |
| C(18B)-C(13B)-C(12B) | 102(2) | C(18B)-C(13B)-C(12B) | 102(2) |
| C(13B)-C(14B)-H(14B) | 120.0 | C(13B)-C(14B)-H(14B) | 120.0 |
| C(13B)-C(14B)-H(14B) | 120.0 | C(13B)-C(14B)-H(14B) | 120.0 |
| C(16B)-C(15B)-C(14B) | 120.0 | C(16B)-C(15B)-C(14B) | 120.0 |
| C(16B)-C(15B)-C(14B) | 120.0 | C(16B)-C(15B)-C(14B) | 120.0 |
| C(14B)-C(15B)-H(15B) | 120.0 | C(14B)-C(15B)-H(15B) | 120.0 |
| C(14B)-C(15B)-H(15B) | 120.0 | C(14B)-C(15B)-H(15B) | 120.0 |
| C(17B)-C(16B)-H(16B) | 120.0 | C(17B)-C(16B)-H(16B) | 120.0 |
| C(17B)-C(16B)-H(16B) | 120.0 | C(17B)-C(16B)-H(16B) | 120.0 |
| C(16B)-C(17B)-C(18B) | 120.0 | C(16B)-C(17B)-C(18B) | 120.0 |
| C(16B)-C(17B)-H(17B) | 120.0 | C(16B)-C(17B)-H(17B) | 120.0 |
| C(18B)-C(17B)-H(17B) | 120.0 | C(18B)-C(17B)-H(17B) | 120.0 |
| C(17B)-C(18B)-H(18B) | 120.0 | C(17B)-C(18B)-H(18B) | 120.0 |
| N(22)-Zn(2)-N(24) | 162.0(3) | N(22)-Zn(2)-N(23) | 89.0(3) |
| N(24)-Zn(2)-N(23) | 89.0(3) | N(22)-Zn(2)-N(21) | 89.0(3) |
| N(24)-Zn(2)-N(21) | 89.0(3) | N(23)-Zn(2)-N(21) | 164.0(3) |
| N(22)-Zn(2)-N(2) | 95.8(3) | N(24)-Zn(2)-N(2) | 102.2(3) |
| N(23)-Zn(2)-N(2) | 105.8(2) | N(21)-Zn(2)-N(2) | 93.8(3) |
| C(2A1)-N(21)-C(2A2) | 107.9(7) | C(2A1)-N(21)-Zn(2) | 126.5(6) |
| C(2A2)-N(21)-Zn(2) | 124.4(6) | C(2A3)-N(22)-C(2A4) | 108.4(8) |
| C(2A3)-N(22)-Zn(2) | 124.1(6) | C(2A4)-N(22)-Zn(2) | 126.3(6) |
| C(2B6)-N(23)-C(2A5) | 107.0(7) | C(2B6)-N(23)-Zn(2) | 126.2(6) |
| C(2A5)-N(23)-Zn(2) | 126.1(6) | C(2A8)-N(24)-C(2A7) | 108.0(7) |
| C(2A8)-N(24)-Zn(2) | 125.8(6) | C(2A7)-N(24)-Zn(2) | 126.1(6) |
| C(2A3)-C(2M1)-C(2A2) | 125.3(8) | C(2A3)-C(2M1)-C(211) | 117.4(8) |
| C(2A2)-C(2M1)-C(211) | 117.3(8) | C(2A4)-C(2M2)-C(2A5) | 125.8(8) |
| Bond                              | Distance  | Bond                              | Distance  |
|----------------------------------|-----------|----------------------------------|-----------|
| C(2A4)-C(2M2)-C(221)            | 116.4(8)  | C(2A5)-C(2M2)-C(221)            | 117.7(8)  |
| C(2B6)-C(2M3)-C(2A7)           | 124.7(8)  | C(2B6)-C(2M3)-C(231)           | 119.0(7)  |
| C(2A7)-C(2M3)-C(231)           | 116.2(7)  | C(2A1)-C(2M4)-C(2A8)           | 123.5(8)  |
| C(2A1)-C(2M4)-C(241)           | 119.8(7)  | C(2A8)-C(2M4)-C(241)           | 116.5(8)  |
| C(2B2)-C(2B1)-C(2A1)           | 105.9(8)  | C(2B2)-C(2B1)-H(2B1)           | 127.1     |
| C(2A1)-C(2B1)-H(2B1)           | 127.1     | N(21)-C(2A2)-C(2M1)           | 125.9(9)  |
| N(21)-C(2A2)-C(2M1)            | 125.9(9)  | N(22)-C(2A3)-C(2M1)           | 125.8(9)  |
| C(2A1)-C(2B1)-H(2B1)           | 127.1     | N(22)-C(2A3)-C(2B1)           | 125.8(9)  |
| N(22)-C(2A3)-C(2M1)            | 127.6(8)  | N(22)-C(2A4)-C(2M2)           | 125.9(8)  |
| C(2M1)-C(2A3)-C(2B3)           | 124.1(9)  | C(2M1)-C(2A4)-C(2B4)           | 126.4     |
| C(2B5)-C(2A6)-H(2A6)           | 126.4     | N(24)-C(2A7)-C(2M3)           | 126.0(8)  |
| N(24)-C(2A7)-C(2M3)            | 126.0(8)  | N(24)-C(2A7)-C(2B7)           | 109.7(8)  |
| C(2M3)-C(2A7)-C(2B7)           | 124.3(8)  | N(24)-C(2B3)-C(2M3)           | 108.5(8)  |
| C(2M3)-C(2A8)-C(2B8)           | 109.9(8)  | C(2M3)-C(2A8)-C(2B7)           | 121.8(8)  |
| N(21)-C(2A1)-C(2M4)            | 126.0(8)  | N(21)-C(2A1)-C(2B1)           | 109.8(8)  |
| C(2M4)-C(2A1)-C(2B1)           | 124.1(8)  | C(2B1)-C(2B2)-C(2A2)           | 108.1(9)  |
| C(2A3)-C(2B3)-H(2B4)           | 126.6     | C(2A2)-C(2B2)-H(2B3)           | 125.9     |
| C(2B3)-C(2B4)-H(2B5)           | 125.8     | C(2B3)-C(2B4)-H(2B5)           | 125.8     |
| C(2A4)-C(2B4)-H(2B5)           | 125.8     | C(2A4)-C(2B4)-H(2B5)           | 125.8     |
| C(2A6)-C(2B5)-C(2A5)           | 107.6(8)  | C(2A6)-C(2B5)-H(2B6)           | 126.2     |
| C(2A5)-C(2B5)-H(2B6)           | 126.2     | N(23)-C(2B6)-C(2M3)           | 126.1(8)  |
| N(23)-C(2B6)-C(2A6)            | 109.2(8)  | C(2M3)-C(2B6)-C(2A6)           | 124.7(8)  |
| C(2B8)-C(2B7)-C(2A7)           | 108.5(8)  | C(2B8)-C(2B7)-H(2B7)           | 125.8     |
| C(2A7)-C(2B7)-H(2B7)           | 125.8     | C(2B7)-C(2B8)-C(2A8)           | 103.9(8)  |
| C(2B7)-C(2B8)-H(2B8)           | 128.1     | C(2A8)-C(2B8)-H(2B8)           | 128.1     |
| C(212)-C(211)-C(216)           | 120.0     | C(212)-C(211)-C(2M1)           | 120.1(5)  |
| C(216)-C(211)-C(2M1)           | 119.8(5)  | C(213)-C(212)-C(211)           | 120.0     |
| C(213)-C(212)-H(212)           | 120.0     | C(211)-C(212)-H(212)           | 120.0     |
| C(212)-C(213)-C(214)           | 120.0     | C(212)-C(213)-H(213)           | 120.0     |
| C(214)-C(213)-H(213)           | 120.0     | C(215)-C(214)-C(213)           | 120.0     |
| C(215)-C(214)-H(214)           | 120.0     | C(213)-C(214)-H(214)           | 120.0     |
| C(214)-C(215)-C(216)           | 120.0     | C(214)-C(215)-H(215)           | 120.0     |
| Bond                              | Angle (°) | Bond                              | Angle (°) |
|-----------------------------------|-----------|-----------------------------------|-----------|
| C(216)-C(215)-H(215)             | 120.0     | C(215)-C(216)-C(211)             | 120.0     |
| C(215)-C(216)-H(216)             | 120.0     | C(211)-C(216)-H(216)             | 120.0     |
| C(226)-C(221)-C(222)             | 116.9(6)  | C(226)-C(221)-C(2M2)             | 122.9(7)  |
| C(222)-C(221)-C(2M2)             | 120.1(7)  | C(221)-C(222)-C(223)             | 121.5(7)  |
| C(221)-C(222)-H(222)             | 119.3     | C(223)-C(222)-H(222)             | 119.3     |
| C(224)-C(223)-C(222)             | 119.6(7)  | C(224)-C(223)-H(223)             | 120.2     |
| C(222)-C(223)-H(223)             | 120.2     | C(225)-C(224)-H(224)             | 120.1     |
| C(225)-C(224)-H(224)             | 120.1     | C(223)-C(224)-H(224)             | 120.1     |
| C(226)-C(225)-H(225)             | 119.2     | C(221)-C(226)-C(225)             | 120.5(7)  |
| C(221)-C(226)-H(226)             | 119.8     | C(225)-C(226)-H(226)             | 119.8     |
| C(232)-C(231)-C(236)             | 117.0(4)  | C(232)-C(231)-C(2M3)             | 121.8(6)  |
| C(236)-C(231)-C(2M3)             | 121.2(6)  | C(233)-C(232)-C(231)             | 120.2(5)  |
| C(233)-C(232)-H(232)             | 119.0     | C(231)-C(232)-H(232)             | 119.0     |
| C(234)-C(233)-C(232)             | 119.5(5)  | C(234)-C(233)-H(233)             | 120.2     |
| C(232)-C(233)-H(233)             | 120.2     | C(233)-C(234)-C(235)             | 121.1(5)  |
| C(233)-C(234)-H(234)             | 119.5     | C(235)-C(234)-H(234)             | 119.5     |
| C(234)-C(235)-C(236)             | 119.2(5)  | C(234)-C(235)-H(235)             | 120.4     |
| C(236)-C(235)-H(235)             | 120.4     | C(235)-C(236)-C(231)             | 121.2(5)  |
| C(235)-C(236)-N(013)             | 121.7(6)  | C(231)-C(236)-N(013)             | 117.1(5)  |
| C(246)-C(241)-C(242)             | 117.2(6)  | C(246)-C(241)-C(2M4)             | 123.2(7)  |
| C(242)-C(241)-C(2M4)             | 119.6(7)  | C(243)-C(242)-C(241)             | 120.2(8)  |
| C(243)-C(242)-H(242)             | 119.9     | C(241)-C(242)-H(242)             | 119.9     |
| C(244)-C(243)-C(242)             | 121.7(8)  | C(244)-C(243)-H(243)             | 119.2     |
| C(242)-C(243)-H(243)             | 119.2     | C(245)-C(244)-C(243)             | 119.0(6)  |
| C(245)-C(244)-H(244)             | 120.5     | C(243)-C(244)-H(244)             | 120.5     |
| C(244)-C(245)-C(246)             | 120.5(8)  | C(244)-C(245)-H(245)             | 119.8     |
| C(246)-C(245)-H(245)             | 119.8     | C(241)-C(246)-C(245)             | 121.5(7)  |
| C(241)-C(246)-H(246)             | 119.3     | C(245)-C(246)-H(246)             | 119.3     |
| C(022)-N(2)-Zn(2)                | 113.2(6)  | C(022)-N(2)-H(2A)                | 108.9     |
| Zn(2)-N(2)-H(2A)                 | 108.9     | C(022)-N(2)-H(2B)                | 108.9     |
| Zn(2)-N(2)-H(2B)                 | 108.9     | H(2A)-N(2)-H(2B)                 | 107.8     |
| C(022)-C(021)-H(02A)             | 109.5     | C(022)-C(021)-H(02B)             | 109.5     |
| H(02A)-C(021)-H(02B)             | 109.5     | C(022)-C(021)-H(02C)             | 109.5     |
| H(02A)-C(021)-H(02C)             | 109.5     | H(02B)-C(021)-H(02C)             | 109.5     |
| Bond                  | Angle (°)  | Bond                  | Angle (°)  |
|-----------------------|------------|-----------------------|------------|
| C(023)-C(022)-C(021)  | 113.5(8)   | C(023)-C(022)-N(2)    | 110.1(7)   |
| C(021)-C(022)-N(2)    | 108.2(8)   | C(023)-C(022)-H(022)  | 108.3      |
| C(021)-C(022)-H(022)  | 108.3      | N(2)-C(022)-H(022)    | 108.3      |
| C(024)-C(023)-C(028)  | 120.0      | C(024)-C(023)-C(022)  | 117.8(5)   |
| C(028)-C(023)-C(022)  | 122.2(5)   | C(023)-C(024)-C(025)  | 120.0      |
| C(023)-C(024)-H(024)  | 120.0      | C(025)-C(024)-H(024)  | 120.0      |
| C(026)-C(025)-C(024)  | 120.0      | C(026)-C(025)-H(025)  | 120.0      |
| C(024)-C(025)-H(025)  | 120.0      | C(025)-C(026)-C(027)  | 120.0      |
| C(025)-C(026)-H(026)  | 120.0      | C(027)-C(026)-H(026)  | 120.0      |
| C(028)-C(027)-C(026)  | 120.0      | C(028)-C(027)-H(027)  | 120.0      |
| C(026)-C(027)-H(027)  | 120.0      | C(027)-C(028)-C(023)  | 120.0      |
| C(027)-C(028)-H(028)  | 120.0      | C(027)-C(028)-H(028)  | 120.0      |
| N(33)-Zn(3)-N(31)     | 158.9(3)   | N(33)-Zn(3)-N(32)     | 88.4(3)    |
| N(31)-Zn(3)-N(32)     | 88.8(3)    | N(33)-Zn(3)-N(34)     | 88.9(3)    |
| N(31)-Zn(3)-N(34)     | 87.9(3)    | N(32)-Zn(3)-N(34)     | 163.5(3)   |
| N(33)-Zn(3)-N(3)      | 102.7(3)   | N(31)-Zn(3)-N(3)      | 98.2(3)    |
| N(32)-Zn(3)-N(3)      | 105.0(3)   | N(34)-Zn(3)-N(3)      | 91.5(3)    |
| C(3A2)-N(31)-C(3A1)   | 105.5(7)   | C(3A2)-N(31)-Zn(3)    | 125.8(6)   |
| C(3A1)-N(31)-Zn(3)    | 128.4(6)   | C(3A4)-N(32)-C(3A3)   | 106.7(7)   |
| C(3A4)-N(32)-Zn(3)    | 126.2(6)   | C(3A3)-N(32)-Zn(3)    | 125.8(6)   |
| C(3A5)-N(33)-C(3A6)   | 104.8(8)   | C(3A5)-N(33)-Zn(3)    | 127.1(6)   |
| C(3A6)-N(33)-Zn(3)    | 126.2(6)   | C(3A7)-N(34)-C(3A8)   | 105.7(8)   |
| C(3A7)-N(34)-Zn(3)    | 126.1(6)   | C(3A8)-N(34)-Zn(3)    | 127.7(6)   |
| C(3A2)-C(3M1)-C(3A3)  | 126.3(8)   | C(3A2)-C(3M1)-C(311)  | 117.0(7)   |
| C(3A3)-C(3M1)-C(311)  | 116.7(7)   | C(3A5)-C(3M2)-C(3A4)  | 124.1(8)   |
| C(3A5)-C(3M2)-C(321)  | 118.1(7)   | C(3A4)-C(3M2)-C(321)  | 117.7(7)   |
| C(3A7)-C(3M3)-C(3A6)  | 127.2(9)   | C(3A7)-C(3M3)-C(31A)  | 115.5(8)   |
| C(3A6)-C(3M3)-C(31A)  | 117.2(8)   | C(3A7)-C(3M3)-C(31B)  | 118.6(8)   |
| C(3A6)-C(3M3)-C(31B)  | 113.6(8)   | C(3A1)-C(3M4)-C(3A8)  | 126.8(8)   |
| C(3A1)-C(3M4)-C(341)  | 116.3(8)   | C(3A8)-C(3M4)-C(341)  | 116.8(7)   |
| N(31)-C(3A1)-C(3M4)   | 123.9(8)   | N(31)-C(3A1)-C(3B1)   | 109.0(8)   |
| C(3M4)-C(3A1)-C(3B1)  | 127.1(8)   | N(31)-C(3A2)-C(3M1)   | 125.7(8)   |
| N(31)-C(3A2)-C(3B2)   | 109.2(7)   | C(3M1)-C(3A2)-C(3B2)  | 125.1(8)   |
| N(32)-C(3A3)-C(3M1)   | 124.2(8)   | N(32)-C(3A3)-C(3B3)   | 109.1(8)   |
| C(3M1)-C(3A3)-C(3B3)  | 126.6(8)   | N(32)-C(3A4)-C(3M2)   | 125.9(8)   |
| Bond                                | Angle (°) | Bond                                | Angle (°) |
|-------------------------------------|-----------|-------------------------------------|-----------|
| N(32)-C(3A4)-C(3B4)                | 109.4(8)  | C(3M2)-C(3A4)-C(3B4)                | 124.7(8)  |
| N(33)-C(3A5)-C(3B5)                | 125.5(8)  | N(33)-C(3A5)-C(3B5)                | 110.5(8)  |
| C(3M2)-C(3A5)-C(3B5)               | 124.0(8)  | C(3B6)-C(3A6)-N(33)                 | 123.5(8)  |
| C(3B6)-C(3A6)-C(3B5)               | 125.9(9)  | N(33)-C(3A6)-C(3M3)                 | 124.5(8)  |
| N(34)-C(3A7)-C(3M3)                | 124.6(8)  | N(34)-C(3A7)-C(3B7)                 | 109.8(8)  |
| C(3M3)-C(3A7)-C(3B7)               | 125.6(9)  | N(34)-C(3A8)-C(3M4)                 | 124.5(8)  |
| N(34)-C(3A8)-C(3B8)                | 108.7(8)  | C(3M4)-C(3A8)-C(3B8)                | 126.8(8)  |
| C(3B2)-C(3B1)-C(3A1)               | 109.8(8)  | C(3B2)-C(3B1)-H(3B1)                | 125.1     |
| C(3A1)-C(3B1)-H(3B1)               | 125.1     | C(3B1)-C(3B2)-C(3A2)                | 106.5(8)  |
| C(3B1)-C(3B2)-H(3B2)               | 126.7     | C(3A2)-C(3B2)-H(3B2)                | 126.7     |
| C(3B4)-C(3B3)-C(3A3)               | 108.0(8)  | C(3B4)-C(3B3)-H(3B3)                | 126.0     |
| C(3A3)-C(3B3)-H(3B3)               | 126.0     | C(3B3)-C(3B4)-C(3A4)                | 106.8(8)  |
| C(3B3)-C(3B4)-H(3B4)               | 126.6     | C(3A4)-C(3B4)-H(3B4)                | 126.6     |
| C(3B6)-C(3B5)-C(3A5)               | 105.6(9)  | C(3B6)-C(3B5)-H(3B5)                | 127.2     |
| C(3A5)-C(3B5)-H(3B5)               | 127.2     | C(3B5)-C(3B6)-C(3A6)                | 108.7(9)  |
| C(3B5)-C(3B6)-H(3B6)               | 125.7     | C(3A6)-C(3B6)-H(3B6)                | 125.7     |
| C(3B8)-C(3B7)-C(3A7)               | 106.8(9)  | C(3B8)-C(3B7)-H(3B7)                | 126.6     |
| C(3A7)-C(3B7)-H(3B7)               | 126.6     | C(3B7)-C(3B8)-C(3A8)                | 108.8(9)  |
| C(3B7)-C(3B8)-H(3B8)               | 125.6     | C(3A8)-C(3B8)-H(3B8)                | 125.6     |
| C(312)-C(311)-C(316)               | 120.0     | C(312)-C(311)-C(3M1)                | 120.0     |
| C(316)-C(311)-C(3M1)               | 120.0     | C(311)-C(312)-C(313)                | 120.0     |
| C(311)-C(312)-H(312)               | 120.0     | C(313)-C(312)-H(312)                | 120.0     |
| C(314)-C(313)-C(312)               | 120.0     | C(314)-C(313)-H(313)                | 120.0     |
| C(312)-C(313)-H(313)               | 120.0     | C(313)-C(314)-C(315)                | 120.0     |
| C(313)-C(314)-H(314)               | 120.0     | C(315)-C(314)-H(314)                | 120.0     |
| C(316)-C(315)-C(314)               | 120.0     | C(316)-C(315)-H(315)                | 120.0     |
| C(314)-C(315)-H(315)               | 120.0     | C(315)-C(316)-C(311)                | 120.0     |
| C(315)-C(316)-N(021)               | 121.8(4)  | C(311)-C(316)-N(021)                | 118.2(4)  |
| C(322)-C(321)-C(326)               | 120.0     | C(322)-C(321)-C(3M2)                | 120.3(5)  |
| C(326)-C(321)-C(3M2)               | 119.6(5)  | C(323)-C(322)-C(321)                | 120.0     |
| C(323)-C(322)-H(32C)               | 120.0     | C(321)-C(322)-H(32C)                | 120.0     |
| C(324)-C(323)-C(322)               | 120.0     | C(324)-C(323)-H(32D)                | 120.0     |
| C(322)-C(323)-H(32D)               | 120.0     | C(323)-C(324)-C(325)                | 120.0     |
| C(323)-C(324)-H(32E)               | 120.0     | C(325)-C(324)-H(32E)                | 120.0     |
| C(326)-C(325)-C(324)               | 120.0     | C(326)-C(325)-H(32F)                | 120.0     |
| Bond                              | Angle (°) |
|----------------------------------|-----------|
| C(324)-C(325)-H(32F)            | 120.0     |
| C(325)-C(326)-H(32G)            | 120.0     |
| C(32A)-C(31A)-C(36A)            | 120.0     |
| C(36A)-C(31A)-C(3M3)            | 117.5(6)  |
| C(31A)-C(32A)-H(32A)            | 120.0     |
| C(34A)-C(33A)-C(32A)            | 120.0     |
| C(32A)-C(33A)-H(33A)            | 120.0     |
| C(33A)-C(34A)-H(34A)            | 120.0     |
| C(36A)-C(35A)-C(34A)            | 120.0     |
| C(34A)-C(35A)-H(35A)            | 120.0     |
| C(35A)-C(36A)-H(36A)            | 120.0     |
| C(32B)-C(31B)-C(36B)            | 120.0     |
| C(36B)-C(31B)-C(3M3)            | 124.5(6)  |
| C(31B)-C(32B)-H(32B)            | 120.0     |
| C(32B)-C(33B)-C(34B)            | 120.0     |
| C(34B)-C(33B)-H(33B)            | 120.0     |
| C(35B)-C(34B)-H(34B)            | 120.0     |
| C(34B)-C(35B)-C(36B)            | 120.0     |
| C(36B)-C(35B)-H(35B)            | 120.0     |
| C(35B)-C(36B)-H(36B)            | 120.0     |
| C(342)-C(341)-C(346)            | 120.0     |
| C(346)-C(341)-C(3M4)            | 119.4(5)  |
| C(341)-C(342)-H(34C)            | 120.0     |
| C(342)-C(343)-C(344)            | 120.0     |
| C(344)-C(343)-H(34D)            | 120.0     |
| C(345)-C(344)-H(34E)            | 120.0     |
| C(344)-C(345)-C(346)            | 120.0     |
| C(346)-C(345)-H(34F)            | 120.0     |
| C(345)-C(346)-H(34G)            | 120.0     |
| C(037)-N(3)-Zn(3)               | 137.2(9)  |
| Zn(3)-N(3)-H(3A)                | 102.8     |
| Zn(3)-N(3)-H(3B)                | 102.8     |
| C(032)-C(031)-C(036)            | 120.0     |
| C(036)-C(031)-C(037)            | 121.9(8)  |
| C(031)-C(032)-H(032)            | 120.0     |

S27
| Bond                          | Distance | Bond                          | Distance |
|-------------------------------|----------|-------------------------------|----------|
| C(032)-C(033)-C(034)         | 120.0    | C(032)-C(033)-H(033)         | 120.0    |
| C(034)-C(033)-H(033)         | 120.0    | C(035)-C(034)-C(033)         | 120.0    |
| C(035)-C(034)-H(034)         | 120.0    | C(033)-C(034)-H(034)         | 120.0    |
| C(034)-C(035)-C(036)         | 120.0    | C(034)-C(035)-H(035)         | 120.0    |
| C(036)-C(035)-H(035)         | 120.0    | C(035)-C(036)-C(031)         | 120.0    |
| C(035)-C(036)-H(036)         | 120.0    | C(031)-C(036)-H(036)         | 120.0    |
| C(038)-C(037)-N(3)           | 118.0(12)| C(038)-C(037)-H(037)         | 108.8    |
| N(3)-C(037)-C(031)           | 102.4(10)| C(038)-C(037)-H(037)         | 108.8    |
| N(3)-C(037)-H(037)           | 108.8    | C(031)-C(037)-H(037)         | 108.8    |
| C(037)-C(038)-H(03A)         | 109.5    | C(037)-C(038)-H(03B)         | 109.5    |
| H(03A)-C(038)-H(03B)         | 109.5    | C(037)-C(038)-H(03C)         | 109.5    |
| H(03A)-C(038)-H(03C)         | 109.5    | H(03B)-C(038)-H(03C)         | 109.5    |
| N(41)-Zn(4)-N(43)            | 159.4(3) | N(41)-Zn(4)-N(42)            | 88.3(3)  |
| N(43)-Zn(4)-N(42)            | 87.8(3)  | N(41)-Zn(4)-N(44)            | 89.4(3)  |
| N(43)-Zn(4)-N(44)            | 87.3(3)  | N(42)-Zn(4)-N(44)            | 160.1(3) |
| N(41)-Zn(4)-N(4)             | 106.3(3) | N(43)-Zn(4)-N(4)             | 94.3(3)  |
| N(42)-Zn(4)-N(4)             | 98.9(3)  | N(44)-Zn(4)-N(4)             | 100.7(3) |
| C(4A2)-N(41)-C(4A1)          | 106.2(7) | C(4A2)-N(41)-Zn(4)           | 127.0(6) |
| C(4A1)-N(41)-Zn(4)           | 125.2(6) | C(4A4)-N(42)-C(4A3)          | 108.2(8) |
| C(4A4)-N(42)-Zn(4)           | 125.8(6) | C(4A3)-N(42)-Zn(4)           | 125.9(6) |
| C(4A5)-N(43)-C(4A6)          | 106.0(7) | C(4A5)-N(43)-Zn(4)           | 124.1(5) |
| C(4A6)-N(43)-Zn(4)           | 128.5(5) | C(4A8)-N(44)-C(4A7)          | 106.8(7) |
| C(4A8)-N(44)-Zn(4)           | 124.4(6) | C(4A7)-N(44)-Zn(4)           | 128.7(5) |
| C(4A2)-C(4M1)-C(4A3)         | 121.8(8) | C(4A2)-C(4M1)-C(411)         | 118.7(8) |
| C(4A3)-C(4M1)-C(411)         | 119.2(8) | C(4A5)-C(4M2)-C(4A4)         | 124.2(8) |
| C(4A5)-C(4M2)-C(421)         | 119.2(8) | C(4A4)-C(4M2)-C(421)         | 116.5(8) |
| C(4A7)-C(4M3)-C(4A6)         | 127.1(8) | C(4A7)-C(4M3)-C(431)         | 118.3(6) |
| C(4A6)-C(4M3)-C(431)         | 114.6(7) | C(4A8)-C(4M4)-C(4A1)         | 124.9(8) |
| C(4A8)-C(4M4)-C(441)         | 119.2(7) | C(4A1)-C(4M4)-C(441)         | 115.8(7) |
| N(41)-C(4A1)-C(4M4)          | 125.3(8) | N(41)-C(4A1)-C(4B1)          | 109.8(8) |
| C(4M4)-C(4A1)-C(4B1)         | 124.8(8) | N(41)-C(4A2)-C(4M1)          | 126.7(8) |
| N(41)-C(4A2)-C(4B2)          | 109.2(8) | C(4M1)-C(4A2)-C(4B2)         | 124.1(9) |
| N(42)-C(4A3)-C(4M1)          | 128.3(8) | N(42)-C(4A3)-C(4B3)          | 109.1(9) |
| C(4M1)-C(4A3)-C(4B3)         | 122.6(9) | N(42)-C(4A4)-C(4M2)          | 126.3(8) |
| N(42)-C(4A4)-C(4B4)          | 109.3(8) | C(4M2)-C(4A4)-C(4B4)         | 124.4(8) |
| Bond                                | Angle (°) | Bond                                | Angle (°) |
|-------------------------------------|-----------|-------------------------------------|-----------|
| N(43)-C(4A5)-C(4M2)                | 126.7(8)  | N(43)-C(4A5)-C(4B5)                | 109.3(7)  |
| C(4M2)-C(4A5)-C(4B5)               | 123.5(8)  | N(43)-C(4A6)-C(4M3)                | 126.9(8)  |
| N(43)-C(4A6)-C(4M3)                | 123.1(7)  | C(4B6)-C(4A6)-C(4M3)               | 126.9(8)  |
| N(44)-C(4A7)-C(4M3)                | 124.0(7)  | N(44)-C(4A7)-C(4B7)                | 109.1(7)  |
| C(4M3)-C(4A7)-C(4B7)               | 126.8(8)  | N(44)-C(4A8)-C(4M4)                | 126.7(8)  |
| N(44)-C(4A8)-C(4B8)                | 108.4(8)  | C(4M4)-C(4A8)-C(4B8)               | 124.8(8)  |
| C(4B2)-C(4B1)-C(4A1)               | 106.9(8)  | C(4B2)-C(4B1)-H(4B1)               | 126.5     |
| C(4A1)-C(4B1)-H(4B1)               | 126.5     | C(4B1)-C(4B2)-C(4A2)               | 107.8(9)  |
| C(4B1)-C(4B2)-H(4B2)               | 126.1     | C(4A2)-C(4B2)-H(4B2)               | 126.1     |
| C(4B4)-C(4B3)-C(4A3)               | 106.4(9)  | C(4B4)-C(4B3)-H(4B3)               | 126.8     |
| C(4A3)-C(4B3)-H(4B3)               | 126.8     | C(4B3)-C(4B4)-C(4A4)               | 107.0(9)  |
| C(4B3)-C(4B4)-H(4B4)               | 126.5     | C(4A4)-C(4B4)-H(4B4)               | 126.5     |
| C(4B6)-C(4B5)-C(4A5)               | 105.9(7)  | C(4B6)-C(4B5)-H(4B5)               | 127.0     |
| C(4A5)-C(4B5)-H(4B5)               | 127.0     | C(4B5)-C(4B6)-C(4A6)               | 108.8(8)  |
| C(4B5)-C(4B6)-H(4B6)               | 125.6     | C(4A6)-C(4B6)-H(4B6)               | 125.6     |
| C(4B8)-C(4B7)-C(4A7)               | 108.1(8)  | C(4B8)-C(4B7)-H(4B7)               | 125.9     |
| C(4A7)-C(4B7)-H(4B7)               | 125.9     | C(4B7)-C(4B8)-C(4A8)               | 107.4(8)  |
| C(4B7)-C(4B8)-H(4B8)               | 126.3     | C(4A8)-C(4B8)-H(4B8)               | 126.3     |
| C(412)-C(411)-C(416)               | 120.0     | C(412)-C(411)-C(4M1)               | 119.8(4)  |
| C(416)-C(411)-C(4M1)               | 120.2(4)  | C(411)-C(412)-C(413)               | 120.0     |
| C(411)-C(412)-H(412)               | 120.0     | C(413)-C(412)-H(412)               | 120.0     |
| C(414)-C(413)-C(412)               | 120.0     | C(414)-C(413)-H(413)               | 120.0     |
| C(412)-C(413)-H(413)               | 120.0     | C(413)-C(414)-C(415)               | 120.0     |
| C(413)-C(414)-H(414)               | 120.0     | C(415)-C(414)-H(414)               | 120.0     |
| C(416)-C(415)-C(414)               | 120.0     | C(416)-C(415)-H(415)               | 120.0     |
| C(414)-C(415)-H(415)               | 120.0     | C(415)-C(416)-C(411)               | 120.0     |
| C(415)-C(416)-H(416)               | 120.0     | C(411)-C(416)-H(416)               | 120.0     |
| C(422)-C(421)-C(426)               | 116.4(5)  | C(422)-C(421)-C(4M2)               | 121.4(6)  |
| C(426)-C(421)-C(4M2)               | 122.2(6)  | C(423)-C(422)-C(421)               | 122.3(6)  |
| C(423)-C(422)-H(422)               | 118.8     | C(421)-C(422)-H(422)               | 118.8     |
| C(424)-C(423)-C(422)               | 120.1(6)  | C(424)-C(423)-H(423)               | 119.9     |
| C(422)-C(423)-H(423)               | 119.9     | C(425)-C(424)-C(423)               | 119.8(6)  |
| C(425)-C(424)-H(424)               | 120.1     | C(423)-C(424)-H(424)               | 120.1     |
| C(424)-C(425)-C(426)               | 120.6(6)  | C(424)-C(425)-H(425)               | 119.7     |
| C(426)-C(425)-H(425)               | 119.7     | C(421)-C(426)-C(425)               | 120.8(6)  |
C(421)-C(426)-H(426)  119.6  
C(432)-C(431)-C(436)  120.0  
C(436)-C(431)-C(4M3)  120.6(3)  
C(433)-C(432)-H(432)  120.0  
C(431)-C(432)-H(432)  120.0  
C(433)-C(432)-H(432)  120.0  
C(434)-C(433)-C(432)  120.0  
C(434)-C(433)-H(433)  120.0  
C(433)-C(434)-H(433)  120.0  
C(435)-C(434)-C(435)  120.0  
C(435)-C(434)-H(435)  120.0  
C(436)-C(435)-C(436)  120.0  
C(435)-C(436)-C(431)  120.0  
C(446)-C(441)-C(442)  120.0  
C(442)-C(441)-C(4M4)  121.5(4)  
N(023)-C(442)-C(441)  115.9(4)  
C(445)-C(444)-C(443)  120.0  
C(445)-C(444)-H(444)  120.0  
C(446)-C(445)-H(445)  120.0  
C(445)-C(446)-H(446)  120.0  
C(047)-N(4)-Zn(4)  125.4(5)  
Zn(4)-N(4)-H(41)  106.0  
Zn(4)-N(4)-H(42)  106.0  
N(4)-C(047)-C(048)  110.6(9)  
C(048)-C(047)-C(048)  110.5(7)  
C(048)-C(047)-H(047)  107.4  
C(047)-C(048)-H(048)  109.5  
H(048)-C(048)-H(048)  109.5  
C(042)-C(041)-C(046)  120.0  
C(046)-C(041)-C(047)  118.9(5)  
C(041)-C(042)-H(042)  120.0  
C(042)-C(043)-C(042)  120.0  
C(042)-C(043)-H(043)  120.0  
C(043)-C(044)-H(044)  120.0  
C(046)-C(045)-C(044)  120.0  
C(046)-C(045)-H(045)  120.0
| Bond                        | Bond Angle | Bond Angle |
|-----------------------------|------------|------------|
| C(044)-C(045)-H(045)       | 120.0      | C(045)-C(046)-C(041) | 120.0 |
| C(045)-C(046)-H(046)       | 120.0      | C(041)-C(046)-H(046) | 120.0 |
| C(18)-N(011)-C(126)        | 134.2(7)   | C(18)-N(011)-H(011) | 112.9 |
| C(126)-N(011)-H(011)       | 112.9      | C(15)-N(012)-H(01D) | 120.0 |
| C(15)-N(012)-H(01E)        | 120.0      | H(01D)-N(012)-H(01E) | 120.0 |
| C(17)-N(013)-C(236)        | 127.4(7)   | C(17)-N(013)-H(013) | 116.3 |
| C(236)-N(013)-H(013)       | 116.3      | C(12)-C(11)-C(16) | 120.0 |
| C(12)-C(11)-C(17)          | 117.2(5)   | C(16)-C(11)-C(17) | 122.7(5) |
| C(13)-C(12)-C(11)          | 120.0      | C(13)-C(12)-H(12) | 120.0 |
| C(11)-C(12)-H(12)          | 120.0      | C(14)-C(13)-C(12) | 120.0 |
| C(14)-C(13)-C(18)          | 117.9(5)   | C(12)-C(13)-C(18) | 122.0(5) |
| C(15)-C(14)-C(13)          | 120.0      | C(15)-C(14)-H(14) | 120.0 |
| C(13)-C(14)-H(14)          | 120.0      | C(14)-C(15)-C(16) | 120.0 |
| C(14)-C(15)-N(012)         | 121.3(5)   | C(16)-C(15)-N(012) | 118.7(5) |
| C(15)-C(16)-C(11)          | 120.0      | C(15)-C(16)-H(16) | 120.0 |
| C(11)-C(16)-H(16)          | 120.0      | O(012)-C(17)-N(013) | 126.0(9) |
| O(012)-C(17)-C(11)         | 121.3(7)   | N(013)-C(17)-C(11) | 112.7(8) |
| O(011)-C(18)-N(011)        | 121.8(9)   | O(011)-C(18)-C(13) | 120.7(9) |
| N(011)-C(18)-C(13)         | 117.5(7)   | C(27)-N(021)-C(316) | 131.3(8) |
| C(27)-N(021)-H(021)        | 114.4      | C(316)-N(021)-H(021) | 114.4 |
| C(21)-N(022)-H(02D)        | 120.0      | C(21)-N(022)-H(02E) | 120.0 |
| H(02D)-N(022)-H(02E)       | 120.0      | C(28)-N(023)-C(442) | 130.1(7) |
| C(28)-N(023)-H(023)        | 115.0      | C(442)-N(023)-H(023) | 115.0 |
| N(022)-C(21)-C(22)         | 120.6(5)   | N(022)-C(21)-C(26) | 119.4(5) |
| C(22)-C(21)-C(26)          | 120.0      | C(23)-C(22)-C(21) | 120.0 |
| C(23)-C(22)-H(22)          | 120.0      | C(21)-C(22)-H(22) | 120.0 |
| C(22)-C(23)-C(24)          | 120.0      | C(22)-C(23)-C(27) | 121.3(5) |
| C(24)-C(23)-C(27)          | 118.7(5)   | C(25)-C(24)-C(23) | 120.0 |
| C(25)-C(24)-H(24A)         | 120.0      | C(23)-C(24)-H(24A) | 120.0 |
| C(24)-C(25)-C(26)          | 120.0      | C(24)-C(25)-C(28) | 123.6(5) |
| C(26)-C(25)-C(28)          | 116.4(5)   | C(25)-C(26)-C(21) | 120.0 |
| C(25)-C(26)-H(26)          | 120.0      | C(21)-C(26)-H(26) | 120.0 |
| O(021)-C(27)-N(021)        | 121.1(9)   | O(021)-C(27)-C(23) | 120.6(8) |
| N(021)-C(27)-C(23)         | 118.3(8)   | O(022)-C(28)-N(023) | 123.0(8) |
| O(022)-C(28)-C(25)         | 122.9(8)   | N(023)-C(28)-C(25) | 114.0(7) |
Fig. S1. FT IR spectrum of [Zn₂-AmBis].

Fig. S2. FT IR spectrum of [Zn₂-AmBis](R-1-PEA)₂.
Fig. S3. FT IR spectrum of [ZnNi-AmBis].

Fig. S4. FT IR spectrum of [ZnNi-AmBis](1-PEA).
Fig. S5. $^1$H NMR spectrum of [Zn2-AmBis] in DMSO (4.1×10$^{-3}$ M).
Fig. S6. $^{13}$C NMR spectrum of [Zn$_2$-AmBis] in DMSO (8.3×10$^{-3}$ M).
Fig. S7. $^1$H NMR spectrum of [ZnNi-AmBis] in DMSO ($4.4 \times 10^{-3}$ M).
Fig. S8. $^{13}$C NMR spectrum of [ZnNi-AmBis] in DMSO ($8.1 \times 10^{-3}$ M).
Fig. S9. UV-Vis spectrum of [Zn$_2$-AmBis] (1.58×10$^{-6}$M).

Fig. S10. UV-Vis spectrum of [ZnNi-AmBis] (2.12×10$^{-6}$M).
Fig. S11: DTA-TG diagram of [ZnNi-AmBis](1-PEA)·2C7H16. The lost of 17.2% weight is caused by the lost of two heptane and one 1-phenylethylamine molecules (calculated lost is 17.4%).

Fig. S12: DTA-TG diagram of [Zn2-AmBis](R-1-PEA)2·C7H16. The lost of 17.6% weight is caused by the lost of one heptane and two 1-phenylethylamine molecules (calculated lost is 18.2%).
Relative energies of DFT-optimized conformer A·R-1-PEA and conformer B·R-1-PEA.

Figure S13. Relative energies of DFT-optimized conformer A·R-1-PEA and conformer B·R-1-PEA.
Relative energies of DFT-optimized conformer A·(R-1-PEA)$_2$ and conformer B·(R-1-PEA)$_2$.

Figure S14. Relative energies of DFT-optimized conformer (A·R-1-PEA)$_2$ and conformer B·(R-1-PEA)$_2$. 
Cartesian coordinates for Geometry Optimized Conformers for all the calculated structures.

Conformer A

\[ \Delta = -8004.81373445 \text{ a.u.} \]

| Atoms | x               | y               | z               |
|-------|-----------------|-----------------|-----------------|
| Zn    | 3.88033200      | 0.17018300      | -0.36843000     |
| N     | 4.04179900      | -1.86280500     | -0.76112600     |
| N     | 3.24714800      | 0.41991600      | -2.30909100     |
| N     | 4.52937500      | 2.13455500      | -0.38599700     |
| N     | 5.05769000      | -0.14651700     | 1.29607600      |
| C     | 4.54406600      | -2.81801800     | 0.07589300      |
| C     | 3.61051900      | -2.52272800     | -1.87962900     |
| C     | 2.83802400      | -0.55409300     | -3.17414300     |
| C     | 3.05291200      | 1.61269000      | -2.94781500     |
| C     | 4.20366000      | 3.08790200      | -1.30754000     |
| C     | 5.12165800      | 2.78308000      | 0.65655300      |
| C     | 5.50640900      | 0.82692500      | 2.14299000      |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 4.657072| 6.495841| -5.182297 |
| C    | 2.528893| 6.252083| -4.963462 |
| H    | 2.283713| 7.106037| -5.588150 |
| C    | 1.515065| 5.486481| -4.393715 |
| H    | 0.473320| 5.739531| -4.569955 |
| C    | 1.831290| 4.393103| -3.594559 |
| H    | 1.041013| 3.801457| -3.143160 |
| C    | 6.104043| 3.102033|  2.908474 |
| C    | 5.380180| 3.371241|  4.073158 |
| H    | 4.407253| 2.907062|  4.209651 |
| C    | 5.895127| 4.220718|  5.048001 |
| H    | 5.320420| 4.421053|  5.947589 |
| C    | 7.141697| 4.814376|  4.869382 |
| H    | 7.542564| 5.479956|  5.628148 |
| C    | 7.871815| 4.550372|  3.713494 |
| H    | 8.847003| 5.006293|  3.569250 |
| C    | 7.357321| 3.698136|  2.741581 |
| H    | 7.925641| 3.487980|  1.839932 |
| N    | -4.207529| 2.314973|  0.120413 |
| N    | -6.378926| 0.454572|  0.239873 |
| N    | -4.559092| -1.673451| -0.411854 |
| N    | -2.498547| 0.239514|  0.880892 |
| C    | -3.037543| 3.026491|  0.088323 |
| C    | -5.175634| 1.751240|  0.568091 |
| C    | -7.071958| 1.580410|  0.590947 |
| N    | -7.251308| -0.595067|  0.374370 |
| C    | -5.655203| -2.435921| -0.094416 |
| C    | -3.558610| -2.550498| -0.748826 |
| C    | -1.817901| -0.875620| -1.307053 |
| C    | -1.612245| 1.280224|  0.953346 |
| C    | -3.266136| 4.364072|  0.584123 |
| H    | -2.511202| 5.129040|  0.692484 |
| C    | -4.590760| 4.465388|  0.845634 |
| H    | -5.129315| 5.330637|  1.204112 |
| C    | -8.435176| 1.236845|  0.915930 |
| H    | -9.193232| 1.936753|  1.236571 |
| C    | -8.544682| -0.107271|  0.785583 |
| H    | -9.410474| -0.724960|  0.976972 |
| C    | -5.321743| -3.830881| -0.187942 |
| H    | -5.998978| -4.648402|  0.013943 |
| C    | -4.021660| -3.902538| -0.574221 |
| H    | -3.431524| -4.797250| -0.734850 |
| C    | -0.499681| -0.497649| -1.752696 |
| H    | 0.252454| -1.161882| -2.150961 |
| C    | -0.372525| 0.833672|  -1.536376 |
| H    | 0.499322| 1.444974|  -1.728081 |
|  | X  | Y  | Z   |
|---|---|---|----|
| C | -1.81747200  | 2.55783700  | -0.40981900|
| C | -6.52606500  | 2.86211400  | 0.74517400 |
| C | -6.92428500  | -1.94560100 | 0.24073200 |
| C | -2.27605600  | -2.19210000 | -1.19638100|
| C | -0.61583800  | 3.43051400  | -0.25283900|
| C | -0.48814100  | 4.64757300  | -0.92219800|
| H | -1.27413900  | 4.95361400  | -1.60667900|
| C | 0.62892800   | 5.45358200  | -0.72909300|
| H | 0.71724400   | 6.39320400  | -1.26465600|
| C | 1.64496000   | 5.03792100  | 0.12287200 |
| H | 2.52607200   | 5.65135900  | 0.26708800 |
| C | 1.54462800   | 3.82503900  | 0.79591900 |
| H | 2.33664400   | 3.48974400  | 1.45726400 |
| C | 0.41174000   | 3.03963200  | 0.62522400 |
| C | -7.44929200  | 3.95547800  | 1.17611000|
| C | -8.40500400  | 4.46013400  | 0.29009700 |
| H | -8.46455200  | 4.05082600  | -0.71443200|
| C | -9.27262200  | 5.47297200  | 0.68735600 |
| H | -10.00944500 | 5.85585400  | -0.01257100|
| C | -9.19319800  | 5.99602100  | 1.97510700 |
| H | -9.87012900  | 6.78649900  | 2.28492700|
| C | -8.24525200  | 5.49851900  | 2.86528500|
| H | -8.18013800  | 5.89908000  | 3.87258400|
| C | -7.38094000  | 4.48266000  | 2.46872700|
| H | -6.64582500  | 4.08793200  | 3.16449200|
| C | -8.00696700  | -2.94724100 | 0.48570600 |
| C | -9.00375500  | -3.15741900 | -0.47017400|
| H | -8.98166000  | -2.58654700 | -1.39414600|
| C | -10.01224900 | -4.08974200 | -0.24519500|
| H | -10.77964000 | -4.24538500 | -0.99770500|
| C | -10.03473100 | -4.82303000 | 0.93803300 |
| H | -10.82019600 | -5.55217600 | 1.11270100|
| C | -9.04583500  | -4.61850900 | 1.89665900 |
| H | -9.05995300  | -5.18309300 | 2.82423200 |
| C | -8.03881900  | -3.68462600 | 1.67206500|
| H | -7.26886400  | -3.51936200 | 2.42057000|
| C | -1.30743900  | -3.29626600 | -1.45855200|
| C | -1.54681600  | -4.27692900 | -2.42723600|
| H | -2.43412900  | -4.20517700 | -3.05035600|
| C | -0.65956500  | -5.33667000 | -2.59131800|
| H | -0.85085900  | -6.08577800 | -3.35378100|
| C | 0.47654800   | -5.42952300 | -1.79225900|
| H | 1.17054400   | -6.25411100 | -1.92373300|
| C | 0.72635400   | -4.45490500 | -0.83102200|
| H | 1.60950200   | -4.51652000 | -0.20393100|
| C | -0.15472100  | -3.39316700 | -0.67209500|
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 0.04409700 | -2.63592900 | 0.07818200 |
| C       | 0.82238600 | -2.68818000 | 2.82106800 |
| C       | 1.31625500 | -1.48898600 | 2.30334700 |
| H       | 2.37901900 | -1.27033700 | 2.26450000 |
| C       | 0.42257300 | -0.52106300 | 1.85578800 |
| C       | -0.95097600 | -0.75271600 | 1.90908400 |
| H       | -1.65569800 | -0.03865800 | 1.49162800 |
| C       | -1.45431400 | -1.95872200 | 2.41719200 |
| C       | -0.54694100 | -2.91122600 | 2.89847200 |
| H       | -0.89981800 | -3.85141300 | 3.31252200 |
| C       | 1.75519700 | -3.77552600 | 3.29153100 |
| C       | 0.99489000 | 0.72699500 | 1.26134400 |
| N       | 2.92333000 | -3.77913400 | 2.58157400 |
| H       | 2.96605800 | -3.11460300 | 1.82290500 |
| N       | -2.82212400 | -2.18281200 | 2.46275000 |
| H       | -3.09061700 | -3.15690100 | 2.49346100 |
| H       | -3.35889800 | -1.69081900 | 1.75848300 |
| N       | 0.23780500 | 1.84345100 | 1.37993400 |
| H       | -0.66291600 | 1.73246400 | 1.82320700 |
| O       | 1.46915900 | -4.55413800 | 4.18490500 |
| O       | 2.09342900 | 0.74204200 | 0.70533800 |
| Zn      | -4.44642100 | 0.35699000 | -0.34610200 |
Conformer B

$\Delta = -8004.81373443 \text{ a.u.}$

| Atoms | x          | y          | z          |
|-------|------------|------------|------------|
| Zn    | -3.88105700 | 0.17016000 | -0.36857000|
| N     | -4.04190100 | -1.86278300| -0.76124900|
| N     | -3.24749300 | 0.42018900 | -2.30907500|
| N     | -4.52999900 | 2.13458500 | -0.38601600|
| N     | -5.05838100 | -0.14671900| 1.29583200 |
| C     | -4.54417800 | -2.81810900| 0.07561900 |
| C     | -3.61071300 | -2.52252600| -1.87987800|
| C     | -2.83836100 | -0.55373400| -3.17420800|
| C     | -3.05302200 | 1.61302200 | -2.94758200|
| C     | -4.20388400 | 3.08808000 | -1.30727100|
| C     | -5.12231000 | 2.78298400 | 0.65658600 |
| C     | -5.50739300 | 0.82662300 | 2.14268600 |
| C     | -5.29665400 | -1.33870400| 1.91632300 |
| C     | -4.43611300 | -4.12347400| -0.53428400|
| H     | -4.77411300 | -5.04756600| -0.08574500|
| C     | -3.86389100 | -3.93875600| -1.74808900|
| H     | -3.62244300 | -4.68408800| -2.49238700|
| C     | -2.31926500 | 0.04212000 | -4.38101400|
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| H   | -1.93896300 | -0.50196400 | -5.23362900 |
| C   | -2.45289800  | 1.38310700  | -4.24238800  |
| H   | -2.20867500  | 2.14604300  | -4.96672900  |
| C   | -4.64723100  | 4.38407100  | -0.84619300  |
| H   | -4.51810700  | 5.31743400  | -1.37468000  |
| C   | -5.20801900  | 4.19728900  | 0.37296600   |
| H   | -5.63344300  | 4.94406700  | 1.02822400   |
| C   | -6.02097700  | 0.22639500  | 3.35557500   |
| H   | -6.45099100  | 0.76717100  | 4.18671000   |
| C   | -5.88029400  | -1.11363900 | 3.21985100   |
| H   | -6.16489700  | -1.88366000 | 3.91789400   |
| C   | -5.07015400  | -2.60163400 | 1.35742500   |
| C   | -3.00571300  | -1.93430600 | -2.99250100  |
| C   | -3.48409300  | 2.86807700  | -2.49106200  |
| C   | -5.54739000  | 2.19473500  | 1.85938200   |
| C   | -5.28267400  | -3.80346700 | 2.22687100   |
| C   | -4.16141700  | -4.37727100 | 2.86256500   |
| C   | -4.30762700  | -5.46587100 | 3.72026800   |
| H   | -3.43312400  | -5.87846800 | 4.20694000   |
| C   | -5.57847000  | -5.98974800 | 3.93993100   |
| H   | -5.69190700  | -6.83618400 | 4.61082500   |
| C   | -6.69334700  | -5.44571900 | 3.31077400   |
| H   | -7.67954000  | -5.86539000 | 3.48276600   |
| C   | -6.53890000  | -4.35508300 | 2.45761900   |
| H   | -7.40079800  | -3.91100300 | 1.96805500   |
| C   | -2.58970600  | -2.82836400 | -4.11704700  |
| C   | -1.24518500  | -3.12641200 | -4.33974400  |
| H   | -0.48888000  | -2.73359200 | -3.66788600  |
| C   | -0.86638000  | -3.94036100 | -5.40295800  |
| H   | 0.18555900   | -4.16298100 | -5.55625300  |
| C   | -1.82853200  | -4.47048300 | -6.25663100  |
| H   | -1.53281600  | -5.10574700 | -7.08652800  |
| C   | -3.17427500  | -4.18398600 | -6.03929500  |
| H   | -3.93256900  | -4.59166800 | -6.70150100  |
| C   | -3.55085000  | -3.36686000 | -4.97834200  |
| H   | -4.59908500  | -3.13669000 | -4.80973700  |
| C   | -3.16306300  | 4.04686800  | -3.34802800  |
| C   | -4.17290600  | 4.81619000  | -3.93470900  |
| H   | -5.21117300  | 4.54529300  | -3.76581600  |
| C   | -3.85839700  | 5.91281200  | -4.73173000  |
| H   | -4.65606200  | 6.49697900  | -5.18130800  |
| C   | -2.52796000  | 6.25271500  | -4.96232400  |
| H   | -2.28253600  | 7.10674200  | -5.58681800  |
| C   | -1.51435400  | 5.48677600  | -4.39263500  |
| H   | -0.47253700  | 5.73964100  | -4.56871400  |
| C   | -1.83088700  | 4.39330600  | -3.59373200  |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | -1.04078000| 3.80140100 | -3.14233400|
| C       | -6.10515300| 3.10164800 | 2.90832500 |
| C       | -5.38147100| 3.37063200 | 4.07317500 |
| H       | -4.40860200| 2.90635900 | 4.20976400 |
| C       | -5.89652100| 4.22001200 | 5.04804700 |
| H       | -5.32196100| 4.42017600 | 5.94777600 |
| C       | -7.14301900| 4.81378600 | 4.86929300 |
| H       | -7.54396700| 5.47928900 | 5.62808200 |
| C       | -7.87295100| 4.55000800 | 3.71323700 |
| H       | -8.84808300| 5.00601800 | 3.56896600 |
| C       | -7.35834700| 3.69787600 | 2.74129800 |
| H       | -7.92651600| 3.48789900 | 1.83950300 |
| N       | 4.20797400 | 2.31494900 | 0.12059500 |
| N       | 6.37940600 | 0.45458500 | 0.23964000 |
| N       | 4.55944900 | -1.67345900| -0.41179200|
| N       | 2.49892200 | 0.23949600 | -0.88037000|
| C       | 3.03797500 | 3.02644800 | 0.08860100 |
| C       | 5.17606800 | 3.17507100 | 0.56384500 |
| C       | 7.07242300 | 1.58038100 | 0.59087000 |
| C       | 7.25178300 | -0.59506400| 0.37405300 |
| C       | 5.65551500 | -2.43593100| -0.09418500|
| C       | 3.55886700 | -2.55049400| -0.74840900|
| C       | 1.81835500 | -0.87555800| -1.30711500|
| C       | 1.61271000 | 1.28028300 | -0.95327300|
| C       | 3.26655400 | 4.36396400 | 0.58456100 |
| H       | 2.51164000 | 5.12893400 | 0.69304400 |
| C       | 4.59118000 | 4.46528200 | 0.84606300 |
| H       | 5.12969300 | 5.33051000 | 1.20465200 |
| C       | 8.43564100 | 1.23680500 | 0.91577900 |
| H       | 9.19370300 | 1.93665900 | 1.23652300 |
| C       | 8.54516100 | -0.10730000| 0.78527700 |
| H       | 9.41097500 | -0.72499700| 0.97660800 |
| C       | 5.32189300 | -3.83089200| -0.18721900|
| H       | 5.99903300 | -4.64844400| 0.01485400 |
| C       | 4.02177000 | -3.90252900| -0.57334900|
| H       | 3.43150000 | -4.79269700| -0.73281700|
| C       | 0.50032800 | -0.49745800| -1.75323800|
| H       | -0.25169800| -1.16153500| -2.15199600|
| C       | 0.37313100 | 0.83383400 | -1.53670300|
| H       | -0.49867700| 1.44515400 | -1.72855900|
| C       | 1.81790100 | 2.55783600 | -0.40959600|
| C       | 6.52651200 | 2.86206100 | 0.74530500 |
| C       | 6.92468900 | -1.94561500| 0.24060500 |
| C       | 2.27638000 | -2.19207200| -1.19619500|
| C       | 0.61632900 | 3.43057400 | -0.25256600|
| C       | 0.48888600 | 4.64786800 | -0.92153500|
|  | X     | Y     | Z     |
|---|-------|-------|-------|
| H | 1.275 | 4.954 | -1.606 |
| C | -0.628 | 5.454 | -0.728 |
| H | -0.716 | 6.394 | -1.264 |
| C | -1.644 | 5.039 | 0.123 |
| H | -2.525 | 5.652 | 0.267 |
| C | -1.544 | 3.824 | 0.796 |
| H | -2.336 | 4.461 | 0.291 |
| C | -0.411 | 3.039 | 0.625 |
| C | 7.449 | 3.955 | 1.176 |
| C | 8.405 | 4.461 | 0.291 |
| H | 8.465 | 4.051 | -0.714 |
| C | 9.273 | 5.473 | 0.688 |
| H | 10.009 | 5.856 | -0.012 |
| C | 9.193 | 5.996 | 1.976 |
| H | 9.870 | 6.786 | 2.286 |
| C | 8.245 | 5.498 | 2.866 |
| H | 8.180 | 5.898 | 3.873 |
| C | 7.381 | 4.482 | 2.469 |
| H | 6.646 | 4.086 | 3.167 |
| C | 8.007 | -2.947 | 0.486 |
| C | 9.004 | -3.157 | -0.470 |
| H | 8.982 | -2.586 | -1.394 |
| C | 10.012 | -4.095 | -0.245 |
| H | 10.780 | -4.245 | -0.998 |
| C | 10.035 | -4.823 | 0.938 |
| H | 10.821 | -5.552 | 1.112 |
| C | 9.046 | -4.619 | 1.896 |
| H | 9.960 | -5.184 | 2.823 |
| C | 8.039 | -3.685 | 1.672 |
| H | 7.269 | -3.519 | 2.420 |
| C | 1.308 | -3.296 | -1.459 |
| C | 1.547 | -4.277 | -2.427 |
| H | 2.436 | -4.205 | -3.049 |
| C | 0.661 | -5.337 | -2.590 |
| H | 0.852 | -6.087 | -3.353 |
| C | -0.476 | -5.429 | -1.792 |
| H | -1.169 | -6.254 | -1.923 |
| C | -0.726 | -4.455 | -0.831 |
| H | -1.609 | -4.516 | -0.204 |
| C | 0.154 | -3.393 | -0.672 |
| H | -0.044 | -2.635 | 0.078 |
| C | -0.823 | -2.689 | 2.820 |
| C | -1.316 | -1.489 | 2.303 |
| H | -2.379 | -1.271 | 2.264 |
| C | -0.423 | -0.521 | 1.855 |
| C | 0.951 | -0.753 | 1.908 |
|  | x         | y         | z         |
|---|-----------|-----------|-----------|
| H | 1.65527600| -0.03889500| 1.49107500|
| C | 1.45400500| -1.95888300| 2.41672500|
| C | 0.54672600| -2.91149800| 2.89796400|
| H | 0.89969600| -3.85159800| 3.31211700|
| C | -1.75543700| -3.77590500| 3.29094900|
| C | -0.99532100| 0.72667400| 1.26078500|
| N | -2.92323600| -3.78021200| 2.58041300|
| H | -2.96581900| -3.11610500| 1.82136200|
| N | 2.82184800| -2.18269800| 2.46242200|
| H | 3.09060100| -3.15669500| 2.49336000|
| H | 3.35860400| -1.69064600| 1.75820900|
| N | -0.23785500| 1.84285500| 1.37918200|
| H | 0.66278400| 1.73154800| 1.82252600|
| O | -1.46969300| -4.55391700| 4.18492900|
| O | -2.09398700| 0.74200200| 0.70505100|
| Zn| 4.44684300| 0.35700000| -0.34601700|
Conformer A·R-1-PEA

$\Delta = -8370.95801458 \text{ a.u.}$

| Atoms | x       | y       | z       |
|-------|---------|---------|---------|
| Zn    | 5.11305300 | 0.27463100 | 0.73522100 |
| N     | 3.83223400 | -0.44073500 | -0.77922000 |
| H     | 4.21873400 | -0.10206700 | -1.65879200 |
| H     | 2.97527700 | 0.09427500  | -0.60541200 |
| C     | 3.49008300 | -1.86748100 | -0.89364800 |
| H     | 3.35673200 | -2.23569300 | 0.13188600  |
| C     | 4.65847300 | -2.62297400 | -1.52617000 |
| H     | 4.45735800 | -3.69768100 | -1.53940700 |
| H     | 5.58167300 | -2.44408600 | -0.96911000 |
| H     | 4.80138800 | -2.29506000 | -2.56320400 |
| C     | 2.19909900 | -2.12380800 | -1.65974300 |
| C     | 1.77639000 | -1.28713200 | -2.69308400 |
| H     | 2.34327500 | -0.39344400 | -2.93814000 |
| C     | 0.60602300 | -1.55841500 | -3.39645600 |
| H     | 0.28498300 | -0.88360900 | -4.18490400 |
| C     | -0.15607700 | -2.67840800 | -3.08300100 |
| H     | -1.07623500 | -2.88467700 | -3.62104200 |
| C     | 0.25739500 | -3.52108900 | -2.05437100 |
|   |   |   |   |
|---|---|---|---|
| H | -0.34766300 | -4.38088000 | -1.78179800 |
| C | 1.42323500 | -3.24244200 | -1.34941500 |
| H | 1.72681900 | -3.89217600 | -0.53113100 |
| N | 5.92683800 | -1.38803100 | 1.65432100 |
| N | 6.87853000 | 0.46879700 | -0.33035500 |
| N | 4.74560100 | 2.30648800 | 0.36326100 |
| N | 3.78969700 | 0.43616300 | 2.32504800 |
| C | 5.29909100 | -2.15892700 | 2.58931700 |
| C | 6.99178400 | -2.11268200 | 1.20069300 |
| C | 7.86585400 | -0.46289800 | -0.44240900 |
| C | 7.21463500 | 1.49830600 | -1.16417600 |
| C | 5.31533100 | 3.02590100 | -0.64631400 |
| C | 3.65694200 | 3.01421000 | 0.78346400 |
| C | 2.91400700 | 1.45726900 | 2.57304200 |
| C | 3.55947300 | -0.51335000 | 3.27282900 |
| C | 5.96428300 | -3.44003400 | 2.69915600 |
| H | 5.66358900 | -4.24512000 | 3.34996900 |
| C | 7.01480100 | -3.40814800 | 1.84603800 |
| H | 7.39828000 | -4.18730500 | 1.65880400 |
| C | 8.87517000 | -0.00059900 | -1.36562100 |
| H | 9.78765000 | -0.52978000 | -1.61338100 |
| C | 8.47411200 | 1.21199800 | -1.81414500 |
| H | 8.98798200 | 1.86986200 | -2.50055500 |
| C | 4.54668200 | 4.22194500 | -0.89446900 |
| H | 4.76540500 | 4.96389100 | -1.64939500 |
| C | 3.51851600 | 4.21462600 | -0.00994000 |
| H | 2.72967500 | 4.94660700 | 0.08557300 |
| C | 2.12158200 | 1.14541100 | 3.74249100 |
| H | 1.37983900 | 1.79324000 | 4.18704800 |
| C | 2.52020700 | -0.07518000 | 4.17490000 |
| H | 2.16425000 | -0.62604600 | 5.03448700 |
| C | 4.20248300 | -1.76351000 | 3.36579400 |
| C | 7.91807700 | -1.69020900 | 0.23962600 |
| C | 6.47741700 | 2.67293300 | -1.35398300 |
| C | 2.79255100 | 2.63777500 | 1.82840200 |
| C | 3.68631300 | -2.73313900 | 4.38061600 |
| C | 2.42332300 | -3.34159000 | 4.22907700 |
| C | 1.97118800 | -4.26428300 | 5.17625500 |
| H | 1.00276100 | -4.72468100 | 5.04333200 |
| C | 2.76553000 | -4.57094800 | 6.27531800 |
| H | 2.40090800 | -5.28813700 | 7.00481000 |
| C | 4.00962300 | -3.97414900 | 6.44343700 |
| H | 4.62604800 | -4.21312600 | 7.30445500 |
| C | 4.45841600 | -3.06238100 | 5.49470700 |
| H | 5.42688000 | -2.58400200 | 5.60760400 |
| C | 9.05055400 | -2.60980100 | -0.07941500 |
|   |   |   |   |   |
|---|---|---|---|---|
| C | -4.76808600 | 4.18504300 | 0.94142600 |
| H | -4.97119300 | 4.94856400 | 1.67843500 |
| C | -8.48522600 | 1.64398100 | 3.94755000 |
| H | -8.86768200 | -0.17243200 | 1.82299400 |
| C | -8.88095200 | -0.79494600 | 2.55513000 |
| H | -9.65078800 | -1.76998800 | 3.47515000 |
| C | -6.28038300 | -0.19806600 | -0.07463000 |
| H | -9.65078800 | -3.37230200 | -2.72645200 |
| C | -2.39258400 | 1.00957900 | -3.63096000 |
| H | -5.46053000 | 1.58649600 | -3.97580100 |
| C | -3.10750900 | 2.55730400 | -1.79122100 |
| H | -6.79562000 | 6.15506000 | -3.35614500 |
| C | -8.12981200 | -1.76221700 | -3.39375000 |
| H | -4.66300700 | 3.32172100 | -1.98856500 |
| C | -1.83626500 | 4.53435400 | -2.66855400 |
| H | -2.70039000 | 4.94269800 | -3.08234300 |
| C | -0.57514300 | 5.21066100 | -2.82198100 |
| H | -0.54533900 | 6.15506000 | -3.35614500 |
| C | 0.58748200 | 4.66578000 | -2.28745500 |
| H | 1.53772700 | 5.17979400 | -2.39940700 |
| C | 0.56116800 | 3.45851600 | -1.59756100 |
| H | 1.46384000 | 3.04050500 | -1.17471900 |
| C | -0.65047300 | 2.78633300 | -1.44656600 |
| C | -7.13916600 | 3.60705800 | 2.54762500 |
| H | -8.33310400 | 4.31177400 | 2.37024300 |
| H | -8.90980500 | 4.15522700 | 1.46308100 |
| C | -8.77876300 | 5.20470300 | 3.33919900 |
| H | -9.70813600 | 5.74539500 | 3.18704100 |
| C | -8.03452400 | 4.40484800 | 4.49861900 |
| H | -8.38090900 | 6.10238700 | 5.25521700 |
| C | -6.84384700 | 4.70741200 | 4.68421800 |
| H | -6.26172400 | 4.85495400 | 5.58893700 |
| C | -6.39956500 | 3.81266000 | 3.71543100 |
| H | -5.47348900 | 3.26378800 | 3.86165900 |
| C | -9.18203600 | 2.27260600 | 0.46025700 |
| C | -10.53386400 | 2.45965100 | 0.22258800 |
| H | -10.81377000 | -1.54231300 | -0.28747000 |
| C | -11.51114200 | -3.36212600 | 0.20365400 |
| H | -12.55789900 | -3.14765700 | 0.43698700 |
| C | -11.14861100 | -4.53820000 | 1.28174000 |
| H | -11.91106700 | -5.24247000 | 1.60040900 |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | -9.804271 | -4.808356 | 1.522931 |
| H       | -9.514704 | -5.721825 | 2.033671 |
| C       | -8.827681 | -3.905817 | 1.114289 |
| H       | -7.778213 | -4.111966 | 1.304383 |
| C       | -4.177385 | -2.750996 | -4.402372|
| H       | -4.369883 | -2.536541 | -5.768918|
| C       | -4.889452 | -1.641239 | -6.098641|
| H       | -3.901681 | -3.459611 | -6.699477|
| C       | -4.059344 | -3.283478 | -7.759320|
| H       | -3.236114 | -4.605686 | -6.273025|
| C       | -2.869360 | -5.324519 | -6.999489|
| C       | -3.041128 | -4.826237 | -4.911929|
| H       | -2.515960 | -5.714257 | -4.573032|
| C       | -3.510423 | -3.905469 | -3.979747|
| H       | -3.344047 | -4.060537 | -2.916048|
| C       | -0.249470 | -2.424756 | 1.713039 |
| C       | 0.289637  | -1.243068 | 1.201050 |
| H       | 1.172362  | -0.769955 | 1.623451 |
| C       | -0.364353 | -0.609587 | 0.144722 |
| C       | -1.517494 | -1.157913 | -0.411993|
| H       | -1.977444 | -0.707563 | -1.287564|
| C       | -2.060144 | -2.340703 | 0.099124 |
| C       | -1.418994 | -2.955312 | 1.174950 |
| H       | -1.821257 | -3.862346 | 1.616084 |
| C       | 0.324716  | -3.175066 | 2.887038 |
| C       | 0.184019  | 0.684970  | -0.371375|
| N       | 1.659984  | -2.980966 | 3.101322 |
| H       | 2.135958  | -2.366928 | 2.456044 |
| N       | -3.177415 | -2.918797 | -0.496390|
| H       | -3.716493 | -3.525526 | 0.106308 |
| H       | -3.777607 | -2.278898 | -1.001065|
| N       | -0.774958 | 1.561913  | -0.768233|
| H       | -1.725917 | 1.266040  | -0.606413|
| O       | -0.381515 | -3.909527 | 3.561865 |
| O       | 1.381580  | 0.944549  | -0.393658|
| Zn      | -5.710092 | 0.470264  | -0.978274|
Conformer B·R-1-PEA

$\Delta = -8370.95716188 \text{ a.u.}$

| Atoms | x        | y        | z        |
|-------|----------|----------|----------|
| Zn    | -4.99943900 | 0.21450400 | 0.70097100 |
| O     | -1.33543300 | 0.66676600 | -1.06147400 |
| O     | 0.55521700  | -4.26552500 | 2.82316900  |
| N     | 0.79995700  | 1.45855800 | -1.10690200 |
| H     | 1.74403300  | 1.21105500 | -0.84924000 |
| N     | -1.54281000 | -3.52600500 | 2.29818400  |
| H     | -2.05999800 | -2.95457300 | 1.64386500  |
| N     | 3.42279400  | -2.90218800 | -1.05686100 |
| H     | 3.94715600  | -3.54959800 | -0.48435600 |
| H     | 4.02559800  | -2.19133400 | -1.45170000 |
| N     | -5.89320500 | -1.48313700 | 1.43974300  |
| N     | -6.85817100 | 0.79106600  | -0.03308500 |
| N     | -4.44897600 | 2.26377000  | 0.63326500  |
| N     | -3.50462300 | -0.00913700 | 2.11322200  |
| N     | 4.94704600  | 2.37483500  | -0.15973500 |
| N     | 7.04365100  | 0.60899600  | 0.68371500  |
| N     | 6.51232800  | -1.09614000 | -1.56997100 |
| N     | 4.45986200  | 0.69803700  | -2.43820900 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 3.15087400| 2.69368900| -1.81241900|
| C       | -6.30121300| 3.07510100| -0.77476700|
| C       | -5.02817000| 3.18710500| -0.77476700|
| C       | 6.35480800 | 2.67608100| 1.83901200 |
| C       | 4.36819300 | -0.21166000| -3.46218600|
| C       | -4.13475700| 4.30639700| -0.37865400|
| H       | -4.33150300| 5.17171500| -0.99572300|
| C       | 3.88357100 | 3.06272600| -0.67987600|
| C       | -3.31111300| -1.10803700| 2.89639400 |
| C       | 6.16174000 | -1.75175600| -2.72214500|
| C       | -4.05626200| -2.29933700| 2.85003200 |
| C       | 5.15658800 | -1.35400400| -3.61140400|
| C       | 8.16526700 | -1.53399300| 0.20492800 |
| C       | -2.32795300| 2.14815200| 1.87304900 |
| C       | 7.12126700 | 1.50914900| 1.71127800 |
| C       | 3.46101500 | 1.60995900| -2.64457200|
| C       | -8.99899100| 0.69972800| -0.87031600|
| H       | -9.98440600| 0.30981200| -1.08176800|
| C       | -3.02428600| 4.04794600| 0.35618600 |
| H       | -2.13288000| 4.65302800| 0.43552300 |
| C       | -2.52353600| 0.88485200| 2.44694800 |
| C       | -7.15773500| 1.97253500| -0.65105200|
| C       | 5.34982300 | 3.06950600| 0.95075600 |
| C       | -3.23597700| 2.76980500| 0.99640800 |
| C       | -5.25633000| -2.46106800| 2.14702200 |
| C       | -2.19367600| -0.89339500| 3.78544700 |
| H       | -1.84851700| -1.59212200| 4.53459800 |
| C       | 3.28334200 | 0.14712000| -4.34202800|
| H       | 2.99818900 | -0.40024700| -5.22906000|
| C       | -8.04909600| -1.34378500| 0.25845200 |
| C       | -1.70574100| 0.33816300| 3.50755200 |
| H       | -0.88635400| 0.84700400| 3.99373600 |
| C       | 6.95096400 | -2.94660400| -2.86967400|
| H       | 6.87275700 | -3.64491800| -3.69082200|
| C       | -7.94992200| -0.01031600| -0.17289600|
| C       | 7.93318500 | -0.39178400| 0.97658000 |
| C       | -0.13541000| 0.49385300| -0.89236300|
| C       | -7.06443600| -2.02254000| 0.98746900 |
| C       | 3.61351300 | 4.23378800| 0.11809200 |
| H       | 2.81763500 | 4.94153200| -0.06257300|
| C       | -0.18827100| -3.57187700| 2.14381600 |
| C       | 4.53881200 | 4.25422600| 1.10649200 |
| H       | 4.66113360 | 4.99616100| 1.88222600 |
| C       | 1.65337700 | -1.25353600| -0.95431200|
| H       | 2.13100800 | -0.71201000| -1.76743600|
| C       | 2.71776600 | 1.26879800| -3.83223100|
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 4.85419000 | -2.25457700| -4.76718300|
| C       | 5.45879400 | -2.05305400| -6.00905000|
| H       | 6.16509300 | -1.23664800| -6.13120100|
| C       | 5.16021100 | -2.89121000| -7.08008500|
| H       | 5.63614600 | -2.72733900| -8.04234900|
| C       | 4.25281900 | -3.93444600| -6.91746500|
| H       | 4.01714000 | -4.58632900| -7.75345000|
| C       | 3.64831700 | -4.14043300| -5.67989000|
| H       | 2.93878900 | -4.95210300| -5.54864200|
| C       | 3.94751000 | -3.30612100| -4.60709000|
| H       | 3.48257000 | -3.46310800| -3.63639500|
| C       | 11.10391800| -4.33268500| 1.60725200 |
| H       | 11.84622300| -5.04226500| 1.96003000 |
| C       | 8.79739900 | -3.72516600| 1.25145000 |
| H       | 7.73869500 | -3.95514800| 1.33074400 |
| N       | -4.10183400| 0.00068700 | -1.21670300|
| H       | -3.10694700| 0.17648700 | -1.05356000|
| H       | -4.46399500| 0.86069100 | -1.62986300|
| C       | -4.21712000| -1.07751000| -2.22480300|
| H       | -3.75756000| -0.72375600| -3.15921600|
| C       | -5.68523600| -1.37463100| -2.50986700|
| H       | -5.77261300| -2.12217100| -3.30418700|
| H       | -6.19623100| -1.75014900| -1.62042500|
| H       | -6.20583000| -0.46327600| -2.82570600|
| C       | -3.41510500| -2.28363900| -1.77335500|
| C       | -2.12321100| -2.47184100| -2.26652200|
| H       | -1.71095600| -1.75102000| -2.96832900|
| C       | -1.35052100| -3.55446600| -1.85789300|
| H       | -0.33940900| -3.67111500| -2.23726500|
| C       | -1.86414000| -4.46602500| -0.94154300|
| H       | -1.25991900| -5.30393800| -0.60641500|
| C       | -3.15060000| -4.28552400| -0.43794300|
| H       | -3.55624400| -4.98236600| 0.29042000 |
| C       | -3.91995900| -3.20207000| -0.85043200|
| H       | -4.91959700| -3.08007400| -0.44836900|
| Zn      | 5.77989400 | 0.67630300 | -0.89612500|

S61
Conformer A·(R-1-PEA)$_2$

$\Delta = -8737.13207946$ a.u.

| Atoms | x                  | y                  | z                  |
|-------|--------------------|--------------------|--------------------|
| Zn    | -5.35875500        | -0.08760300        | -0.83471600        |
| N     | -3.89288700        | -0.26815900        | -2.28711300        |
| N     | -5.10933300        | 1.95865900         | -0.92508500        |
| N     | -7.27783400        | 0.24952900         | -0.11367200        |
| N     | -6.02708300        | -1.99600000        | -1.44202400        |
| C     | -2.98478700        | 2.02847600         | -2.15527900        |
| C     | -7.05333600        | 2.64400500         | 0.42040500         |
| C     | -8.13612100        | -2.06065700        | -0.17079900        |
| C     | -4.16463700        | -2.64281700        | -2.91350000        |
| C     | -3.51149800        | -1.40100700        | -2.95689200        |
| C     | -2.98748700        | 0.70014100         | -2.61237800        |
| C     | -4.00197700        | 2.60779400         | -1.39028900        |
| C     | -5.84581400        | 2.88633200         | -0.24194500        |
| C     | -7.70731900        | 1.40210900         | 0.47238500         |
| C     | -8.18055000        | -0.71804000        | 0.22816700         |
| C     | -7.14882700        | -2.62962200        | -0.99055300        |
| C     | -5.36261500        | -2.89343300        | -2.22252700        |
| C     | -2.31261400        | -1.13146000        | -3.71995300        |
H  -8.00852200  -4.10813000  1.59920900
C  -3.53889700  -3.78356800  -3.64858200
C  -3.34722700  -3.73956000  -5.03367500
H  -3.69998300  -2.87505100  -5.58813400
C  -2.71415900  -4.78439800  -6.77437900
H  -2.15107000  -3.53889700  -5.69532000
C  -3.10998900  -4.89054000  -2.95676500
H  -3.28128800  -6.58813400  -1.88595600
N  -4.57999200  -1.06947700  0.94038200
H  -5.35341100  -1.73489800  0.97789700
H  -3.78848600  -1.63808700  0.61905800
C  -3.15039300  0.31406100  2.44986700
C  -2.11310500  0.04403400  3.34202300
H  -2.09577500  -0.89271600  3.89411300
C  -1.07662600  0.95840200  3.52127000
H  -0.27015200  0.72856400  4.21213700
C  -1.06001000  2.14841700  2.80345100
H  -0.25212200  2.85987500  2.93980900
C  -2.08721500  2.42022800  1.90232300
H  -2.09169900  3.34453900  1.33162600
C  -3.12620700  1.51273500  1.73346300
H  -3.93457600  1.74411500  1.05132300
C  -4.33018200  -0.63059400  2.33604200
H  -4.09465700  -1.51888800  2.93971200
C  -5.60207100  0.00609600  2.89629800
H  -5.84713600  0.92261300  2.35196000
H  -5.46083700  0.25698600  3.95133200
H  -6.45742900  -0.67451000  2.81157900
Zn  5.42634400  0.45936300  0.54185900
N  -6.25425500  -0.83266900  1.92228900
N  -7.08160900  0.11911700  -0.66599000
N  -5.15529700  2.26347300  -0.49277800
N  -4.27469600  1.26364800  2.06095000
C  -8.08430600  -1.76480500  0.56440100
C  -6.67585900  1.84124000  -2.38299200
C  -3.44240100  3.29368600  0.94594800
C  -4.63902900  -0.49617500  3.74683700
C  -5.67836000  -1.18356400  3.10896100
C  -7.25143300  -1.73809100  1.68887300
C  -8.00590600  -0.86938500  -0.51674700
C  -7.36098300  0.74147300  -1.85087800
C  -5.64772100  2.54564000  -1.73356900
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| C    | 4.21357200   | 3.21082500   | -0.22422100  |
| C    | 3.49126100   | 2.38391800   | 2.00418300   |
| C    | 4.03240000   | 0.67801700   | 3.26508300   |
| C    | 6.31479300   | -2.37213100  | 3.63495500   |
| H    | 6.04566100   | -2.86987300  | 4.55576500   |
| C    | 7.29094200   | -2.71090400  | 2.76057100   |
| H    | 7.97492600   | -3.54526200  | 2.82215600   |
| C    | 8.91798400   | -0.86675800  | -1.63909600  |
| H    | 9.76551900   | -1.52642500  | -1.75877900  |
| C    | 8.51574000   | 0.12703400   | -2.46709600  |
| H    | 9.97492600   | 0.44103400   | -3.39534900  |
| C    | 4.09264400   | 4.11959700   | -1.34015700  |
| H    | 4.21357200   | 4.95963000   | -1.39223000  |
| C    | 3.72667500   | 2.50699100   | 3.22456700   |
| H    | 2.05775700   | 3.32237600   | 3.46205400   |
| C    | 3.05248500   | 1.44466200   | 4.00232000   |
| H    | 2.69701000   | 1.21207300   | 4.99695400   |
| C    | 9.10953400   | -2.84757000  | 0.48429200   |
| C    | 10.19369400  | -2.88342300  | 1.36588800   |
| H    | 10.28957100  | -2.10418400  | 2.11664700   |
| C    | 11.14107300  | -3.89968400  | 1.28393400   |
| H    | 11.97855700  | -3.91533000  | 1.97543200   |
| C    | 11.01891400  | -4.89373700  | 0.31684900   |
| H    | 11.75983500  | -5.68506400  | 0.25206900   |
| C    | 9.94328500   | -4.86706100  | -0.56693700  |
| H    | 9.83945200   | -5.64029000  | -1.32266600  |
| C    | 8.99585000   | -3.85218300  | -0.48199300  |
| H    | 8.15481900   | -3.83072000  | -1.16963700  |
| C    | 7.10368500   | 2.32888700   | -3.72876200  |
| C    | 7.74090000   | 3.56556700   | -3.86923100  |
| H    | 7.92558300   | 4.16673500   | -2.98363600  |
| C    | 8.13924600   | 4.02051500   | -5.12206900  |
| H    | 8.63573700   | 4.98207000   | -5.21387800  |
| C    | 7.90648700   | 3.24384000   | -6.25415500  |
| H    | 8.21704700   | 3.59889300   | -7.23242700  |
| C    | 7.27633900   | 2.00918300   | -6.12531800  |
| H    | 7.09002700   | 1.39839200   | -7.00392000  |
| C    | 6.87838500   | 1.55573400   | -4.87136700  |
| H    | 6.38674600   | 0.59239400   | -4.76887400  |
| C    | 2.50023200   | 4.44846800   | 1.05606200   |
| C    | 2.99033700   | 5.74032400   | 1.26740200   |
| H    | 4.06115500   | 5.88844700   | 1.37342600   |
| C    | 2.12163100   | 6.82495400   | 1.33956700   |
| H    | 2.51849300   | 7.82209300   | 1.50648200   |
|   | C         | H         | C         |
|---|-----------|-----------|-----------|
| 1 | -0.88201000 | -1.15344600 | -0.19405100 |
| 2 | -1.36077500 | -0.91444300 | -1.13879700 |
| 3 | 0.15296300  | -0.36270600 | 0.28735400  |
| 4 | 0.81826800  | -0.69587700 | 1.46636300  |
| 5 | 1.58738000  | -0.02644400 | 1.84340200  |
| 6 | 0.38356600  | -1.80781400 | 2.18699100  |
| 7 | -0.65951600 | -2.59798500 | 1.70922600  |
| 8 | -0.99677800 | -3.43373500 | 2.31556700  |
| 9 | 0.54604700  | 0.86187200  | -0.47651200 |
|10 | 0.87323800  | -2.12636500 | 3.57229700  |
Conformer B·(R-1-PEA)$_2$

$\Delta = -8737.13127748$ a.u.

| Atoms | x        | y        | z        |
|-------|----------|----------|----------|
| Zn    | -5.37519300 | 0.45845300 | 0.36820300 |
| N     | -6.94515800 | 0.62337300 | -0.98782800 |
| N     | -6.23561700 | -1.27815700 | 1.05778600 |
| N     | -4.37813300 | 0.61488000 | 2.17514400 |
| N     | -5.12374500 | 2.54887000 | 0.16017300 |
| C     | -7.90218300 | -1.62795400 | -0.72426800 |
| C     | -4.85311600 | -1.63661200 | 3.06365500 |
| C     | -3.53161100 | 2.92396100 | 1.99708000 |
| C     | -6.48143400 | 2.88046400 | -1.86590000 |
| C     | -7.15931800 | 1.65361200 | -1.85958600 |
| C     | -7.81433900 | -0.36542100 | -1.33319600 |
| C     | -7.14644100 | -2.04033600 | 0.37926600 |
| C     | -5.77048800 | -2.04611600 | 2.08672400 |
| C     | -4.24972600 | -0.36797400 | 3.11066900 |
| C     | -3.64766900 | 1.67962800 | 2.62439100 |
| C     | -4.21022200 | 3.30519000 | 0.82813700 |
| C     | -5.52858400 | 3.28507800 | -0.91537400 |
| C     | -8.22227900 | 1.30705000 | -2.77765200 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| H       | -8.61705900  | 1.95152800   | -3.55012900  |
| C       | -8.63097700  | 0.05816500   | -2.44814300  |
| H       | -9.42228400  | -0.52169500  | -2.90147000  |
| C       | -7.22288700  | -3.35629100  | 0.97454700   |
| H       | -7.84891700  | -4.16518600  | 0.62579100   |
| C       | -6.37383000  | -3.35968800  | 2.03023200   |
| H       | -6.17129900  | -4.17061700  | 2.71531700   |
| C       | -3.40618600  | 0.08589900   | 4.19433800   |
| H       | -3.16130300  | -0.48607700  | 5.07854000   |
| C       | -3.03259700  | 1.35230900   | 3.89217600   |
| H       | -2.42554400  | 2.02173500   | 4.48492600   |
| C       | -4.01469100  | 4.56418300   | 0.14594300   |
| H       | -3.33583300  | 5.34677900   | 0.45536000   |
| C       | -4.82544400  | 4.54752800   | -0.94213800  |
| H       | -4.94084400  | 5.31601500   | -1.69331200  |
| C       | -8.87787400  | -2.60447000  | -1.29574200  |
| H       | -10.03222700 | -2.95160900  | -0.58806300  |
| C       | -10.21237200 | -2.49723800  | 0.38200200   |
| H       | -10.94080000 | -3.86337800  | -1.11639700  |
| C       | -11.83496000 | -4.12042900  | -0.55587800  |
| H       | -10.70735100 | -4.44036100  | -2.36180000  |
| C       | -11.41603000 | -5.15268000  | -2.77399800  |
| H       | -9.56130200  | -4.10011000  | -3.07570600  |
| C       | -9.37138700  | -4.54892400  | -4.04636300  |
| H       | -8.65351900  | -3.18805400  | -2.54599100  |
| C       | -7.75708600  | -2.92223600  | -3.09966900  |
| C       | -4.56443800  | -2.59260800  | 4.17971900   |
| C       | -5.57719000  | -2.91267600  | 5.08535700   |
| H       | -6.54978600  | -2.44827700  | 4.95184600   |
| C       | -5.35907200  | -3.79429300  | 6.13760400   |
| H       | -6.16130700  | -4.02400800  | 6.83184300   |
| C       | -4.10328800  | -4.37037400  | 6.29140000   |
| H       | -3.91534700  | -5.06341600  | 7.10617000   |
| C       | -3.07330600  | -4.07465100  | 5.40604200   |
| H       | -2.09441700  | -4.51800800  | 5.52200200   |
| C       | -3.29619300  | -3.18387000  | 4.35208600   |
| C       | -2.64913400  | 3.94276200   | 2.63852000   |
| C       | -1.26381200  | 3.76469300   | 2.69625000   |
| H       | -0.82771100  | 2.88266900   | 2.23648200   |
| C       | -0.45732500  | 4.70583300   | 3.32961900   |
| H       | 0.61572500   | 4.55157300   | 3.38686800   |
| C       | -1.02107500  | 5.84319500   | 3.90055700   |
| H       | -0.38915100  | 6.57464100   | 4.39549200   |
| C       | -2.39775600  | 6.03673700   | 3.83438600   |
| H       | -2.84655300  | 6.92066200   | 4.27796600   |
| C       | -3.20506100  | 5.09144500   | 3.21018300   |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -4.281111 | 5.233287 | 3.167256 |
| C    | -6.815970  | 3.844255 | -2.956730 |
| C    | -7.465824  | 5.048562 | -2.669494 |
| H    | -7.728011  | 5.273005 | -1.639573 |
| C    | -7.776809  | 5.947107 | -3.684897 |
| H    | -8.284731  | 6.876721 | -3.451990 |
| C    | -7.444440  | 5.653340 | -5.004768 |
| H    | -7.688505  | 6.354412 | -5.797378 |
| C    | -6.799637  | 4.455974 | -5.302643 |
| H    | -6.536899  | 4.220090 | -6.329787 |
| C    | -6.483800  | 3.559260 | -4.285900 |
| H    | -5.985794  | 2.623629 | -4.516299 |
| C    | -2.817575  | -1.978027 | -1.275830 |
| C    | -3.506761  | -2.785291 | -0.367750 |
| H    | -4.560287  | -2.612436 | -0.179900 |
| C    | -2.855511  | -3.821574 | 0.292544 |
| H    | -3.409363  | -4.435421 | 0.997476 |
| C    | -1.506365  | -4.071347 | 0.046407 |
| H    | -0.999564  | -4.881521 | 0.563049 |
| C    | -0.811357  | -3.270730 | -0.852992 |
| H    | 0.241488   | -3.446201 | -1.050820 |
| C    | -1.464814  | -2.226342 | -1.499750 |
| H    | -0.907977  | -1.589483 | -2.182071 |
| Zn   | 5.361945   | -0.019289 | -1.075259 |
| N    | 5.838867   | -1.926084 | -1.774503 |
| N    | 7.422548   | 0.316308  | -0.833023 |
| N    | 5.109813   | 2.025959  | -1.061057 |
| N    | 3.579468   | -0.177425 | -2.106157 |
| C    | 8.193518   | -2.015738 | -1.048910 |
| C    | 7.318852   | 2.690039  | -0.188358 |
| C    | 2.767464   | 2.133237  | -1.808080 |
| C    | 3.651335   | -2.570765 | -2.698103 |
| C    | 5.637782   | -4.107121 | -2.482072 |
| H    | 5.191030   | -4.991547 | -2.914133 |
| C    | 7.021929   | -2.578836 | -1.580742 |
| C    | 8.362581   | -0.665749 | -0.700675 |
| C    | 7.971898   | 1.452251  | -0.318860 |
| C    | 5.992973   | 2.942698  | -0.562131 |
| C    | 4.077685   | 4.077936  | -0.894322 |
| H    | 3.303249   | 4.828173  | -0.967192 |
| C    | 2.637916   | 0.803665  | -2.237619 |
| C    | 3.029117   | -1.317966 | -2.626464 |
| C    | 4.978451   | -2.832202 | -2.318853 |
| C    | 6.904804   | -3.950030 | -2.026184 |
| H    | 7.699232   | -4.682434 | -2.014908 |
| C    | 9.555052   | -0.126628 | -0.083147 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| H       | 1.59973800   | -4.91529500  | -6.16730300  |
| C       | 1.29388900   | -5.81816500  | -4.23737900  |
| H       | 0.68626800   | -6.63088100  | -4.62336600  |
| C       | 1.56532600   | -5.73554300  | -2.87504000  |
| H       | 1.16788100   | -6.48031400  | -2.19210700  |
| C       | 2.34063800   | -4.69040500  | -2.38277700  |
| H       | 2.54658800   | -4.62395800  | -1.31776000  |
| N       | 5.33016000   | -0.72234000  | 0.94429500   |
| H       | 4.57252600   | -1.37805200  | 1.16543300   |
| H       | 6.17508600   | -1.29073500  | 0.88178300   |
| C       | 6.42721200   | -0.24265000  | 3.12755400   |
| H       | 6.04153200   | -1.16233500  | 3.58094700   |
| H       | 6.54440900   | 0.50538100   | 3.91738100   |
| H       | 7.41826800   | -0.45272100  | 2.70836400   |
| C       | 5.50198700   | 0.27655000   | 2.02685500   |
| H       | 5.98536100   | 1.14740100   | 1.57532500   |
| C       | 4.14051000   | 0.71236800   | 2.52731400   |
| C       | 3.62800500   | 1.95374900   | 2.15078400   |
| H       | 4.21749200   | 2.60727400   | 1.51379500   |
| C       | 2.37190600   | 2.36475000   | 2.58973800   |
| H       | 1.98278900   | 3.32405400   | 2.26131900   |
| C       | 1.61353400   | 1.53947500   | 3.41471800   |
| H       | 0.63201100   | 1.85570000   | 3.75570900   |
| C       | 2.11498300   | 0.29622300   | 3.79175100   |
| H       | 1.52040600   | -0.36549100  | 4.41392400   |
| C       | 3.36677800   | -0.11370500  | 3.34714100   |
| H       | 3.73572500   | -1.09490800  | 3.63499600   |
| N       | -2.28689000  | -2.84142600  | 3.43406000   |
| H       | -2.60845700  | -2.34580100  | 2.61267200   |
| N       | 3.10065000   | -2.76170500  | 0.76576900   |
| H       | 3.30831400   | -2.62235700  | -0.21952600  |
| H       | 3.21743000   | -3.73696400  | 1.01227600   |
| N       | 0.66861200   | 1.70037900   | -0.02816600  |
| H       | 1.62937300   | 1.45255200   | 0.16457300   |
| O       | -0.38094500  | -3.65656100  | 4.42462000   |
| O       | -1.48205000  | 1.05573400   | 0.31856100   |
| C       | 0.23129600   | -0.44618900  | 0.99441300   |
| C       | -0.57410600  | -1.07923800  | 1.93800000   |
| H       | -1.50667600  | -0.60386500  | 2.22569700   |
| C       | -0.13975700  | -2.26926000  | 2.51005300   |
| C       | 1.08542600   | -2.82347800  | 2.14139100   |
| H       | 1.40424800   | -3.74412800  | 2.62232100   |
| C       | 1.86510600   | -2.21862100  | 1.16010700   |
| C       | 1.43535000   | -1.01502600  | 0.59578500   |
| H       | 2.05200800   | -0.55411700  | -0.16933400  |
| C       | -0.27982500  | 0.82609000   | 0.40008700   |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -0.93487300 | -2.99407500 | 3.55875400 |
| C       | -4.77175800  | -1.31720100  | -2.75192300  |
| H       | -4.51916300  | -2.07809700  | -3.49654100  |
| H       | -5.49644900  | -1.74054700  | -2.05144700  |
| H       | -5.25636500  | -0.47475100  | -3.25866100  |
| C       | -3.51215200  | -0.85702300  | -2.02253200  |
| H       | -2.80052800  | -0.48647900  | -2.77528200  |
| N       | -3.83848900  | 0.25241700   | -1.10184300  |
| H       | -2.99024400  | 0.52325600   | -0.59596800  |
| H       | -4.09510900  | 1.06437700   | -1.66340300  |