

Supporting Information

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

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

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)

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(2BA)	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

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(7A)-N(1A)-Zn(1)	124(2)	C(7A)-N(1A)-H(1A)	120.0
Zn(1)-N(1A)-H(1A)	57.1	C(7A)-N(1A)-H(1B)	120.0
Zn(1)-N(1A)-H(1B)	89.4	H(1A)-N(1A)-H(1B)	120.0
N(1A)-C(7A)-C(8A)	109.0(17)	N(1A)-C(7A)-C(1A)	112.5(19)
C(8A)-C(7A)-C(1A)	115.9(10)	N(1A)-C(7A)-H(7A)	106.2
C(8A)-C(7A)-H(7A)	106.2	C(1A)-C(7A)-H(7A)	106.2
C(7A)-C(8A)-H(8A)	109.5	C(7A)-C(8A)-H(8B)	109.5
H(8A)-C(8A)-H(8B)	109.5	C(7A)-C(8A)-H(8C)	109.5
H(8A)-C(8A)-H(8C)	109.5	H(8B)-C(8A)-H(8C)	109.5
C(2A)-C(1A)-C(6A)	120.0	C(2A)-C(1A)-C(7A)	120.1(10)
C(6A)-C(1A)-C(7A)	119.6(10)	C(1A)-C(2A)-C(3A)	120.0

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)

C(1M2)-C(1A3)-C(1B3) 125.3(3)	N(12)-C(1A4)-C(1M3) 125.8(3)
N(12)-C(1A4)-C(1B4) 109.4(3)	C(1M3)-C(1A4)-C(1B4) 124.8(3)
N(13)-C(1A5)-C(1M3) 125.5(3)	N(13)-C(1A5)-C(1B5) 110.0(2)
C(1M3)-C(1A5)-C(1B5) 124.3(3)	N(13)-C(1A6)-C(1M4) 125.5(3)
N(13)-C(1A6)-C(1B6) 109.3(2)	C(1M4)-C(1A6)-C(1B6) 125.1(3)
N(14)-C(1A7)-C(1M4) 125.4(3)	N(14)-C(1A7)-C(1B7) 109.1(3)
C(1M4)-C(1A7)-C(1B7) 125.4(3)	N(14)-C(1A8)-C(1M1) 125.6(3)
N(14)-C(1A8)-C(1B8) 109.4(3)	C(1M1)-C(1A8)-C(1B8) 124.9(3)
C(1B2)-C(1B1)-C(1A1) 107.3(3)	C(1B2)-C(1B1)-H(1BF) 126.4
C(1A1)-C(1B1)-H(1BF) 126.4	C(1B1)-C(1B2)-C(1A2) 107.9(3)
C(1B1)-C(1B2)-H(1BH) 126.1	C(1A2)-C(1B2)-H(1BH) 126.1
C(1B4)-C(1B3)-C(1A3) 107.7(3)	C(1B4)-C(1B3)-H(1BB) 126.2
C(1A3)-C(1B3)-H(1BB) 126.2	C(1B3)-C(1B4)-C(1A4) 107.2(3)
C(1B3)-C(1B4)-H(1BG) 126.4	C(1A4)-C(1B4)-H(1BG) 126.4
C(1B6)-C(1B5)-C(1A5) 106.8(3)	C(1B6)-C(1B5)-H(1BA) 126.6
C(1A5)-C(1B5)-H(1BA) 126.6	C(1B5)-C(1B6)-C(1A6) 107.7(3)
C(1B5)-C(1B6)-H(1BC) 126.2	C(1A6)-C(1B6)-H(1BC) 126.2
C(1B8)-C(1B7)-C(1A7) 107.4(3)	C(1B8)-C(1B7)-H(1BE) 126.3
C(1A7)-C(1B7)-H(1BE) 126.3	C(1B7)-C(1B8)-C(1A8) 107.5(3)
C(1B7)-C(1B8)-H(1BD) 126.3	C(1A8)-C(1B8)-H(1BD) 126.3
C(1A8)-C(1M1)-C(1A1) 125.4(3)	C(1A8)-C(1M1)-C(111) 118.8(3)
C(1A1)-C(1M1)-C(111) 115.7(3)	C(1A3)-C(1M2)-C(1A2) 124.9(3)
C(1A3)-C(1M2)-C(121) 118.1(3)	C(1A2)-C(1M2)-C(121) 116.9(3)
C(1A5)-C(1M3)-C(1A4) 124.5(3)	C(1A5)-C(1M3)-C(131) 118.2(3)
C(1A4)-C(1M3)-C(131) 117.2(3)	C(1A7)-C(1M4)-C(1A6) 124.9(3)
C(1A7)-C(1M4)-C(141) 117.9(2)	C(1A6)-C(1M4)-C(141) 117.1(3)
C(116)-C(111)-C(112) 118.8(3)	C(116)-C(111)-C(1M1) 120.0(3)
C(112)-C(111)-C(1M1) 121.0(3)	C(113)-C(112)-C(111) 119.7(3)
C(113)-C(112)-N(011) 123.4(3)	C(111)-C(112)-N(011) 116.8(3)
C(112)-C(113)-C(114) 119.9(4)	C(112)-C(113)-H(11A) 120.0
C(114)-C(113)-H(11A) 120.0	C(115)-C(114)-C(113) 120.7(3)
C(115)-C(114)-H(11B) 119.7	C(113)-C(114)-H(11B) 119.7
C(114)-C(115)-C(116) 119.2(4)	C(114)-C(115)-H(11C) 120.4
C(116)-C(115)-H(11C) 120.4	C(115)-C(116)-C(111) 121.6(4)
C(115)-C(116)-H(11D) 119.2	C(111)-C(116)-H(11D) 119.2

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)

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(2M2)-C(2A3)-C(2B3)	124.6(3)
N(22)-C(2A3)-C(2B3)	109.3(3)	N(22)-C(2A4)-C(2M3)	125.7(3)
N(22)-C(2A4)-C(2B4)	110.3(3)	C(2M3)-C(2A4)-C(2B4)	123.9(3)
N(23)-C(2A5)-C(2M3)	125.3(3)	N(23)-C(2A5)-C(2B5)	110.3(3)
C(2M3)-C(2A5)-C(2B5)	124.1(3)	N(23)-C(2A6)-C(2M4)	125.9(3)
N(23)-C(2A6)-C(2B6)	110.2(3)	C(2M4)-C(2A6)-C(2B6)	123.9(3)
C(2M4)-C(2A7)-N(24)	126.1(3)	C(2M4)-C(2A7)-C(2B7)	123.8(3)
N(24)-C(2A7)-C(2B7)	110.0(3)	N(24)-C(2A8)-C(2M1)	126.3(2)
N(24)-C(2A8)-C(2B8)	109.9(2)	C(2M1)-C(2A8)-C(2B8)	123.8(3)
C(2B2)-C(2B1)-C(2A1)	107.5(3)	C(2B2)-C(2B1)-H(2BC)	126.2
C(2A1)-C(2B1)-H(2BC)	126.2	C(2B1)-C(2B2)-C(2A2)	107.2(3)
C(2B1)-C(2B2)-H(2BD)	126.4	C(2A2)-C(2B2)-H(2BD)	126.4
C(2B4)-C(2B3)-C(2A3)	107.8(3)	C(2B4)-C(2B3)-H(2BG)	126.1
C(2A3)-C(2B3)-H(2BG)	126.1	C(2B3)-C(2B4)-C(2A4)	107.4(3)
C(2B3)-C(2B4)-H(2BH)	126.3	C(2A4)-C(2B4)-H(2BH)	126.3
C(2B6)-C(2B5)-C(2A5)	107.5(3)	C(2B6)-C(2B5)-H(2BF)	126.2
C(2A5)-C(2B5)-H(2BF)	126.2	C(2B5)-C(2B6)-C(2A6)	106.7(3)
C(2B5)-C(2B6)-H(2BB)	126.6	C(2A6)-C(2B6)-H(2BB)	126.6
C(2B8)-C(2B7)-C(2A7)	107.5(3)	C(2B8)-C(2B7)-H(2BA)	126.3
C(2A7)-C(2B7)-H(2BA)	126.3	C(2B7)-C(2B8)-C(2A8)	107.4(3)
C(2B7)-C(2B8)-H(2BE)	126.3	C(2A8)-C(2B8)-H(2BE)	126.3
C(2A8)-C(2M1)-C(2A1)	122.7(2)	C(2A8)-C(2M1)-C(211)	118.2(2)
C(2A1)-C(2M1)-C(211)	119.0(2)	C(2A3)-C(2M2)-C(2A2)	123.1(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)	118.5(3)
C(2A5)-C(2M3)-C(231)	118.0(3)	C(2A7)-C(2M4)-C(2A6)	122.5(3)
C(2A7)-C(2M4)-C(241)	117.8(3)	C(2A6)-C(2M4)-C(241)	119.8(3)
C(212)-C(211)-C(216)	118.7(2)	C(212)-C(211)-C(2M1)	120.8(3)
C(216)-C(211)-C(2M1)	120.5(3)	C(213)-C(212)-C(211)	121.4(3)
C(213)-C(212)-H(21A)	119.3	C(211)-C(212)-H(21A)	119.3
C(214)-C(213)-C(212)	119.3(3)	C(214)-C(213)-H(21B)	120.4

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

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.

Zn(1)-N(11)	2.062(8)	Zn(1)-N(14)	2.068(7)
Zn(1)-N(13)	2.081(7)	Zn(1)-N(12)	2.085(7)
Zn(1)-N(1B)	2.12(3)	Zn(1)-N(1A)	2.151(15)
N(11)-C(1A2)	1.388(11)	N(11)-C(1A1)	1.394(12)
N(12)-C(1A3)	1.362(12)	N(12)-C(1A4)	1.369(11)
N(13)-C(1A5)	1.372(11)	N(13)-C(1A6)	1.383(12)
N(14)-C(1A7)	1.353(11)	N(14)-C(1A8)	1.378(11)
C(1M1)-C(1A2)	1.381(14)	C(1M1)-C(1A3)	1.400(14)
C(1M1)-C(111)	1.530(10)	C(1M2)-C(1A4)	1.388(13)
C(1M2)-C(1A5)	1.405(12)	C(1M2)-C(121)	1.506(9)
C(1M3)-C(1A7)	1.387(11)	C(1M3)-C(1A6)	1.411(12)
C(1M3)-C(131)	1.516(9)	C(1M4)-C(1A1)	1.383(13)
C(1M4)-C(1A8)	1.436(12)	C(1M4)-C(141)	1.509(9)
C(1A1)-C(1B1)	1.443(13)	C(1A2)-C(1B2)	1.429(13)
C(1A3)-C(1B3)	1.417(15)	C(1A4)-C(1B4)	1.423(14)
C(1A5)-C(1B5)	1.448(12)	C(1A6)-C(1B6)	1.470(12)
C(1A7)-C(1B7)	1.475(11)	C(1A8)-C(1B8)	1.401(13)
C(1B1)-C(1B2)	1.342(14)	C(1B1)-H(1B1)	0.9400
C(1B2)-H(1B2)	0.9400	C(1B3)-C(1B4)	1.363(14)
C(1B3)-H(1B3)	0.9400	C(1B4)-H(1B4)	0.9400
C(1B5)-C(1B6)	1.377(14)	C(1B5)-H(1B5)	0.9400
C(1B6)-H(1B6)	0.9400	C(1B7)-C(1B8)	1.365(12)
C(1B7)-H(1B7)	0.9400	C(1B8)-H(1B8)	0.9400
C(111)-C(112)	1.3900	C(111)-C(116)	1.3900
C(112)-C(113)	1.3900	C(112)-H(112)	0.9400
C(113)-C(114)	1.3900	C(113)-H(113)	0.9400
C(114)-C(115)	1.3900	C(114)-H(114)	0.9400
C(115)-C(116)	1.3900	C(115)-H(115)	0.9400
C(116)-H(116)	0.9400	C(121)-C(122)	1.3896
C(121)-C(126)	1.3905	C(122)-C(123)	1.3906
C(122)-H(122)	0.9400	C(123)-C(124)	1.3897
C(123)-H(123)	0.9400	C(124)-C(125)	1.3900
C(124)-H(124)	0.9400	C(125)-C(126)	1.3903

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)

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(211)	1.515(9)
C(2M2)-C(2A4)	1.397(13)	C(2M2)-C(2A5)	1.403(12)
C(2M2)-C(221)	1.504(11)	C(2M3)-C(2B6)	1.398(12)
C(2M3)-C(2A7)	1.408(12)	C(2M3)-C(231)	1.490(10)
C(2M4)-C(2A1)	1.392(12)	C(2M4)-C(2A8)	1.409(12)
C(2M4)-C(241)	1.497(11)	C(2B1)-C(2B2)	1.364(13)
C(2B1)-C(2A1)	1.470(13)	C(2B1)-H(2B1)	0.9400
C(2A2)-C(2B2)	1.464(13)	C(2A3)-C(2B3)	1.474(12)
C(2A4)-C(2B4)	1.456(13)	C(2A5)-C(2B5)	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(2B2)-H(2B3)	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(211)-C(212)	1.3900
C(211)-C(216)	1.3900	C(212)-C(213)	1.3900
C(212)-H(212)	0.9400	C(213)-C(214)	1.3900
C(213)-H(213)	0.9400	C(214)-C(215)	1.3900
C(214)-H(214)	0.9400	C(215)-C(216)	1.3900
C(215)-H(215)	0.9400	C(216)-H(216)	0.9400
C(221)-C(226)	1.386(9)	C(221)-C(222)	1.392(9)
C(222)-C(223)	1.398(9)	C(222)-H(222)	0.9400
C(223)-C(224)	1.362(10)	C(223)-H(223)	0.9400
C(224)-C(225)	1.342(10)	C(224)-H(224)	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(236)	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)

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

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)

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

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

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)

C(1M1)-C(1A3)-C(1B3) 125.9(9)	N(12)-C(1A4)-C(1M2) 125.9(8)
N(12)-C(1A4)-C(1B4) 108.9(9)	C(1M2)-C(1A4)-C(1B4) 125.1(8)
N(13)-C(1A5)-C(1M2) 124.8(8)	N(13)-C(1A5)-C(1B5) 110.9(7)
C(1M2)-C(1A5)-C(1B5) 124.2(8)	N(13)-C(1A6)-C(1M3) 126.1(8)
N(13)-C(1A6)-C(1B6) 109.5(8)	C(1M3)-C(1A6)-C(1B6) 124.4(9)
N(14)-C(1A7)-C(1M3) 128.4(7)	N(14)-C(1A7)-C(1B7) 109.3(7)
C(1M3)-C(1A7)-C(1B7) 122.3(8)	N(14)-C(1A8)-C(1B8) 110.0(8)
N(14)-C(1A8)-C(1M4) 123.3(8)	C(1B8)-C(1A8)-C(1M4) 126.6(8)
C(1B2)-C(1B1)-C(1A1) 107.0(8)	C(1B2)-C(1B1)-H(1B1) 126.5
C(1A1)-C(1B1)-H(1B1) 126.5	C(1B1)-C(1B2)-C(1A2) 108.2(8)
C(1B1)-C(1B2)-H(1B2) 125.9	C(1A2)-C(1B2)-H(1B2) 125.9
C(1B4)-C(1B3)-C(1A3) 107.2(9)	C(1B4)-C(1B3)-H(1B3) 126.4
C(1A3)-C(1B3)-H(1B3) 126.4	C(1B3)-C(1B4)-C(1A4) 107.1(9)
C(1B3)-C(1B4)-H(1B4) 126.5	C(1A4)-C(1B4)-H(1B4) 126.5
C(1B6)-C(1B5)-C(1A5) 106.5(8)	C(1B6)-C(1B5)-H(1B5) 126.7
C(1A5)-C(1B5)-H(1B5) 126.7	C(1B5)-C(1B6)-C(1A6) 106.6(8)
C(1B5)-C(1B6)-H(1B6) 126.7	C(1A6)-C(1B6)-H(1B6) 126.7
C(1B8)-C(1B7)-C(1A7) 105.1(8)	C(1B8)-C(1B7)-H(1B7) 127.5
C(1A7)-C(1B7)-H(1B7) 127.5	C(1B7)-C(1B8)-C(1A8) 108.5(7)
C(1B7)-C(1B8)-H(1B8) 125.8	C(1A8)-C(1B8)-H(1B8) 125.8
C(112)-C(111)-C(116) 120.0	C(112)-C(111)-C(1M1) 120.7(4)
C(116)-C(111)-C(1M1) 119.2(4)	C(111)-C(112)-C(113) 120.0
C(111)-C(112)-H(112) 120.0	C(113)-C(112)-H(112) 120.0
C(114)-C(113)-C(112) 120.0	C(114)-C(113)-H(113) 120.0
C(112)-C(113)-H(113) 120.0	C(113)-C(114)-C(115) 120.0
C(113)-C(114)-H(114) 120.0	C(115)-C(114)-H(114) 120.0
C(116)-C(115)-C(114) 120.0	C(116)-C(115)-H(115) 120.0
C(114)-C(115)-H(115) 120.0	C(115)-C(116)-C(111) 120.0
C(115)-C(116)-H(116) 120.0	C(111)-C(116)-H(116) 120.0
C(122)-C(121)-C(126) 120.0	C(122)-C(121)-C(1M2) 119.3(3)
C(126)-C(121)-C(1M2) 120.2(3)	C(121)-C(122)-C(123) 120.0
C(121)-C(122)-H(122) 120.0	C(123)-C(122)-H(122) 120.0
C(124)-C(123)-C(122) 119.9	C(124)-C(123)-H(123) 120.0
C(122)-C(123)-H(123) 120.0	C(123)-C(124)-C(125) 120.1
C(123)-C(124)-H(124) 120.0	C(125)-C(124)-H(124) 120.0

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

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
Zn(1)-N(1B)-H(1BX) 100.1	H(1B9)-N(1B)-H(1BX) 104.2
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
H(11D)-C(11B)-H(11F) 109.5	H(11E)-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) 105(2)	N(1B)-C(12B)-H(12B) 103.7
C(13B)-C(12B)-H(12B) 103.7	C(11B)-C(12B)-H(12B) 103.7
C(14B)-C(13B)-C(18B) 120.0	C(14B)-C(13B)-C(12B) 138(2)
C(18B)-C(13B)-C(12B) 102(2)	C(13B)-C(14B)-C(15B) 120.0
C(13B)-C(14B)-H(14B) 120.0	C(15B)-C(14B)-H(14B) 120.0
C(16B)-C(15B)-C(14B) 120.0	C(16B)-C(15B)-H(15B) 120.0
C(14B)-C(15B)-H(15B) 120.0	C(17B)-C(16B)-C(15B) 120.0
C(17B)-C(16B)-H(16B) 120.0	C(15B)-C(16B)-H(16B) 120.0
C(16B)-C(17B)-C(18B) 120.0	C(16B)-C(17B)-H(17B) 120.0
C(18B)-C(17B)-H(17B) 120.0	C(17B)-C(18B)-C(13B) 120.0
C(17B)-C(18B)-H(18B) 120.0	C(13B)-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) 88.5(3)	N(22)-Zn(2)-N(21) 89.0(3)
N(24)-Zn(2)-N(21) 88.5(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) 102.2(3)	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)

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(2B2) 108.2(8)	C(2M1)-C(2A2)-C(2B2) 125.8(9)
N(22)-C(2A3)-C(2M1) 127.6(8)	N(22)-C(2A3)-C(2B3) 108.2(8)
C(2M1)-C(2A3)-C(2B3) 124.1(9)	N(22)-C(2A4)-C(2M2) 125.9(8)
N(22)-C(2A4)-C(2B4) 108.2(8)	C(2M2)-C(2A4)-C(2B4) 125.6(9)
N(23)-C(2A5)-C(2M2) 125.2(8)	N(23)-C(2A5)-C(2B5) 108.9(7)
C(2M2)-C(2A5)-C(2B5) 125.9(8)	C(2B5)-C(2A6)-C(2B6) 107.3(8)
C(2B5)-C(2A6)-H(2A6) 126.4	C(2B6)-C(2A6)-H(2A6) 126.4
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(2A8)-C(2M4) 128.3(8)
N(24)-C(2A8)-C(2B8) 109.9(8)	C(2M4)-C(2A8)-C(2B8) 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(2B1)-C(2B2)-H(2B3) 125.9	C(2A2)-C(2B2)-H(2B3) 125.9
C(2B4)-C(2B3)-C(2A3) 106.9(9)	C(2B4)-C(2B3)-H(2B4) 126.5
C(2A3)-C(2B3)-H(2B4) 126.6	C(2B3)-C(2B4)-C(2A4) 108.3(9)
C(2B3)-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

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)-C(223)	119.8(6)
C(225)-C(224)-H(224)	120.1	C(223)-C(224)-H(224)	120.1
C(224)-C(225)-C(226)	121.7(7)	C(224)-C(225)-H(225)	119.2
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)	122.0(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

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(023)-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)

N(32)-C(3A4)-C(3B4) 109.4(8)	C(3M2)-C(3A4)-C(3B4) 124.7(8)
N(33)-C(3A5)-C(3M2) 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) 110.5(8)
C(3B6)-C(3A6)-C(3M3) 125.9(9)	N(33)-C(3A6)-C(3M3) 123.5(9)
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(4)
C(316)-C(311)-C(3M1) 120.0(4)	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

C(324)-C(325)-H(32F) 120.0	C(325)-C(326)-C(321) 120.0
C(325)-C(326)-H(32G) 120.0	C(321)-C(326)-H(32G) 120.0
C(32A)-C(31A)-C(36A) 120.0	C(32A)-C(31A)-C(3M3) 122.5(6)
C(36A)-C(31A)-C(3M3) 117.5(6)	C(31A)-C(32A)-C(33A) 120.0
C(31A)-C(32A)-H(32A) 120.0	C(33A)-C(32A)-H(32A) 120.0
C(34A)-C(33A)-C(32A) 120.0	C(34A)-C(33A)-H(33A) 120.0
C(32A)-C(33A)-H(33A) 120.0	C(33A)-C(34A)-C(35A) 120.0
C(33A)-C(34A)-H(34A) 120.0	C(35A)-C(34A)-H(34A) 120.0
C(36A)-C(35A)-C(34A) 120.0	C(36A)-C(35A)-H(35A) 120.0
C(34A)-C(35A)-H(35A) 120.0	C(35A)-C(36A)-C(31A) 120.0
C(35A)-C(36A)-H(36A) 120.0	C(31A)-C(36A)-H(36A) 120.0
C(32B)-C(31B)-C(36B) 120.0	C(32B)-C(31B)-C(3M3) 115.4(6)
C(36B)-C(31B)-C(3M3) 124.5(6)	C(31B)-C(32B)-C(33B) 120.0
C(31B)-C(32B)-H(32B) 120.0	C(33B)-C(32B)-H(32B) 120.0
C(32B)-C(33B)-C(34B) 120.0	C(32B)-C(33B)-H(33B) 120.0
C(34B)-C(33B)-H(33B) 120.0	C(35B)-C(34B)-C(33B) 120.0
C(35B)-C(34B)-H(34B) 120.0	C(33B)-C(34B)-H(34B) 120.0
C(34B)-C(35B)-C(36B) 120.0	C(34B)-C(35B)-H(35B) 120.0
C(36B)-C(35B)-H(35B) 120.0	C(35B)-C(36B)-C(31B) 120.0
C(35B)-C(36B)-H(36B) 120.0	C(31B)-C(36B)-H(36B) 120.0
C(342)-C(341)-C(346) 120.0	C(342)-C(341)-C(3M4) 120.5(5)
C(346)-C(341)-C(3M4) 119.4(5)	C(341)-C(342)-C(343) 120.0
C(341)-C(342)-H(34C) 120.0	C(343)-C(342)-H(34C) 120.0
C(342)-C(343)-C(344) 120.0	C(342)-C(343)-H(34D) 120.0
C(344)-C(343)-H(34D) 120.0	C(345)-C(344)-C(343) 120.0
C(345)-C(344)-H(34E) 120.0	C(343)-C(344)-H(34E) 120.0
C(344)-C(345)-C(346) 120.0	C(344)-C(345)-H(34F) 120.0
C(346)-C(345)-H(34F) 120.0	C(345)-C(346)-C(341) 120.0
C(345)-C(346)-H(34G) 120.0	C(341)-C(346)-H(34G) 120.0
C(037)-N(3)-Zn(3) 137.2(9)	C(037)-N(3)-H(3A) 102.8
Zn(3)-N(3)-H(3A) 102.8	C(037)-N(3)-H(3B) 102.8
Zn(3)-N(3)-H(3B) 102.8	H(3A)-N(3)-H(3B) 105.0
C(032)-C(031)-C(036) 120.0	C(032)-C(031)-C(037) 117.8(8)
C(036)-C(031)-C(037) 121.9(8)	C(031)-C(032)-C(033) 120.0
C(031)-C(032)-H(032) 120.0	C(033)-C(032)-H(032) 120.0

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)-C(031)	109.7(12)
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)

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(4B6) 109.9(7)
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(425)-C(426)-H(426)	119.6
C(432)-C(431)-C(436)	120.0	C(432)-C(431)-C(4M3)	119.2(3)
C(436)-C(431)-C(4M3)	120.6(3)	C(433)-C(432)-C(431)	120.0
C(433)-C(432)-H(432)	120.0	C(431)-C(432)-H(432)	120.0
C(434)-C(433)-C(432)	120.0	C(434)-C(433)-H(433)	120.0
C(432)-C(433)-H(433)	120.0	C(433)-C(434)-C(435)	120.0
C(433)-C(434)-H(434)	120.0	C(435)-C(434)-H(434)	120.0
C(434)-C(435)-C(436)	120.0	C(434)-C(435)-H(435)	120.0
C(436)-C(435)-H(435)	120.0	C(435)-C(436)-C(431)	120.0
C(435)-C(436)-H(436)	120.0	C(431)-C(436)-H(436)	120.0
C(446)-C(441)-C(442)	120.0	C(446)-C(441)-C(4M4)	118.3(4)
C(442)-C(441)-C(4M4)	121.5(4)	N(023)-C(442)-C(443)	124.1(4)
N(023)-C(442)-C(441)	115.9(4)	C(443)-C(442)-C(441)	120.0
C(442)-C(443)-C(444)	120.0	C(442)-C(443)-H(443)	120.0
C(444)-C(443)-H(443)	120.0	C(445)-C(444)-C(443)	120.0
C(445)-C(444)-H(444)	120.0	C(443)-C(444)-H(444)	120.0
C(446)-C(445)-C(444)	120.0	C(446)-C(445)-H(445)	120.0
C(444)-C(445)-H(445)	120.0	C(445)-C(446)-C(441)	120.0
C(445)-C(446)-H(446)	120.0	C(441)-C(446)-H(446)	120.0
C(047)-N(4)-Zn(4)	125.4(5)	C(047)-N(4)-H(41)	106.0
Zn(4)-N(4)-H(41)	106.0	C(047)-N(4)-H(42)	106.0
Zn(4)-N(4)-H(42)	106.0	H(41)-N(4)-H(42)	106.3
N(4)-C(047)-C(048)	110.6(9)	N(4)-C(047)-C(041)	113.3(6)
C(048)-C(047)-C(041)	110.5(7)	N(4)-C(047)-H(47A)	107.4
C(048)-C(047)-H(47A)	107.4	C(041)-C(047)-H(47A)	107.4
C(047)-C(048)-H(48A)	109.5	C(047)-C(048)-H(48B)	109.5
H(48A)-C(048)-H(48B)	109.5	C(047)-C(048)-H(48C)	109.5
H(48A)-C(048)-H(48C)	109.5	H(48B)-C(048)-H(48C)	109.5
C(042)-C(041)-C(046)	120.0	C(042)-C(041)-C(047)	121.1(5)
C(046)-C(041)-C(047)	118.9(5)	C(041)-C(042)-C(043)	120.0
C(041)-C(042)-H(042)	120.0	C(043)-C(042)-H(042)	120.0
C(044)-C(043)-C(042)	120.0	C(044)-C(043)-H(043)	120.0
C(042)-C(043)-H(043)	120.0	C(043)-C(044)-C(045)	120.0
C(043)-C(044)-H(044)	120.0	C(045)-C(044)-H(044)	120.0
C(046)-C(045)-C(044)	120.0	C(046)-C(045)-H(045)	120.0

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)

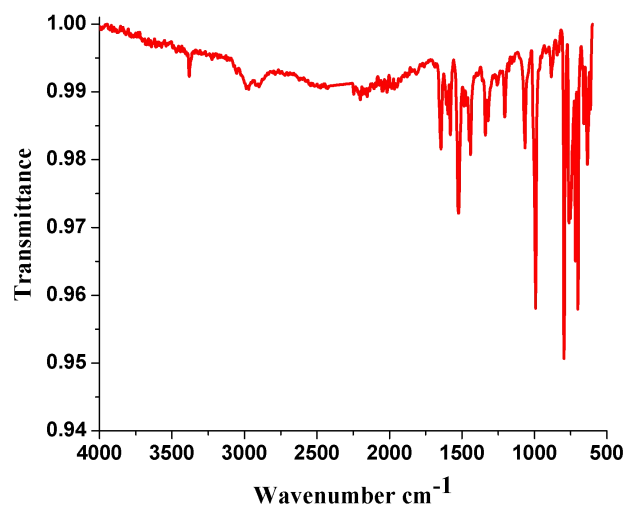


Fig. S1. FT IR spectrum of [Zn₂-AmBis].

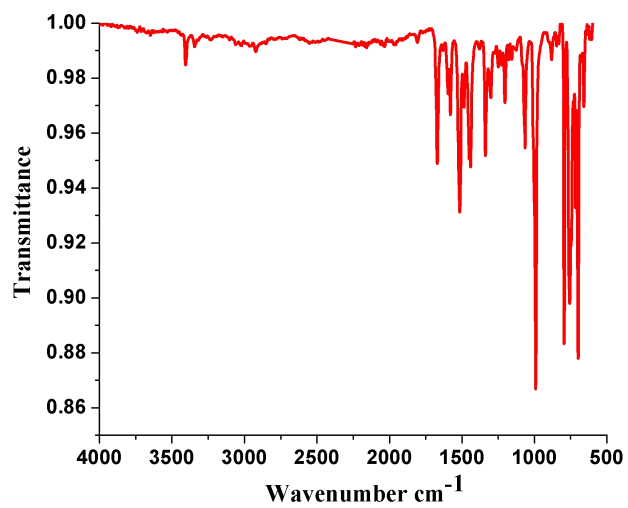


Fig. S2. FT IR spectrum of [Zn₂-AmBis](R-1-PEA)₂.

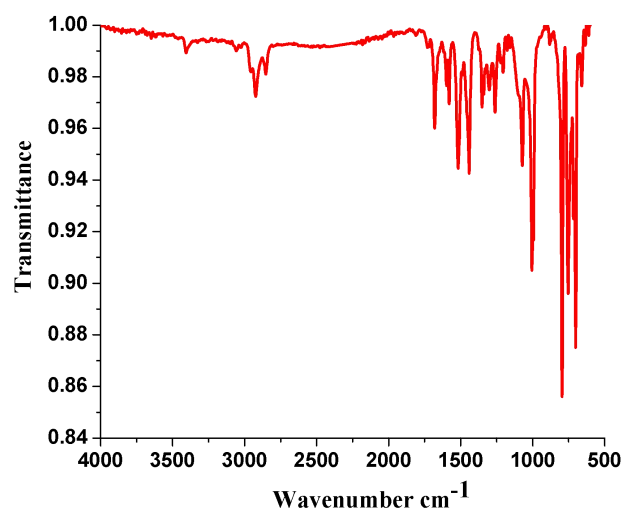


Fig. S3. FT IR spectrum of [ZnNi-AmBis].

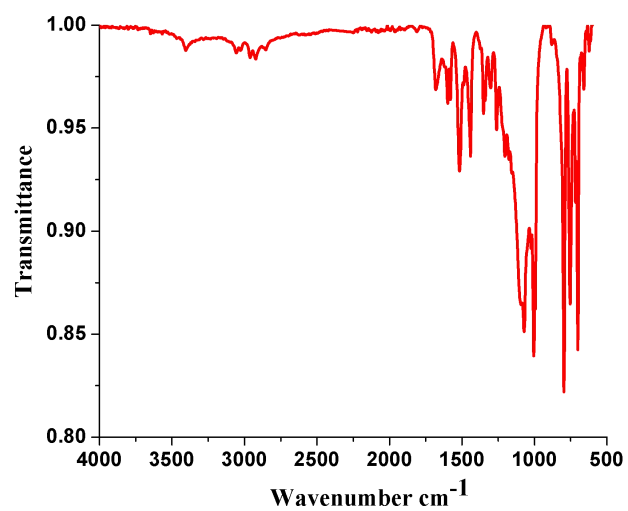


Fig. S4. FT IR spectrum of [ZnNi-AmBis](1-PEA).

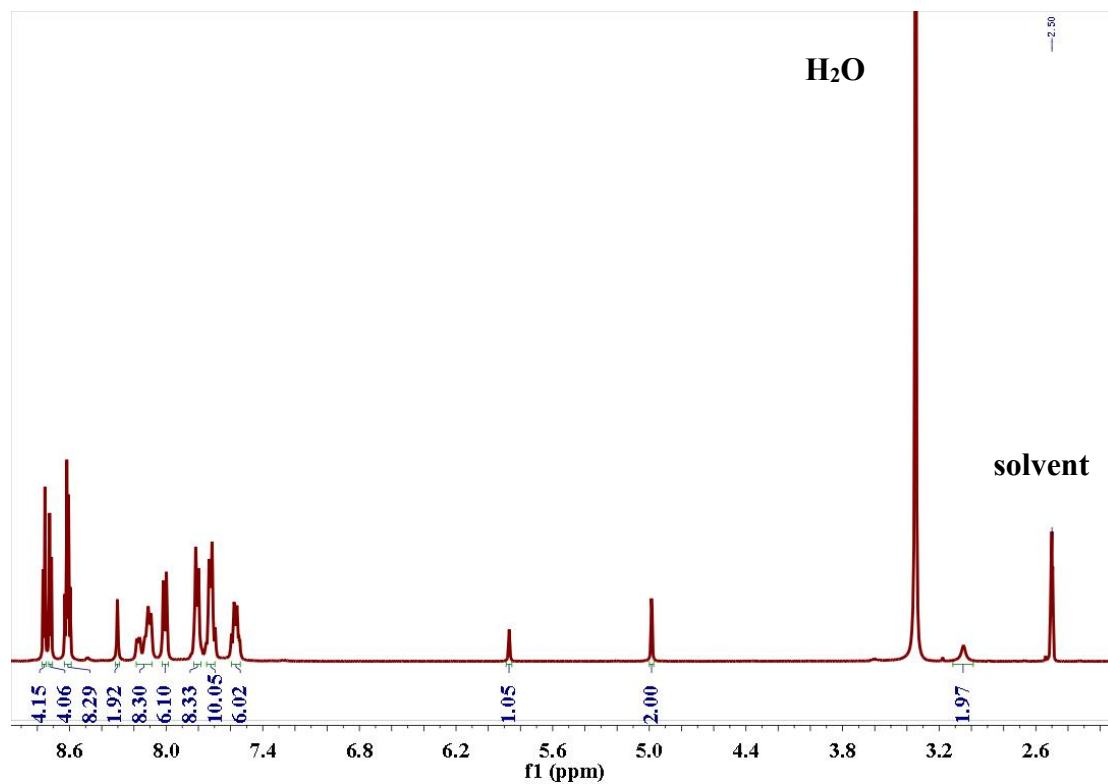


Fig. S5. ¹H NMR spectrum of [Zn₂-AmBis] in DMSO (4.1×10^{-3} M).

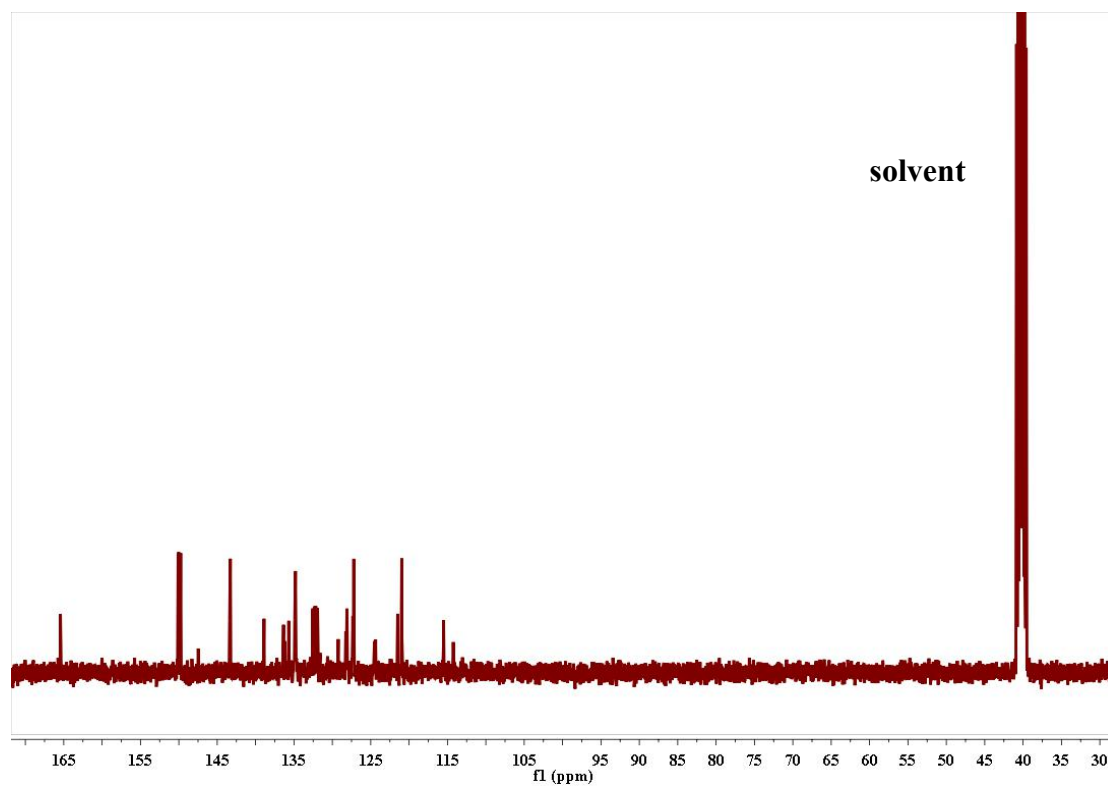


Fig. S6. ^{13}C NMR spectrum of $[\text{Zn}_2\text{-AmBis}]$ in DMSO (8.3×10^{-3} M).

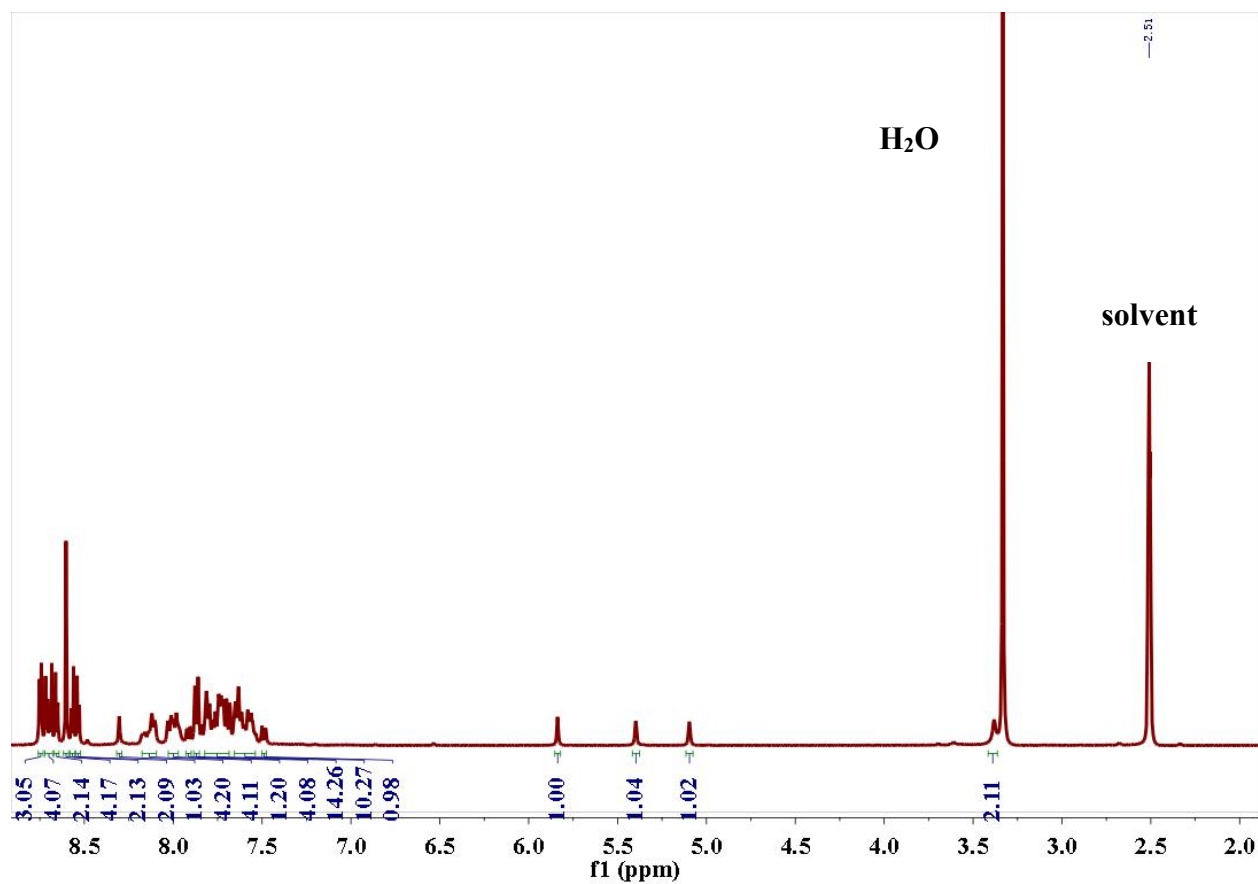


Fig. S7. ¹H NMR spectrum of [ZnNi-AmBis] in DMSO (4.4×10^{-3} M).

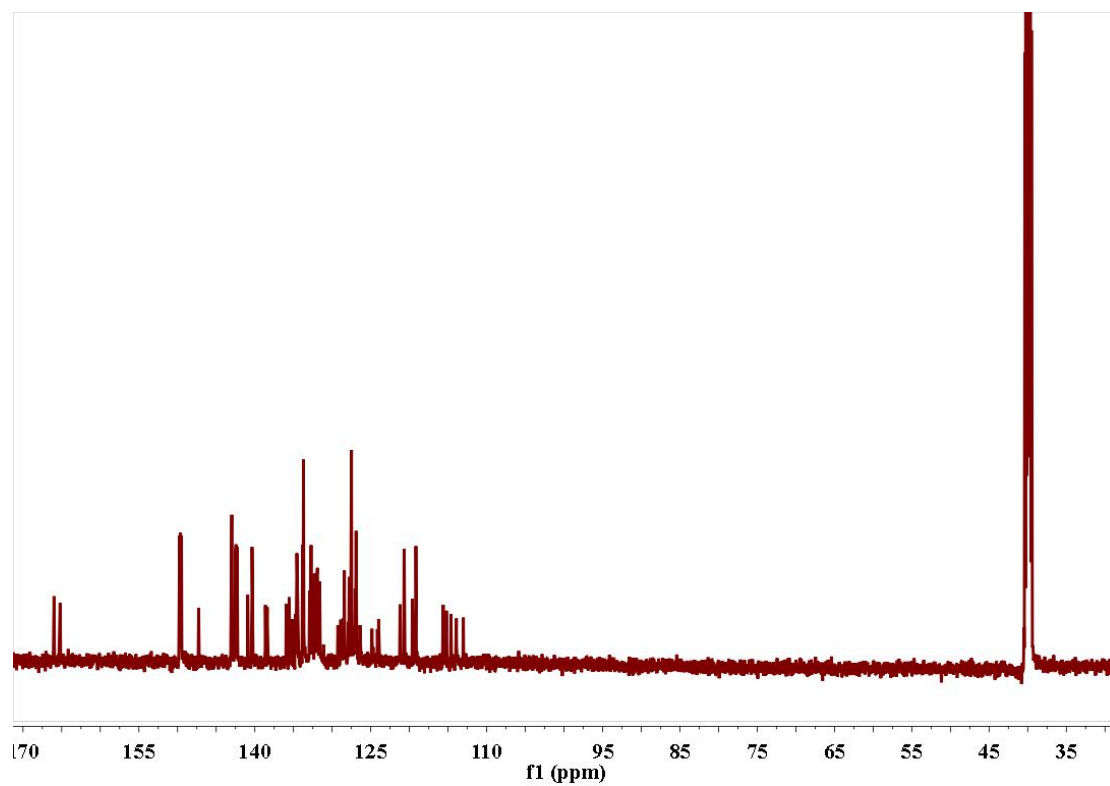


Fig. S8. ^{13}C NMR spectrum of $[\text{ZnNi-AmBis}]$ in DMSO (8.1×10^{-3} M).

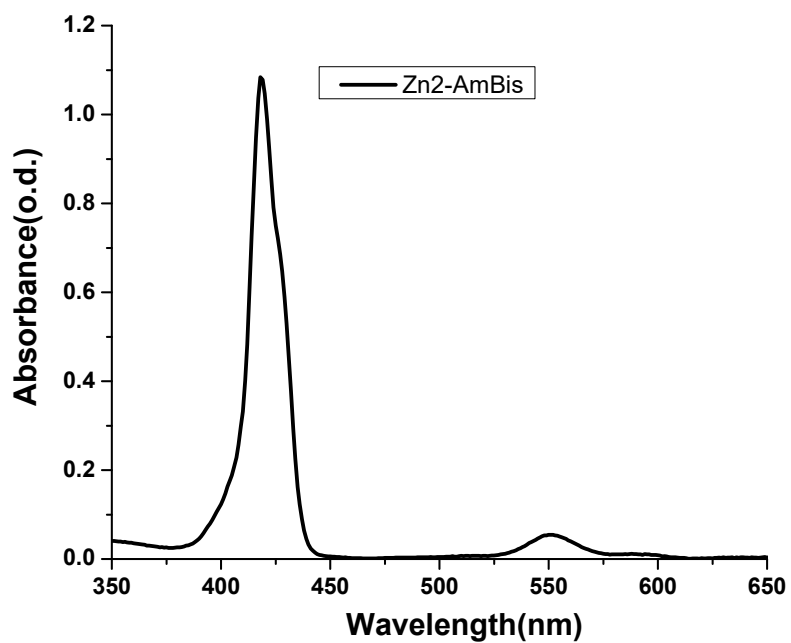


Fig. S9. UV-Vis spectrum of [Zn₂-AmBis] (1.58×10^{-6} M).

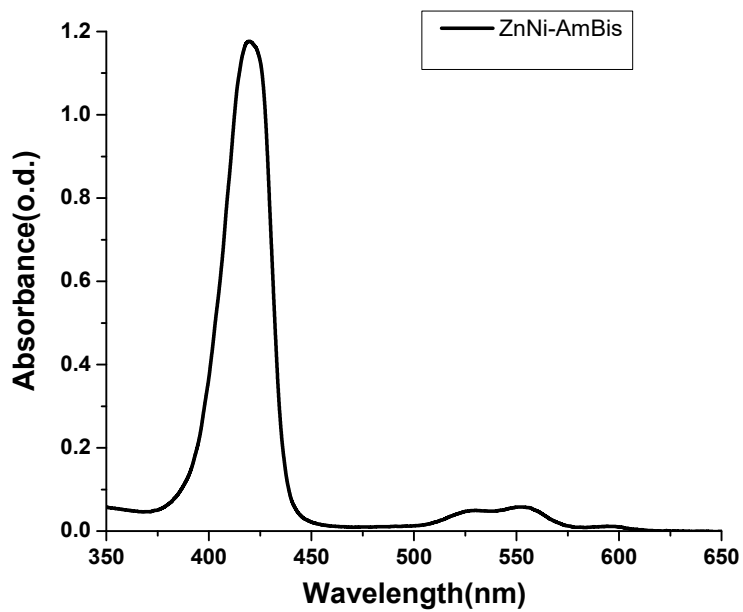


Fig. S10. UV-Vis spectrum of [ZnNi-AmBis] (2.12×10^{-6} M).

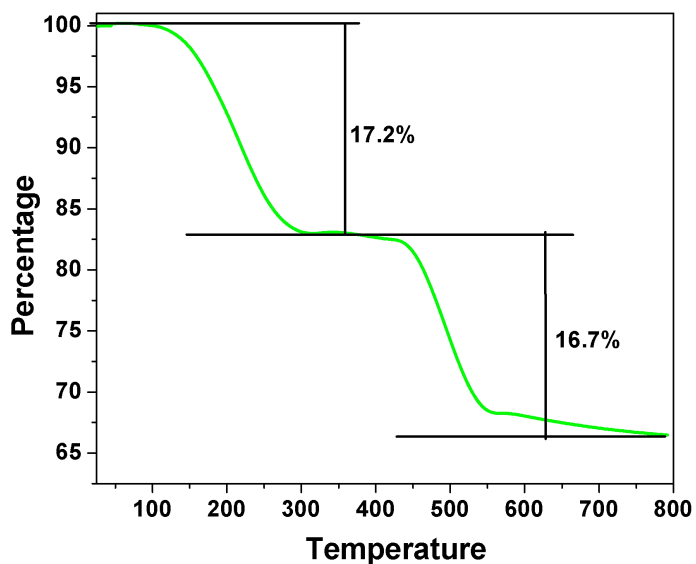


Fig. S11: DTA-TG diagram of $[\text{ZnNi-AmBis}] \cdot (1\text{-PEA}) \cdot 2\text{C}_7\text{H}_{16}$. the lost of 17.2% weight is caused by the lost of two heptane and one 1-phenylethylamine molecules (calculated lost is 17.4%)

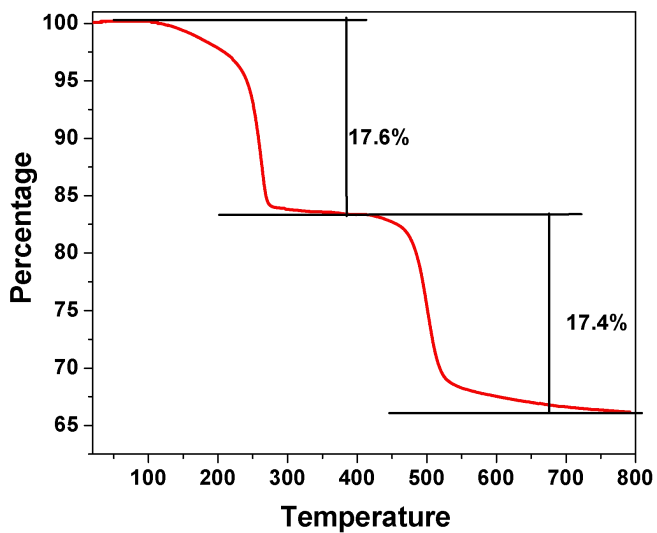


Fig. S12: DTA-TG diagram of $[\text{Zn}_2\text{-AmBis}] \cdot (\text{R-1-PEA})_2 \cdot \text{C}_7\text{H}_{16}$. The lost of 17.6% weight is caused by the lost of one heptane and two 1-phenylethylamine molecules (calculated lost is 18.2%).

Relative energies of DFT -optimized conformer A·R-1-PEA and conformer B·R-1-PEA.

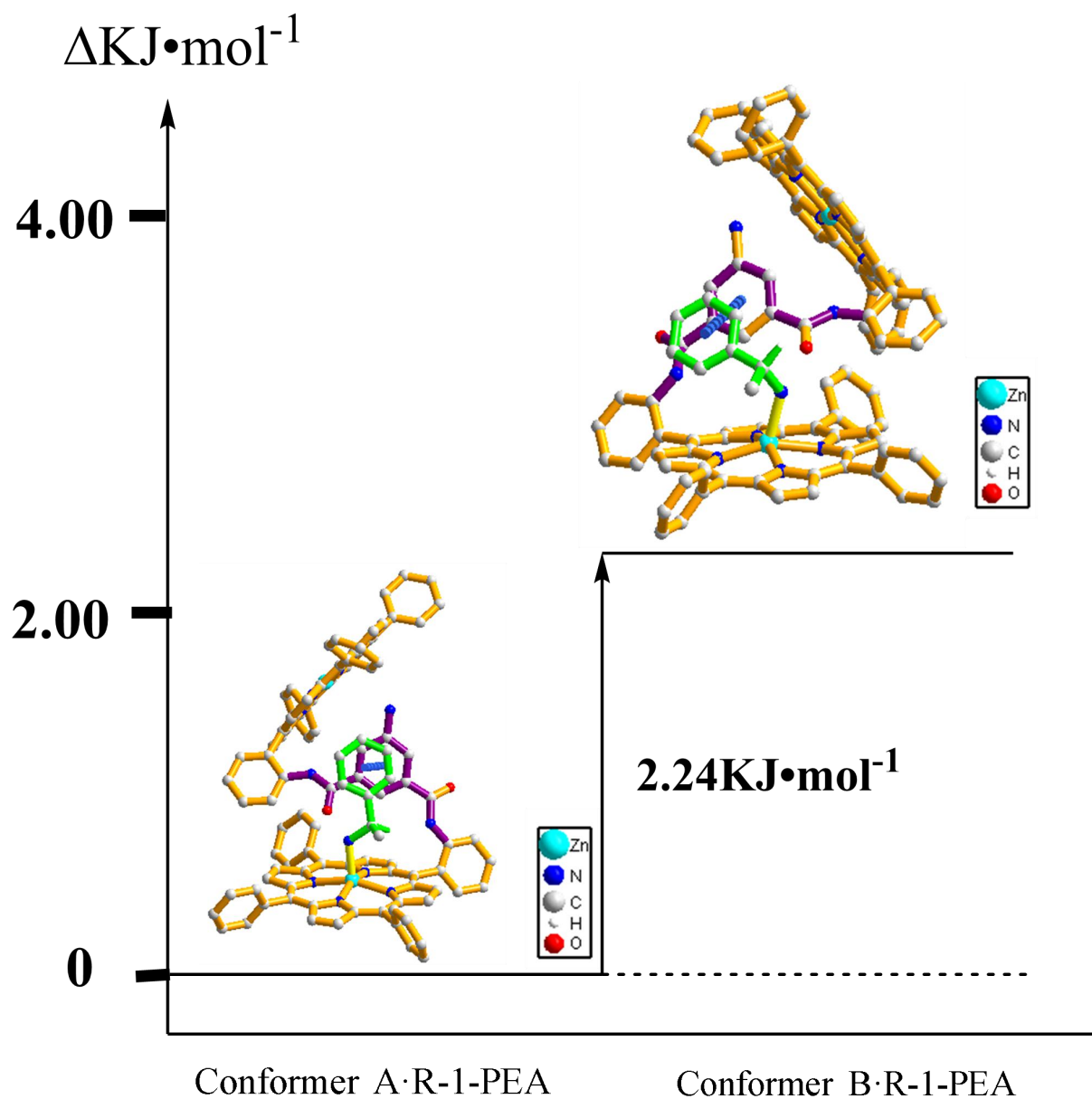


Figure S13. Relative energies of DFT-optimized conformer A·R-1-PEA and conformer B·R-1-PEA.

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

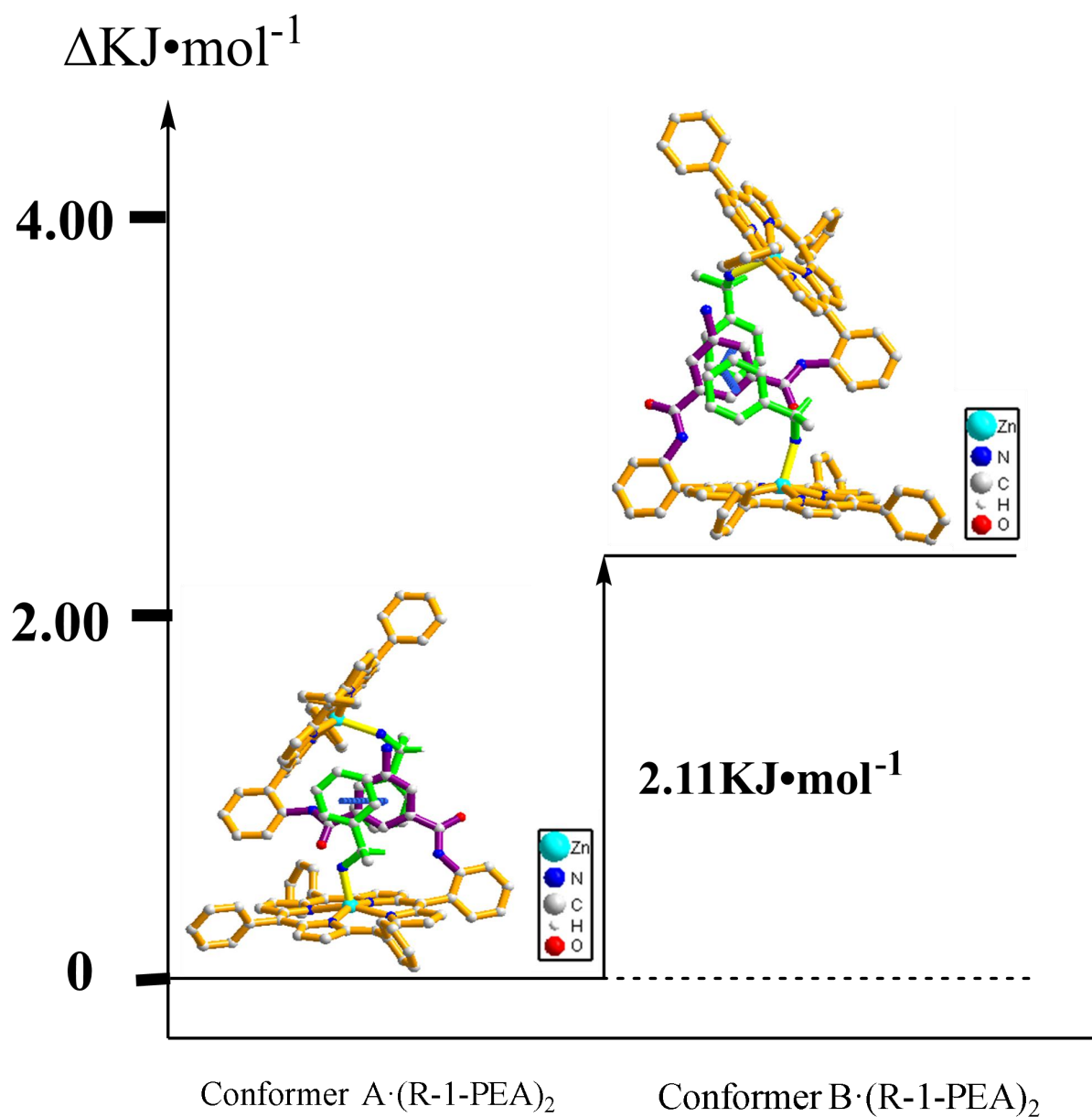
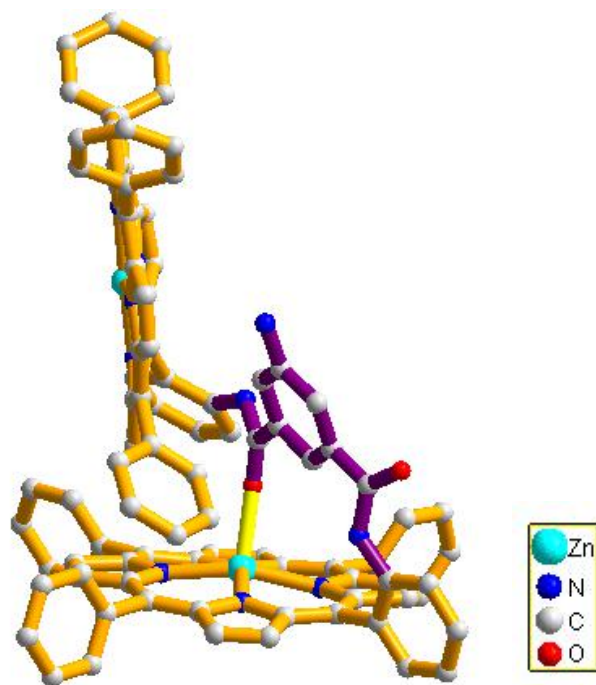


Figure S14. Relative energies of DFT-optimized conformer (A·R-1-PEA)₂ and conformer B·(R-1-PEA)₂.

Cartesian coordinates for Geometry Optimized Conformers for all the calculated structures.



Conformer A

$$\Delta = -8004.81373445 \text{ a.u.}$$

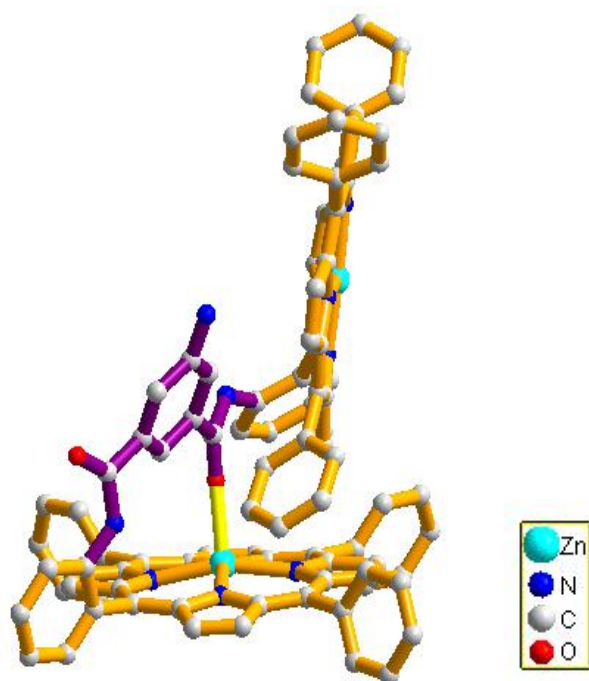
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	y	z		
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N	4.52937500	2.13455500	-0.38599700	
N	5.05769000	-0.14651700	1.29607600	
C	4.54406600	-2.81801800	0.07589300	
C	3.61051900	-2.52272800	-1.87962900	
C	2.83802400	-0.55409300	-3.17414300	
C	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	

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C	2.45292400	1.38267100	-4.24263500
H	2.20894000	2.14552800	-4.96714500
C	4.64718500	4.38390000	-0.84670000
H	4.51833500	5.31717400	-1.37541100
C	5.20773500	4.19728600	0.37260100
H	5.63318100	4.94413500	1.02776200
C	6.01989700	0.22680900	3.35597500
H	6.44969100	0.76766600	4.18717100
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C	5.28255400	-3.80321800	2.22717100
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C	4.17344000	4.81543200	-3.93538100
H	5.21163200	4.54435100	-3.76632200
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H	1.04101300	3.80145700	-3.14311600
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H	7.54256400	5.47995600	5.62814800
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C	1.31625500	-1.48898600	2.30334700
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C	0.42257300	-0.52106300	1.85578800
C	-0.95097600	-0.75271600	1.90908400
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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

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

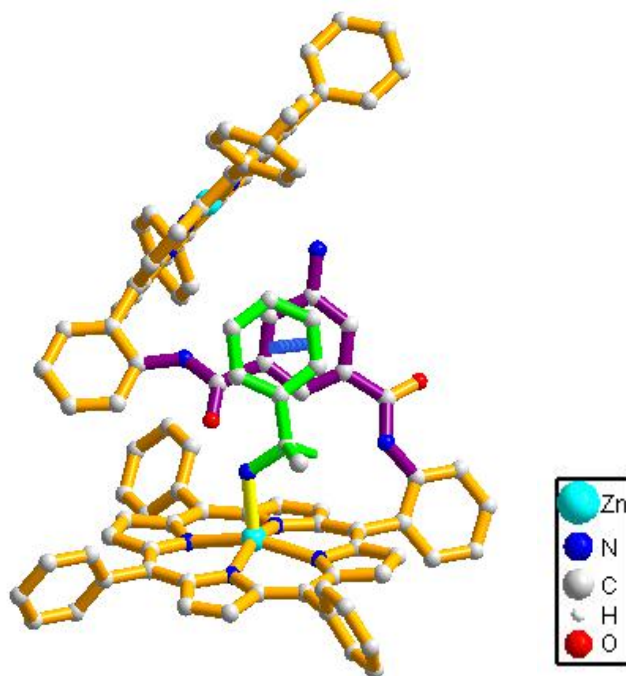
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y	z				
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N	-4.52999900	2.13458500	-0.38601600		
N	-5.05838100	-0.14671900	1.29583200		
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C	-3.61071300	-2.52252600	-1.87987800		
C	-2.83836100	-0.55373400	-3.17420800		
C	-3.05302200	1.61302200	-2.94758200		
C	-4.20388400	3.08808000	-1.30727100		
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H	-2.20867500	2.14604300	-4.96672900
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H	-1.04078000	3.80140100	-3.14233400
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C	-5.89652100	4.22001200	5.04804700
H	-5.32196100	4.42017600	5.94777600
C	-7.14301900	4.81378600	4.86929300
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H	-8.84808300	5.00601800	3.56889600
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H	-7.92651600	3.48789900	1.83950300
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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
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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

H	1.27503800	4.95406300	-1.60576900
C	-0.62814800	5.45391600	-0.72839300
H	-0.71626000	6.39373100	-1.26365400
C	-1.64436100	5.03808800	0.12325900
H	-2.52543400	5.65156900	0.26751200
C	-1.54432000	3.82495200	0.79589600
H	-2.33650200	3.48975200	1.45696000
C	-0.41148100	3.03949200	0.62517400
C	7.44971500	3.95536600	1.17643800
C	8.40549100	4.46013500	0.29056500
H	8.46511300	4.05097000	-0.71401600
C	9.27309700	5.47291000	0.68803200
H	10.00997700	5.85587100	-0.01179300
C	9.19359000	5.99577200	1.97584700
H	9.87051700	6.78618700	2.28584100
C	8.24556400	5.49816300	2.86588800
H	8.18039100	5.89858600	3.87323800
C	7.38127000	4.48237700	2.46912500
H	6.64608900	4.08756300	3.16477200
C	8.00737000	-2.94725000	0.48559200
C	9.00435600	-3.15718200	-0.47014100
H	8.98241200	-2.58611800	-1.39400000
C	10.01283000	-4.08952300	-0.24518000
H	10.78036500	-4.24497400	-0.99758600
C	10.03512100	-4.82308200	0.93788500
H	10.82057400	-5.55224400	1.11253000
C	9.04604500	-4.61879600	1.89637500
H	9.06001800	-5.18356200	2.82384100
C	8.03904200	-3.68489400	1.67179600
H	7.26895000	-3.51982100	2.42020500
C	1.30773000	-3.29622400	-1.45829200
C	1.54749000	-4.27729800	-2.42651400
H	2.43505800	-4.20576400	-3.04929200
C	0.66039600	-5.33717300	-2.59046300
H	0.85207000	-6.08663100	-3.35248200
C	-0.47602000	-5.42974200	-1.79178200
H	-1.16990900	-6.25444300	-1.92312900
C	-0.72628800	-4.45466700	-0.83114200
H	-1.60968700	-4.51605000	-0.20438300
C	0.15467400	-3.39279500	-0.67231100
H	-0.04447600	-2.63526100	0.07758600
C	-0.82261200	-2.68862100	2.82035800
C	-1.31660800	-1.48951100	2.30252200
H	-2.37940800	-1.27106500	2.26355900
C	-0.42301500	-0.52148400	1.85502500
C	0.95057500	-0.75298200	1.90849000

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

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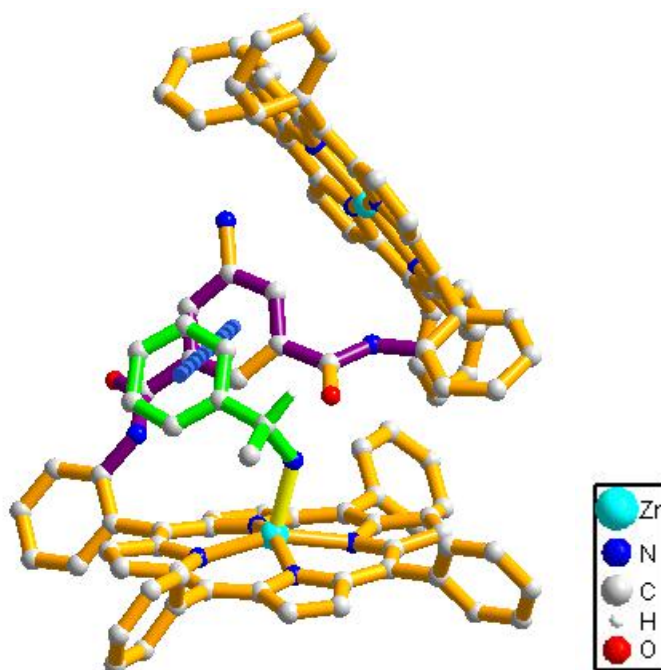
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y	z			
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H	2.97527700	0.09427500	-0.60541200	
C	3.49008300	-1.86748100	-0.89364800	
H	3.35673200	-2.23569300	0.13188600	
C	4.65847300	-2.62297400	-1.52617000	
H	4.45735800	-3.69768100	-1.53940700	
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	3.01424100	0.78346400
C	2.91400700	1.45726900	2.57304200
C	3.55947300	-0.51533500	3.27282900
C	5.96428300	-3.44003400	2.69915600
H	5.66358900	-4.24851200	3.34999600
C	7.01480100	-3.40814800	1.84603800
H	7.73982800	-4.18730500	1.65880400
C	8.87851700	-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	4.54688200	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	1.14544100	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	2.42323300	-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	9.14798200	-3.21613700	-1.33548100
H	8.38574100	-3.00984100	-2.08181900
C	10.20298600	-4.07460300	-1.62952800
H	10.26264900	-4.54067800	-2.60876600
C	11.17648600	-4.33969000	-0.66995800
H	11.99909000	-5.01077300	-0.89905500
C	11.08920200	-3.74108600	0.58400500
H	11.84661700	-3.93976400	1.33668600
C	10.03446000	-2.88204100	0.87592100
H	9.96571400	-2.41048100	1.85198200
C	6.98320500	3.64473800	-2.36970900
C	7.49482300	4.88401600	-1.97248400
H	7.52369700	5.12726500	-0.91425300
C	7.96667200	5.79207000	-2.91486200
H	8.36644500	6.74788300	-2.58877600
C	7.93274700	5.47414700	-4.27012900
H	8.29986300	6.18326600	-5.00623000
C	7.42695000	4.24244600	-4.67672200
H	7.39463100	3.98846400	-5.73231800
C	6.95676400	3.33467700	-3.73250600
H	6.56108000	2.37340000	-4.04820500
C	1.63812800	3.53336500	2.13354000
C	0.33014200	3.04296200	2.04637800
H	0.17522400	1.99642800	1.81224600
C	-0.76505400	3.87374900	2.25338900
H	-1.77049300	3.47353700	2.15597200
C	-0.57080700	5.21540500	2.56790400
H	-1.42379700	5.86960400	2.72481600
C	0.72474100	5.71120300	2.69116800
H	0.88712500	6.75236200	2.95452700
C	1.81833700	4.87750100	2.47841400
H	2.82667200	5.26877700	2.57814700
N	-5.03168400	2.25403400	-0.28716100
N	-7.15964200	0.47239200	0.43575500
N	-6.25643200	-1.40854500	-1.54362900
N	-4.24207700	0.44515600	-2.38074900
C	-3.93577300	2.94196600	-0.73397400
C	-5.55840000	2.99228500	0.73946800
C	-7.40359700	1.45568300	1.35478200
C	-8.05022500	-0.53568200	0.70083400
C	-7.29555000	-2.14248500	-1.03377900
C	-5.74220200	-2.14050800	-2.58321500
C	-3.97524900	-0.55060200	-3.28809600
C	-3.28253900	1.40313400	-2.56777800
C	-3.75140400	4.14224900	0.04740100
H	-2.95026000	4.85535900	-0.08695200

C	-4.76808600	4.18504300	0.94142600
H	-4.97119300	4.94856400	1.67843500
C	-8.48522600	1.05934800	2.22352400
H	-8.86768200	1.64398100	3.04765500
C	-8.88095200	-0.17243200	1.82299400
H	-9.65078800	-0.79494600	2.25551300
C	-7.43484600	-3.37262300	-1.76998800
H	-8.18628600	-4.12699300	-1.58675400
C	-6.47280300	-3.37230200	-2.72645200
H	-6.28038300	-4.12670000	-3.47551500
C	-2.81920200	-0.19800600	-4.07468300
H	-2.38997700	-0.80756700	-4.85697600
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H	-1.54605300	1.58649600	-3.97580100
C	-3.10750900	2.55730400	-1.79122100
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C	-8.12981200	-1.75575400	0.02373400
C	-4.66300700	-1.76221700	-3.39375000
C	-1.83626500	3.32172100	-1.98856500
C	-1.78282600	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
C	-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	5.40484800	4.49861900
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H	-6.26172400	4.85495400	5.58893700
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H	-5.47348900	3.26337800	3.86165900
C	-9.18203600	-2.72260600	0.46025700
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H	-10.81377000	-1.54231300	-0.28747000
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C	-9.80427100	-4.80835600	1.52293100
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C	-8.82768100	-3.90581700	1.11428900
H	-7.77821300	-4.11196600	1.30438300
C	-4.17738500	-2.75099600	-4.40237200
C	-4.36988300	-2.53654100	-5.76891800
H	-4.88945200	-1.64123900	-6.09864100
C	-3.90168100	-3.45961100	-6.69947700
H	-4.05934400	-3.28347800	-7.75932000
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H	-2.86939600	-5.32451900	-6.99948900
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C	-3.51042300	-3.90546900	-3.97974700
H	-3.34404700	-4.06053700	-2.91604800
C	-0.24947000	-2.42475600	1.71303900
C	0.28963700	-1.24306800	1.20105000
H	1.17236200	-0.76995500	1.62345100
C	-0.36435300	-0.60958700	0.14472200
C	-1.51749400	-1.15791300	-0.41199300
H	-1.97744400	-0.70756300	-1.28756400
C	-2.06014400	-2.34070300	0.09912400
C	-1.41899400	-2.95531200	1.17495000
H	-1.82125700	-3.86234600	1.61608400
C	0.32471600	-3.17506600	2.88703800
C	0.18401900	0.68497000	-0.37137500
N	1.65998400	-2.98096600	3.10132200
H	2.13595800	-2.36692800	2.45604400
N	-3.17741500	-2.91879700	-0.49639000
H	-3.71649300	-3.52552600	0.10630800
H	-3.77760700	-2.27889800	-1.00106500
N	-0.77495800	1.56191300	-0.76823300
H	-1.72591700	1.26604000	-0.60641300
O	-0.38151500	-3.90952700	3.56186500
O	1.38158000	0.94454900	-0.39365800
Zn	-5.71009200	0.47026400	-0.97827400



Conformer B·R-1-PEA

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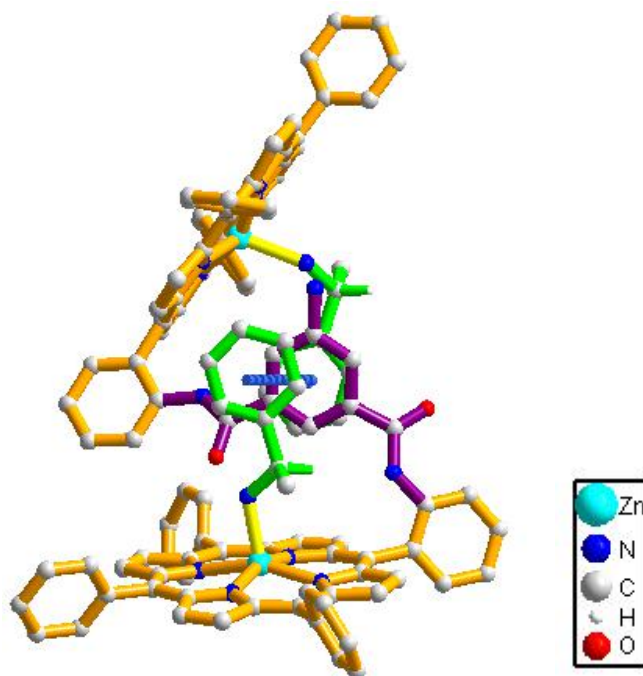
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O	0.55521700	-4.26552500	2.82316900	
N	0.79995700	1.45855800	-1.10690200	
H	1.74403300	1.21105500	-0.84924000	
N	-1.54281000	-3.52600500	2.29818400	
H	-2.05999800	-2.95457300	1.64386500	
N	3.42279400	-2.90218800	-1.05686100	
H	3.94715600	-3.54959800	-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	

C	3.15087400	2.69368900	-1.81241900
C	-6.30121300	3.07510100	-0.77476700
C	-5.02817000	3.18710500	-0.18746700
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	-5.22920600
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	4.66133600	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

H	1.87647700	1.82750800	-4.21771400
C	0.44902200	-0.80238200	-0.41345500
C	-0.21410400	-1.53387500	0.57251900
H	-1.14928800	-1.15137400	0.97251800
C	0.37355800	-2.71226300	1.03844900
C	7.50381800	-1.84261400	-0.98998400
C	-6.02427500	-3.68578700	2.09153700
H	-5.74127800	-4.62519400	2.54449500
C	7.78377800	-3.00134400	-1.79993200
H	8.52920600	-3.75077500	-1.57557200
C	8.08437600	1.05834800	2.68669000
H	8.32386400	1.56900600	3.60808400
C	-8.50769100	1.92619900	-1.16939900
H	-9.01469400	2.73866400	-1.67001500
C	2.24319800	-2.43263900	-0.48819400
C	-7.14295800	-3.41387700	1.37643300
H	-7.94966500	-4.08926600	1.12969300
C	8.58586300	-0.11535800	2.23229500
H	9.31792400	-0.75337100	2.70626500
C	1.59219000	-3.14368800	0.52152200
H	2.03120400	-4.04750000	0.93305600
C	-3.54840500	-3.45622000	3.64505800
C	-2.30023000	-4.05087400	3.36450600
C	-1.85269600	-5.13058800	4.13104200
H	-0.89164800	-5.57190700	3.90903900
C	-2.63275700	-5.61111400	5.17666600
H	-2.26850600	-6.44813900	5.76495200
C	-3.86257500	-5.03248900	5.46844900
H	-4.46823100	-5.40361700	6.28933800
C	-4.30742100	-3.96253000	4.70179800
H	-5.25957500	-3.48925300	4.92250100
C	-9.28137400	-2.10036300	-0.11303900
C	-9.55015800	-2.39727600	-1.45311000
H	-8.85028400	-2.06840500	-2.21639500
C	-10.69345700	-3.10545700	-1.80878000
H	-10.88490300	-3.32914900	-2.85426100
C	-11.58653900	-3.52847200	-0.82796000
H	-12.47997900	-4.08064100	-1.10435900
C	-11.32896300	-3.23867300	0.50922100
H	-12.02334700	-3.56121600	1.27954800
C	-10.18538500	-2.52909800	0.86333800
H	-9.98588900	-2.29891700	1.90603600
C	-6.78184300	4.23022100	-1.59042400
C	-7.02732200	5.47177100	-0.99541100
H	-6.87049700	5.58519600	0.07331600
C	-7.47004900	6.54901900	-1.75648600

H	-7.65864200	7.50537400	-1.27754700
C	-7.67583000	6.40026800	-3.12554900
H	-8.02213100	7.24066300	-3.71992400
C	-7.43782200	5.16809500	-3.72820300
H	-7.59526700	5.04316500	-4.79553200
C	-6.99397600	4.09222700	-2.96564100
H	-6.80804900	3.13024700	-3.43512000
C	-1.07019200	2.86961000	2.22041200
C	0.17180800	2.25798100	2.01117800
H	0.20346100	1.24791700	1.61714300
C	1.35719900	2.92027300	2.30558600
H	2.30995900	2.43271100	2.11901400
C	1.32309200	4.20876400	2.83142000
H	2.25029900	4.72785000	3.05682200
C	0.09582100	4.82160400	3.06813400
H	0.05785000	5.81911300	3.49629800
C	-1.08947700	4.15780000	2.76673100
H	-2.04494700	4.63569700	2.96166200
C	1.85074600	3.39263900	-2.05623500
C	1.77169500	4.66295500	-2.61897000
H	2.69127100	5.16028500	-2.91398200
C	0.54049300	5.28724800	-2.80198100
H	0.49334800	6.27744600	-3.24393200
C	-0.62292500	4.63138500	-2.41496700
H	-1.59052700	5.10801300	-2.54153100
C	-0.57314500	3.36035400	-1.85194500
H	-1.47696200	2.85543200	-1.54207900
C	0.66131900	2.73865000	-1.67200500
C	6.60127200	3.54034300	3.03216500
C	7.80249600	4.24195700	3.16537000
H	8.55663100	4.15479400	2.38835000
C	8.03232300	5.04654500	4.27713600
H	8.97015500	5.58662100	4.36669600
C	7.06252400	5.16065000	5.26941000
H	7.24196600	5.78794900	6.13737300
C	5.86240200	4.46521800	5.14591700
H	5.10330400	4.54441900	5.91833600
C	5.63394400	3.65905600	4.03526200
H	4.69987800	3.11170400	3.94100000
C	9.19038800	-2.50513200	0.69519200
C	10.55279200	-2.20993300	0.60221600
H	10.86197200	-1.26324300	0.16843200
C	11.50434200	-3.11901900	1.05481000
H	12.56046900	-2.88058300	0.97123600
C	9.74812800	-4.63357600	1.70600700
H	9.42857800	-5.57595500	2.14065000

C	4.85419000	-2.25457700	-4.76718300
C	5.45879400	-2.05305400	-6.00905000
H	6.16509300	-1.23664800	-6.13120100
C	5.16021100	-2.89112100	-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



Conformer A·(R-1-PEA)₂

$$\Delta = -8737.13207946 \text{ a.u.}$$

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	

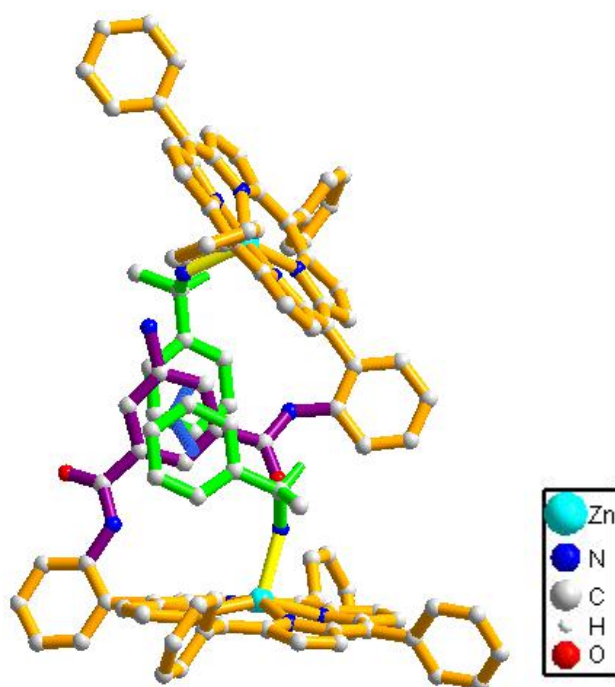
H	-1.79153700	-1.84021700	-4.34446500
C	-1.99303500	0.16765800	-3.51139800
H	-1.16567800	0.72345400	-3.92985800
C	-4.02914700	3.99299800	-0.97708100
H	-3.27598100	4.73098300	-1.21506500
C	-5.17829300	4.16923500	-0.28192500
H	-5.55194700	5.08170200	0.15990300
C	-8.91745700	1.15719500	1.22408400
H	-9.46015600	1.89610800	1.79597000
C	-9.20820700	-0.15726200	1.07675000
H	-10.03736600	-0.70336200	1.50317400
C	-7.20028300	-3.97628700	-1.51085000
H	-7.99559800	-4.68663000	-1.33521800
C	-6.09502700	-4.13852900	-2.27856800
H	-5.81475600	-5.00772700	-2.85630900
C	-1.79216100	2.86359200	-2.50467200
C	-1.87427200	3.88193600	-3.45252900
H	-2.83354800	4.07324300	-3.92472800
C	-0.75314400	4.62701800	-3.80554300
H	-0.83532900	5.41234400	-4.55032700
C	0.47057400	4.34660300	-3.20787500
H	1.35686700	4.91250000	-3.47910700
C	0.58308300	3.34294100	-2.25225700
H	1.53528500	3.12783200	-1.78643900
C	-0.54744600	2.60680700	-1.89445900
C	-7.69157400	3.78896000	1.13657300
C	-7.11970100	4.31045900	2.30060500
H	-6.20262400	3.87036900	2.68335400
C	-7.71614100	5.37939100	2.96288000
H	-7.26202100	5.77409600	3.86697100
C	-8.89241300	5.93853800	2.47024200
H	-9.35696200	6.77351900	2.98626500
C	-9.46999700	5.42382000	1.31265500
H	-10.38511100	5.85762500	0.92043400
C	-8.87263600	4.35613400	0.65032400
H	-9.31861000	3.95414100	-0.25496800
C	-9.24738500	-2.95332000	0.27733500
C	-10.54002800	-2.78792400	-0.22838400
H	-10.72744300	-2.00017900	-0.95237700
C	-11.57336700	-3.62398300	0.18244800
H	-12.57094000	-3.48637400	-0.22414300
C	-11.32800000	-4.63664100	1.10606400
H	-12.13397900	-5.28977000	1.42699100
C	-10.04395500	-4.80968600	1.61549100
H	-9.84561500	-5.59471000	2.33924900
C	-9.01099500	-3.97402400	1.20209700

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	-5.69953200
H	-2.57094400	-4.72688800	-6.77437900
C	-2.27206000	-5.90086400	-4.99477100
H	-1.77559200	-6.71466400	-5.51419300
C	-2.48107600	-5.97166500	-3.62048200
H	-2.15107000	-6.84296100	-3.06252100
C	-3.10998900	-4.92291800	-2.95676500
H	-3.28128800	-4.99054000	-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	3.52122700
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

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	6.04556100	-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	8.97140900	0.44103400	-3.39534900
C	4.97300600	3.69913300	-2.28262100
H	5.15376400	4.12919500	-3.25730200
C	4.09264400	4.11959700	-1.34015700
H	3.41372200	4.95963000	-1.39223000
C	2.72667500	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
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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
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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	0.75017500	6.63274000	1.19501100
H	0.07162900	7.47937700	1.24237600
C	0.25328600	5.34985000	0.98482400
H	-0.81356500	5.19380700	0.85350000
C	1.12218700	4.26486700	0.92145800
H	0.73409900	3.26645500	0.75226700
C	4.10856700	-1.06454400	5.02416800
C	2.85935600	-1.71682300	5.03627800
C	2.35847200	-2.25960400	6.22112200
H	1.39931700	-2.75812600	6.21122100
C	3.09982900	-2.14668800	7.39300000
H	2.70109700	-2.56994800	8.31018400
C	4.33356300	-1.50572700	7.39806200
H	4.90592900	-1.41943100	8.31633600
C	4.82860600	-0.97053900	6.21287100
H	5.78933900	-0.46433300	6.19516100
N	3.99183900	-0.57457000	-0.62662700
H	3.16452800	0.03246400	-0.57147400
H	4.36971700	-0.45324300	-1.56588100
C	3.60396000	-1.97845600	-0.43118100
H	3.35168200	-2.08719100	0.63122200
C	4.79949500	-2.88114000	-0.74011100
H	5.08872200	-2.77439500	-1.79267800
H	4.54691200	-3.93055500	-0.56503900
H	5.65345700	-2.61532500	-0.11417000
C	2.39239900	-2.40529800	-1.25146500
C	2.00739700	-1.73251200	-2.41114300
H	2.52285900	-0.82722600	-2.71630600
C	0.94216600	-2.19096600	-3.18027400
H	0.66163800	-1.64927800	-4.07876600
C	0.24357100	-3.33423200	-2.80624500
H	-0.58020800	-3.70342700	-3.41045700
C	0.61282900	-4.00637500	-1.64413400
H	0.06639800	-4.89403100	-1.33626600
C	1.67370200	-3.54221400	-0.87356600
H	1.94695100	-4.06524000	0.04030600
N	-0.51413800	1.57987700	-0.93097600
H	-1.42022600	1.27215600	-0.60199300
N	-2.36614700	-3.03915100	0.02749500
H	-2.47296300	-2.99618500	-0.98052500
H	-2.38702900	-3.99697100	0.35334300
N	2.16856300	-1.77957800	3.81149600
H	2.67980800	-1.39093300	3.03096000
O	1.71713600	1.17650000	-0.67076200
O	0.12791200	-2.64439300	4.39374600
C	-1.28137700	-2.29286300	0.50372500

C	-0.88201000	-1.15344600	-0.19405100
H	-1.36077500	-0.91444300	-1.13879700
C	0.15296300	-0.36270600	0.28735400
C	0.81826800	-0.69587700	1.46636300
H	1.58738000	-0.02644400	1.84340200
C	0.38356600	-1.80781400	2.18699100
C	-0.65951600	-2.59798500	1.70922600
H	-0.99677800	-3.43373500	2.31556700
C	0.54604700	0.86187200	-0.47651200
C	0.87323800	-2.12636500	3.57229700



Conformer B·(R-1-PEA)₂

$$\Delta = -8737.13127748 \text{ a.u.}$$

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	

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	-3.33588300	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
C	-10.03222700	-2.95160900	-0.58806300
H	-10.21237200	-2.49723800	0.38200200
C	-10.94080000	-3.86337800	-1.11639700
H	-11.83496000	-4.12042900	-0.55587800
C	-10.70735100	-4.44036100	-2.36180000
H	-11.41603000	-5.15268000	-2.77399800
C	-9.56130200	-4.10011000	-3.07570600
H	-9.37138700	-4.54892400	-4.04636300
C	-8.65351900	-3.18805400	-2.54599100
H	-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

H	-4.28111100	5.23328700	3.16725600
C	-6.81597000	3.84425500	-2.95673000
C	-7.46582400	5.04856200	-2.66949400
H	-7.72801100	5.27300500	-1.63957300
C	-7.77680900	5.94710700	-3.68489700
H	-8.28473100	6.87672100	-3.44519900
C	-7.44444000	5.65333400	-5.00476800
H	-7.68850500	6.35441200	-5.79737800
C	-6.79963700	4.45597400	-5.30264300
H	-6.53689900	4.22009000	-6.32978700
C	-6.48838000	3.55892600	-4.28559000
H	-5.98579400	2.62362900	-4.51629900
C	-2.81757500	-1.97802700	-1.27588300
C	-3.50676100	-2.78529100	-0.36777500
H	-4.56028700	-2.61243600	-0.17989000
C	-2.85551100	-3.82157400	0.29254400
H	-3.40936300	-4.43542100	0.99747600
C	-1.50636500	-4.07134700	0.04640700
H	-0.99956400	-4.88152100	0.56304900
C	-0.81135700	-3.27078300	-0.85299200
H	0.24148800	-3.44620100	-1.05082000
C	-1.46481400	-2.22634200	-1.49975000
H	-0.90797700	-1.58948300	-2.18207100
Zn	5.36194500	-0.01928900	-1.07525900
N	5.83886700	-1.92608400	-1.77450300
N	7.42254800	0.31630800	-0.83302300
N	5.10981300	2.02595900	-1.06105700
N	3.57946800	-0.17742500	-2.10615700
C	8.19351800	-2.01573800	-1.04891000
C	7.31885200	2.69003900	-0.18835800
C	2.76746400	2.13323700	-1.80808000
C	3.65133500	-2.57076500	-2.69810300
C	5.63778200	-4.10712100	-2.48207200
H	5.19103000	-4.99154700	-2.91413300
C	7.02192900	-2.57883600	-1.58074200
C	8.36258100	-0.66574900	-0.70065700
C	7.97189800	1.45225100	-0.31880600
C	5.99297300	2.94269800	-0.56213100
C	4.07768500	4.07793600	-0.89433200
H	3.30324900	4.82817300	-0.96719200
C	2.63791600	0.80366500	-2.23761900
C	3.02911700	-1.31796600	-2.62646400
C	4.97845100	-2.83220200	-2.31885300
C	6.90480400	-3.95003000	-2.02618400
H	7.69923200	-4.68243400	-2.01490800
C	9.55505200	-0.12662800	-0.08314700

H	10.45032400	-0.68531900	0.14936700
C	9.31275900	1.18545400	0.15298800
H	9.97038000	1.90682300	0.61647400
C	5.35206400	4.23658100	-0.46281300
H	5.82690100	5.14436300	-0.11925200
C	3.93883600	2.69142100	-1.28020100
C	1.44889600	0.26614800	-2.85682300
H	0.55554200	0.83080500	-3.08617400
C	1.68804700	-1.04716900	-3.09103600
H	1.03019700	-1.77095800	-3.55146800
C	9.34691000	-2.93659800	-0.81766700
C	10.52492000	-2.81839900	-1.56083400
H	10.59476500	-2.04695200	-2.32226500
C	11.59413800	-3.67982200	-1.33391400
H	12.50204700	-3.57774100	-1.92096000
C	11.50013500	-4.67118400	-0.36080300
H	12.33432100	-5.34362300	-0.18445600
C	10.33072300	-4.79805700	0.38390100
H	10.25061700	-5.56718000	1.14637800
C	9.26287500	-3.93645600	0.15593500
H	8.34913100	-4.03443500	0.73566700
C	8.07290400	3.80740100	0.45454600
C	7.69494000	4.26420500	1.72121200
H	6.85133800	3.79671400	2.22248100
C	8.38509300	5.30368100	2.33560200
H	8.08003200	5.64666500	3.31988400
C	9.46563800	5.89992700	1.69084300
H	10.00438300	6.71283300	2.16848900
C	9.85141600	5.45087400	0.43061500
H	10.69156800	5.91395900	-0.07842800
C	9.15941400	4.41129600	-0.18389100
H	9.45532200	4.06232600	-1.16919800
C	1.53981000	2.98838500	-1.86207300
C	1.39349500	4.01072000	-2.79823400
H	2.20197600	4.19327700	-3.50035800
C	0.22791200	4.77027800	-2.85213600
H	0.12683100	5.55431800	-3.59611600
C	-0.80459100	4.51194800	-1.95626200
H	-1.72383700	5.08923900	-1.98963600
C	-0.67888600	3.50893000	-1.00128500
H	-1.47933400	3.31185100	-0.30041300
C	0.48851000	2.74696600	-0.95680900
C	2.84649200	-3.70941500	-3.23978700
C	2.57404200	-3.80589800	-4.60685500
H	2.96869600	-3.04992700	-5.27969300
C	1.80284000	-4.85297400	-5.10237800

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

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