

Supporting Information Available

Table S1.- Distances (Å) between O atoms connected via H bonds for NiPB5.5, calculated by PLATON program.⁽ⁱ⁾

	O(1W)	O(2W)	O(3W)	O(4W)	O(5W)	O3	O6	O8	O10
O(1W)				2.752(17)		2.907(8)		2.869(6)	
O(2W)							2.775(6)	2.765(8)	2.762(7)
O(3W)					2.928(17)	3.000(15)			3.297(11)
O(4W)	2.752(17)				2.954(18) 2.768(21)				
O(5W)			2.928(17)	2.954(18) 2.768(21)					

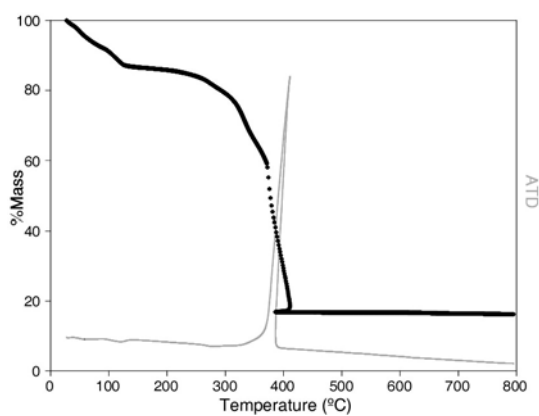


Figure S1.- TG diagram for NiPB5.5.

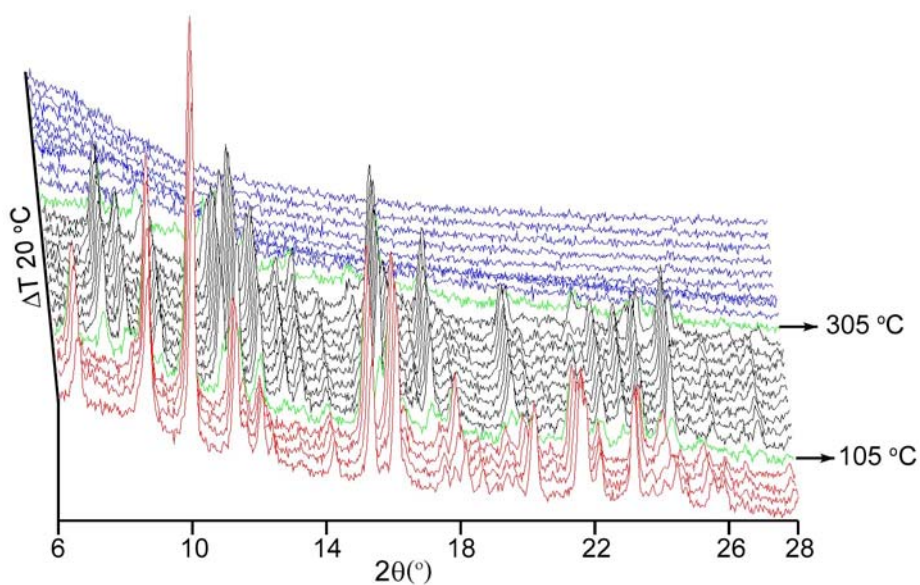


Figure S2.- TDX diagrams for NiPB5.5 from 25°C to 450°C at steps of 20°C.

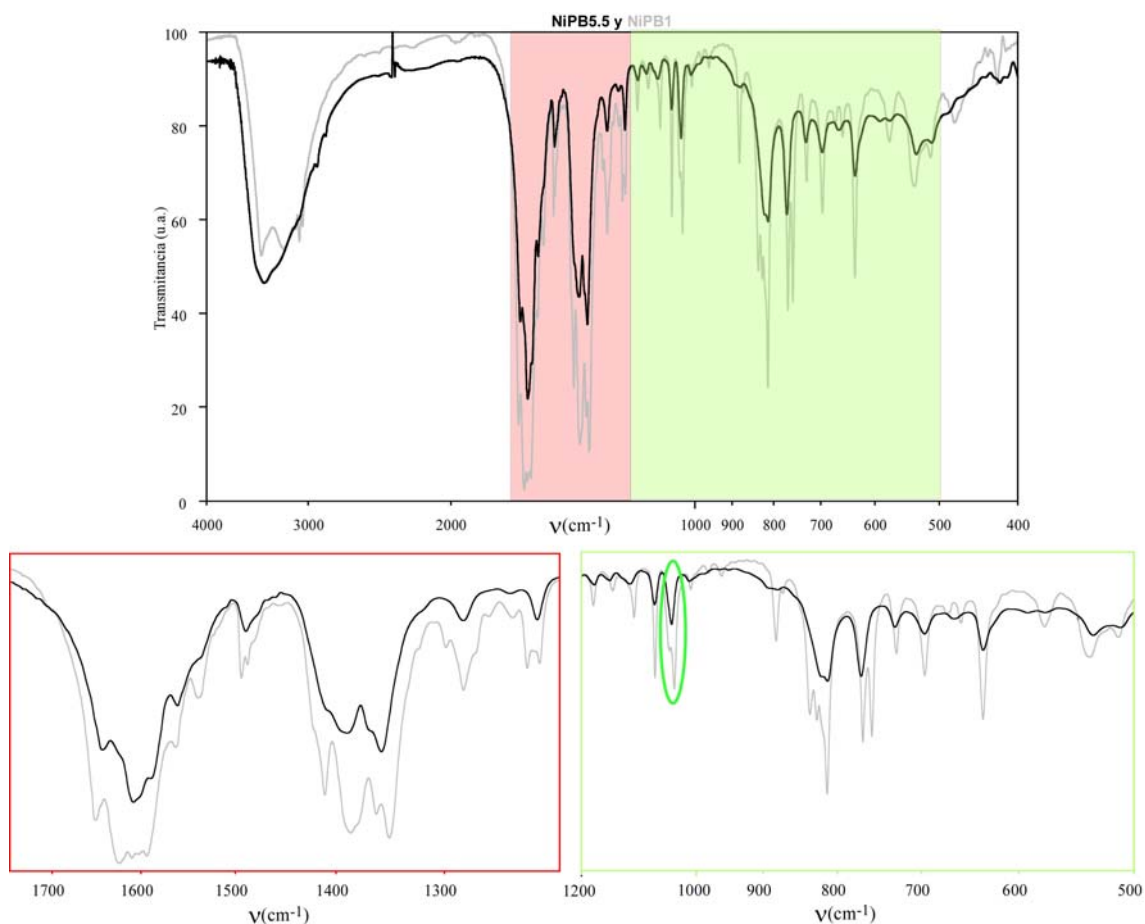


Figure S3.- IR spectra for NiPB5.5 and NiPB1. Pink zone corresponds to carboxylate groups. Green zone has been marked as it is the most significant for these compounds. Green circle is the carboxylate band. This band is split for NiPB1 because of the new metal-carboxylate bond.

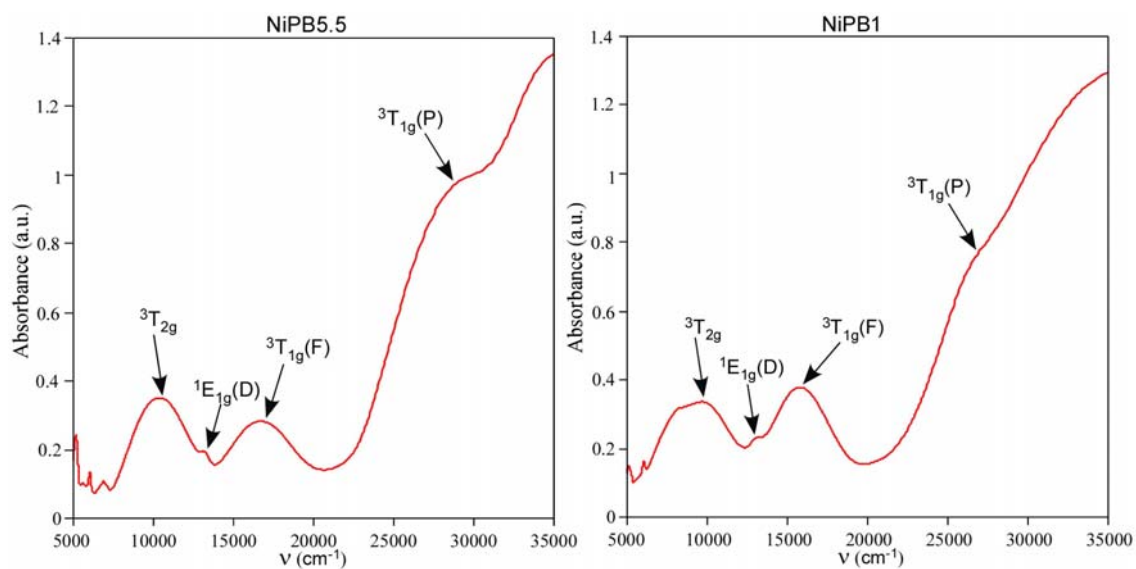


Figure S4.- UV-Vis spectra for NiPB5.5 (right) and NiPB1 (left).

Table S2.- Distances (Å) between O atoms connected via H bonds for NiPB1

	O(2)	O(3)	O(6)	O(8)	O(10)
O(2)					2.66(3)
O(3)			2.85(5)		
O(6)		2.85(5)		2.79(6)	
O(8)			2.79(6)		
O(10)	2.66(3)				

Table S3.- Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) for NiPB5.5.

Átomo	x	y	z	U _{eq} , Å ²	Occ(<1)
Ni1	-0.27580 (7)	-0.30598 (8)	-0.22185 (5)	0.0131 (3)	
Ni2	0.07255 (7)	-0.03851 (8)	-0.09494 (5)	0.0136 (3)	
N1	-0.2779 (4)	-0.3495 (5)	-0.1296 (3)	0.0160 (6)	
N2	-0.2821 (5)	-0.2467 (5)	0.1870 (3)	0.0160 (6)	
N3	-0.3308 (4)	-0.1465 (5)	-0.2100 (3)	0.0147 (5)	
N4	0.2286 (4)	-0.0079 (5)	-0.0626 (3)	0.0203 (9)	
N5	0.0826 (4)	-0.1970 (5)	-0.1327 (3)	0.0196 (5)	
O1	-0.1408 (3)	-0.2207 (4)	-0.1704 (2)	0.0147 (5)	
O2	-0.0779 (3)	-0.0513 (4)	-0.1197 (2)	0.0147 (5)	
O1W	0.3416 (4)	-0.1562 (5)	-0.3807 (3)	0.0431 (17)*	
O3	-0.6241 (3)	-0.0624 (4)	-0.2499 (2)	0.0147 (5)	
O2W	0.0707 (4)	-0.4017 (4)	0.1213 (2)	0.0234 (14)*	
O4	-0.5823 (3)	0.1239 (4)	-0.2270 (2)	0.0147 (5)	
O4W	-0.2857 (9)	-0.7652 (11)	-0.2890 (6)	0.072 (4)*	0.5
O5	0.0544 (3)	0.1139 (4)	-0.0489 (2)	0.0152 (9)	
O3W	0.4232 (9)	-0.0761 (12)	-0.4640 (6)	0.070 (4)*	0.5
O6	-0.2038 (3)	-0.4593 (4)	-0.2253 (2)	0.0152 (9)	
O5W	0.4075 (10)	-0.0909 (12)	-0.5938 (7)	0.085 (5)*	0.5
O7	0.1035 (4)	-0.1336 (4)	-0.0098 (2)	0.0196 (5)	
O8	0.1305 (3)	-0.3148 (4)	0.0275 (2)	0.0196 (5)	
O9	-0.0284 (3)	-0.4620 (4)	-0.3119 (2)	0.0196 (5)	
O10	0.0484 (3)	-0.3046 (4)	-0.3240 (2)	0.0196 (5)	
C1	-0.1899 (6)	-0.3589 (6)	-0.0706 (4)	0.0160 (6)	
C2	-0.1894 (6)	-0.3514 (6)	-0.0079 (4)	0.0160 (6)	
C3	-0.2794 (5)	-0.3297 (6)	-0.0028 (4)	0.0160 (6)	
C4	-0.3695 (5)	-0.3261 (6)	-0.0624 (3)	0.0160 (6)	
C5	-0.3674 (6)	-0.3369 (6)	-0.1240 (4)	0.0160 (6)	
C6	-0.1962 (6)	-0.2460 (6)	0.1796 (4)	0.0160 (6)	
C7	-0.1924 (6)	-0.2767 (6)	0.1193 (3)	0.0160 (6)	
C8	-0.2810 (5)	-0.3084 (6)	0.0633 (3)	0.0160 (6)	
C9	-0.3702 (5)	-0.3107 (6)	0.0711 (4)	0.0160 (6)	
C10	-0.3663 (5)	-0.2810 (6)	0.1334 (3)	0.0160 (6)	
C11	-0.2556 (5)	-0.0722 (6)	-0.1762 (3)	0.0147 (5)	
C12	-0.2746 (5)	0.0373 (6)	-0.1598 (3)	0.0147 (5)	
C13	-0.3749 (5)	0.0696 (6)	-0.1798 (3)	0.0147 (5)	
C14	-0.4512 (5)	-0.0077 (6)	-0.2127 (3)	0.0147 (5)	
C15	-0.4263 (6)	-0.1149 (6)	-0.2292 (4)	0.0147 (5)	
C16	-0.5625 (5)	0.0208 (7)	-0.2323 (3)	0.0147 (5)	
C17	-0.1494 (6)	-0.1174 (6)	-0.1540 (4)	0.0147 (5)	
C18	0.2752 (5)	-0.0183 (6)	-0.1029 (4)	0.0203 (9)	
C19	0.3795 (5)	-0.0158 (6)	-0.0801 (4)	0.0203 (9)	
C20	0.4428 (5)	-0.0023 (6)	-0.0135 (4)	0.0203 (9)	
C21	0.3957 (5)	0.0112 (6)	0.0280 (4)	0.0203 (9)	
C22	0.2913 (5)	0.0091 (6)	0.0020 (4)	0.0203 (9)	

C23	0.0262 (6)	-0.3715 (7)	-0.2883 (4)	0.0196 (5)
C24	0.0678 (5)	-0.2285 (7)	-0.1943 (4)	0.0196 (5)
C25	0.0567 (5)	-0.3449 (7)	-0.2156 (4)	0.0196 (5)
C26	0.0942 (5)	-0.2814 (7)	-0.0868 (4)	0.0196 (5)
C27	0.0657 (5)	-0.4274 (7)	-0.1689 (3)	0.0196 (5)
C28	0.0883 (5)	-0.3979 (7)	-0.1034 (4)	0.0196 (5)
C29	0.1129 (6)	-0.2404 (7)	-0.0177 (4)	0.0196 (5)

Table S4.- Atomic displacement parameters (Å²) for NiPB5.5.

Átomo	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C2	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C3	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C4	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C5	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C6	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C7	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C8	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C9	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C10	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
C11	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C12	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C13	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C14	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C15	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C16	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C17	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
C18	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
C19	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
C20	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
C21	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
C22	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
C23	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C24	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C25	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C26	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C27	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C28	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
C29	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
N1	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
N2	0.0185 (13)	0.0137 (13)	0.0167 (16)	-0.0011 (11)	0.0085 (12)	-0.0044 (12)
N3	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
N4	0.0136 (19)	0.034 (2)	0.0111 (17)	-0.0037 (17)	0.0031 (15)	-0.0028 (17)
N5	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
O1	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
O2	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
O3	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
O4	0.0179 (13)	0.0099 (13)	0.0175 (12)	-0.0013 (9)	0.0089 (11)	-0.0007 (10)
O5	0.026 (2)	0.004 (2)	0.018 (2)	0.0031 (17)	0.0118 (19)	-0.0026 (18)
O6	0.026 (2)	0.004 (2)	0.018 (2)	0.0031 (17)	0.0118 (19)	-0.0026 (18)
O7	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
O8	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
O9	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
O10	0.0272 (12)	0.0184 (13)	0.0165 (13)	0.0001 (10)	0.0126 (11)	0.0019 (10)
Ni1	0.0147 (6)	0.0102 (6)	0.0145 (6)	0.0017 (5)	0.0066 (5)	0.0011 (5)
Ni2	0.0159 (6)	0.0105 (6)	0.0153 (7)	-0.0014 (5)	0.0078 (5)	-0.0001 (5)

Table S5.- Geometric parameters (Å, °) for NiPB5.5.

C1—N1	1.373 (8)	C20—C21	1.372 (9)
C1—C2	1.378 (9)	C20—C20 ⁱ	1.511 (13)
C2—C3	1.393 (9)	C21—C22	1.375 (8)
C3—C4	1.392 (9)	C22—N4	1.325 (8)
C3—C8	1.485 (9)	C23—O10	1.246 (8)
C4—C5	1.375 (8)	C23—O9	1.282 (8)
C5—N1	1.376 (8)	C23—C25	1.490 (9)
C6—N2	1.336 (8)	C24—N5	1.326 (8)
C6—C7	1.398 (8)	C24—C25	1.416 (9)
C7—C8	1.388 (9)	C25—C27	1.368 (9)
C8—C9	1.390 (8)	C26—N5	1.363 (8)
C9—C10	1.390 (8)	C26—C28	1.393 (10)
C10—N2	1.337 (8)	C26—C29	1.498 (9)
C11—N3	1.336 (8)	C27—C28	1.372 (9)
C11—C12	1.381 (9)	C29—O8	1.255 (8)
C11—C17	1.503 (9)	C29—O7	1.267 (8)
C12—C13	1.385 (8)	N1—Ni ⁱ	2.104 (6)
C13—C14	1.364 (9)	N2—Ni ⁱⁱ	2.060 (6)
C14—C15	1.389 (9)	N3—Ni ⁱ	2.079 (6)
C14—C16	1.524 (9)	N4—Ni ⁱⁱ	2.100 (6)
C15—N3	1.321 (8)	N5—Ni ⁱⁱ	2.050 (6)
C16—O4	1.248 (8)	O1—Ni ⁱ	2.046 (4)
C16—O3	1.260 (8)	O2—Ni ⁱⁱ	2.026 (5)
C17—O2	1.248 (7)	O4—Ni ⁱⁱⁱ	2.045 (5)
C17—O1	1.274 (7)	O5—Ni ⁱⁱ	2.112 (4)
C18—N4	1.342 (8)	O6—Ni ⁱ	2.085 (4)
C18—C19	1.381 (9)	O7—Ni ⁱⁱ	2.046 (5)
C19—C20	1.354 (9)	O9—Ni ^{iv}	2.060 (5)

N1—C1—C2	122.1 (7)	C1—N1—C5	117.1 (6)
C1—C2—C3	120.3 (7)	C1—N1—Ni ⁱ	121.7 (5)
C4—C3—C2	117.8 (7)	C5—N1—Ni ⁱ	118.7 (4)
C4—C3—C8	120.1 (7)	C6—N2—C10	116.4 (6)
C2—C3—C8	122.2 (6)	C6—N2—Ni ⁱⁱ	118.4 (5)
C5—C4—C3	120.2 (7)	C10—N2—Ni ⁱⁱ	125.2 (5)
C4—C5—N1	122.3 (7)	C15—N3—C11	119.5 (7)
N2—C6—C7	123.1 (7)	C15—N3—Ni ⁱ	128.3 (5)
C8—C7—C6	119.9 (7)	C11—N3—Ni ⁱ	112.1 (5)
C7—C8—C9	117.1 (7)	C22—N4—C18	114.2 (6)
C7—C8—C3	120.2 (7)	C22—N4—Ni ⁱⁱ	121.6 (5)
C9—C8—C3	122.5 (6)	C18—N4—Ni ⁱⁱ	123.7 (5)
C8—C9—C10	118.9 (7)	C24—N5—C26	118.1 (7)
N2—C10—C9	124.5 (7)	C24—N5—Ni ⁱⁱ	130.7 (5)
N3—C11—C12	121.9 (7)	C26—N5—Ni ⁱⁱ	110.6 (5)
N3—C11—C17	115.7 (7)	C17—O1—Ni ⁱ	114.8 (5)
C12—C11—C17	122.3 (7)	C17—O2—Ni ⁱⁱ	136.9 (5)
C11—C12—C13	118.2 (7)	C16—O4—Ni ⁱⁱⁱ	123.4 (5)
C14—C13—C12	119.7 (7)	C29—O7—Ni ⁱⁱ	113.3 (5)
C13—C14—C15	118.6 (7)	C23—O9—Ni ^{iv}	128.5 (5)
C13—C14—C16	122.0 (7)	O4 ^v —Ni ⁱ —O1	174.27 (19)
C15—C14—C16	119.4 (6)	O4 ^v —Ni ⁱ —N2 ^{vi}	89.0 (2)
N3—C15—C14	121.9 (7)	O1—Ni ⁱ —N2 ^{vi}	90.8 (2)
O4—C16—O3	126.8 (7)	O4 ^v —Ni ⁱ —N3	93.9 (2)
O4—C16—C14	116.4 (6)	O1—Ni ⁱ —N3	80.4 (2)
O3—C16—C14	116.8 (7)	N2 ^{vi} —Ni ⁱ —N3	90.3 (2)

O2—C17—O1	126.0 (7)	O4 ^v —Ni1—O6	92.70 (18)
O2—C17—C11	117.0 (7)	O1—Ni1—O6	93.03 (18)
O1—C17—C11	117.0 (7)	N2 ^{vi} —Ni1—O6	91.4 (2)
N4—C18—C19	124.0 (7)	N3—Ni1—O6	173.2 (2)
C20—C19—C18	121.0 (7)	O4 ^v —Ni1—N1	89.6 (2)
C19—C20—C21	115.4 (6)	O1—Ni1—N1	90.2 (2)
C19—C20—C20 ⁱ	122.6 (8)	N2 ^{vi} —Ni1—N1	175.4 (2)
C21—C20—C20 ⁱ	121.9 (9)	N3—Ni1—N1	85.5 (2)
C20—C21—C22	120.9 (7)	O6—Ni1—N1	93.0 (2)
N4—C22—C21	124.4 (7)	O2—Ni2—O7	89.00 (19)
O10—C23—O9	122.9 (7)	O2—Ni2—N5	95.1 (2)
O10—C23—C25	120.7 (7)	O7—Ni2—N5	82.0 (2)
O9—C23—C25	116.3 (7)	O2—Ni2—O9 ^{vii}	86.37 (18)
N5—C24—C25	122.9 (7)	O7—Ni2—O9 ^{vii}	171.9 (2)
C27—C25—C24	117.4 (7)	N5—Ni2—O9 ^{vii}	91.7 (2)
C27—C25—C23	123.1 (7)	O2—Ni2—N4	173.2 (2)
C24—C25—C23	119.2 (7)	O7—Ni2—N4	90.7 (2)
N5—C26—C28	121.9 (7)	N5—Ni2—N4	91.6 (2)
N5—C26—C29	115.6 (7)	O9 ^{vii} —Ni2—N4	94.7 (2)
C28—C26—C29	122.5 (7)	O2—Ni2—O5	80.75 (19)
C25—C27—C28	120.9 (8)	O7—Ni2—O5	92.09 (19)
C27—C28—C26	118.5 (7)	N5—Ni2—O5	172.9 (2)
O8—C29—O7	124.1 (7)	O9 ^{vii} —Ni2—O5	93.78 (18)
O8—C29—C26	117.8 (7)	N4—Ni2—O5	92.5 (2)
O7—C29—C26	117.9 (7)		

Table S6.- Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) for NiPB1.

Átomo	x	y	z	Uiso, Å ²
Ni1	-0.1199(11)	-0.2202(11)	0.1750(10)	0.119
Ni2	0.1623(8)	-0.2201(12)	0.0912(8)	0.119
N1	-0.2191(22)	-0.2355(20)	0.0806(16)	0.119
N2	-0.5298(18)	-0.2701(25)	-0.2332(17)	0.119
N3	-0.1088(11)	-0.0286(12)	0.1770(6)	0.119
N4	0.2958(16)	-0.1655(11)	0.0520(18)	0.119
N5	0.2112(9)	-0.3986(15)	0.1190(10)	0.119
O1	0.0014(8)	-0.1972(19)	0.1207(5)	0.119
O10	0.3284(12)	-0.4716(26)	0.3110(15)	0.119
O2	0.0847(11)	-0.0495(19)	0.0680(6)	0.119
O3	-0.1978(17)	0.3934(21)	0.2170(9)	0.119
O4	-0.2756(10)	0.2336(28)	0.2600(6)	0.119
O6	-0.0940(34)	-0.3972(29)	0.1716(27)	0.119
O7	0.1068(8)	-0.3216(21)	0.0018(12)	0.119
O8	0.0983(9)	-0.5179(28)	-0.0349(13)	0.119
O9	0.2740(16)	-0.6697(23)	0.3066(18)	0.119
C1	-0.3024(23)	-0.3053(17)	0.0752(16)	0.119
C2	-0.3634(19)	-0.3122(13)	0.0149(17)	0.119
C3	-0.3422(16)	-0.2470(15)	-0.0434(15)	0.119
C4	-0.2579(18)	-0.1760(12)	-0.0389(16)	0.119
C5	-0.1991(17)	-0.1718(15)	0.0222(18)	0.119
C6	-0.5390(16)	-0.3461(20)	-0.1802(20)	0.119
C7	-0.4791(17)	-0.3402(14)	-0.1181(18)	0.119
C8	-0.4059(16)	-0.2526(14)	-0.1091(15)	0.119
C9	-0.3959(17)	-0.1737(14)	-0.1637(16)	0.119
C10	-0.4589(20)	-0.1866(20)	-0.2233(16)	0.119
C11	-0.1618(10)	0.0602(18)	0.2042(6)	0.119
C12	-0.1484(10)	0.1850(17)	0.1922(6)	0.119
C13	-0.0778(11)	0.2222(18)	0.1509(6)	0.119
C14	-0.0213(10)	0.1335(18)	0.1218(6)	0.119

C15	-0.0397(10)	0.0112(17)	0.1366(6)	0.119
C16	0.0211(10)	-0.0869(18)	0.1056(6)	0.119
C17	-0.2121(11)	0.2803(20)	0.2256(6)	0.119
C18	0.2943(10)	-0.1165(13)	-0.0117(16)	0.119
C19	0.3737(8)	-0.0519(11)	-0.0319(11)	0.119
C20	0.4564(6)	-0.0353(6)	0.0115(7)	0.119
C21	0.4588(16)	-0.0856(9)	0.0770(8)	0.119
C22	0.3771(19)	-0.1488(9)	0.0936(13)	0.119
C23	0.2507(10)	-0.4247(20)	0.1819(11)	0.119
C24	0.2363(10)	-0.5394(21)	0.2114(11)	0.119
C25	0.1804(11)	-0.6251(18)	0.1746(12)	0.119
C26	0.1386(10)	-0.5966(14)	0.1083(12)	0.119
C27	0.1560(7)	-0.4813(14)	0.0821(10)	0.119
C28	0.1170(7)	-0.4379(20)	0.0109(10)	0.119
C29	0.2848(11)	-0.5628(23)	0.2840(11)	0.119

Table S7.- Geometric parameters (Å, °) for NiPB1.

A1	A2	dist
Ni1		
Ni1	O1	2.05(2)
Ni1	N3	2.08(2)
Ni1	N1	2.18(3)
Ni1	N2	2.07(3)
Ni1	O4	2.04(2)
Ni1	O6	1.95(3)
Ni2		
Ni2	O1	2.32(2)
Ni2	O2	2.16(2)
Ni2	C16	2.44(2)
Ni2	O9	2.15(4)
Ni2	O7	2.13(2)
Ni2	N5	2.10(2)
Ni2	N4	2.11(3)
Bipy2		
N4	C18	1.34(4)
N4	C22	1.32(4)
C18	C19	1.37(2)
C19	C20	1.35(2)
C20	C21	1.37(2)
C21	C22	1.37(3)
C20	C20	1.51(1)
Bipy1		
N1	C1	1.36(4)
N1	C5	1.37(4)
C1	C2	1.37(4)
C2	C3	1.38(4)
C3	C4	1.38(3)
C4	C5	1.37(4)

C3	C8	1.47(4)
C6	C7	1.39(5)
C7	C8	1.38(3)
C8	C9	1.37(4)
C9	C10	1.38(4)
N2	C10	1.32(4)
N2	C6	1.33(5)
PDC1		
C11	C12	1.39(3)
C12	C13	1.36(2)
C13	C14	1.38(2)
C14	C15	1.38(3)
C15	C16	1.50(2)
N3	C11	1.34(2)
N3	C15	1.34(2)
O1	C16	1.27(3)
O2	C16	1.25(2)
C12	C17	1.53(2)
O3	C17	1.26(3)
O4	C17	1.24(2)
PDC2		
C23	C24	1.39(3)
C24	C25	1.36(3)
C25	C26	1.39(3)
C26	C27	1.38(2)
C27	C28	1.50(3)
N5	C23	1.31(3)
N5	C27	1.34(2)
O7	C28	1.28(3)
O8	C28	1.25(3)
C24	C29	1.52(3)
O9	C29	1.25(4)
O10	C29	1.24(3)

A1	A2	A3	angle
Ni1			
N2	Ni1	O6	83(2)
O6	Ni1	N1	90(2)
N1	Ni1	N3	97(1)
N3	Ni1	N2	90(1)
O4	Ni1	N2	82(1)
O4	Ni1	O6	85(1)
O4	Ni1	N1	95(1)
O4	Ni1	N3	106.7(9)

O1	Ni1	N2	90(1)
O1	Ni1	O6	87(1)
O1	Ni1	N1	93(1)
O1	Ni1	N3	80.1(8)
N1	Ni1	N2	172(1)
N3	Ni1	O6	165(2)
O1	Ni1	O4	169(1)
Ni2			
O9	Ni2	N5	85(1)
N5	Ni2	O7	79.2(8)
O7	Ni2	O2	98.2(8)
O2	Ni2	O1	60.3(6)
O2	Ni2	O9	97(1)
O1	Ni2	O9	93.5(9)
O1	Ni2	O7	88.8(8)
O1	Ni2	N5	108.7(8)
O2	Ni2	N4	96.0(9)
O7	Ni2	N4	96(1)
N4	Ni2	O9	88(1)
N5	Ni2	N4	95.0(9)
O9	Ni2	O7	164(1)
N5	Ni2	O2	168.9(9)
N4	Ni2	O1	156(1)
C16	Ni2	N5	138.7(8)
C16	Ni2	N4	125.8(9)

i <http://www.chem.gla.ac.uk/~louis/software/platon/>