

ANEXO II
Estructuras Cristalinas

II. 1. Estructura Cristalina del complejo $[\text{Co}(\text{HL}^0)_2\text{Cl}(\text{H}_2\text{O})]\text{Cl} \cdot \text{H}_2\text{O}$

Datos Cristalográficos:

Fórmula $[\text{Co}(\text{C}_{14}\text{H}_{11}\text{N}_3)_2\text{Cl}(\text{H}_2\text{O})]\text{Cl} \cdot \text{H}_2\text{O}$

Peso molecular 608,390 g/mol

Parámetros de celda $a = 10,466(4) \text{ \AA}$

$b = 10,918(5) \text{ \AA}$

$c = 13,436(4) \text{ \AA}$

$= 74,99(3)^\circ$

$= 78,02(3)^\circ$

$= 72,77(4)^\circ$

Volumen de la celda $1402,0(1) \text{ \AA}^3$

Moléculas por celda $Z = 2$

Grupo espacial $P\bar{1}$

Sistema Triclínico

Valor de R(F) $R(F) = 0,035$

$R_w(F^2) = 0,103$

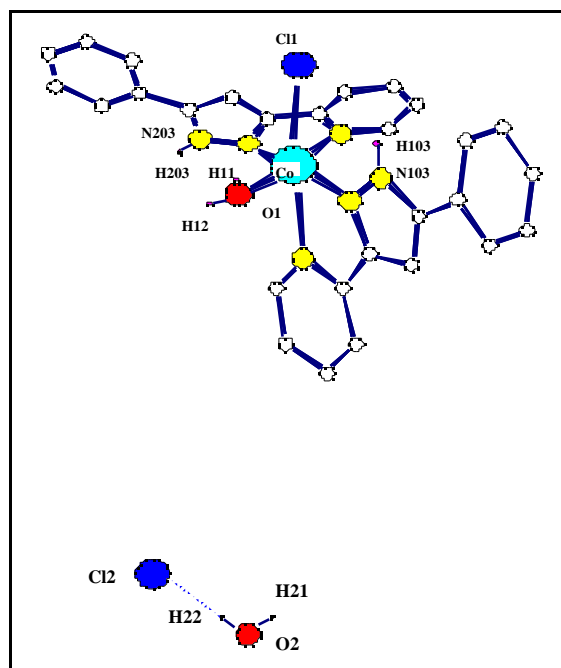


Tabla 1. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del complejo $[\text{Co}(\text{HL}^0)_2\text{Cl}(\text{H}_2\text{O})]\text{Cl} \cdot \text{H}_2\text{O}$, (excepto los átomos de hidrógeno).

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 | Beq (Å^2) |
|-------|---------------|---------------|---------------|----------------------|
| Co | 4000(0) | 7512(0) | 6715(0) | 3,01(1) |
| Cl1 | 4261(0) | 9686(0) | 6464(0) | 3,83(2) |
| O1 | 2597(2) | 8066(2) | 5677(1) | 4,40(5) |
| N101 | 4189(2) | 5453(2) | 6809(1) | 3,46(*) |
| N102 | 5705(2) | 6947(2) | 5628(1) | 3,22(*) |
| N103 | 6672(2) | 7495(2) | 5032(1) | 3,31(*) |
| C101 | 3333(3) | 4763(2) | 7366(2) | 4,24(8) |
| C102 | 3563(2) | 3441(2) | 7458(2) | 4,76(9) |
| C103 | 4743(3) | 2791(2) | 6941(2) | 4,66(10) |
| C104 | 5633(3) | 3489(2) | 6341(2) | 3,94(8) |
| C105 | 5333(2) | 4820(2) | 6286(2) | 3,22(6) |
| C106 | 6195(2) | 5660(2) | 5657(2) | 3,08(6) |
| C107 | 7451(2) | 5409(2) | 5061(2) | 3,35(7) |

| | | | | |
|------|----------|---------|----------|----------|
| C108 | 7740(2) | 6607(2) | 4663(2) | 3,35(6) |
| C109 | 8920(2) | 6976(2) | 4000(2) | 3,56(7) |
| C110 | 9836(2) | 6101(3) | 3425(2) | 4,51(8) |
| C111 | 10972(3) | 6442(3) | 2823(2) | 5,40(9) |
| C112 | 11222(3) | 7600(3) | 2785(2) | 5,42(10) |
| C113 | 10335(3) | 8464(3) | 3347(2) | 5,58(11) |
| C114 | 9184(3) | 8158(3) | 3953(2) | 4,58(9) |
| N201 | 5172(2) | 6952(2) | 8000(1) | 3,31(5) |
| N202 | 2543(2) | 7551(2) | 8063(1) | 3,40(6) |
| N203 | 1198(2) | 7981(2) | 8266(1) | 3,72(6) |
| C201 | 6518(2) | 6683(2) | 7918(2) | 4,06(8) |
| C202 | 7184(3) | 6409(3) | 8754(2) | 5,35(10) |
| C203 | 6442(3) | 6392(3) | 9726(2) | 6,14(12) |
| C204 | 5061(3) | 6666(3) | 9833(2) | 5,02(10) |
| C205 | 4449(2) | 6958(2) | 8952(2) | 3,46(7) |
| C206 | 2989(2) | 7337(2) | 8963(2) | 3,38(7) |
| C207 | 1929(2) | 7629(2) | 9739(2) | 3,80(7) |
| C208 | 776(2) | 8054(2) | 9276(2) | 3,66(7) |
| C209 | -636(2) | 8602(2) | 9667(2) | 3,98(7) |
| C210 | -994(3) | 8719(2) | 10699(2) | 4,80(9) |
| C211 | -2292(3) | 9289(3) | 11076(3) | 5,72(10) |
| C212 | -3255(3) | 9755(3) | 10448(3) | 6,53(13) |
| C213 | -2938(3) | 9662(4) | 9416(3) | 7,07(14) |
| C214 | -1623(3) | 9075(3) | 9029(2) | 5,60(10) |
| Cl2 | 225(0) | 2422(0) | 3376(0) | 5,20(2) |
| O2 | 2726(2) | -22(2) | 3930(2) | 6,38(8) |

Tabla 2. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos de hidrógeno del complejo $[\text{Co}(\text{HL}^0)_2\text{Cl}(\text{H}_2\text{O})]\text{Cl} \cdot \text{H}_2\text{O}$.

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 |
|-------|---------------|---------------|---------------|
| H11 | 2592(31) | 8715(26) | 5153(21) |
| H12 | 1780(24) | 8016(30) | 5837(24) |
| H103 | 6616(2) | 8322(2) | 4900(1) |
| H101 | 2532(3) | 5203(2) | 7712(2) |
| H10A | 2938(3) | 2993(2) | 7860(2) |
| H133 | 4937(3) | 1889(2) | 6997(2) |
| H104 | 6427(3) | 3069(2) | 5975(2) |
| H107 | 7990(2) | 4596(2) | 4951(2) |
| H110 | 9682(2) | 5297(3) | 3448(2) |
| H111 | 11575(3) | 5864(3) | 2437(2) |

| | | | |
|------|----------|----------|----------|
| H112 | 11994(3) | 7811(3) | 2379(2) |
| H113 | 10507(3) | 9260(3) | 3320(2) |
| H114 | 8585(3) | 8750(3) | 4329(2) |
| H203 | 664(2) | 8187(2) | 7807(1) |
| H201 | 7024(2) | 6683(2) | 7261(2) |
| H20A | 8120(3) | 6238(3) | 8667(2) |
| H233 | 6873(3) | 6196(3) | 10308(2) |
| H204 | 4546(3) | 6655(3) | 10487(2) |
| H207 | 1984(2) | 7553(2) | 10436(2) |
| H210 | -339(3) | 8404(2) | 11142(2) |
| H211 | -2512(3) | 9357(3) | 11770(3) |
| H212 | -4137(3) | 10141(3) | 10710(3) |
| H213 | -3603(3) | 9990(4) | 8982(3) |
| H214 | -1409(3) | 9002(3) | 8336(2) |
| H21 | 3451(25) | 235(30) | 3737(25) |
| H22 | 2051(26) | 632(27) | 3818(26) |

AII. 2. Estructura cristalina del complejo $[\text{Ni}(\text{HL}^0)_2\text{Cl}(\text{H}_2\text{O})][\text{Ni}(\text{HL}^0)_2(\text{H}_2\text{O})_2]\text{Cl}_3 \cdot \text{CH}_3\text{OH} \cdot \text{H}_2\text{O}$

Datos cristalográficos:

| | |
|---------------------|--|
| Fórmula | $[\text{Ni}(\text{C}_{14}\text{H}_{11}\text{N}_3)_2\text{Cl}(\text{H}_2\text{O})][\text{Ni}(\text{C}_{14}\text{H}_{11}\text{N}_3)_2(\text{H}_2\text{O})_2]\text{Cl}_3 \cdot \text{CH}_3\text{OH} \cdot \text{H}_2\text{O}$ |
| Peso molecular | 1239,280 g/mol |
| Parámetros de celda | $a = 9,374(2) \text{ \AA}$ $b = 13,257(5) \text{ \AA}$ $c = 23,269(7) \text{ \AA}$ $\alpha = 87,89(3)^\circ$ $\beta = 85,80(2)^\circ$ $\gamma = 87,81(3)^\circ$ |
| Volumen de la celda | $2880,0(2) \text{ \AA}^3$ |
| Moléculas por celda | $Z = 2$ |
| Grupo espacial | $P \bar{1}$ |
| Sistema | Triclínico |
| Valor de R(F) | $R(F) = 0,059$ |
| | $R_w(F^2) = 0,175$ |

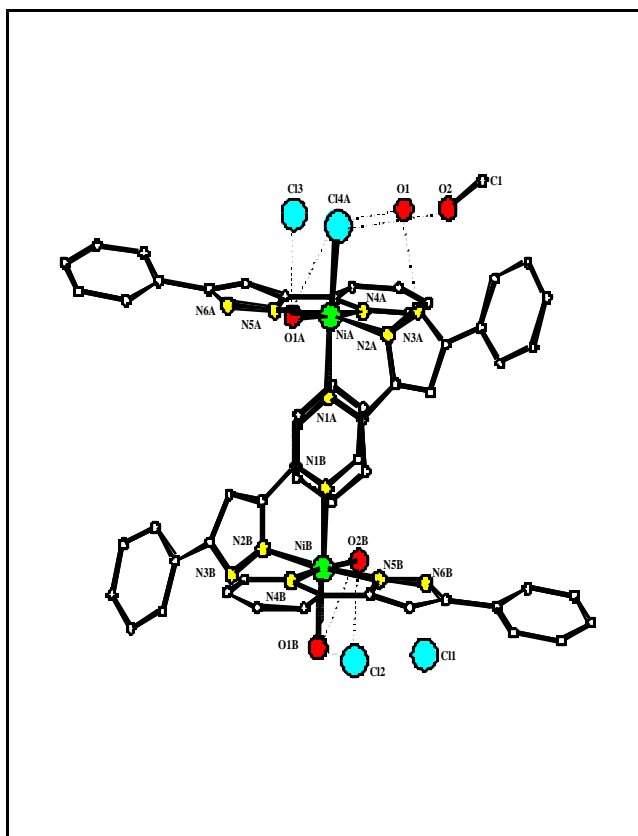


Tabla 3. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del **cation (A)** $[\text{Ni}(\text{HL}^0)_2\text{Cl}(\text{H}_2\text{O})]^+$, (excepto para los átomos de hidrógeno).

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 | Ueq (\AA^2) |
|-------|---------------|---------------|---------------|------------------------|
| NiA | 2014(1) | 3900(1) | 1472(1) | 37(1) |
| O1A | 1319(3) | 3145(2) | 2247(1) | 50(1) |
| Cl4A | -124(1) | 4928(1) | 1563(1) | 58(1) |
| N1A | 3997(3) | 3056(2) | 1470(1) | 41(1) |
| N2A | 3207(3) | 4759(2) | 1964(1) | 42(1) |
| N3A | 22984(3) | 5562(2) | 2300(1) | 42(1) |
| N4A | 2511(3) | 4612(2) | 671(1) | 42(1) |
| N5A | 1149(3) | 2941(2) | 913(1) | 41(1) |
| N6A | 363(3) | 2106(2) | 945(1) | 42(1) |
| C1A | 4317(4) | 2172(3) | 1215(2) | 53(1) |
| C2A | 5609(5) | 1661(3) | 1260(2) | 57(1) |
| C3A | 6632(4) | 2061(3) | 1576(2) | 58(1) |
| C4A | 6329(4) | 2979(3) | 1826(2) | 49(1) |
| C5A | 4995(3) | 3454(3) | 1768(1) | 39(1) |
| C6A | 4530(3) | 4392(2) | 2047(1) | 38(1) |
| C7A | 5174(4) | 4961(3) | 2440(2) | 43(1) |
| C8A | 4149(3) | 5707(2) | 2597(1) | 40(1) |
| C9A | 4174(4) | 6517(3) | 3008(2) | 43(1) |
| C10A | 5270(4) | 6515(3) | 3382(2) | 54(1) |
| C11A | 5277(5) | 7257(4) | 3787(2) | 65(1) |
| C12A | 4212(5) | 7995(4) | 3821(2) | 65(1) |
| C13A | 3137(5) | 8021(3) | 3447(2) | 62(1) |
| C14A | 3126(4) | 7281(3) | 3039(2) | 54(1) |
| C15A | 3248(4) | 5458(3) | 568(2) | 54(1) |
| C16A | 3351(5) | 5954(3) | 38(2) | 65(1) |
| C17A | 2659(5) | 5579(3) | -410(2) | 63(1) |
| C18A | 1914(4) | 4709(3) | -316(2) | 52(1) |
| C19A | 1859(3) | 4239(2) | 227(1) | 40(1) |
| C20A | 1085(3) | 3314(2) | 377(1) | 39(1) |
| C21A | 259(4) | 2716(3) | 58(1) | 42(1) |
| C22A | -191(3) | 1945(3) | 438(1) | 41(1) |
| C23A | -1099(3) | 1088(3) | 358(2) | 43(1) |
| C24A | -1932(5) | 1112(3) | -118(2) | 58(1) |
| C25A | -2803(5) | 312(4) | -195(2) | 69(1) |
| C26A | -2870(5) | -493(3) | 193(2) | 68(1) |
| C27A | -2056(5) | -526(3) | 658(2) | 62(1) |
| C28A | -1167(4) | 263(3) | 746(2) | 51(1) |

| | | | | |
|------|---------|---------|---------|-----|
| HN3A | 2176(4) | 5875(3) | 2309(2) | --- |
| HN6A | 271(4) | 1733(3) | 1300(2) | --- |

Tabla 4. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del **cation (B)** $[\text{Ni}(\text{HL}^0)_2(\text{H}_2\text{O})_2]^{2+}$, (excepto para los átomos de hidrógeno).

| átomo | (x/a). 10 ⁴ | (y/b). 10 ⁴ | (z/c). 10 ⁴ | Ueq (Å ²) |
|-------|------------------------|------------------------|------------------------|-----------------------|
| NiB | 7809(1) | 1111(1) | 3649(1) | 36(1) |
| O1B | 9742(3) | 235(2) | 3461(1) | 49(1) |
| O2B | 8282(3) | 1918(2) | 2878(1) | 51(1) |
| N1B | 5854(3) | 1962(2) | 3656(1) | 40(1) |
| N2B | 6556(3) | 211(2) | 3205(1) | 42(1) |
| N3B | 6793(3) | -614(2) | 2879(1) | 42(1) |
| N4B | 7539(3) | 341(2) | 4445(1) | 40(1) |
| N5B | 8818(3) | 2029(2) | 4177(1) | 40(1) |
| N6B | 9581(3) | 2873(2) | 4129(1) | 41(1) |
| C1B | 5555(4) | 2848(3) | 3907(2) | 49(1) |
| C2B | 4363(4) | 3448(3) | 3786(2) | 55(1) |
| C3B | 3438(4) | 3128(3) | 3402(2) | 55(1) |
| C4B | 3732(4) | 2217(3) | 3145(2) | 46(1) |
| C5B | 4949(3) | 1653(2) | 3281(1) | 38(1) |
| C6B | 5382(3) | 683(2) | 3021(1) | 37(1) |
| C7B | 4836(3) | 155(3) | 2584(1) | 40(1) |
| C8B | 5765(3) | -678(2) | 2505(1) | 39(1) |
| C9B | 5798(3) | -1490(2) | 2089(1) | 40(1) |
| C10B | 6871(4) | -2240(3) | 2075(2) | 51(1) |
| C11B | 6918(4) | -2984(3) | 1670(2) | 59(1) |
| C12B | 5874(5) | -2976(3) | 1280(2) | 64(1) |
| C13B | 4788(5) | -2257(4) | 1303(2) | 68(1) |
| C14B | 4744(4) | -1502(3) | 1700(2) | 55(1) |
| C15B | 6827(4) | -516(3) | 4559(2) | 52(1) |
| C16B | 6791(5) | -1011(3) | 5094(2) | 63(1) |
| C17B | 7523(5) | -632(3) | 5526(2) | 61(1) |
| C18B | 8246(4) | 248(3) | 5417(2) | 49(1) |
| C19B | 8230(3) | 722(2) | 4874(1) | 36(1) |
| C20B | 8954(3) | 1661(2) | 4714(1) | 36(1) |
| C21B | 9795(4) | 2272(2) | 5015(1) | 40(1) |
| C22B | 10179(3) | 3050(2) | 4624(1) | 38(1) |
| C23B | 11070(3) | 3925(2) | 4687(2) | 41(1) |
| C24B | 11115(4) | 4726(3) | 4282(2) | 48(1) |

| | | | | |
|------|----------|----------|---------|-------|
| C25B | 11997(5) | 5529(3) | 4345(2) | 57(1) |
| C26B | 12805(5) | 5541(3) | 4814(2) | 63(1) |
| C27B | 12754(5) | 4769(4) | 5222(2) | 67(1) |
| C28B | 11884(4) | 3951(3) | 5162(2) | 55(1) |
| HN3B | 7443(4) | -1095(3) | 3012(2) | --- |
| HN6B | 9552(4) | 3274(3) | 3813(2) | --- |

Tabla 5. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos de **cloro**, **metanol** y **H₂O** no coordinados.

| átomo | (x/a). 10 ⁴ | (y/b). 10 ⁴ | (z/c). 10 ⁴ | Ueq (Å ²) |
|-------|------------------------|------------------------|------------------------|-----------------------|
| Cl1 | 10908(1) | 1981(1) | 6511(1) | 56(1) |
| Cl2 | 10826(1) | 871(1) | 2144(1) | 64(1) |
| Cl3 | -1332(1) | 4127(1) | 3062(1) | 63(1) |
| O1 | 190(5) | 6275(3) | 2640(2) | 104(1) |
| O2 | 1052(5) | 7201(4) | 1292(2) | 112(2) |
| C1 | 770(9) | 8095(6) | 1650(4) | 123(3) |

AII. 3. Estructura cristalina del complejo [Ni(HL¹)₂(H₂O)₂] Br₂

Datos cristalográficos:

| | |
|------------------------|--|
| Fórmula | [Ni(C ₁₅ H ₁₃ N ₃) ₂ (H ₂ O) ₂] Br ₂ |
| Peso molecular | 725,124 g/mol |
| Parámetros de la celda | a = 12,199 Å b = 17,152 Å c = 19,878 Å = 90,00 ° = 91,32 ° = 90,00 ° |
| Volumen de la celda | 4158,11 Å ³ |
| Moléculas por celda | Z = 4 |
| Grupo espacial | P 2 ₁ / n |
| Sistema | Monoclínico |
| Valor de R(F) | R(F) = 0,063 R _w (F ²) = 0,198 |

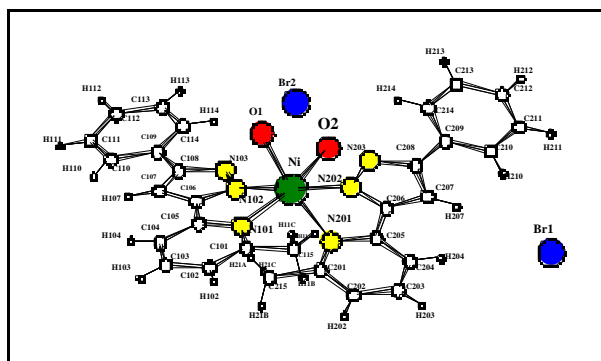


Tabla 6. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del complejo [Ni(HL¹)₂(H₂O)₂]
Br₂, (incluso los átomos de hidrógeno).

| átomo | (x/a). 10 ⁴ | (y/a). 10 ⁴ | (z/a). 10 ⁴ | Ueq (Å ²) |
|-------|------------------------|------------------------|------------------------|-----------------------|
| Br1 | 1289(1) | 1799(0) | 1568(0) | 647(3) |

| | | | | |
|------|----------|----------|----------|---------|
| Br2 | -1137(1) | -3096(1) | 2479(0) | 653(3) |
| Ni | 324(1) | -2525(0) | 416(0) | 347(2) |
| N101 | 1586(4) | 3341(3) | 716(2) | 367(12) |
| N102 | 264(4) | -3317(3) | -344(2) | 345(12) |
| N103 | -390(4) | -3428(3) | -899(2) | 373(12) |
| N201 | 1338(4) | -1630(3) | -18(3) | 389(13) |
| N202 | 288(4) | -1668(3) | 1141(3) | 407(13) |
| N203 | -251(4) | -1555(3) | 1724(2) | 408(13) |
| O1 | -802(4) | -3268(2) | 891(2) | 462(11) |
| O2 | -1040(3) | -1922(3) | 19(2) | 474(11) |
| C101 | 2327(6) | -3309(4) | 1225(4) | 490(17) |
| C102 | 3044(5) | -3910(4) | 1376(4) | 536(19) |
| H102 | 3536(5) | -3871(4) | 1739(4) | --- |
| C103 | 3015(7) | -4575(4) | 976(4) | 532(19) |
| H103 | 3496(6) | -4985(4) | 1065(4) | --- |
| C104 | 2267(5) | -4621(4) | 447(3) | 456(17) |
| H104 | 2234(5) | -5060(4) | 172(3) | --- |
| C105 | 1560(5) | -3989(4) | 331(3) | 365(14) |
| C106 | 792(5) | -3974(4) | -235(3) | 357(14) |
| C107 | 505(5) | -4522(4) | -723(3) | 376(15) |
| H107 | 770(5) | -5029(4) | -758(3) | --- |
| C108 | -249(5) | -4162(3) | -1144(3) | 332(14) |
| C109 | -864(5) | -4443(3) | -1734(3) | 384(15) |
| C110 | -594(6) | -5156(4) | -2022(3) | 503(18) |
| H110 | -13(6) | -5448(4) | -1845(3) | --- |
| C111 | -1199(7) | -5431(5) | -2579(4) | 680(24) |
| H111 | -1000(7) | -5899(5) | -2778(4) | --- |
| C112 | -2090(7) | -5021(5) | -2842(4) | 647(22) |
| H112 | -2507(7) | -5224(5) | -3198(4) | --- |
| C113 | -2343(7) | -4314(4) | -2569(4) | 633(22) |
| H113 | -2919(7) | -4023(4) | -2753(4) | --- |
| C114 | 1751(7) | -4029(4) | -2021(3) | 464(17) |
| H114 | -1946(6) | -3551(4) | -1837(3) | --- |
| C115 | 2316(8) | -2598(5) | 1681(5) | 798(27) |
| H11A | 1781(8) | -2232(5) | 1514(5) | --- |
| H11B | 3028(8) | -2359(5) | 1689(5) | --- |
| H11C | 2133(8) | -2755(5) | 2128(5) | --- |
| C201 | 1897(6) | -1619(4) | -589(3) | 494(17) |
| C202 | 2289(6) | -935(4) | -876(4) | 567(19) |
| H202 | 2690(6) | -954(4) | -1267(4) | --- |
| C203 | 2083(7) | -252(5) | -582(4) | 691(23) |

| | | | | |
|------|----------|----------|---------|----------|
| H203 | 2300(7) | 213(5) | -780(4) | --- |
| C204 | 1523(6) | -250(4) | 41(4) | 568(20) |
| H204 | 1400(6) | 215(4) | 269(4) | --- |
| C205 | 1173(5) | -936(4) | 296(3) | 366(15) |
| C206 | 604(5) | -972(3) | 933(3) | 360(14) |
| C207 | 279(5) | -400(4) | 1367(3) | 426(16) |
| H207 | 398(5) | 133(4) | 1330(3) | --- |
| C208 | -260(5) | -784(4) | 1872(3) | 402(15) |
| C209 | -781(6) | -471(4) | 2477(3) | 466(17) |
| C210 | -674(8) | 296(5) | 2626(4) | 723(25) |
| H210 | -259(8) | 619(5) | 2357(4) | --- |
| C211 | -1196(8) | 599(5) | 3193(7) | 868(31) |
| H211 | -1114(8) | 1124(5) | 3297(5) | --- |
| C212 | -1816(8) | 142(5) | 3589(5) | 885(31) |
| H212 | -2151(8) | 347(5) | 3965(5) | --- |
| C213 | -1938(9) | -627(6) | 3423(5) | 1030(39) |
| H213 | -2372(9) | -948(6) | 3684(5) | --- |
| C214 | -1423(9) | -923(5) | 2876(5) | 887(32) |
| H214 | -1511(9) | -1448(5) | 2772(5) | --- |
| C215 | 2174(7) | -2401(4) | -915(4) | 619(22) |
| H21A | 1852(7) | -2817(4) | -663(4) | --- |
| H21B | 2956(7) | -2467(4) | -916(4) | --- |
| H21C | 1890(7) | -2410(4) | -369(4) | --- |

AII. 4. Estructura cristalina del complejo $[\text{Cu}_2(\text{CIL}^1)_2\text{Cl}_2(\text{DMF})_2]$

Datos cristalográficos:

| | |
|---------------------|---|
| Fórmula | $[\text{Cu}_2(\text{ClC}_{15}\text{H}_{11}\text{N}_3)_2\text{Cl}_2(\text{DMF})_2]$ |
| Peso molecular | 881,637 g/mol |
| Parámetros de celda | $a = 9,487(7) \text{ \AA}$ $b = 9,523(3) \text{ \AA}$ $c = 20,915(8) \text{ \AA}$ $\alpha = 90,00(0)^\circ$ $\beta = 99,00(3)^\circ$ $\gamma = 90,00(0)^\circ$ |
| Volumen de la celda | $1866,3(2) \text{ \AA}^3$ |
| Moléculas por celda | $Z = 2$ |
| Grupo espacial | $P2_1/c$ |
| Sistema | Monoclínico |
| Valor de R(F) | $R(F) = 0,094$ |
| | $R_w(F^2) = 0,286$ |

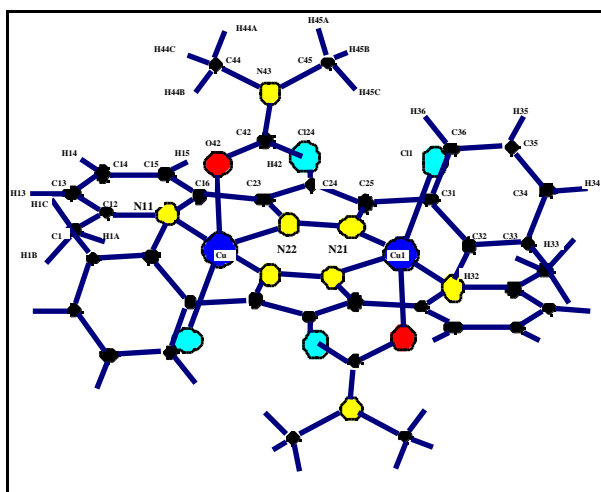


Tabla 7. Coordenadas fraccionarias y factores equivalente de temperatura para los átomos del complejo $[\text{Cu}_2(\text{CIL}^1)_2\text{Cl}_2(\text{DMF})_2]$, (incluso los átomos de hidrógeno).

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 | Ueq (\AA^2) |
|-------|---------------|---------------|---------------|------------------------|
| Cu | 4554(1) | 1008(1) | 9177(0) | 359(4) |
| Cl1 | 6033(3) | 144(2) | 8501(1) | 530(8) |
| C1 | 3789(13) | 2985(11) | 7935(5) | 677(41) |
| H1A | 3535(13) | 2073(11) | 8075(5) | --- |
| H1B | 4247(13) | 2891(11) | 7559(5) | --- |
| H1C | 2945(13) | 3547(11) | 7830(5) | --- |
| N11 | 5129(7) | 2994(7) | 9026(3) | 401(22) |
| C12 | 4774(10) | 3668(9) | 8458(4) | 429(29) |
| C13 | 5304(11) | 5012(11) | 8374(5) | 585(37) |
| H13 | 5078(11) | 5469(11) | 7978(5) | --- |
| C14 | 6174(11) | 5664(11) | 8888(5) | 571(37) |
| H14 | 6542(11) | 6555(11) | 8840(5) | --- |
| C15 | 6475(11) | 4960(10) | 9467(5) | 538(34) |
| H15 | 7042(11) | 5387(10) | 9816(5) | --- |
| C16 | 5953(9) | 3647(8) | 9536(4) | 384(29) |
| N21 | 6190(7) | 842(6) | 10681(3) | 328(22) |
| N22 | 5747(7) | 1482(8) | 10089(3) | 366(21) |
| C23 | 6271(8) | 2797(8) | 10116(4) | 354(26) |
| C24 | 7030(8) | 3038(9) | 10725(4) | 399(27) |
| C25 | 6972(8) | 1789(8) | 11074(4) | 354(25) |
| Cl24 | 7970(7) | 4455(6) | 10988(3) | 1593(31) |
| C31 | 7652(8) | 1419(9) | 11743(4) | 390(26) |
| C32 | 8332(10) | 180(10) | 11878(4) | 517(34) |
| H32 | 8341(10) | -475(10) | 11549(4) | --- |
| C33 | 9009(12) | -133(12) | 12489(5) | 627(38) |
| H33 | 9519(12) | -964(12) | 12575(5) | --- |
| C34 | 8904(13) | 844(14) | 12979(5) | 729(45) |
| H34 | 9292(13) | 619(14) | 13403(5) | --- |
| C35 | 8279(12) | 2063(13) | 12863(5) | 649(41) |
| H35 | 8296(12) | 2721(13) | 13193(5) | --- |
| C36 | 7587(10) | 2365(11) | 12240(5) | 531(29) |
| H36 | 7083(10) | 3200(11) | 12159(5) | --- |
| O42 | 2575(6) | 1894(6) | 9417(3) | 465(22) |
| C42 | 2221(9) | 1571(10) | 9947(4) | 431(28) |

| | | | | |
|------|----------|----------|----------|----------|
| H42 | 2869(9) | 1071(10) | 10242(4) | --- |
| N43 | 985(8) | 1900(8) | 10113(4) | 520(28) |
| C44 | -101(13) | 2617(16) | 9663(6) | 939(57) |
| H44A | -929(13) | 2772(16) | 9865(6) | --- |
| H44B | -355(13) | 2049(16) | 9283(6) | --- |
| H44C | 265(13) | 3502(16) | 9543(6) | --- |
| C45 | 13(13) | 1566(16) | 10747(6) | 819(52) |
| H45A | -334(13) | 1896(16) | 10769(6) | --- |
| H45B | 1277(13) | 2014(16) | 11078(6) | --- |
| H45C | 652(13) | 567(16) | 10811(6) | --- |

AII. 5. Estructura Cristalina del complejo $[\text{Cu}(\text{HL}^0)(\text{NO}_3)(\text{H}_2\text{O})_2](\text{NO}_3)$

Datos Cristalográficos:

Fórmula $[\text{Cu}(\text{C}_{14}\text{H}_{11}\text{N}_3)(\text{NO}_3)(\text{H}_2\text{O})_2](\text{NO}_3)$

Peso molecular 444,847 g/mol

Parámetros de celda $a = 8,349(3) \text{ \AA}$

$b = 10,362(1) \text{ \AA}$

$c = 10,689(1) \text{ \AA}$

$= 66,52(1)^\circ$

$= 88,12(1)^\circ$

$= 88,98(1)^\circ$

Volumen de la celda $847,7(3) \text{ \AA}^3$

Moléculas por celda $Z = 2$

Grupo espacial $P \bar{1}$

Sistema Triclínico

Valor de R(F) $R(F)=0,034$

$R_w(F^2)=0,095$

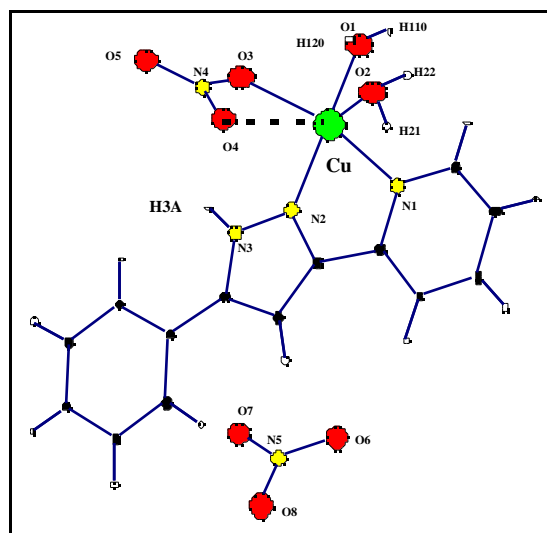


Tabla 8. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del complejo $[\text{Cu}(\text{HL}^0)(\text{NO}_3)(\text{H}_2\text{O})_2](\text{NO}_3)$, (incluso los átomos de hidrógeno).

| átomo | $(x/a) \cdot 10^4$ | $(y/b) \cdot 10^4$ | $(z/c) \cdot 10^4$ | $U_{eq} (\text{Å}^2)$ |
|-------|--------------------|--------------------|--------------------|-----------------------|
| Cu | 2167(3) | 7546(2) | 6183(2) | 299(11) |

| | | | | |
|------|-----------|-----------|-----------|---------|
| C1 | 3813(27) | 4704(23) | 7233(23) | 368(83) |
| H1 | 4109(27) | 4891(23) | 7975(23) | --- |
| N1 | 2897(23) | 5641(18) | 6281(18) | 314(63) |
| C5 | 2458(24) | 5356(21) | 5209(21) | 302(66) |
| C4 | 2942(26) | 4148(22) | 5053(23) | 358(75) |
| H4 | 2635(26) | 3975(22) | 4306(23) | --- |
| C3 | 3902(27) | 3195(23) | 6047(25) | 395(86) |
| H3 | 4253(27) | 2373(23) | 5967(25) | --- |
| C2 | 4326(28) | 3474(24) | 7141(24) | 407(83) |
| H2 | 4956(28) | 2838(24) | 7815(24) | --- |
| N2 | 952(22) | 7454(18) | 4667(18) | 328(65) |
| N3 | 33(22) | 8337(18) | 3665(18) | 330(69) |
| H3A | -403(22) | 9093(18) | 3670(18) | --- |
| C8 | -119(25) | 7883(22) | 2646(21) | 314(77) |
| C7 | 777(26) | 6656(23) | 3017(21) | 340(71) |
| H7 | 918(26) | 6093(23) | 2527(21) | --- |
| C6 | 1421(25) | 6438(22) | 4261(21) | 307(77) |
| C9 | -1106(26) | 8612(23) | 1457(22) | 340(79) |
| C10 | -1875(30) | 9873(26) | 1248(25) | 433(92) |
| H10 | -1755(30) | 10291(26) | 1864(25) | --- |
| C11 | -2822(33) | 10510(29) | 126(28) | 521(10) |
| H11 | -3326(33) | 11362(29) | -13(28) | --- |
| C12 | -3021(32) | 9808(31) | -770(26) | 516(11) |
| H12 | -3664(32) | 10347(31) | -1519(27) | --- |
| C13 | -2277(33) | 8648(32) | -582(27) | 523(11) |
| H13 | -2424(33) | 8234(32) | -1199(27) | --- |
| C14 | -1316(29) | 8004(27) | 523(24) | 432(91) |
| H14 | -805(29) | 7159(27) | 647(24) | --- |
| N4 | 2903(22) | 10246(18) | 4569(18) | 353(68) |
| O3 | 1830(19) | 9657(15) | 5518(15) | 361(56) |
| O4 | 3834(21) | 9483(18) | 4254(19) | 479(64) |
| O5 | 2953(24) | 11540(17) | 4024(20) | 545(78) |
| O1 | 3782(23) | 7679(20) | 7426(18) | 415(68) |
| H110 | 3774(424) | 7275(383) | 8083(354) | --- |
| H120 | 4593(415) | 7877(366) | 7193(357) | --- |
| O2 | 277(24) | 7135(23) | 7712(19) | 549(86) |
| H21 | -318(382) | 6607(339) | 7587(359) | --- |
| H22 | 660(413) | 6658(347) | 8432(271) | --- |
| N5 | 2815(25) | 5193(22) | 650(20) | 426(78) |

| | | | | |
|----|----------|----------|----------|-----------|
| O6 | 2894(27) | 4306(22) | 1825(18) | 643(88) |
| O7 | 3846(32) | 6115(24) | 132(21) | 784(102) |
| O8 | 1737(32) | 5111(34) | -61(29) | 1139(146) |

AII. 6. Estructura cristalina del complejo $[\text{Cu}(\text{L}^0)_2]$

Datos cristalográficos:

| | |
|---------------------|--|
| Fórmula | $[\text{Cu}(\text{C}_{14}\text{H}_{10}\text{N}_3)_2]$ |
| Peso molecular | 504,054 g/mol |
| Parámetros de celda | $a=13,045(1) \text{ \AA}$ $b=5,2963(6) \text{ \AA}$ $c=16,384(3) \text{ \AA}$ $\alpha=90,00(0)^\circ$ $\beta=103,36(1)^\circ$ $\gamma=90,00(0)^\circ$ |
| Volumen de la celda | $1101,3 \text{ \AA}^3$ |
| Molécula por celda | $Z=2$ |
| Grupo espacial | $P2_1/c$ |
| Sistema | monoclínico |
| Valor de R(F) | $R(F)=0,025$ $R_w(F^2)=0,083$ |

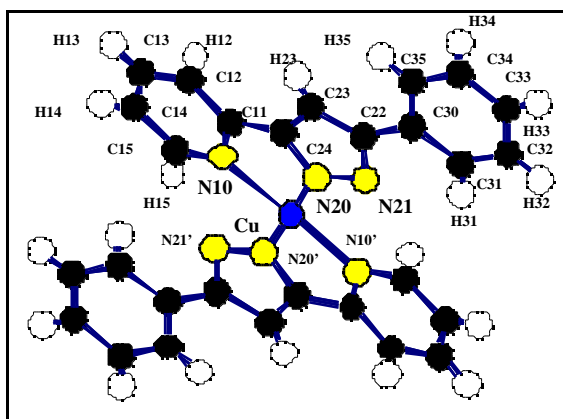


Tabla 9. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos del complejo $[\text{Cu}(\text{L}^0)_2]$, (excepto para los átomos de hidrógeno).

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 | Beq (Å^2) |
|-------|---------------|---------------|---------------|----------------------|
| Cu | 5000(0) | 0000(0) | 5000(0) | 4,64 |
| N10 | 3875(1) | 2579(3) | 5115(1) | 4,75 |
| C11 | 4190(2) | 4159(4) | 5779(1) | 4,63 |
| C12 | 3538(2) | 6085(4) | 5937(1) | 5,61 |
| C13 | 2565(2) | 6387(4) | 5411(1) | 6,19 |
| C14 | 2253(2) | 4793(4) | 4734(2) | 6,01 |
| C15 | 2923(2) | 2915(4) | 4606(1) | 5,42 |
| N20 | 5747(1) | 1681(3) | 6020(1) | 5,08 |
| N21 | 6739(1) | 1552(3) | 6506(1) | 5,26 |
| C22 | 6845(2) | 3481(3) | 7056(1) | 4,75 |
| C23 | 5913(2) | 4861(3) | 6934(1) | 4,89 |
| C24 | 5236(1) | 3667(3) | 6267(1) | 4,64 |
| C30 | 7863(2) | 3927(4) | 7644(1) | 4,78 |
| C31 | 8701(2) | 2296(4) | 7667(1) | 6,09 |
| C32 | 9661(2) | 2697(5) | 8215(2) | 6,99 |

| | | | | |
|-----|---------|---------|---------|------|
| C33 | 9806(2) | 4725(4) | 8759(2) | 6,62 |
| C34 | 8990(2) | 6365(4) | 8734(1) | 6,53 |
| C35 | 8025(2) | 6001(4) | 8180(1) | 5,84 |

Tabla 10. Coordenadas fraccionarias y factores equivalentes de temperatura para los átomos de hidrógeno del complejo $[\text{Cu}(\text{L}^0)_2]$.

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 |
|-------|---------------|---------------|---------------|
| H12 | 3760(2) | 7155(4) | 6394(1) |
| H13 | 2118(2) | 7661(4) | 5509(1) |
| H14 | 1596(2) | 4987(4) | 4369(1) |
| H15 | 2708(1) | 1837(4) | 4150(1) |
| H23 | 5774(2) | 6264(3) | 7233(1) |
| H31 | 8614(2) | 912(4) | 7309(1) |
| H32 | 10215(2) | 1591(4) | 8218(1) |
| H33 | 10450(2) | 4972(4) | 9137(1) |
| H34 | 9085(2) | 7745(4) | 9094(1) |
| H35 | 7482(2) | 7149(4) | 8166(1) |

AII. 7. Estructura Cristalina del complejo $[\text{Pd}_2(\text{L}^1)_4]$

Datos Cristalográficos:

| | |
|---------------------|--|
| Fórmula | [Pd₂(C₁₅H₁₂N₃)₄] |
| Peso molecular | 1149,920 g/mol |
| Parámetros de celda | a = 13,448(2) Å b = 21,605(1) Å c = 18,855(1) Å = 90,00(0) ° = 110,02(7) ° = 90,00(0) ° |
| Volumen de la celda | 5147,2(8) Å ³ |
| Molécula por celda | Z = 4 |
| Grupo espacial | P2 ₁ /c |
| Sistema | monoclínico |
| Valor de R(F) | R(F) = 0,097 |
| | R _w (F ²) = 0,244 |

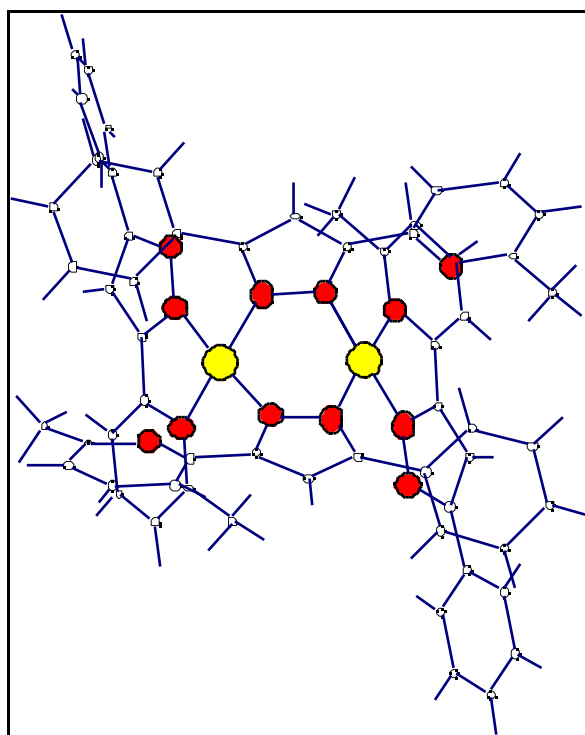


Tabla 11. Coordinadas fraccionarias y factores equivalentes de temperatura para los átomos del complejo [Pd₂(L¹)₄], (excepto los átomos de hidrógeno).

| átomo | (x/a). 10 ⁴ | (y/b). 10 ⁴ | (z/c). 10 ⁴ | U _{eq} (Å ²) |
|-------|------------------------|------------------------|------------------------|-----------------------------------|
| Pd1 | 2341(1) | 490(0) | 1652(0) | 489(3) |
| Pd2 | 1646(1) | 66(0) | 2980(0) | 496(4) |
| C101 | -1923(6) | 1262(4) | 3004(5) | 641(52) |
| C102 | -1533(5) | 1767(4) | 3475(5) | 805(62) |
| C103 | -2220(8) | 2228(4) | 3537(7) | 875(75) |
| C104 | -3295(8) | 2185(4) | 3128(6) | 861(74) |
| C105 | -3685(5) | 1681(5) | 2657(5) | 874(70) |
| C106 | -2999(7) | 1220(4) | 2595(4) | 754(61) |
| N111 | 211(8) | 324(5) | 2918(6) | 598(47) |
| N112 | -185(8) | 870(5) | 3003(5) | 605(48) |
| C113 | -1211(9) | 762(6) | 2942(7) | 600(49) |
| C114 | -1462(11) | 129(7) | 2823(7) | 725(63) |
| C115 | -519(9) | -145(7) | 2800(7) | 580(52) |
| N121 | 856(9) | -800(5) | 2732(5) | 605(44) |
| C122 | -148(11) | -749(6) | 2721(7) | 602(56) |
| C123 | -834(12) | -1270(8) | 2587(8) | 840(72) |

| | | | | |
|------|----------|----------|----------|----------|
| C124 | -465(17) | -1825(8) | 2489(10) | 983(95) |
| C125 | 570(15) | -1882(7) | 2515(8) | 846(73) |
| C126 | 1232(11) | -1353(7) | 2633(6) | 600(55) |
| C127 | 2299(13) | -1439(6) | 2583(8) | 864(72) |
| C201 | 2924(7) | -1375(4) | -99(5) | 566(47) |
| C202 | 3632(8) | -1737(5) | 456(4) | 908(84) |
| C203 | 3982(8) | -2297(5) | 265(6) | 1162(10) |
| C204 | 3624(10) | -2495(4) | -482(7) | 970(92) |
| C205 | 2916(9) | -2133(5) | -1037(5) | 1043(91) |
| C206 | 2566(7) | -1573(5) | -846(5) | 916(81) |
| N211 | 2213(8) | -113(5) | 843(5) | 567(43) |
| N212 | 2757(10) | -640(5) | 843(6) | 755(53) |
| C213 | 2512(11) | -820(6) | 108(7) | 635(54) |
| C214 | 1786(11) | -365(6) | -332(8) | 691(58) |
| C215 | 1688(8) | 78(5) | 168(6) | 494(46) |
| N221 | 1102(8) | 889(4) | 752(5) | 543(41) |
| C222 | 1031(10) | 599(6) | 96(7) | 660(60) |
| C223 | 303(12) | 829(8) | -582(8) | 862(64) |
| C224 | -306(14) | 1313(8) | -597(9) | 987(81) |
| C225 | -273(10) | 1592(7) | 63(9) | 857(73) |
| C226 | 471(10) | 1362(6) | 762(7) | 612(55) |
| C227 | 437(10) | 1651(7) | 1464(7) | 821(65) |
| C301 | 4975(6) | -120(4) | 1996(4) | 584(50) |
| C302 | 4798(7) | 380(4) | 1505(5) | 774(63) |
| C303 | 5299(9) | 407(6) | 972(5) | 1066(93) |
| C304 | 5977(8) | -66(7) | 930(5) | 1239(11) |
| C305 | 6154(7) | -567(6) | 1421(7) | 1105(10) |
| C306 | 5653(7) | -594(4) | 1955(6) | 713(60) |
| N311 | 3152(6) | -146(4) | 3036(5) | 427(33) |
| N312 | 3441(7) | -2(4) | 2445(5) | 438(35) |
| C313 | 4447(9) | -189(5) | 2573(7) | 484(43) |
| C314 | 4805(9) | -449(5) | 3284(6) | 533(48) |
| C315 | 4017(9) | -427(5) | 3573(6) | 491(42) |
| N321 | 2958(9) | -678(5) | 4318(6) | 728(55) |
| C322 | 3913(11) | -635(5) | 4287(6) | 548(49) |
| C323 | 4839(12) | -784(6) | 4906(7) | 807(70) |
| C324 | 4664(18) | -959(7) | 5566(9) | 1014(88) |

| | | | | |
|------|----------|----------|----------|----------|
| C325 | 3671(20) | -984(7) | 5597(9) | 1008(96) |
| C326 | 2788(14) | -847(8) | 4946(10) | 927(76) |
| C327 | 1670(20) | -951(13) | 4903(11) | 1807(15) |
| C401 | 2021(7) | 1366(5) | 4253(4) | 724(58) |
| C402 | 1614(8) | 1885(4) | 4496(6) | 874(70) |
| C403 | 1320(8) | 1849(6) | 5133(7) | 1242(12) |
| C404 | 1431(9) | 1295(8) | 5527(5) | 1282(11) |
| C405 | 1838(10) | 777(6) | 5285(6) | 1157(11) |
| C406 | 2132(8) | 812(4) | 4648(6) | 818(64) |
| N411 | 2176(7) | 940(4) | 3073(5) | 503(35) |
| N412 | 2529(7) | 1129(4) | 2499(5) | 489(34) |
| C413 | 2940(10) | 1716(5) | 2667(8) | 594(57) |
| C414 | 2768(9) | 1890(6) | 3314(7) | 549(48) |
| C415 | 2313(9) | 1409(6) | 3557(7) | 573(51) |
| N421 | 3176(9) | 1765(5) | 1458(7) | 689(50) |
| C422 | 3324(10) | 2045(6) | 2133(9) | 651(66) |
| C423 | 3774(12) | 2608(6) | 2295(10) | 857(79) |
| C424 | 4185(16) | 2886(8) | 1737(16) | 1196(13) |
| C425 | 4044(18) | 2619(11) | 1099(13) | 1202(12) |
| C426 | 3539(14) | 2048(8) | 961(10) | 953(84) |
| C427 | 3384(17) | 1726(10) | 226(10) | 1358(11) |

Tabla 12. Coordinadas fraccionarias y factores equivalentes de temperatura para los átomos de hidrógeno del complejo $[Pd_2(L^1)_4]$.

| átomo | (x/a). 10^4 | (y/b). 10^4 | (z/c). 10^4 |
|-------|---------------|---------------|---------------|
| H102 | -814(6) | 1796(6) | 3749(7) |
| H103 | -1959(11) | 2566(4) | 3852(7) |
| H104 | -3754(10) | 2494(5) | 3169(8) |
| H105 | -4404(5) | 1652(7) | 2383(7) |
| H106 | -3259(10) | 882(5) | 2280(6) |
| H114 | -2102(11) | -64(7) | 2771(7) |
| H123 | -1530(12) | -1225(8) | 2567(8) |
| H124 | -902(17) | -2171(8) | 2404(10) |
| H125 | 834(15) | 2268(7) | 2455(8) |
| H12A | 2669(13) | -1051(6) | 2673(8) |
| H12B | 2233(13) | -1587(6) | 2089(8) |

| | | | |
|------|----------|-----------|----------|
| H12C | 2687(13) | -1735(6) | 2955(8) |
| H202 | 3872(12) | -1604(7) | 955(4) |
| H203 | 4456(11) | -2539(6) | 636(8) |
| H204 | 3858(13) | -2870(5) | -610(10) |
| H205 | 2676(13) | -2266(7) | -1536(6) |
| H206 | 2092(10) | -1331(7) | -1217(6) |
| H214 | 1446(11) | -368(6) | -853(8) |
| H223 | 248(12) | 634(8) | -1033(8) |
| H224 | -757(14) | 1464(8) | -1056(9) |
| H225 | -719(10) | 1922(7) | 61(9) |
| H22A | 963(10) | 1464(7) | 1891(7) |
| H22B | -251(10) | 1591(7) | 1501(7) |
| H22C | 577(10) | 2086(7) | 1457(7) |
| H302 | 4344(10) | 696(5) | 1533(8) |
| H303 | 5180(13) | 741(7) | 643(7) |
| H304 | 6312(11) | -48(10) | 573(7) |
| H305 | 6608(10) | -883(7) | 1393(10) |
| H306 | 5771(11) | -928(5) | 2283(8) |
| H314 | 5477(9) | -612(5) | 3523(6) |
| H323 | 5513(12) | -766(6) | 4873(7) |
| H324 | 5238(18) | -1061(7) | 5992(9) |
| H325 | 3570(20) | 1092(7) | 6045(9) |
| H32A | 1197(20) | -827(13) | 4415(11) |
| H32B | 1528(20) | -710(13) | 5286(11) |
| H32C | 1567(20) | -1382(13) | 4981(11) |
| H402 | 1540(12) | 2255(5) | 4232(9) |
| H403 | 1048(12) | 2195(8) | 5295(10) |
| H404 | 1234(13) | 1271(11) | 5954(7) |
| H405 | 1912(14) | 406(7) | 5549(9) |
| H406 | 2404(11) | 466(5) | 4485(9) |
| H414 | 2934(9) | 2273(6) | 3549(7) |
| H423 | 3823(12) | 2813(6) | 2740(10) |
| H424 | 4552(16) | 3259(8) | 1846(16) |
| H425 | 4275(18) | 2804(11) | 739(13) |
| H42A | 3026(17) | 1340(10) | 215(10) |
| H42B | 4060(17) | 1650(10) | 176(10) |
| H42C | 2966(17) | 1983(10) | -183(10) |

