**SUPPLEMENTARY MATERIAL**



M. Alcolea Palafoxa\*, Nataliya P. Belskayab, Lozan Todorovc, Irena P. Kostovac

*a Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense, Madrid-28040, Spain* (alcolea@ucm.es)

*b Department of Technology for Organic Synthesis, Ural Federal University, 19 Mira Str., Yekaterinburg 620012, Russia; n.p.belskaya@urfu.ru*

*cDepartment of Chemistry, Faculty of Pharmacy, Medical University – Sofia, 2 Dunav Str., Sofia, Bulgaria*

*III*

*II*

*I*

*E* = -528.387053 AU (*G* = -528.502017 AU)

**Figure S1.** Labeling of the atoms and plot of the optimized La(**2b**)3 structure with **2b**: sodium 2-(4-chlorophenyl)-5-(pyrrolidineidin-1-yl)-2*H*-1,2,3-triazole-4-carboxylate at the B3LYP/Cep-4g level.







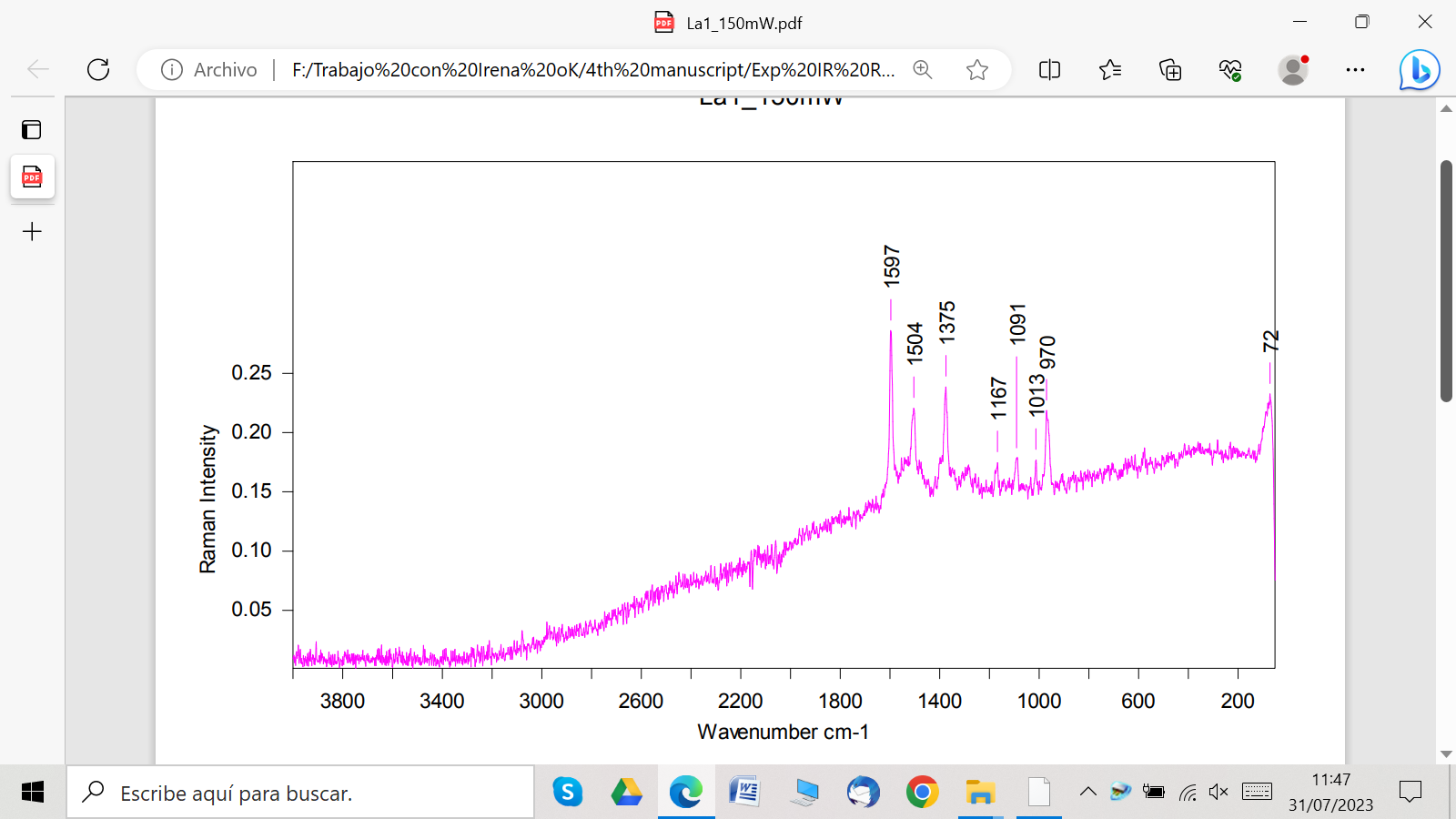


**Figure S2.** Comparison of the theoretical scaled IR spectra with the experimental ones in the 3750-400 cm-1 range.









**Figure S3.** Comparison of the theoretical scaled Raman spectra with the experimental ones

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**Figure S4.**  Comparison of the scaled Raman spectra in the 3400-2600 cm-1 range by three DFT methods.







**Figure S5.**  Comparison of the scaled Raman spectra in the 1800-1000 cm-1 range by three DFT methods.





**Figure S6.**  Comparison of the scaled Raman spectra in the 1000-50 cm-1 range by three DFT methods.

**Table S1.** Calculated, scaled and experimental wavenumbers (ν, cm-1) in the La(2b)3 complex. Relative infrared intensity (A) in %, relative Raman intensity (S) in %, and Raman depolarization ratios for plane (DP) and unpolarized incident light (DU). For each vibration of the tetramer, the wavenumber with the highest IR intensity is indicated in bold type and that with the highest Raman intensity is indicated in italic type. The relative IR and Raman intensities were shown only for these wavenumbers. DP and DU values were from most intense Raman line. The number of the ring mode corresponds to Wilson’s notation [27].

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Calculated at M06-2X/Lanl2dz | | | | | scaled | Experimental | | Characterization |
| ν | A | S | DP | DU | IR | Raman |
| 3287, 3287, 3287  3283, 3282, *3281*  3266, ***3266***, 3265  3265, ***3264***, 3264  3188, 3187, ***3187***  3177, ***3177***, 3176  3168, 3167, ***3167***  3144, 3143, ***3143***  ***3116***, 3116, 3114  3107, ***3107***, 3106  **3103**, 3103, 3102  3068, **3067**, 3067  1687, 1687, *1686*  1677, ***1677***, 1676  **1666**, *1663*, 1662  *1607*, 1596, **1596**  1550, 1550, 1550  1549, *1544*, **1543**  1539, ***1538***, 1538  ***1527***, 1527, 1526  1522, ***1522***, 1521  **1471**, 1471, 1470  **1461**, 1455, *1454*  -  1441, *1440*, **1440**  *1426,* **1422**, 1422  1404, **1402**, *1401*  **1392**, *1391*, 1391  1369, 1368, *1367*  1366, 1366, 1366  1363, 1363, 1363  *1344*, 1343, **1341**  1326, ***1322***, 1321  *1291*, **1291**, 1290  1285, ***1283***, 1283  1276, ***1275***, 1275  *1254*, **1253**, 1252  1235, **1233**, *1232*  **1219**, 1218, *1216*  1209, **1208**, *1207*  1205, 1205, 1205  *1167*, 1167, **1166**  1149, ***1148***, 1146  1127, **1127**, *1126*  1123, 1123, 1123  1099, 1099, 1099  1041, 1041, 1040  *1037*, 1037, **1036**  1031, 1031, 1030  1016, 1016, 1016  **1005**, 1004, *1004*  981, 981, 981  954, 953, 953  *947*, **946**, 946  900, 900, 900  **896**, 895, 894  888, *888*, **887**  886, 886, 884  *830*, **828**, 827  *826*, **819**, 818  *766*, **764**, 764  750, 750, 750  743, 743, 743  **726**, *726*, 724  675, *675*, **674**  **668**, *668*, 667  *648*, 647, 647  *596*, **593**, 592  588, 588, 588  ***538***, 538, 537  511, ***507***, 507  *472*, **469**, 468  432, 432, 431  ***415***, 415, 414  **406**, 403, *402*  *366*, **365**, 363  *326*, 325, 325  302, *301*, 299  *264*, 263, 262  251, 250, *250*  *241*, 238, 234  230, *229*, 225  198, *196*, 195  180, 175, *169*  *167*, 167, 147  145, 143, *120*  113, *106*, 104  *87*, 84, 78  *75*, 74, 70  67, 61, *60*  58, *52*, 51  49, *39*, 39  38, *36*, 35  *31*, 30, 27  8, *7*, 6  *5*, 4, 3 | 0  0  0  0  6  2  0  2  4  2  2  4  --  0  0  100  46  4  83  18  4  0  2  28  --  8  32  14  0  0  2  2  0  42  2  22  0  4  --  22  0  14  0  0  0  2  8  0  0  2  0  0  2  --  10  0  2  0  8  0  0  4  16  6  0  0  --  0  2  2  0  4  0  2  8  12  0  4  10  2  0  4  0  0  2  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0 | 4  2  3  3  3  4  2  3  4  3  4  3  --  55  0  24  100  9  5  2  0  1  0  0  --  21  16  2  1  0  1  0  0  12  4  2  0  0  --  0  2  1  0  0  0  0  5  1  0  1  0  1  0  --  17  0  1  0  0  1  0  3  3  0  0  0  --  0  0  0  1  2  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 | 0.13  0.11  0.57  0.65  0.72  0.32  0.57  030  0.03  0.19  0.15  0.10  0.39  0.75  0.06  0.08  0.48  0.75  0.75  0.47  0.73  0.64  0.75  -  0.32  0.37  0.75  0.45  0.13  0.38  0.38  0.75  0.75  0.65  0.75  0.23  0.73  0.75  0.29  0.75  0.67  0.23  0.55  0.49  0.02  0.62  0.45  0.22  0.72  0.75  0.47  0.07  0.65  0.10  0.09  0.74  0.09  0.19  0.04  0.04  0.09  0.68  0.22  0.24  0.73  0.73  0.75  0.13  0.26  0.72  0.74  0.34  0.70  0.68  0.74  0.70  0.51  0.70  0.38  0.67  0.73  0.17  0.43  0.32  0.71  0.22  0.72  0.71  0.75  0.71  0.73  0.74  0.75  0.74  0.75  0.75 | 0.23  0.20  0.73  0.79  0.84  0.48  0.73  0.46  0.06  0.33  0.27  0.18  0.56  0.86  0.12  0.15  0.65  0.86  0.86  0.64  0.85  0.78  0.86  -  0.48  0.53  0.85  0.62  0.23  0.55  0.55  0.86  0.86  0.79  0.86  0.37  0.84  0.86  0.44  0.86  0.80  0.37  0.71  0.66  0.04  0.76  0.62  0.36  0.84  0.86  0.64  0.14  0.79  0.18  0.17  0.85  0.17  0.32  0.07  0.07  0.16  0.81  0.36  0.38  0.85  0.84  0.86  0.22  0.42  0.84  0.85  0.50  0.83  0.81  0.85  0.82  0.67  0.82  0.55  0.81  0.84  0.29  0.60  0.49  0.83  0.36  0.84  0.83  0.86  0.83  0.84  0.85  0.86  0.85  0.86  0.86 | 3063  3060, 3059  3044  3043  2973  2963  2955  2933  2907  2899  2895  2863  --  1600  1591  **1581**, *1578*  *1527*, **1516**  1475  1474, ***1470***  1465  1454  1449  1402  **1393**, 1388  -  1375  1361  1341, **1340**  1330  1309, 1307  1306  1304  1286, **1283**  1270, ***1267***  1238  1232, **1230**  1224  1204, **1202**  1186, **1184**  **1172**, *1169*  1163, **1162**  1159  1124  1108, **1107**  1088  1084  1062  1009  1005  1000  986  976  954  929  923, **922**  880  876, 874  869  867  *816*, **814**  812, **805**  757, **755**  743  736  721  674  668  650  *602*, **599**  595  549  524, **520**  489, **486**  452  436  **428**, *424*  392, 389  355  333, 330  *298*, 296  286  *277*, 270  267, 262  238, 235  221, 210  *210*, 190  189, *163*  160, 151  *136*, 127  *125*, 120  118, *111*  110, 103  102, 92  92, 89  *85*, 81  64, 62  61, 58 | 3401.6 br, s  2968.1 s  2872.2 m  1895.1 vw  1577.8 br, vs  1500.2 s  1484.5 vs  1418.0 w  1398.1 m  -  1372.3 vs  1347.5 s  1302.0 vs  1285.5 s  1246.8 m  1218.0 m  1178.2 m  1150 sh  1091.2 vs  1011.8 m  969.0 vs  914.3 w  829.7 vs  805.4 m  754.3 w  698.8 vw  654 m  647.1 m  576.7 w  508.9 m  466.5 m | 1597 vs  1504 s  -  1375 vs  1167 w  1091 m  1013 w  970 s  72 br m | ν(O-H) H2O bonded  2, ν(C3-H) in aryl (100)  20b, ν(C5-H) in aryl (100)  7b, ν(C6-H) in aryl (100)  20a, ν(C2-H) in aryl (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C18H2, C17H2 pyrrolidine (100)  νas(C-H) in C15H2 in pyrrolidine (100)  νs(C-H) in C18H2 in pyrrolidine (100)  νs(C-H) in C16H2 in pyrrolidine (100)  νs(C-H) in C17H2 in pyrrolidine (100)  νs(C-H) in C15H2 in pyrrolidine (100)  Combination band  8a, ν(C=C) in aryl (89)  8b, ν(C=C) in aryl (82)  ν(C8-N14) (73) + νs(N7CC) (15)  νs(COO) (49) + ν(C9-C11)  δ(C-H) in-phase in pyrrolidine (92)  19a, ν(CC)(35) + δ(CH) in pyrrolidine (15)  δs(C-H) out-of-phase in pyrrolidine (88)  δs(C-H) out-of-phase in pyrrolidine (85)  δs(C-H) in pyrrolidine  19a,ν(CC,CH) in aryl + ν(C4N) + νs(COO)  νas(CCOO) + νs(NNN) + ν(C-N)  -  νas(COO) + νs(NNN) + δs(CC,CH)  14, ν(CC) + ν(CO12) + ν(NNC)  δ(C-H) in pyrrolidine (30)  γ(C-H) in pyrrolidine (73) + νas(NNN)  γas(CH) in pyrrolidine  14, ν(CC) + ν(NN) + δ(C-H) in pyrrolidine  Γ(pyrrolidine)  3, δ(C-H) in aryl  ν(NN,CN) + γas(CC,CH) in pyrrolidine  νas(NN,CN)+3,δ(CH) in aryl+δ(pyrrolidine)  γas(C-H) out-of-phase in pyrrolidine  γas(C-H) in pyrrolidine  γas(C-H) out-of-phase in pyrrolidine (70)  γas(C-H) in pyrrolidine  9a, δ(C-H) in aryl  γas(C-H) in pyrrolidine (93)  γas(C-H) in pyrrolidine  γas(C-H) in pyrrolidine  15, δ(C-H) in aryl  18a, δ(C-H) in aryl  12, δ(CC,CH) in aryl (96)  δ(CC,CH) in pyrrolidine (73)  17a, γ(C-H) in aryl  18a, δ(CC, CH) in aryl (98)  5, γ(C-H) in aryl (99)  γ(CC,CH) in pyrrolidine + δ(CN)  γas(CC,C-H) in pyrrolidine (86) + δ(CN)  νas(NNN) + 18a, δ(CC,CH) in aryl  γas(C-H) in pyrrolidine (99)  γas(C-H) in pyrrolidine (97)  γas(C-H) in pyrrolidine  17b, γ(C-H) in aryl (100)  γas(C-H) in pyrrolidine  10a, γ(C-H) in aryl  γs(COO) + γ(triazole)  δas(COO) + γ(C9-C11)  δs(COO) + 6a, δ(CC) in aryl  4, γ(CC) in aryl (98)  6a,δ(CCC) in aryl + γas(C-H) in pyrrolidine  γas(NNN) (58) + γs(COO) (22)  γs(NNN) + δas(COO)  Γ(triazol) (65) + δas(COO) (18)  6b, δ(CCC) in aryl  δ(NNN) + ν(CCL) + δ(COO) + 6b, δ(CCC)  γas(C-H) in pyrrolidine  16b, γ(CCC) in aryl (35) + γ(NNN)(28)  δas(NNN) +δ(CCL) +Γ(CC) aryl +δas(COO)  δas(COO) in phase + 6b, δ(CCC) in aryl +La  10a, γ(CH,CC) in aryl (100)  δas(COO) in-phase + δ(triazol) + Γ(ring) |

**Table S2.** Vibrational assignment at the M06-2X/Lanl2mb level.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Calculated at M06-2X/Lanl2mb | | | scaled | Experimental | | Characterization |
| ν | A | S | IR | Raman |
| 3556, 3556, 3556  3555, 3555, 3555  3553, 3553, 3553  3549, 3549, 3548  3541, 3541, 3540  3536, 3536, 3536  *3499*, 3498, 3489  3488, 3468, ***3453***  3439, 3439, 3439  3437, 3437, *3435*  *3387*, **3387**, 3383  3380, 3367, ***3350***  1773, 1773, 1773  1769, 1769, 1769  ***1716***, 1701, 1700  *1697*, 1692, **1689**  ***1686***, 1681, 1680  1679, **1671**, *1670*  ***1669***, 1668, 1668  1640, 1640, 1639  1616, *1602*, **1595**  ***1576***, 1562, 1555  1550, *1548*, **1547**  *1518*, **1510**, 1509  1501, ***1500***, 1498  1494, **1491**, *1486*  1484, ***1477***, 1475  *1474*, **1469**, 1468  ***1433***, 1425, 1424  1399, **1394**, *1390*  1389, 1387, ***1386***  *1367*, **1365**, 1362  ***1351***, 1348, 1347  1343, 1343, 1343  1339, ***1337***, 1336  *1327*, **1318**, 1316  1312, 1311, 1311  1280, 1278, ***1274***  **1269**, *1259*, 1256  1230, 1229, 1229  ***1225***, 1219, 1216  1186, 1186, 1186  1170, 1170, 1170  ***1165***, 1165, 1163  1155, 1154, **1153**  1074, 1073, 1073  ***1071***, 1070, 1068  1068, 1067, 1067  **1054**, *1050*, 1050  1047, 1047, 1046  1035, ***1016***, 1016  1006, 1004, ***1003***  974, 973, 973  ***953***, 941, 941  ***917***, 904***,*** *889*  907, 906, 906  902, 901, **901**  *846*, **842**, 840  799, ***792***, 789  *777*, 745, **773**  *766*, 764, **761**  753, 753, 753  **687**, *685*, 679  658, 658, 658  **638**, *636*, 633  630, 580, ***576***  621, 618,***583***  559, ***559***, 556  521, 521, 521  **504**, *500*, 489  *462*, **460**, 457  436, 435, 435  ***421***, 411, 399  *388*, **385**, 382  364, **362**, *354*  326, *323*, **318**  *316*, 292, **283**  277, *272*, **267**  **260**, 251, 243  237, **234**, 226  225, 219, ***213***  **198**, *187*, 178  *167*, 161, **159**  ***155***, 153, 145  138, 131, ***129***  125, ***121***, 112  100, 95, 84  80, 74, 70  66, 62, 59  56, 50, *46*  41, 41, *37*  *35*, 33, *32*  31, *27*, 23  15, 11, 9  7, 4, 4 | 3  1  26  0  1  4  0  14  0  0  1  16  --  0  9  83  32  18  15  11  55  100  17  6  14  7  4  19  71  15  94  --  9  50  48  2  82  11  17  16  22  --  1  2  35  1  1  3  1  1  0  3  0  0  1  --  36  3  1  0  9  36  26  1  7  0  3  0  --  2  2  5  1  0  32  13  0  20  2  1  1  --  7  2  1  0  1  2  1  1  1  1  0  0  0  0  0  0  0  0  0 | --  11  11  3  4  5  1  3  16  8  3  4  14  --  1  97  22  14  9  2  4  100  80  14  9  2  16  25  33  18  1  16  --  5  16  7  1  8  3  0  2  1  --  5  1  2  0  1  1  3  3  0  1  1  1  3  --  24  5  1  1  0  3  1  1  2  0  1  1  --  0  2  2  0  0  3  1  0  1  1  1  0  --  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0 | --  2958  2957  2956  2953  2948  2944  2919  2911, ***2892***  2878  2876  2842  2837  --  1621  1617  ***1574***, 1560  *1558*, **1552**  ***1549***, 1544  1543, ***1536***  1535  1511  1491, *1477*, **1472**  ***1458***, 1441  1436. ***1433***  *1409*. **1401**  ***1395***, 1392  1389, **1386**, *1382*  1380, ***1375***, 1373  *1372*, **1368**  ***1337***, 1329  1309, **1304**, *1301*  1300, ***1297***  *1281*, **1279**, 1276  ***1268***, 1265  1261  1258, ***1256***  *1247*, **1239**, 1237  1234  1207, 1205, ***1202***  **1198**, *1189*, 1186  1164  ***1160***, 1154, 1151  1126  1112  ***1108***, 1106  1099, **1097**  1029  ***1026***, 1023  1023  **1011**, *1007*  1005  994, ***977***  969, ***966***  941  ***922***, 912  ***890***, 882  881, ***879***, 877  **876**, *874*  *827*, **824**, 822  785, ***779***, 777  *766*, **763**  *756*, 754, **752**  744  **684**, *682*, 676  658  **640**, *638*, 635  63***3***, 583, ***579***  624, 621 ***590***  ***568***, 565  533  **518**, *514*, 503  *479*, **477**, 474  455  ***441***, 431, 419  *411*, **408**, 405  388  353 | 3401.6 br, s  2968.1 s  2872.2 m  1895.1 vw  1577.8 br, vs  1500.2 s  1484.5 vs  1418.0 w  1398.1 m  1372.3 vs  1347.5 s  1302.0 vs  1285.5 s  1246.8 m  1218.0 m  1178.2 m  1150 sh  1091.2 vs  1011.8 m  969.0 vs  914.3 w  829.7 vs  805.4 m  754.3 w  698.8 vw  654 m  647.1 m  576.7 w  508.9 m  466.5 m | 1597 vs  1504 s  1375 vs  1167 w  1091 m  1013 w  970 s  72 br m | ν(O-H) H2O bonded  2, ν(C3-H) in aryl (100)  7b, ν(C5-H) in aryl (100)  20b, ν(C6-H) in aryl (100)  20a, ν(C2-H) in aryl (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C18H2, C17H2 pyrrolidine (100)  νas(C-H) in C15H2 pyrrolidine (100)  νs(C-H) in C18H2 pyrrolidine (100)  νs(C-H) in C16H2 pyrrolidine (100)  νs(C-H) in C17H2 pyrrolidine (100)  νs(C-H) in C15H2 pyrrolidine (100)  Combination band  8b, ν(C=C) in aryl (91)  8a, ν(C=C) in aryl (93)  ν(C8-N14) + νs(N7CC)  δ(C-H) in pyrrolidine + ν(C8-N14)  δ(C-H) in pyrrolidine + ν(C8-N14)  δs(C-H) in pyrrolidine  δs(C-H) out-of-phase in pyrrolidine (85)  19a, ν(CC,CH) + ν(C4-N4) +ν(C9-C11)  νas(COO)+νs(CCN)triazol+ν(C9-C11)+19a,ν(CC)  νas(COO) + νs(CCN) in triazol  19b, ν(CC,CH) + νs(NNN) + νas(COO)  δs(C-H) in pyrrolidine + νs(NNN) + νas(COO)  δs(C-H) in pyrrolidine + νs(NNN)  δs(C-H) in pyrrolidine + νs(NNN)  νs(NNN) + νs(COO) + γs(C-H) in pyrrolidine  νs(COO) +νs(NNN) + δs(CC,CH) +19a, ν(CC)  Γ(C-H) in pyrrolidine  νas(NNN)(36) + δ(C-H) in pyrrolidine (30)  3, δ(C-H) + ν(triazol) + δ(C-H) in pyrrolidine  δas(C-H) in pyrrolidine + ν(triazol)  ν(triazol) + 3, δ(CH)+ δ(C-H) in pyrrolidine  ν(pyrrolidine)  ν(triazol)+ 3, δ(C-H) +δ(C-H) in pyrrolidine  δ(CC,CH) in pyrrolidine  14,ν(CC) in aryl +νas(NN)+δ(C-H) pyrrolidine  νs(COO) + δ(triazole) + δas(C-H) pyrrolidine  ν(triazole) + γas(C-H) in pyrrolidine+νs(COO)  9a, δ(C-H) in aryl  δas(C-H) in pyrrolidine  18a, δ(C-H) in aryl  15, δ(C-H) in aryl  δas(C-H) in pyrrolidine  νs(NNN) + 18a, δ(C-H) in aryl  δas(C-H) in pyrrolidine  18a, δ(C-H) in aryl  12, δ(CC, CH) in aryl + δ(CH) + νs(triazol)  νas(triazol)+δ(CC,CH) pyrrolidine +δs(COO)  17a, γ(C-H) in aryl  γ(C-H) in pyrrolidine  γ(C-H) in pyrrolidine  νas(NNN, CC) in triazol +18a, δ(C-H) in aryl  γas(CC,C-H) in pyrrolidine  γas(CC,C-H) in pyrrolidine  10a, γ(C-H) in aryl  17b, γ(C-H) in aryl  δas(COO) + γas(C-H) pyrrolidine +ν(triazol)  δas(COO) + γas(C-H) pyrrolidine +ν(triazol)  γas(C-H) in pyrrolidine + 6a, δ(CCC) in aryl  γs(C9-C11-C8) + γs(COO)  4, γ(CCC) in aryl  γs(COO) + γ(C8-C9)  6a, δ(CC) in aryl  Γ(triazol) + γas(COO) + γ(C-H) pyrrolidine  Γ(triazol) + γas(COO) + γ(C-H) pyrrolidine  γ(C-H) in pyrrolidine  γs(NNN)  16b, γ(CCC) in aryl  δas(COO)phase+δas(triazol)+ν(CCL)+6b,δ(CCC)  ν(CCL) + δas(COO) + δ(NNN) + 6b,δ(CCC)  16a, γ(CCC) in aryl  δ(COO) + δ(triazol) + Γ(CC) in aryl  δ(COO) + δ(triazol) + Γ(CC) in aryl  γ(COO) + γ(triazol) + γ(CC) in aryl  τ(aryl) + γ(CCN)  La |

**Table S3.** Vibrational assignment at the B3LYP/Cep-4G level.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Calculated at B3LYP/Cep-4G | | | scaled | Experimental | | Characterization |
| ν | A | S | IR | Raman |
| 3324, 3323, 3323  3314, 3313, 3313  3302, 3302, 3302  3296, 3296, 3296  3285, ***3283***, 3282  *3282*, 3279, **327**8  **3277**, 3276, *3271*  **3275**, 3275, **3273**  3211, 3210, 3210  3204, 3203, ***3202***  **3181**, 3178, *3171*  3169, *3169*, **3167**  1596, 1595, 1595  1595, *1593*, **1593**  *1593*, **1591**, 1586  *1505*, **1495**, 1493  ***1462***, 1458, 1457  *1443*, 1440, **1438**  1437, *1435*, **1435**  1428, 1427, 1427  1421, 1420, 1420  1373, 1373, 1373  1370, *1363*, **1356**  1336, **1334**, 1334  1328, **1327**, *1326*  ***1307***, 1305, 1304  *1304*, 1302, **1301**  1295, 1295, 1294  1284, 1282, ***1282***  *1271*, **1270**, 1267  *1234*, **1232**, 1231  *1220*, **1218**, 1216  1187, **1186**, *1185*  1182, *1180*, **1179**  *1173*, **1173**, 1171  1154, 1153, **1152**  1148, 1147, ***1146***  *1119*, **1118**, 1114  1084, *1079*, **1078**  1062, 1062, 1062  *1061*, **1060**, 1058  1032, 1032, 1031  1026, 1026, 1026  1001, 1001, 1000  *983*, 982, **981**  945, 944, ***943***  913, 913, 913  902, 901, 901  **882**, *879*, 878  873, *872*, **871**  820, ***819***, 817  815, 815, 815  811, 810, 810  806, 806, 806  804, 803, 803  744, 744, 744  711, 710, 710  *703*, **699**, 698  *653*, **650**, 649  649, *648*, **645**  **586**, *584*, 583  *544*, 543, **542**  533, 533, 533  533, 533, 532  522, 522, 522  *519*, **515**, 511  498, 496, ***495***  452, 452, 451  **443**, 440, *433*  **403**, *401*, 400  390, 390, 389  *366*, 358, **354**  339, 338, ***334***  326, 326, 326  303, ***302***, 301  265, **264**, *260*  256, **253**, *251*  ***233***, 231, 226  **220**, 217,*216*  ***204***, 202, 200  197, *194*, **191**  **168**, 167, *163*  150, 149, 149  **142**, *140*, 134  133, 130, *127*  *110*, **106**, 103  87, ***84***, 75  71, **63**, *60*  53, 50, *46*  45, 44, **42**  **40**, 36, *32*  **31**, 30, **27**  ***26***, 26, 23  **17**, 11, *9*  6, 4, *4* | --  5  1  8  52  10  3  3  13  8  2  1  4  --  35  13  35  57  2  19  100  7  1  1  6  2  5  3  3  2  2  18  --  10  35  1  23  2  1  10  1  2  0  1  1  3  1  --  5  1  2  2  0  1  3  0  5  0  1  0  20  5  2  15  2  1  1  1  0  6  2  0  25  2  --  1  4  2  0  1  0  1  2  1  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0 | --  2  2  5  1  1  2  1  1  5  2  4  1  --  1  100  58  58  2  18  16  1  0  1  0  1  0  12  9  6  1  1  --  0  3  1  0  1  0  0  0  1  4  1  0  1  0  --  1  0  0  1  0  1  3  0  11  0  1  0  0  5  3  1  0  0  0  0  0  2  0  0  1  0  --  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 | 2906  2899  2891  2886  2879, **2877**  2876, **2874**  **2873**, **2869**  2871, **2870**  2826  2821, **2820**  **2804**, 2797  2795, **2793**  --  1512  1511, ***1509***  *1509*, **1507**, 1503  *1429*, **1420**, 1418  ***1389***, 1386  *1372*, 1370, **1368**  1366, ***1364***  1358  1351  1307  1304, *1298*, **1292**  1272, **1270**  1265, ***1264***  ***1245***, 1243  *1242*, **1240**  1234  1223, ***1221***  ***1211***, 1208  *1176*, **1174**  *1163*, **1161**, 1159  1131, ***1129***  1127, ***1125***  ***1118***, 1116  1100, **1098**  1094, ***1092***  ***1066***, 1062  1032, ***1027***  1011  ***1010***, 1008  982  976  952  *934*, **932**  897, ***895***  866  855  **835**, *832*  *826*, **824**  ***773***, 771  768  764  759  757  697  664  *656*, **653**  *605*, **602**  *601*, **597**  **537**, *535*  *494*, **492**  483  483  471  *468*, **464**  446, ***443***  399  389  348  334  309  281  267  243  202  193  168  154  137  130  99  80  71  61  36  12 | 3401.6 br,s  2968.1 s  2872.2 m  1895.1 vw  1577.8br,vs  1500.2 s  1484.5 vs  1418.0 w  1398.1 m  1372.3 vs  1347.5 s  1302.0 vs  1285.5 s  1246.8 m  1218.0 m  1178.2 m  1150 sh  1091.2 vs  1011.8 m  969.0 vs  914.3 w  829.7 vs  805.4 m  754.3 w  698.8 vw  654 m  647.1 m  576.7 w  508.9 m  466.5 m | 1597 vs  1504 s  1375 vs  1167 w  1091 m  1013 w  970 s  72 br m | ν(O-H) H2O bonded  2, ν(C3-H) in aryl (100)  7b, ν(C5-H) in aryl (100)  20b, ν(C6-H) in aryl (100)  20a, ν(C2-H) in aryl (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C16H2, C17H2 (100)  νas(C-H) in C18H2, C17H2 pyrrolidine (100)  13, ν(C-H) in aryl  νs(C-H) in C16H2. C17H2 pyrrolidine (100)  νs(C-H) in C16H2 pyrrolidine (100)  νs(C-H) in C18H2 pyrrolidine (100)  νs(C-H) in C15H2 pyrrolidine (100)  Combination band  ν(C8-N14) +8a, ν(C=C) in aryl  8a, ν(C=C) in aryl + ν(C8-N14)  8b, ν(C=C) in aryl + ν(C8-N14) + νs(N7CC)  νs(COO) (49) + ν(C9-C11)  δ(C-H) in-phase in pyrrolidine (92)  δ(C-H) in pyrrolidine  ν(C4-N4), 19a,ν(CC) + δs(C-H) in pyrrolidine  19a, ν(CC,CH) in aryl  νas(COO) + νs(CCN) in triazol +19a, ν(CC)  ν(C4-N) + νs(COO)  νas(CCOO) + νs(NNN) + ν(C-N)  19b, ν(CC,CH)+ ν(triazol)+δs(C-H) pyrrolidine  δ(CH)pyrrolidine +ν(N7-C)+19b, ν(CC,CH)  ν(CNN) + 3,δ(CH) + δ(CH) in pyrrolidine  δ(C-H) in pyrrolidine + δ(C8-N14)  δs(CC,CH) in pyrrolidine  ν(NNC)+ δs(CC,CH) pyrrolidine +14, ν(CC)  δ(CN) + γ(C-H) in pyrrolidine  δ(C-H) in pyrrolidine + νas(NNN)  νs(triazol) + δ(C-H) in pyrrolidine  14, ν(CC) + ν(NN) + δ(C-H) in pyrrolidine  νs(NNC) + 3, δ(C-H) in aryl  γas(C-H) in pyrrolidine (98)  ν(NN,CN)(68) + γas(CC,CH) in pyrrolidine  3, δ(C-H) in aryl + δas(CNN)  γas(C-H) out-of-phase in pyrrolidine (96)  γas(C-H) in pyrrolidine + νs(CN) + νs(COO)  9a, δ(C-H) in aryl  γas(C-H) in pyrrolidine  γas(C-H) in pyrrolidine  18a, δ(C-H) in aryl  18b, δ(C-H) in aryl  νs(NNN) + 18a, δ(C-H) in aryl  15, δ(C-H) in aryl  γ(C-H) in pyrrolidine + ν(CN)  18a, δ(CH) + ν(CN) + γ(C-H) in pyrrolidine  δ(CC,CH) in pyrrolidine (73)  17a, γ(C-H) in aryl  γ(C-H) in pyrrolidine  5, γ(C-H) in aryl (95)  νs(NNN, CC) in triazol +18a, δ(CC, C-H)  γas(CC,C-H) in pyrrolidine + δ(CN)  νs(NNN) + 18a, δ(CC,CH) in aryl  γas(C-H) in pyrrolidine (93)  17b, γ(C-H) in aryl  δas(COO) +γas(C-H) pyrrolidine + ν(triazol)  δas(COO) + ν(triazol) + γas(C-H) pyrrolidine  δas(COO) +νas(triazol)+ γas(C-H) pyrrolidine  10a, γ(C-H) in aryl  δ(CC) + δs(COO) + δ(triazole)  γs(C-H) in pyrrolidine  γs(C-H) in pyrrolidine + 6a, δ(CC) in aryl  4, γ(CCC) in aryl  γ(COO) in phase + 6b, δ(CCC) + δ(CN)  γas(NNN) + γs(COO)  γs(NNN) + δas(COO)  δas(COO) + La + γ(triazol)  γ(triazol) + ν(CCL) + 6b, δ(CCC) in aryl  δ(NNN) + ν(CCL) + 6b, δ(CC) in aryl  γas(C-H) in pyrrolidine  δas(COO) phase +δ(NNN) +ν(CCL) + Γ(ring)  δ(NNN) + δ(CCL) + δ(CC) aryl + δ(COO)  δ(COO) structure + δ(aryl) + δ(NNN) + La  10a, γ(CC) in aryl  La |