**Synthesis of a Cd(II) metal complex template with 2-amino-5-methylpyridinium organic cation, (C6H9N2)2[CdCl4]: Structure, DFT-calculated descriptors and molecular docking survey**

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**Figure captions**

**Fig. S1.** Observed, and calculated X-ray diffraction patterns of (C6H9N2)2[CdCl4].

**Fig. S2.** SEM images of (C6H9N2)2[CdCl4] compound with different magnifications (a 500×, b 1000×, c 2000×, and d 5000×).

**Fig. S3.** 2D fingerprint plots of the primary intercontacts of (C6H9N2)2[CdCl4] displaying the percentage distribution of various intermolecular contacts engaged in the Hirshfeld surface.

**Fig. S4.** DFT-calculated, and experimental IR spectrum of (C6H9N2)2[CdCl4].

**Fig. S5.** Theoretical TD-DFT UV-Visible spectra of (C6H9N2)2[CdCl4] at BLYP and B3LYP levels.

**Fig. S6.** Solid-state UV-Vis spectrum (a) of (C6H9N2)2[CdCl4] and the corresponding energy gap (b) determined using the Tauc model.

**Fig. S7.** Comparative visualization of the frontier molecular orbitals of the (C6H9N2)2[CdCl4] molecule in the gaseous phase and across various solvents.

**Fig. S8.** Molecular electrostatic potential surfaces (MEPs) of (C6H9N2)2[CdCl4] in the gaseous phase and across various solvents.

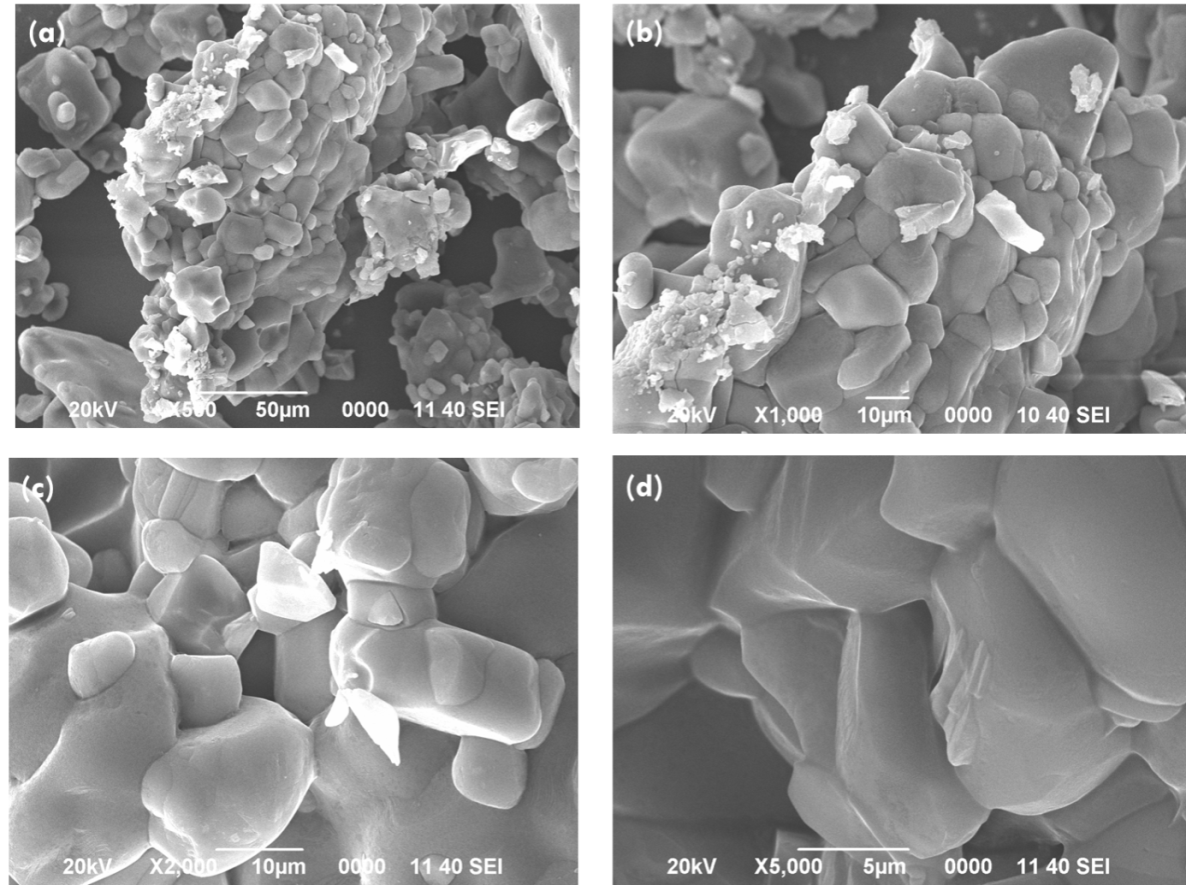
**Fig. S9.** AIM molecular graph screening the different bond critical points (BCPs) of (C6H9N2)2[CdCl4]. The BCPs are depicted as small orange spheres and the connecting paths by orange lines.

**Fig. S10.** Lowest energy docked poses of the ligands: FC1, H4B, HBI and (C6H9N2)2[CdCl4] with iNOS protein.

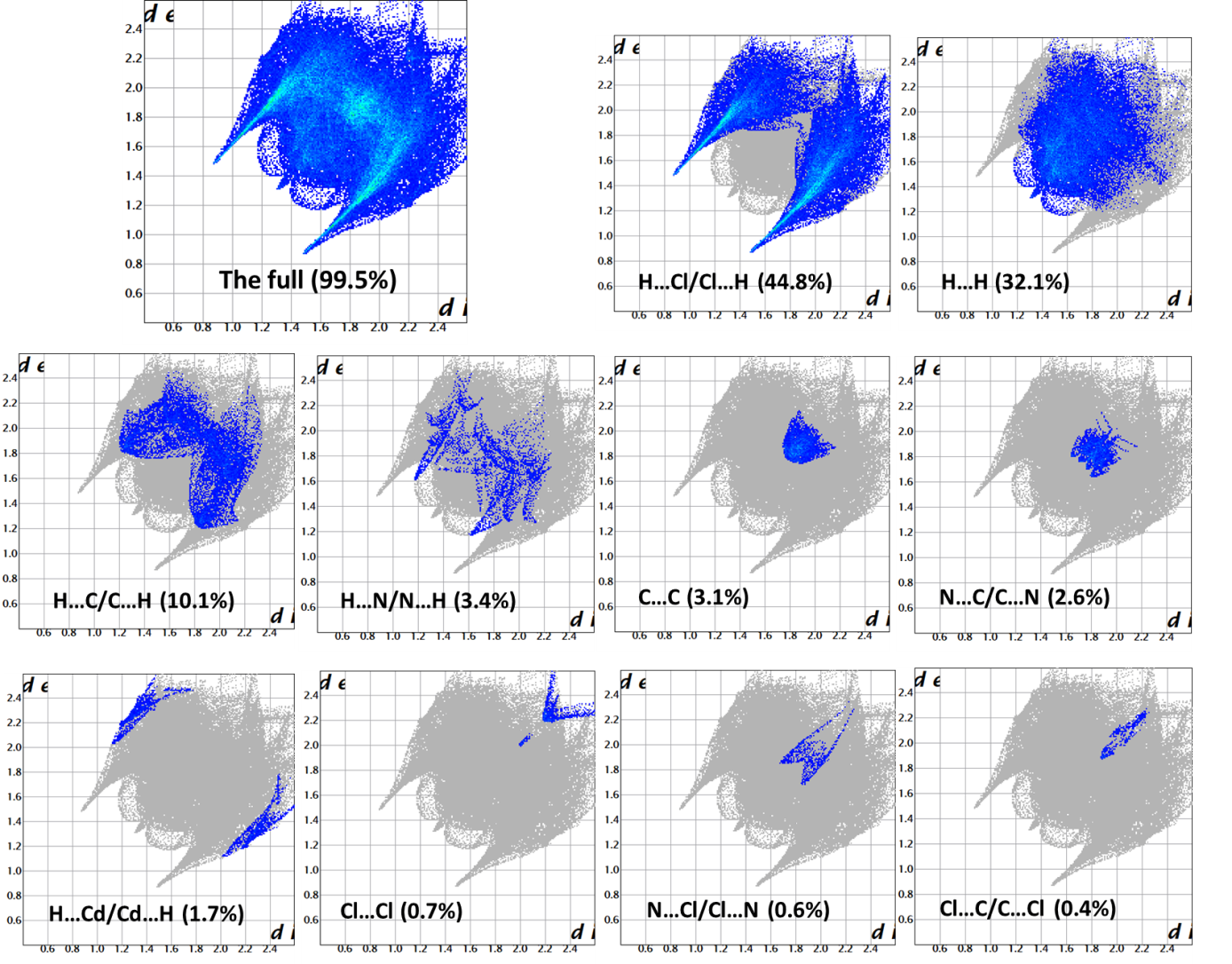
**Fig. S11.** Different types of interactions between the HBI (a), H4B (b) and FC1 (c) ligands and active site residues of the iNOS protein.



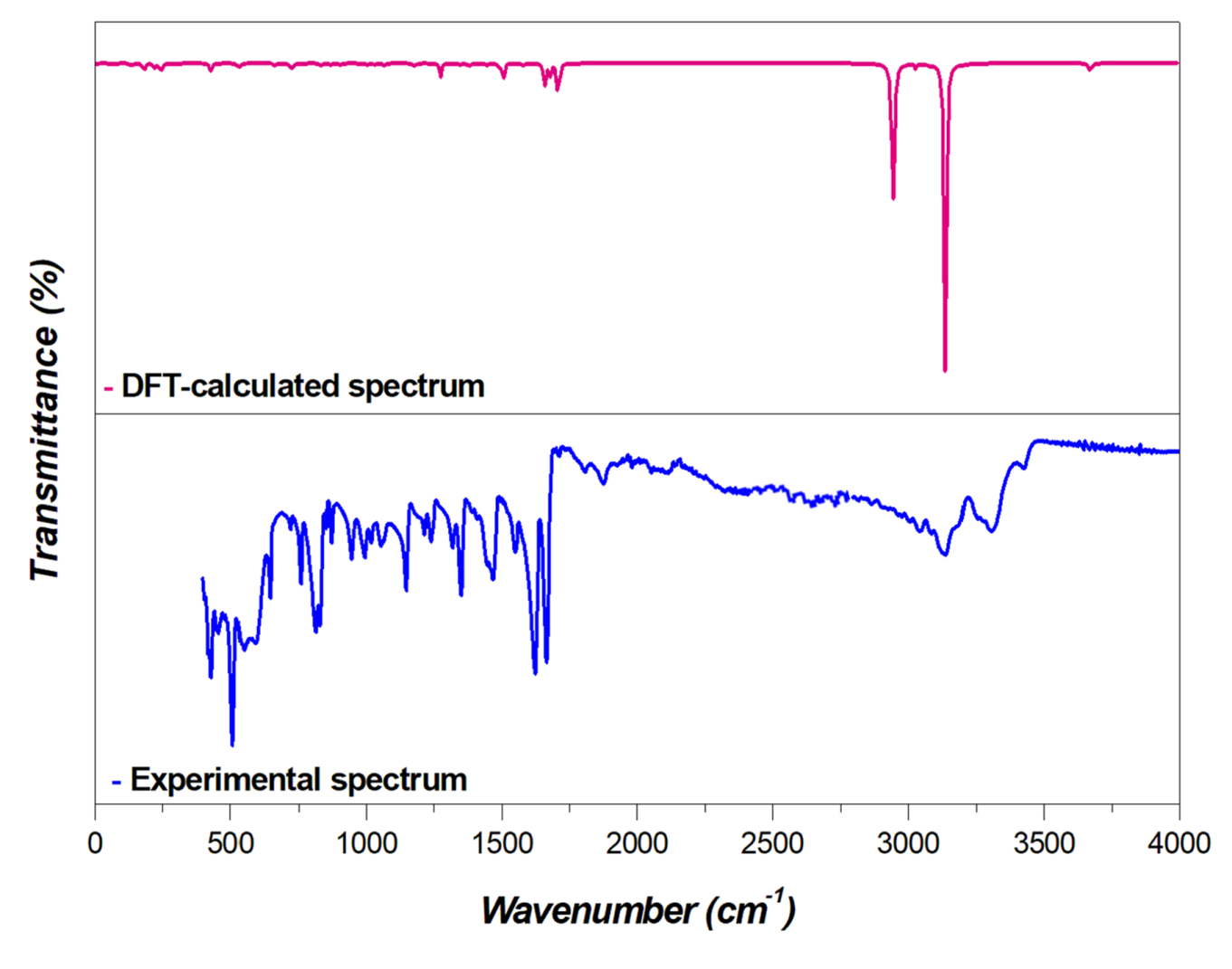
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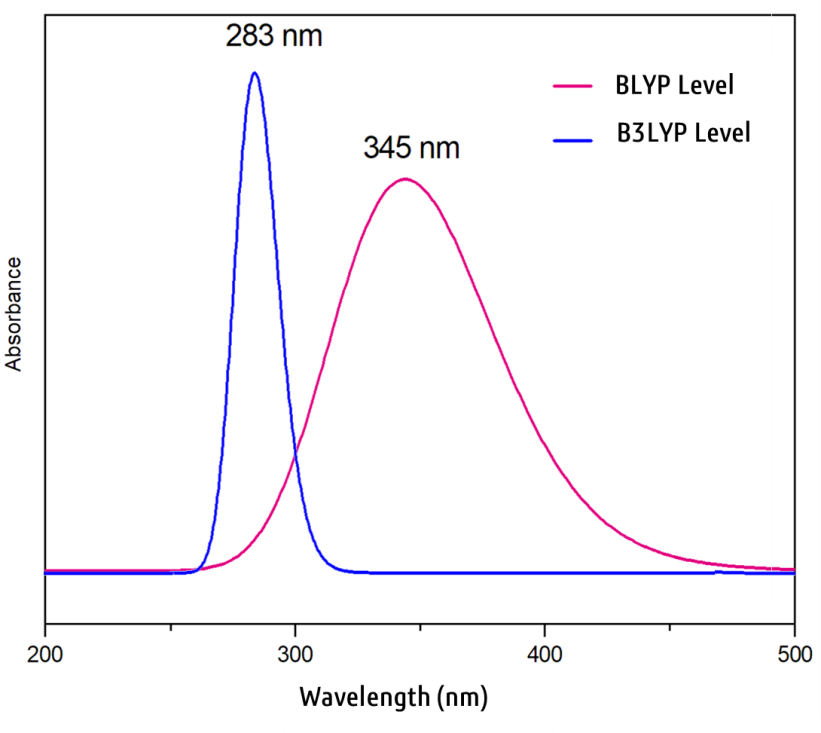
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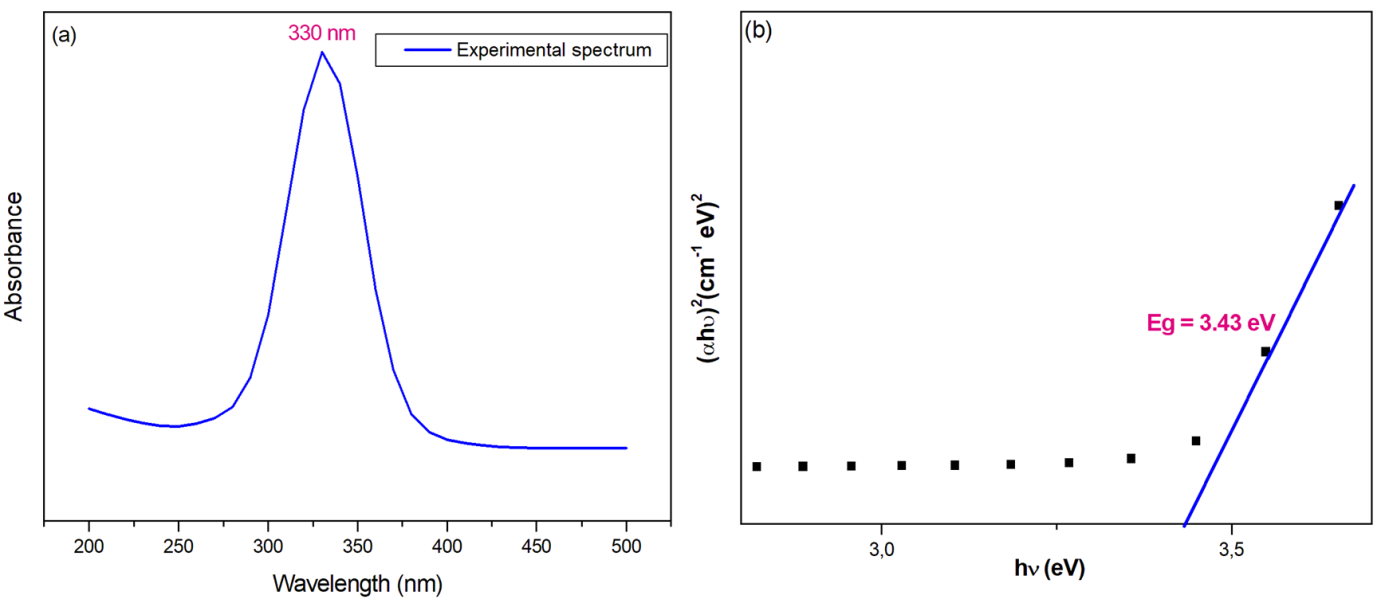
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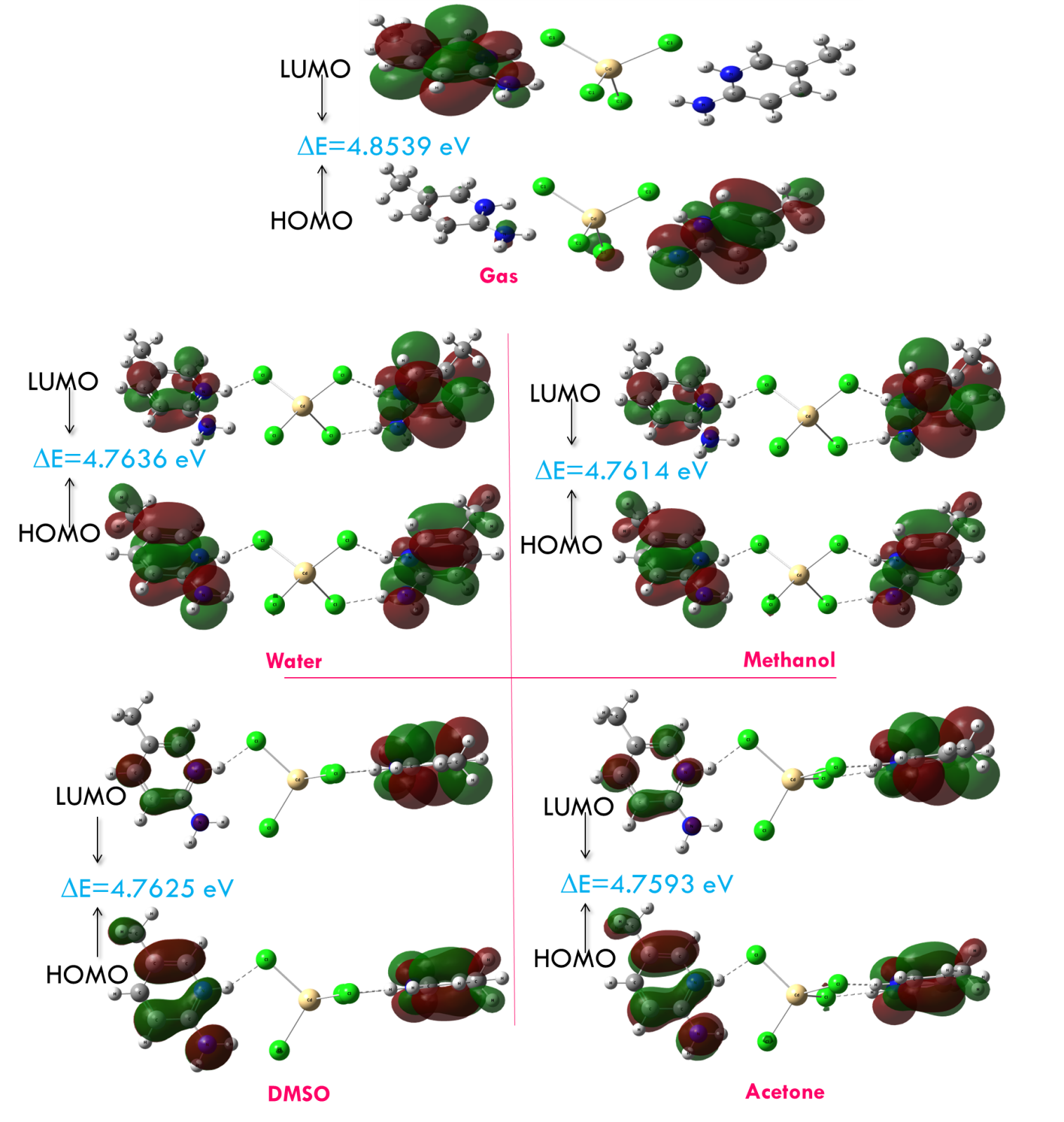
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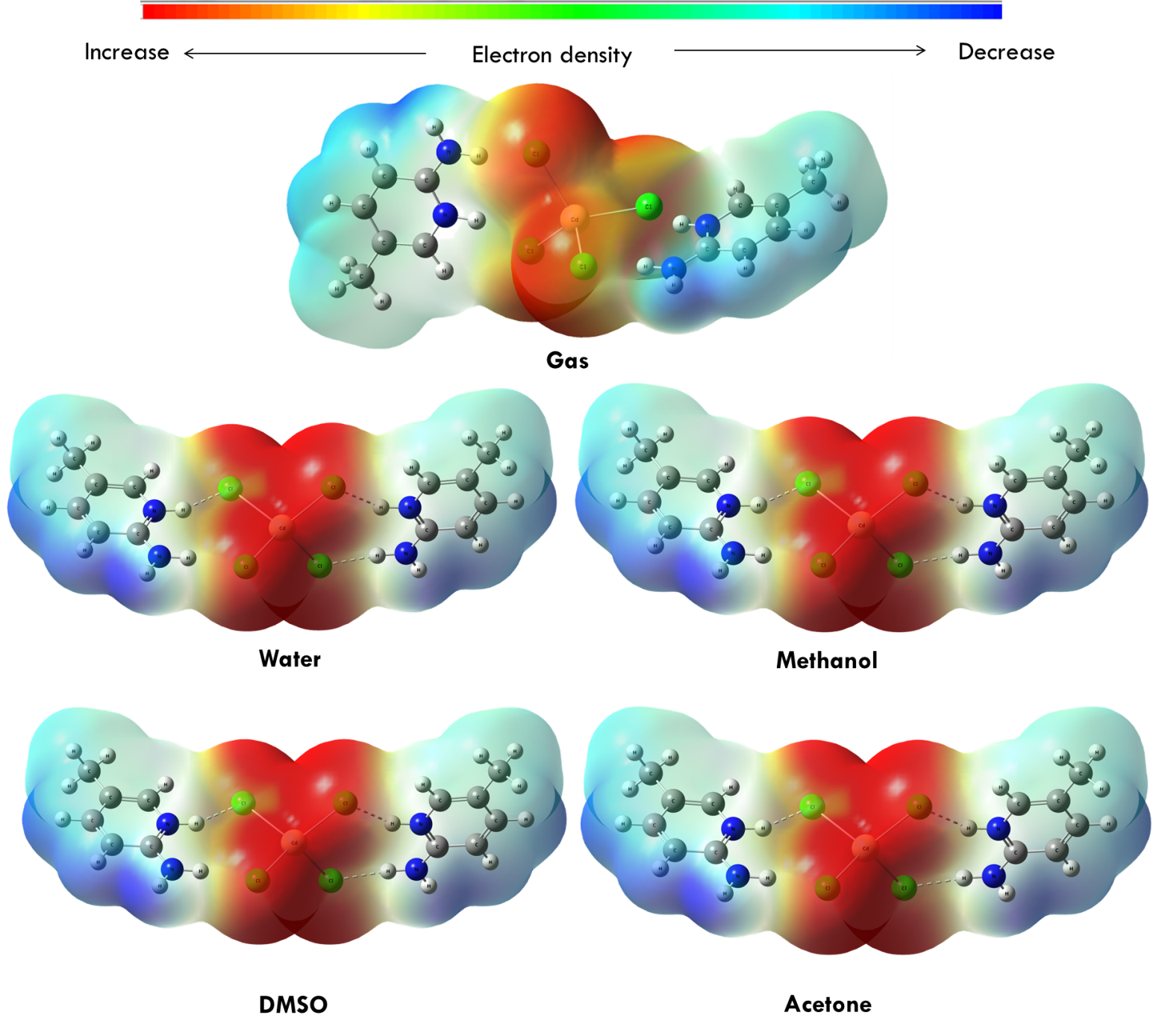
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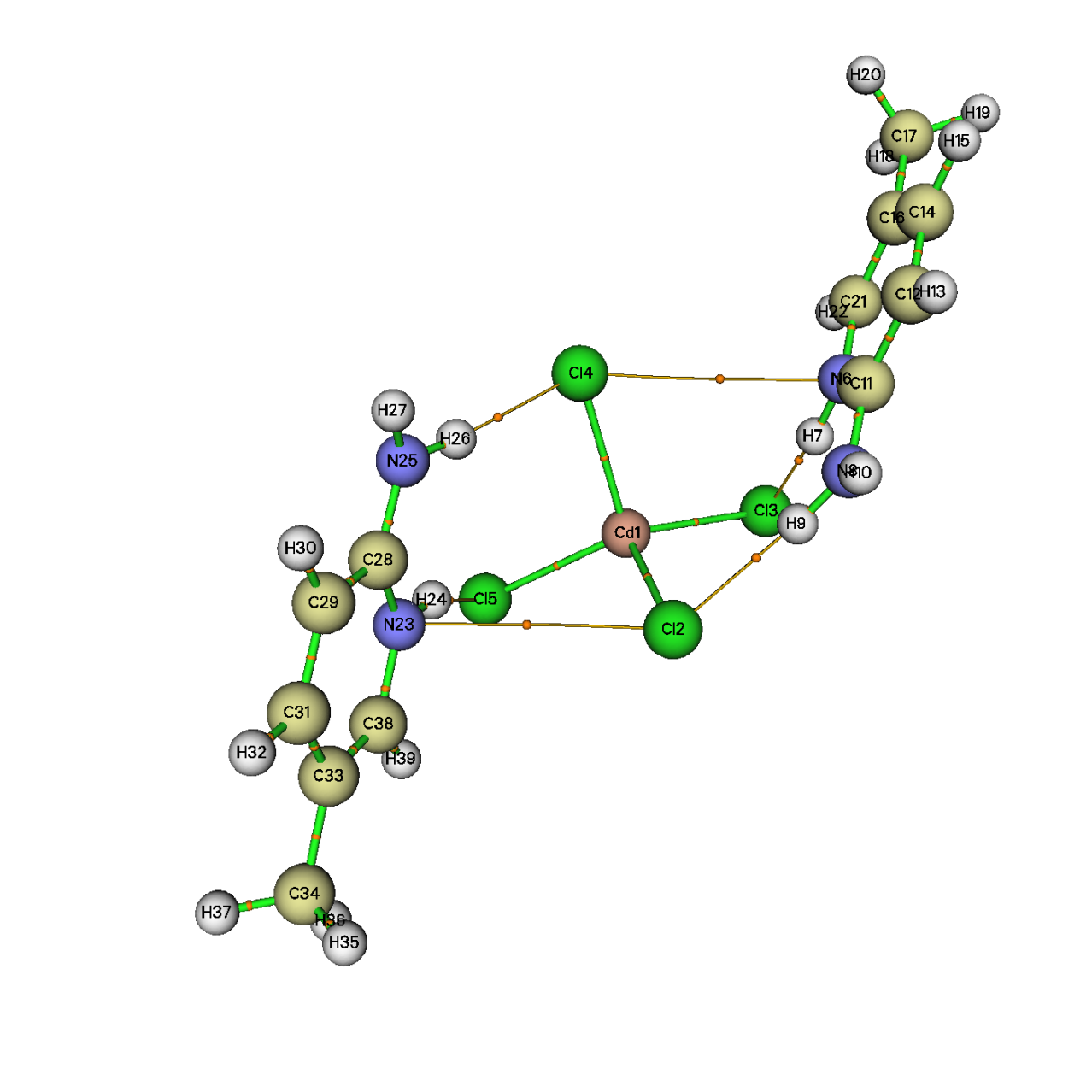
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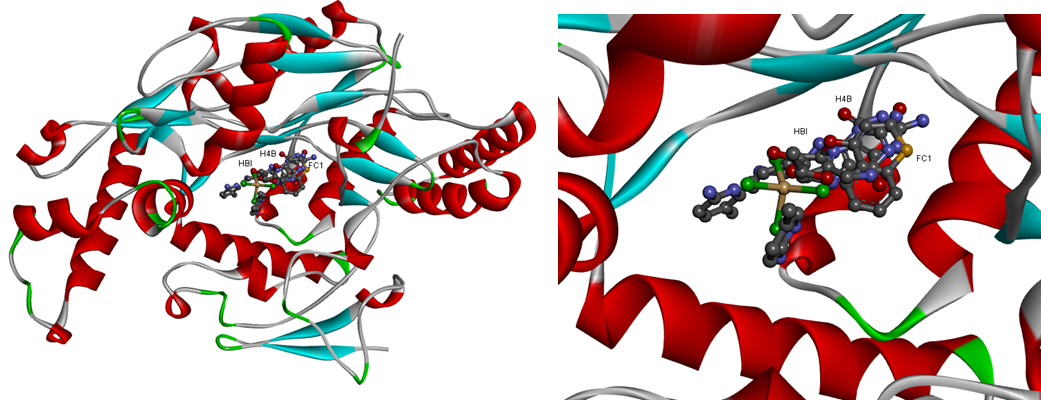
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**Fig. S8.** Molecular electrostatic potential surface (MEPs) of (C6H9N2)2[CdCl4] in the gaseous phase and across various solvents.

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**Fig. S9.** AIM molecular graph screening the different bond critical points (BCPs) of (C6H9N2)2[CdCl4]. The BCPs are depicted as small orange spheres and the connecting paths by orange lines.



**Fig. S10.** Lowest energy docked poses of the ligands: FC1, H4B, HBI and (C6H9N2)2[CdCl4] with iNOS protein.

|  |  |
| --- | --- |
| **(a)** |  |
| **(b)** |  |
| **(c)** |  |

**Fig. S11.** Different types of interactions between the HBI (a), H4B (b) and FC1 (c) ligands and active site residues of the iNOS protein.

**Table captions**

**Table S1.** Selected intermolecular distances (Å) and bond angles (°) in (C6H9N2)2[CdCl4], obtained from X-ray data (with estimated standard deviation in parentheses) and theoretical calculations.

**Table S2.** Hydrogen-bonds details (Å, °) of (C6H9N2)2[CdCl4].

**Table S3.** Observed and calculated wavenumbers (cm-1) and assignments for (C6H9N2)2[CdCl4].

**Table S4.** Global reactivity descriptors and calculated frontier molecular orbital parameters of (C6H9N2)2[CdCl4] calculated using DFT/LANL2DZ level.

**Table S1.** Selected intermolecular distances (Å) and bond angles (°) in (C6H9N2)2[CdCl4], obtained from X-ray data (with estimated standard deviation in parentheses) and theoretical calculations.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Bond lengths(Å)** | | | | **Bond angles(°)** | | |
| Calculated  B3LYP  /LanL2DZ | | | X-Ray | Calculated  B3LYP  /LanL2DZ | | X-Ray |
| **Inorganic atom position** | | |  |  | | |
| Cd1—Cl1 | 2.5444 | | 2.4745 (15) | Cl1—Cd1—Cl4 | 112.89 | 107.41 (6) |
| Cd1—Cl2 | 2.5670 | | 2.4356 (16) | Cl2—Cd1—Cl1 | 102.41 | 103.79 (6) |
| Cd1—Cl3 | 2.5442 | | 2.4236 (15) | Cl2—Cd1—Cl4 | 113.05 | 109.00 (6) |
| Cd1—Cl4 | 2.5667 | | 2.4934 (15) | Cl3—Cd1—Cl1 | 113.01 | 115.27 (6) |
|  |  | |  | Cl3—Cd1—Cl2 | 113.48 | 117.20 (7) |
|  |  | |  | Cl3—Cd1—Cl4 | 102.42 | 103.80 (6) |
| **Organic atom position** | | |  |  | |  |
| N1—C1 | | 1.354 | 1.340 (8) | C1—N1—C6 | 123.4 | 123.4 (5) |
| N1—C6 | | 1.359 | 1.357 (9) | N1—C1—C2 | 116.6 | 117.1 (6) |
| N2—C1 | | 1.333 | 1.328 (8) | N2—C1—N1 | 119.9 | 119.7 (6) |
| C1—C2 | | 1.420 | 1.407 (8) | N2—C1—C2 | 123.4 | 123.2 (6) |
| C2—C3 | | 1.371 | 1.367 (9) | C3—C2—C1 | 120.1 | 119.4 (6) |
| C3—C4 | | 1.417 | 1.397 (9) | C2—C3—C4 | 121.9 | 122.1 (6) |
| C4—C5 | | 1.505 | 1.499 (10) | C3—C4—C5 | 121.8 | 121.8 (6) |
| C4—C6 | | 1.370 | 1.356 (9) | C6—C4—C3 | 116.1 | 116.6 (6) |
| N3—C7  N3—C12  N4—C7  C7—C8  C8—C9  C9—C10  C10—C11  C10—C12 | | 1.354  1.358  1.333  1.419  1.371  1.417  1.505  1.370 | 1.335 (8)  1.382 (9)  1.333 (8)  1.401 (9)  1.347 (10)  1.404 (11)  1.494 (10)  1.332 (11) | C6—C4—C5  C4—C6—N1  C7—N3—C12  N3—C7—C8  N4—C7—N3  N4—C7—C8  C9—C8—C7  C8—C9—C10  C9—C10—C11  C12—C10—C9  C12—C10—C11  C10—C12—N3 | 122.1  121.9  123.4  116.6  119.8  123.4  120  121.8  121.8  116  122.1  121.9 | 121.6 (6)  121.4 (6)  121.8 (6)  117.7 (6)  119.4 (6)  122.9 (6)  119.5 (6)  122.9 (7)  121.7 (8)  115.8 (6)  122.6 (8)  122.4 (7) |

**Table S2.** Hydrogen-bonds details (Å, °) of (C6H9N2)2[CdCl4].

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***D—H···A*** | ***D—H(Å)*** | ***H···A(Å)*** | ***D···A(Å)*** | ***D—H···A(°)*** |
| ***N1—H1···Cl2*** | 0.86 | 2.33 | 3.174 (5) | 167 |
| ***N2—H2A···Cl1*** | 0.86 | 2.78 | 3.433 (6) | 134 |
| ***N2—H2B···Cl4i*** | 0.86 | 2.52 | 3.378 (7) | 174 |
| ***N3—H3A···Cl4*** | 0.86 | 2.30 | 3.134 (6) | 162 |
| ***N4—H4A···Cl3*** | 0.86 | 2.51 | 3.286 (6) | 150 |
| ***N4—H4B···Cl1ii*** | 0.86 | 2.50 | 3.350 (7) | 170 |
| ***C9—H9···Cl1iii*** | 0.93 | 2.75 | 3.670 (7) | 168 |

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*−1, *y*, *z*; (iii) −*x*, −*y*+1, −*z*.

**Table S3.** Observed and calculated wavenumbers (cm-1) and assignments for (C6H9N2)2[CdCl4].

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Calculated frequencies | |  |  |
| Experimental  IR | Unscaled | **Scaled** | **Ii** | Vibrational assignments (% **PED**) |
| 3421 | 3660 | 3506 | 93.59 | ʋNH (30) |
| 3318 | 3660 | 3506 | 35.22 | δHCCC (27) |
| 3140 | 3247 | 3111 | 2807.88 | ʋNH (35) βHNH (10) δHNCN (26) |
| 3140 | 3244 | 3107 | 395.05 | ʋNH (17) δCNHCl (37) |
| 3082 | 3214 | 3079 | 5.05 | ʋNH (20) δHNCN (12) δCNHCl (15) δHNCC (16) |
| 3082 | 3214 | 3079 | 5.39 | ʋNH (49) |
| 3042 | 3199 | 3064 | 1.77 | βHNC (29) δHNCN (10) |
| 3042 | 3199 | 3064 | 1.89 | ʋNH (13) βHNC (26) δCNHCl (17) |
| 3042 | 3168 | 3035 | 9.51 | ʋCH (16) βHNH (32) βHCC (12) δCNHCl (17) |
| 3042 | 3168 | 3035 | 11.97 | ʋNH (17) ʋCH (38) βHCC (28) |
| 2967 | 3113 | 2983 | 11.30 | ʋNH (11) βHNC (10) βHCC (18) βClHN (26) δClCdClH (10) |
| 2967 | 3113 | 2983 | 10.45 | ʋClH (15) βCdClH (10) δHCCC (36) |
| 2967 | 3080 | 2951 | 12.01 | ʋCH (20) βHNH (14) βHCC (11) |
| 2967 | 3079 | 2951 | 11.52 | βHCC (15) δCNHCl (13) δHCCC (30) |
| 2907 | 3037 | 2910 | 1654.06 | ʋCH (29) βHCH (15) δHCCC (11) |
| 2907 | 3030 | 2903 | 98.67 | βHCH (37) δHCCC (25) |
| 2907 | 3029 | 2902 | 33.61 | δHCCC (28) |
| 2907 | 3027 | 2900 | 823.32 | βHCC (10) δHCCC (53) |
| 1667 | 1707 | 1635 | 52.89 | βHCC (53) |
| 1667 | 1707 | 1636 | 515.21 | ʋCH (11) βHCH (28) δHCCC (16) |
| 1667 | 1678 | 1650 | 121.77 | γHCCC (17) |
| 1667 | 1677 | 1648 | 0.88 | δNHClCd (11) |
| 1622 | 1663 | 1635 | 165.00 | ʋCH (29) βHNH (11) |
| 1662 | 1663 | 1634 | 143.70 | ʋCH (33) |
| 1552 | 1581 | 1554 | 21.14 | ʋCH (44) |
| 1552 | 1581 | 1554 | 14.02 | βHNH (25) |
| 1464 | 1508 | 1482 | 61.53 | ʋCH (24) δHCCC (12) |
| 1464 | 1508 | 1482 | 65.23 | βHCC (23) |
| 1464 | 1494 | 1468 | 20.50 | βHCC(12) δHNHCl (11) |
| 1464 | 1494 | 1468 | 51.11 | ʋNH (10) δHNHCl (21) |
| 1464 | 1486 | 1461 | 9.07 | ʋClH (10) δNHClCd (11) |
| 1464 | 1486 | 1461 | 8.24 | δHCCC (19) |
| 1464 | 1436 | 1411 | 11.81 | βHCC (12) δHCCC (12) |
| 1464 | 1436 | 1411 | 28.41 | βHNC |
| 1350 | 1423 | 1398 | 5.86 | βHCH (11) |
| 1350 | 1423 | 1398 | 4.31 | ʋCH (45) δHCCC (10) |
| 1350 | 1379 | 1355 | 11.36 | βNHCl |
| 1350 | 1379 | 1355 | 52.59 | ʋCH (12) δHCCC (10) |
| 1350 | 1350 | 1327 | 13.65 | ʋCH (10) δHCCC (28) |
| 1350 | 1350 | 1326 | 16.74 | ʋCH (29) |
|  | 1278 | 1256 | 47.76 | βHClCd (18) |
|  | 1277 | 1255 | 70.89 | βHCC (20) |
|  | 1242 | 1221 | 1.82 | βHCH |
| 1222 | 1242 | 1221 | 1.53 | ʋCC (14) βCNC (22) |
| 1151 | 1177 | 1157 | 10.70 | γNNCC (17) |
| 1151 | 1177 | 1157 | 36.96 | ʋNC (31) |
|  | 1080 | 1061 | 17.07 | ʋNC (18) δCNHCl (14) γNNCC (10) |
|  | 1079 | 1061 | 3.40 | ʋNC (25) |
|  | 1070 | 1052 | 1.81 | ʋNC (20) βNCC (17) |
|  | 1070 | 1052 | 2.39 | δCNCC (16) |
|  | 1036 | 1018 | 5.45 | βCCC (25) δCNHCl (21) |
|  | 1036 | 1018 | 6.91 | βCCN |
| 989 | 1007 | 990 | 5.11 | δHCCC |
| 989 | 1007 | 990 | 16.67 | δHCCC |
| 989 | 1002 | 985 | 7.58 | βHCH (16) |
| 989 | 1002 | 985 | 3.42 | ʋCH (10) |
| 989 | 980 | 963 | 0.87 | ʋClH (15) |
| 989 | 980 | 963 | 32.25 | ʋNC (24) |
|  | 902 | 886 | 3.74 | ʋNC (12) βNHCl (12) |
|  | 901 | 886 | 43.04 | ʋClH (20) |
|  | 870 | 856 | 7.93 | δHNCN (11) δCCCN(10) γNNCC (13) |
|  | 870 | 855 | 0.24 | δCCCN(15) δHNCC(13) |
| 810 | 831 | 816 | 2.82 | δHClCdCl |
| 810 | 830 | 816 | 59.26 | δClHNC |
| 763 | 773 | 760 | 1.08 | ʋCC (11) βCCC (46) |
| 763 | 773 | 760 | 5.03 | ʋCdCl (10) γNNCC (10) |
| 763 | 732 | 720 | 0.17 | ʋCdCl (18) γNNCC (14) |
| 763 | 732 | 719 | 0.12 | δCCCC |
|  | 680 | 668 | 37.42 | δHCCC(12) |
|  | 675 | 664 | 226.22 | ʋCC (10) βHCC (20) δHCCC(11) |
|  | 661 | 650 | 8.79 | βHCC (11) βCNH (12) |
|  | 661 | 649 | 35.09 | ʋCC (14) |
| 507 | 528 | 519 | 1.98 | βCNH (11) |
| 507 | 527 | 518 | 67.41 | ʋCH (18) βHCC (19) |
| 507 | 485 | 476 | 1.21 | ʋCH (36) ʋCC (12) |
| 484 | 484 | 476 | 0.24 | ʋCH (14) |
| 447 | 448 | 441 | 1.86 | δHCCC(16) |
| 447 | 447 | 439 | 98.36 | γCCCC (27) |
|  | 376 | 370 | 1.94 | δHCCC(15) |
|  | 335 | 329 | 9.66 | γCCCC (16) |
|  | 270 | 265 | 0.05 | ʋClH (11) δCNHCl (10) |
|  | 237 | 233 | 0.04 | βCCC (11) |
|  | 177 | 174 | 3.80 | ʋCdCl (18) βClCdCl (27) |
|  | 152 | 149 | 0.63 | ʋCC (11) ʋCdCl (19) βClHN (11) |
|  | 143 | 141 | 0.32 | δCNHCl |
|  | 134 | 132 | 1.43 | δClCdClH (16) |
|  | 130 | 128 | 61.57 | ʋClH (44) |
|  | 128 | 126 | 0.99 | βNCC (11) δCNHCl (16) |
|  | 120 | 118 | 49.71 | ʋCH (34) |
|  | 117 | 115 | 36.06 | ʋCC (16) δCCCC (10) |
|  | 116 | 114 | 43.34 | ʋNC (39) βNCC (21) |
|  | 113 | 111 | 108.91 | βCCC (11) |
|  | 110 | 108 | 7.19 | βCCC (16) |
|  | 109 | 107 | 4.43 | ʋCH (10) ʋCC (24) βCCC (13) |
|  | 108 | 106 | 0.00 | βHCH (10) δHCCC (12) δCNCC (14) |
|  | 100 | 98 | 6.62 | ʋCC (13) ʋNC (15) βNCC (19) |
|  | 97 | 95 | 0.48 | ʋCC (35) |
|  | 95 | 93 | 0.54 | βHCC (10) |
|  | 90 | 88 | 10.46 | ʋNH (14) ʋCH (10) ʋNC (10) |
|  | 88 | 86 | 1.02 | βCCC (14) δCCCC (15) |
|  | 85 | 83 | 1.27 | ʋNC (20) |
|  | 69 | 68 | 0.34 | ʋClH (12) |
|  | 66 | 65 | 0.33 | δCNHCl |
|  | 64 | 63 | 4.08 | γCCCC |
|  | 45 | 44 | 1.59 | ʋCC (46) |
|  | 39 | 38 | 2.96 | ʋNC (16) |
|  | 29 | 28 | 1.51 | ʋCH (12) βCCC (21) |
|  | 21 | 21 | 3.06 | ʋCC (23) |
|  | 17 | 17 | 0.14 | βCCC (16) |
|  | 13 | 13 | 2.38 | ʋCC (20) |
|  | 11 | 11 | 0.89 | δHCCC (15) |

**Ii**: infrared intensity (km.mol-1). ʋ, β, δ and γ denote stretching, in-plane bending, torsion and out-of-plane bending modes, respectively.

**PED**: potential energy distribution data are taken fromVEDA4

**Scaling factor**: from 4000 to 1700 cm-1 are scaled with 0.983 and lower than 1700 cm-1 are scaled with 0.958.

**Table S4.** Global reactivity descriptors and calculated frontier molecular orbital parameters of (C6H9N2)2[CdCl4] calculated using DFT/LANL2DZ level.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | EHOMO (eV) | ELUMO (eV) | |EHOMO-ELUMO| (eV) | I | A | χ | η | S | μ | ω |
| Gas | -6.5462 | -2.3266 | 4.2196 | 6.5462 | 2.3266 | 4.4364 | 2.1098 | 0.2369 | -4.4364 | 4.6643 |
| Water | -6.3362 | -1.5725 | 4.7636 | 6.3362 | 1.5725 | 3.9543 | 2.3818 | 0.2099 | -3,9543 | 3,2825 |
| Methanol | -6.3459 | -1.5845 | 4.7614 | 6.3459 | 1.5845 | 3.9652 | 2.3807 | 0.2100 | -3,9652 | 3,3021 |
| DMSO | -6.3408 | -1.5783 | 4.7625 | 6.3408 | 1.5783 | 3.9595 | 2.3812 | 0.2099 | -3,9595 | 3,2919 |
| Acetone | -6.3557 | -1.5965 | 4.7692 | 6.3557 | 1.5965 | 3.9761 | 2.3796 | 0.2101 | -3,9761 | 3,3218 |

(I): Ionization potential; (A): Electron affinity ; (ω): Global electrophilicity; (χ): Electronegativity; (μ): Global chemical potential; (η): Global hardness; (S): Global softness.