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# Development of $Hg^{2+}$ sensor based on N'-[1-(pyridin-2-yl)ethylidene]benzenesulfono -hydrazide (PEBSH) fabricated silver electrode for environmental remediation.

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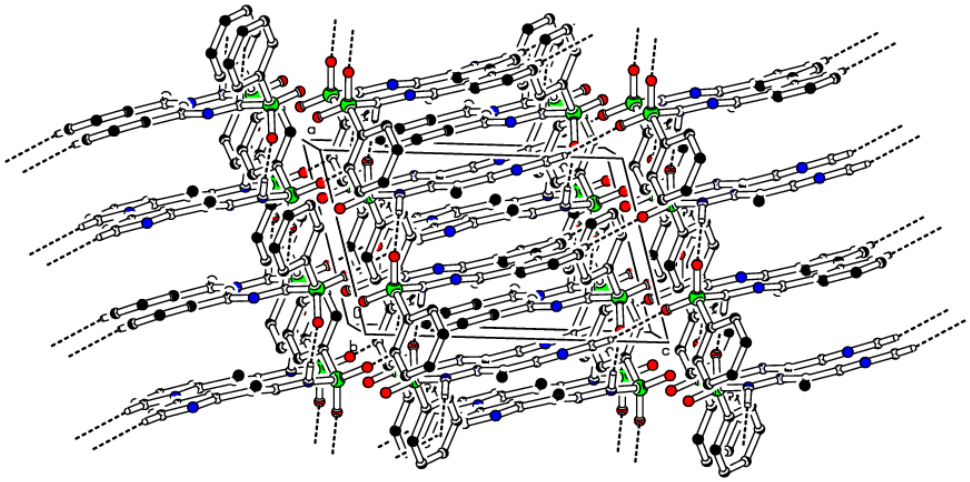

Figure S1 : Unit cell packing diagram of 1.

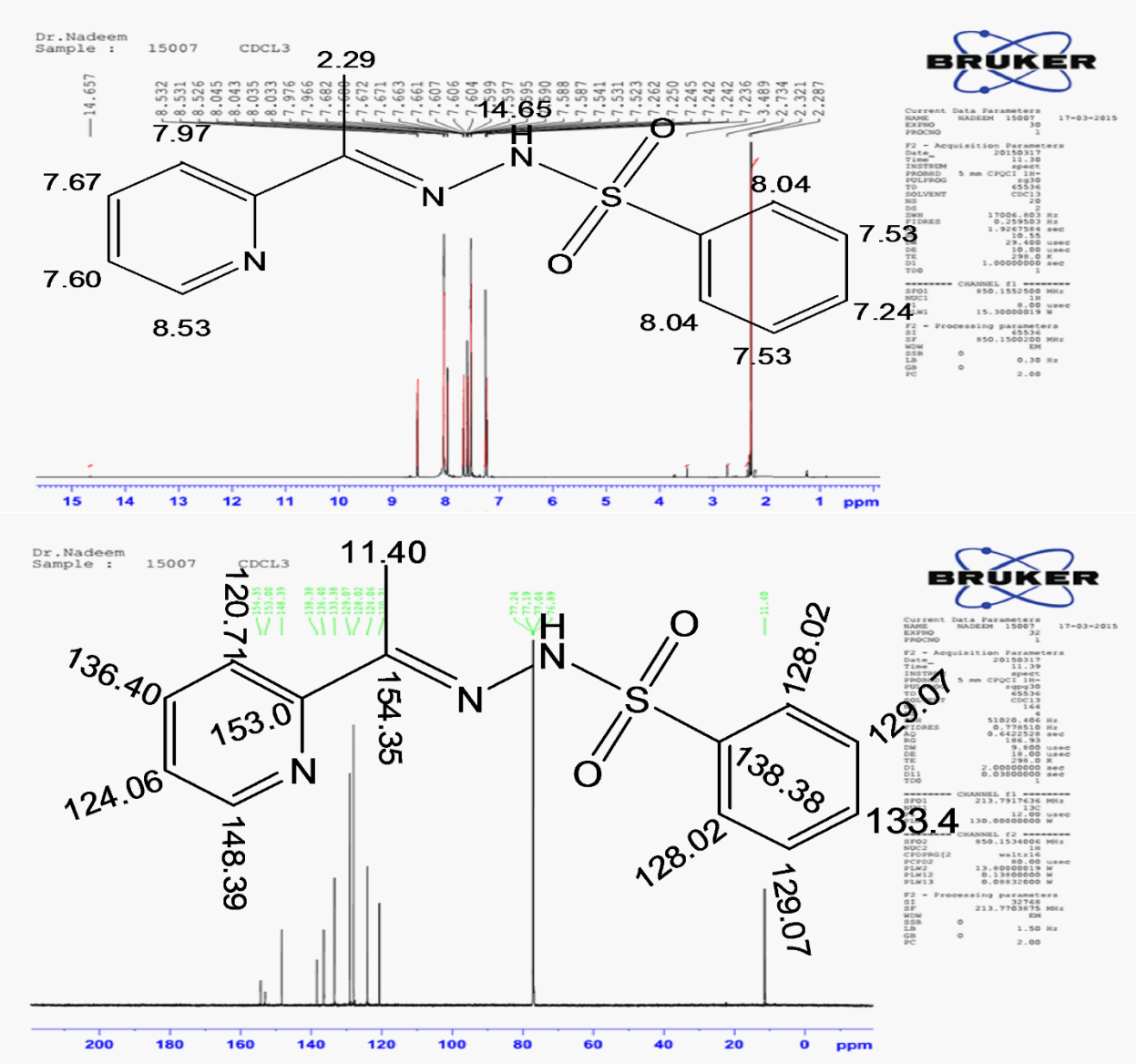


Figure S2: Proton & C-13 NMR spectra of PEBSH and characterization of respective $^{1}H$ and $^{13}C$ positions.

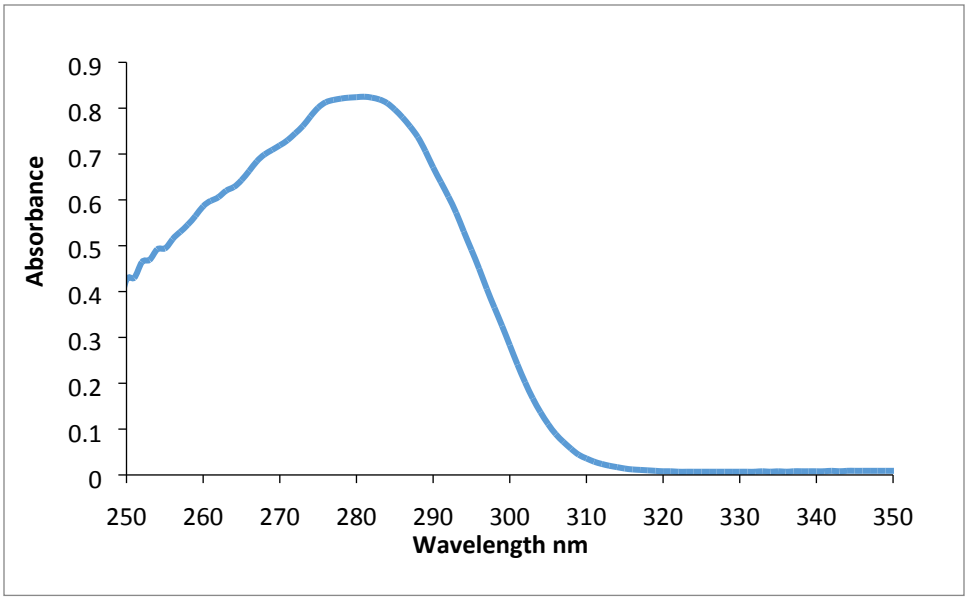


Figure S3: UV/VIS spectrum of PEBSH

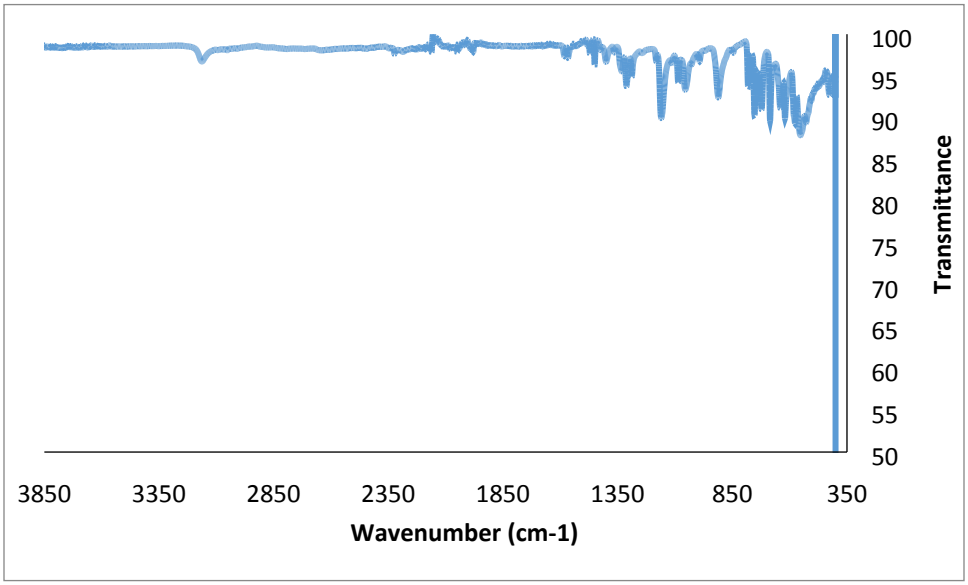


Figure S4: FTIR spectrum of PEBSH

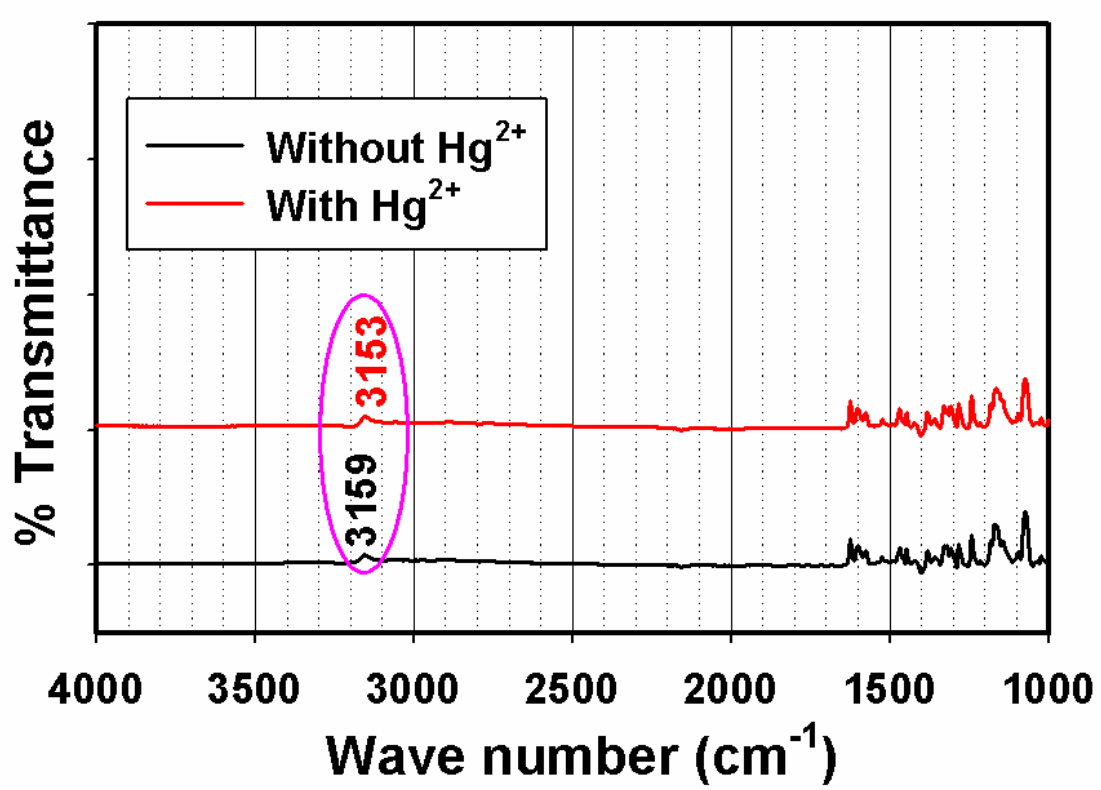


Figure S5: Comparative FTIR spectrums of PEBSH. Red color: In presence of $Hg^{2+}$; Black color: In absence of $Hg^{2+}$ ion

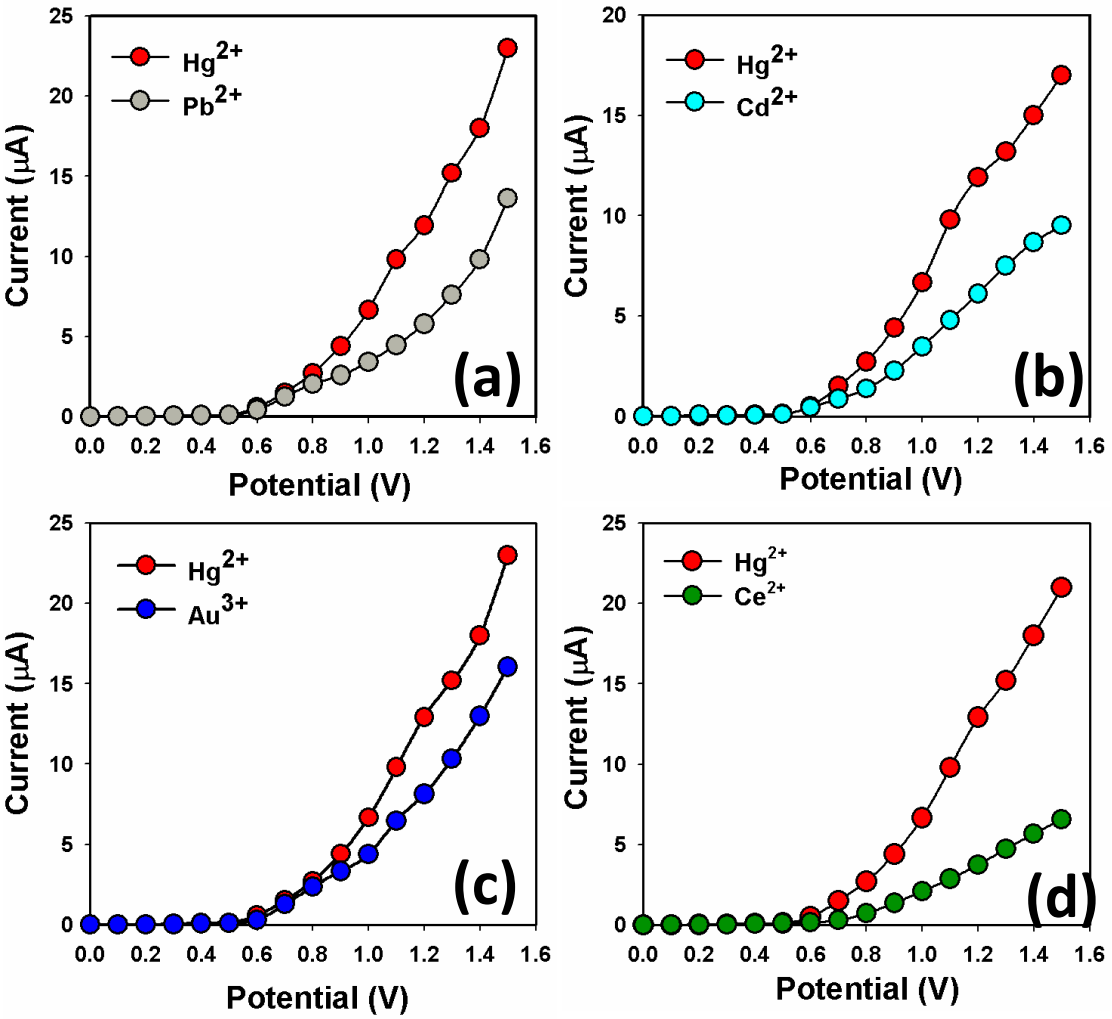


Figure S6: Here, it is investigated the I-V response of dual or complex matrices with and without $Hg^{2+}$ in presence of other metallic ions. (a) $Hg^{2+}$ and $Pb^{2+}$, (b) $Hg^{2+}$ and $Cd^{2+}$, (c) $Hg^{2+}$ and $Au^{3+}$, and (d) $Hg^{2+}$ and $Ce^{2+}$

| **Table S1 Crystal data and structure refinement for PEBSH.** | |
|---|---|
| CCDC number | 1063027 |
| Empirical formula | $C_{13}H_{13}N_3O_2S$ |
| Formula weight | 275.32 |
| Temperature/K | 293(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/a$ |
| a/Å | 7.4145(6) |
| b/Å | 16.0955(16) |
| c/Å | 11.8314(10) |
| α/° | 90 |
| β/° | 105.632(9) |
| γ/° | 90 |
| Volume/Å$^3$ | 1359.7(2) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.345 |
| μ/mm$^{-1}$ | 0.239 |
| F(000) | 576.0 |
| Crystal size/mm$^3$ | 0.14× 0.17 × 0.43 |
| Radiation | MoKα (λ = 0.71073) |
| 2θ range for data collection/° | 6.198 to 58.728 |
| Index ranges | $-9 \leq h \leq 10$, $-22 \leq k \leq 19$, $-13 \leq l \leq 15$ |
| Reflections collected | 7815 |
| Independent reflections | 3293 [$R_{int}$ = 0.0264, $R_{sigma}$ = 0.0354] |
| Data/restraints/parameters | 3293/0/175 |
| Goodness-of-fit on $F^2$ | 1.069 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0493, $wR_2$ = 0.1193 |
| Final R indexes [all data] | $R_1$ = 0.0735, $wR_2$ = 0.1369 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.22/-0.33 |

| Table S2 Selected bond lengths for PEBSH | | |
|---|---|---|
| **Atom** | **Atom** | **Length/Å** |
| C1 | S1 | 1.757(2) |
| C7 | N2 | 1.283(3) |
| C8 | N3 | 1.335(3) |
| C12 | N3 | 1.338(3) |
| N1 | N2 | 1.402(2) |
| N1 | S1 | 1.6461(18) |
| O1 | S1 | 1.4234(16) |
| O2 | S1 | 1.4295(17) |

| Table S3 Selected bond angles for PEBSH | | | |
|---|---|---|---|
| **Atom** | **Atom** | **Atom** | **Angle/°** |
| C2 | C1 | S1 | 118.98(17) |
| N2 | C7 | C8 | 114.54(19) |
| N2 | C7 | C13 | 125.67(18) |
| N3 | C8 | C7 | 116.1(2) |
| N3 | C8 | C9 | 122.41(19) |
| N3 | C12 | C11 | 124.8(3) |
| N2 | N1 | S1 | 112.77(14) |
| C7 | N2 | N1 | 116.68(18) |
| C8 | N3 | C12 | 116.7(2) |
| N1 | S1 | C1 | 108.42(9) |
| O1 | S1 | C1 | 109.58(10) |
| O1 | S1 | N1 | 104.67(10) |
| O1 | S1 | O2 | 119.90(11) |
| O2 | S1 | C1 | 107.46(11) |
| O2 | S1 | N1 | 106.31(10) |