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Electronic Supplementary Information

Dative and Noncovalent Tetrel Bonding in Hemidirected Pb(II) Complexes with Thiosemicarbazone and Hydrazone Ligands: Significance in Crystal Packing and Computational Insights into Pb···N/S/O Interactions

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Table S1 Crystallographic Data and Details of Refinements for Pb(II) complexes **1** and **2**.

Identification code	Complex **1**	Complex **2**
Empirical formula	$C_{18}H_{23}ClN_8O_4PbS_2$	$C_{30}H_{32}SN_6O_9Pb_2$
Formula weight	722.2	1067.05
Temperature/K	100(2)	100(2)
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a/Å	10.4182(10)	11.4145(3)
b/Å	10.9215(10)	15.5121(5)
c/Å	12.9047(12)	18.7691(6)
α/°	78.837(4)	90
β/°	69.941(4)	100.922(2)
γ/°	61.540(4)	90
Volume/Å^3	1211.8(2)	3263.11(17)
Z	2	4
ρ_{calc}g/cm^3	1.979	2.172
μ/mm^{-1}	7.287	10.433
F(000)	700.0	2024.0
Crystal size/mm^3	0.22 × 0.09 × 0.03	0.04 × 0.04 × 0.005
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.362 to 64.296	3.432 to 50.694
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19	-13 ≤ h ≤ 13, -18 ≤ k ≤ 18, -22 ≤ l ≤ 22
Reflections collected	48194	11602
Independent reflections	8509 [R_{int} = 0.0607, R_{sigma} = 0.0387]	5968 [R_{int} = 0.0403, R_{sigma} = 0.0511]
Data/restraints/parameters	8509/0/321	5968/12/444
Goodness-of-fit on F^2	1.057	1.015
Final R indexes [I≥ 2σ (I)]	R_1 = 0.0210, wR_2 = 0.0507	R_1 = 0.0356, wR_2 = 0.0816
Final R indexes [all data]	R_1 = 0.0223, wR_2 = 0.0512	R_1 = 0.0575, wR_2 = 0.0889
Largest diff. peak/hole / e Å^{-3}	1.25/-1.40	1.89/-1.75

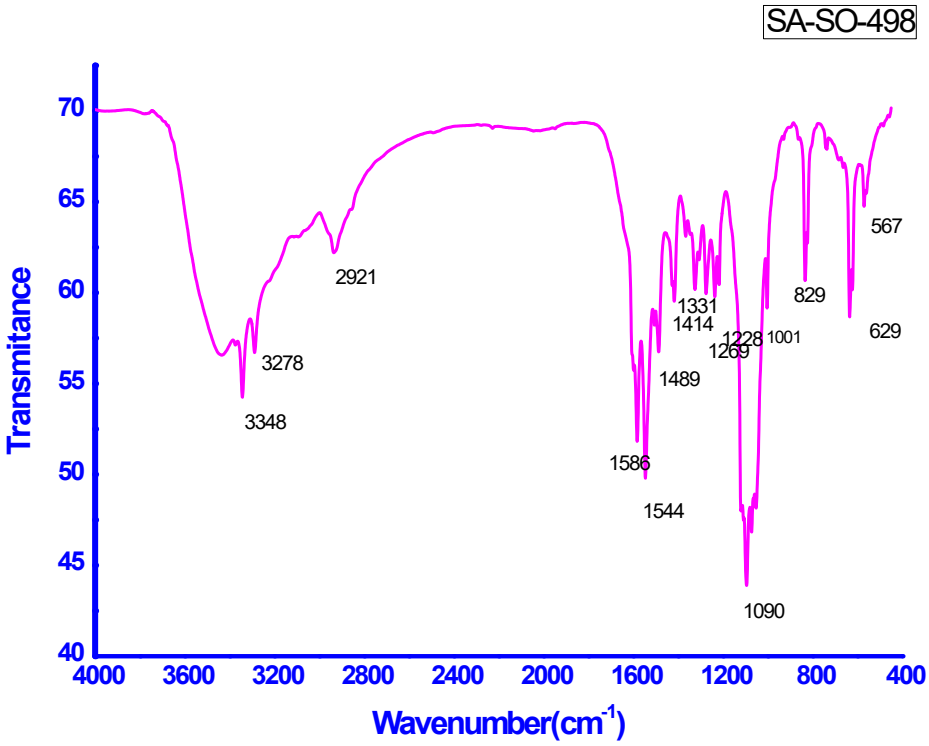

Fig. S1 FT-IR spectrum of Pb(II) complex **1**.

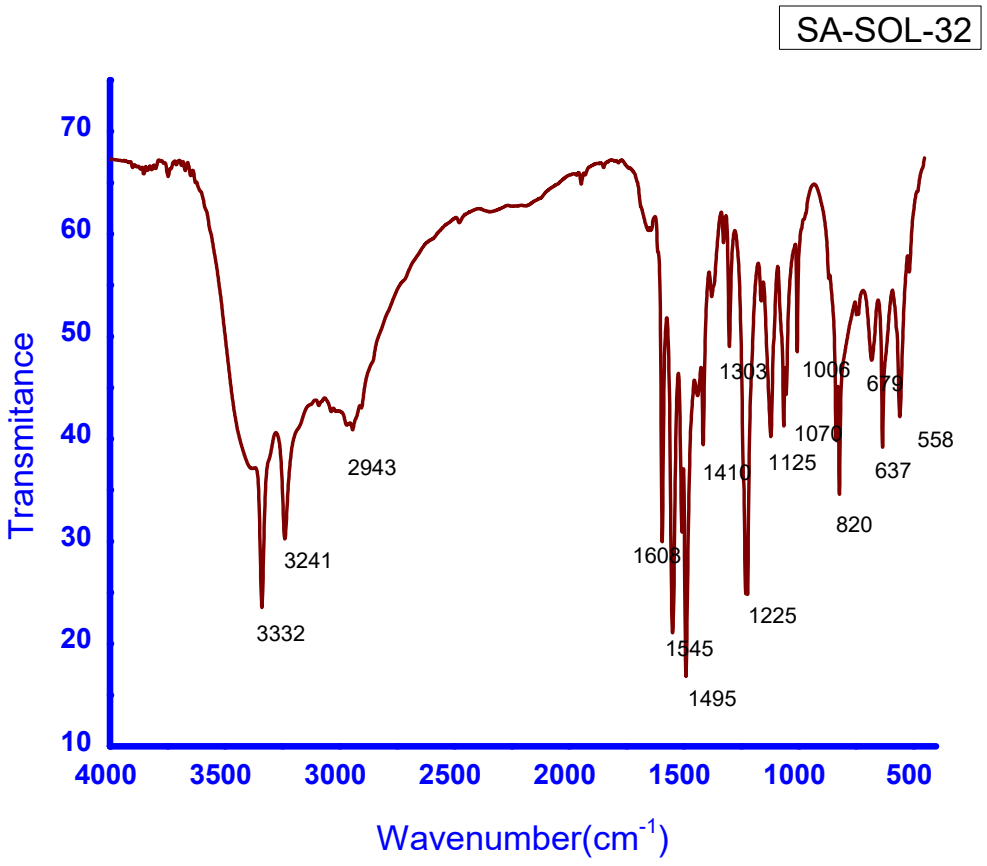

Fig. S2 FT-IR spectrum of thiosemicarbazone-based ligand (H_2L^1).

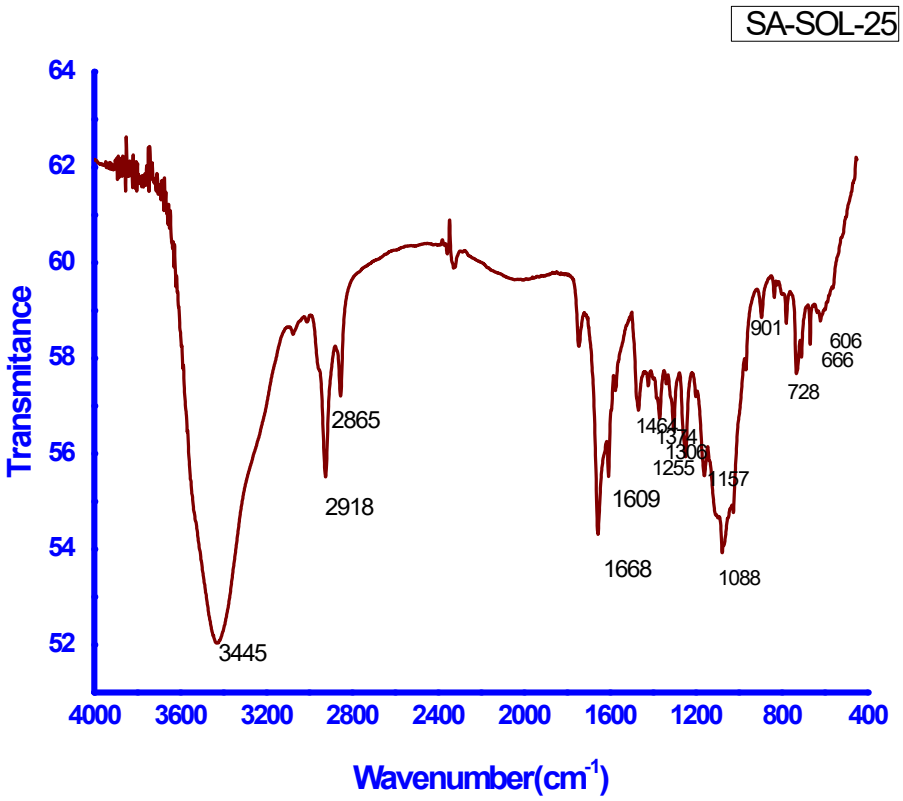

Fig. S3. FT-IR spectrum of hydrazone-based ligand (H_2L^2).

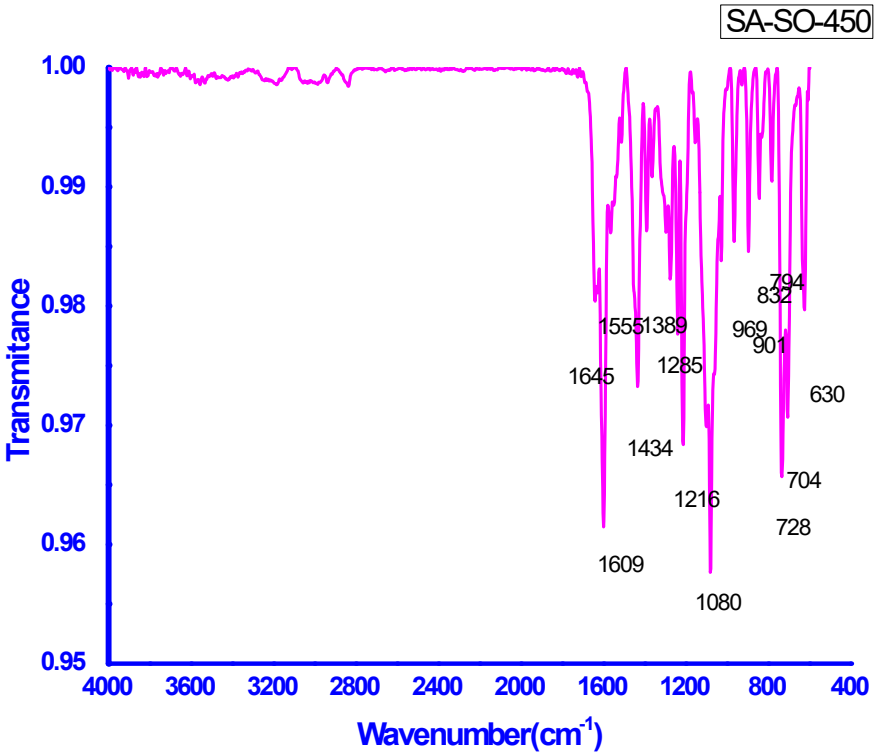

Fig. S4 FT-IR spectrum of Pb(II) complex **2**.

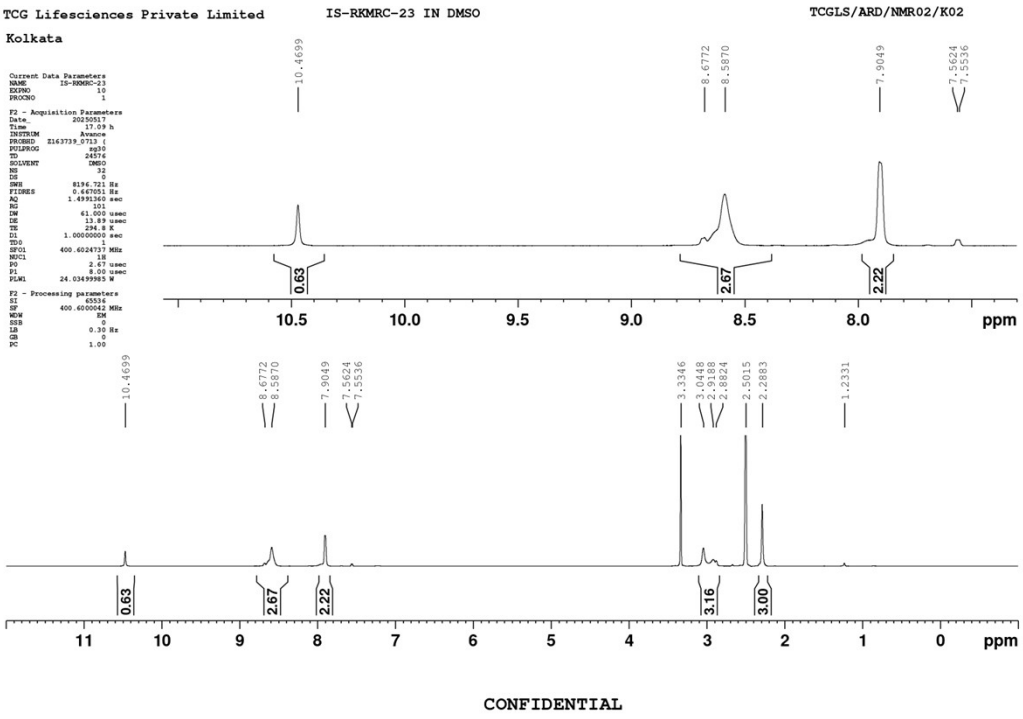

Fig. S5 ^{1}H NMR spectrum of Pb(II) complex **1** in DMSO-d_6.

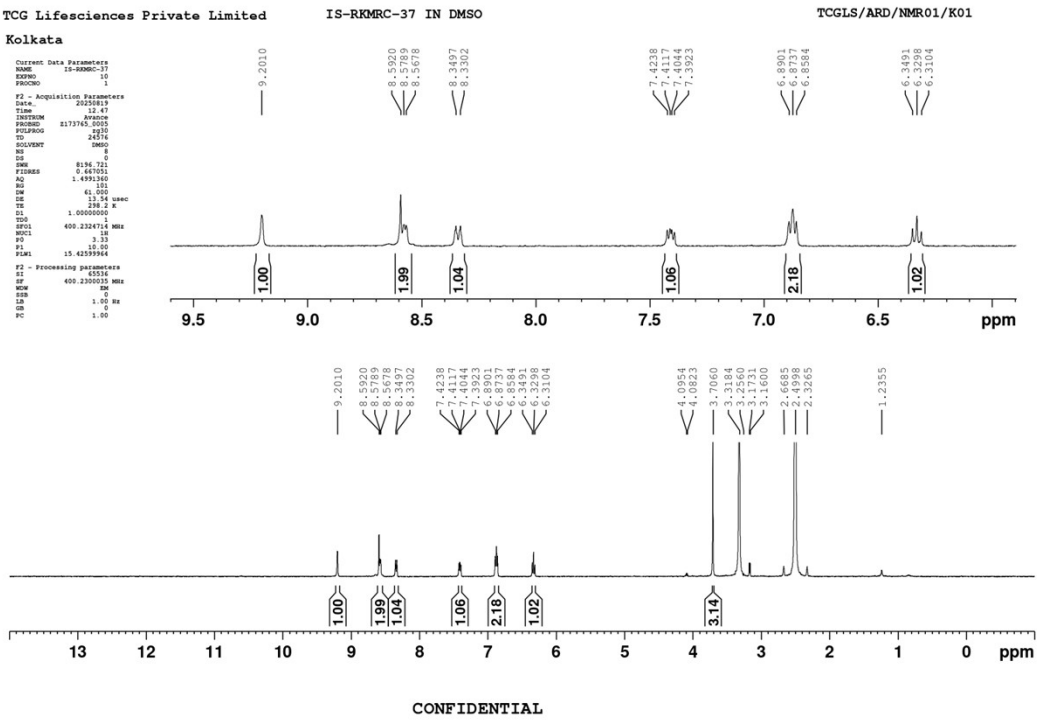

Fig. S6 ^{1}H NMR spectrum of Pb(II) complex **2** in DMSO-d_6.

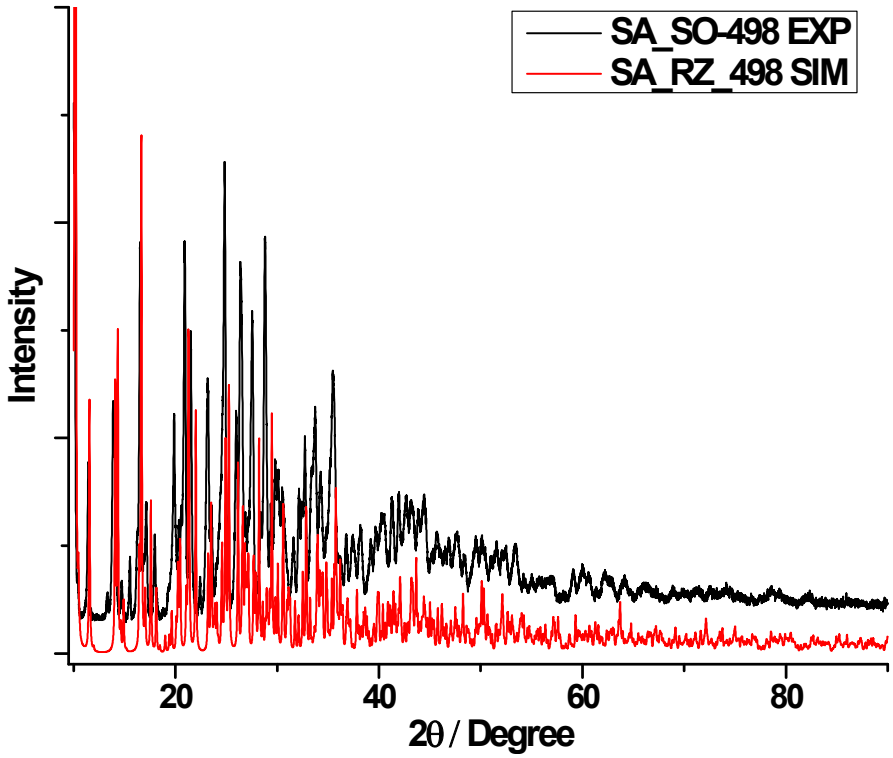

Fig. S7 Powder X-ray diffraction pattern of Pb(II) complex **1**. The red line represents the pattern simulated from the CIF and the black line represents the experimental pattern.

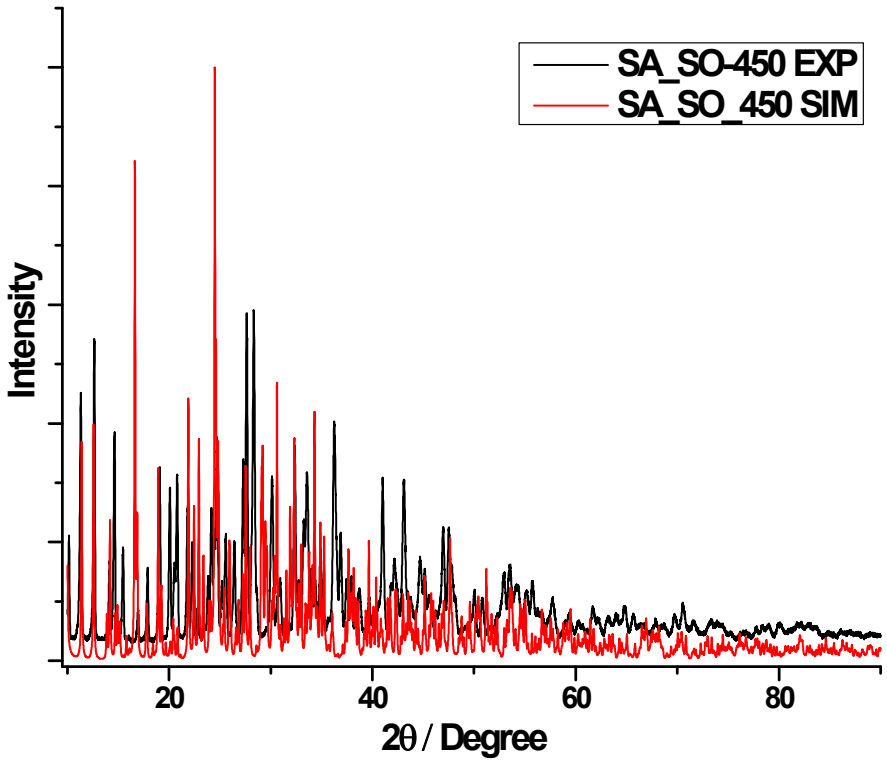

Fig. S8 Powder X-ray diffraction pattern of Pb(II) complex **2**. The red line represents the pattern simulated from the CIF and the black line represents the experimental pattern.