Supporting Information

A neutral heteroleptic molybdenum cluster *trans*-[{Mo_6I_8}$(py)_2I_4$]

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Table S1. Selected crystallographic parameters of the single-crystal X-ray diffraction structural analysis for $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$

Compound	$(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$
Empirical formula	$C_{19}H_{19.2}I_{12.2}Mo_6N_{3.8}$
Formula weight	2424.60
Temperature, K	150(2)
Crystal system	monoclinic
Space group	$P\,2_1/c$
a, Å	12.276(3)
b, Å	14.563(3)
c, Å	12.586(3)
β, °	104.640(6)
V, Å^3	2177.0(8)
Z	2
ϱ_{calc}, g/cm^3	3.699
μ, mm^{-1}	10.345
F (000)	2117
Crystal size	0.12 × 0.08 × 0.02
2Θ range for data collection, °	2.180 – 26.372
Index ranges	$-15 \le h \le 14$ $-18 \le k \le 16$ $-15 \le l \le 13$
Reflections collected	12938
Independent reflections; [R_{int}]	4445; [0.0800]
Parameters refined	193
Goodness-of-fit on F^2	0.935
R_1 / wR_2(I > 2σ(I))	0.0574 / 0.1139
R_1 / wR_1 (all data)	0.1238 / 0.1298
$\Delta\varrho_{max}/\Delta\varrho_{min}$ (e·Å^{-3})	2.360 / –1.464

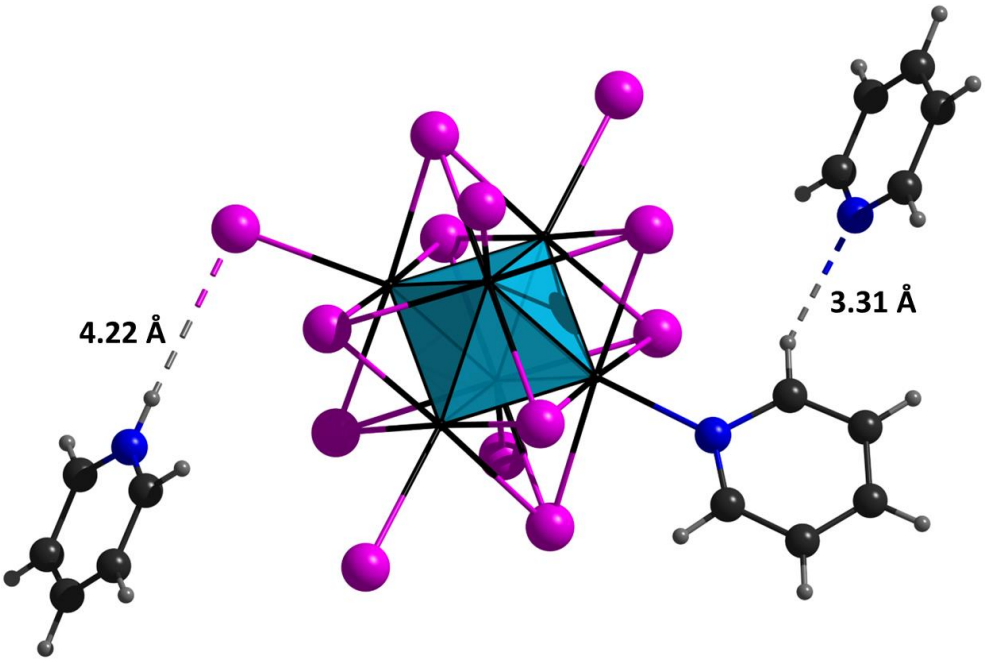

Figure S1. Illustration of $py^{solv}\cdots py^{coord}$ and $pyH\cdots I^a$ interactions. Color code: light blue octahedron – Mo_6, purple – iodine, blue – nitrogen, black – carbon, gray – hydrogen.

Table S2. Crystal lattice parameters for $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$ and $[\{Mo_6X_8\}(py)_2X_4]$ (X = Cl, Br)

Compound	Crystal system	*a*, Å	*b*, Å	*c*, Å	*β*, °
$(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$	monoclinic	12.276(3)	14.563(3)	12.586(3)	104.640(6)
$[\{Mo_6Cl_8\}(py)_2Cl_4]$	orthorhombic	17.412(1)	20.376(2)	12.074(1)	90
$[\{Mo_6Cl_8\}(py)_2Br_4]$		17.780(2)	20.691(2)	12.282(1)	
$[\{Mo_6Br_8\}(py)_2Cl_4]$		17.761(8)	20.594(10)	12.536(6)	
$[\{Mo_6Br_8\}(py)_2Br_4]$		18.143(4)	21.102(6)	12.686(3)	

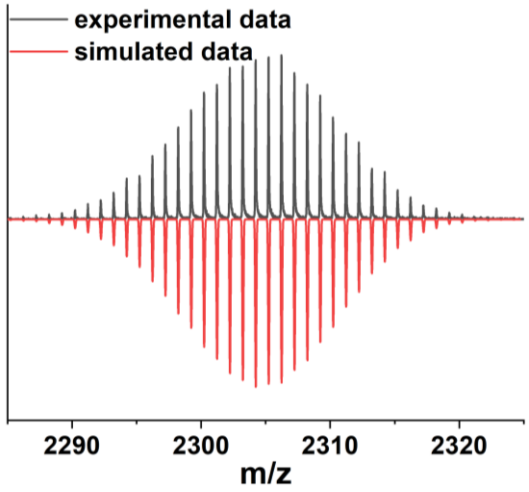

Figure S2. Fragment of ESI-MS of mother liquor illustrating the presence of $[\{Mo_6I_8\}(py)I_5]^-$.

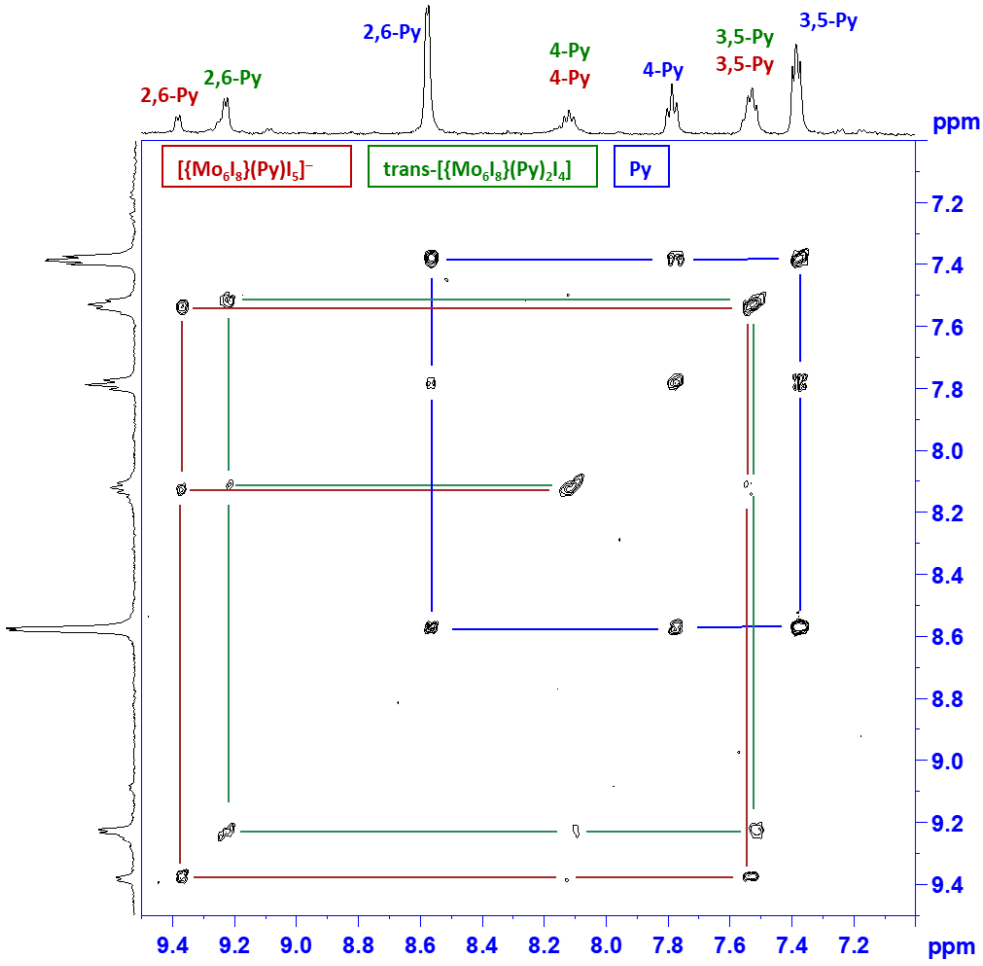

Figure S3. ^{1}H-COSY NMR spectrum of $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$.

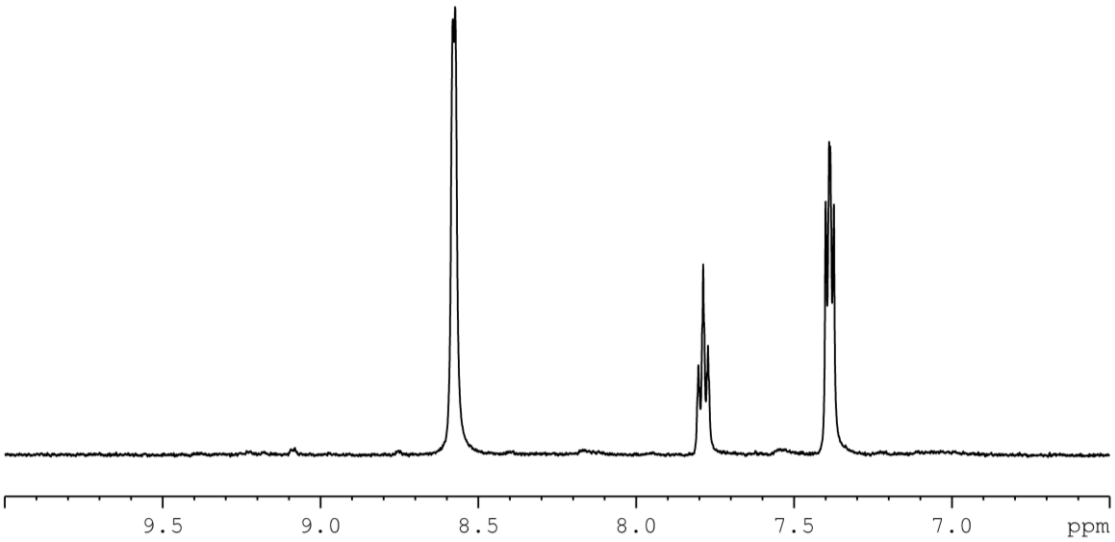

Figure S4. ^{1}H-NMR spectrum of $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$ after heating in DMSO-d_6.

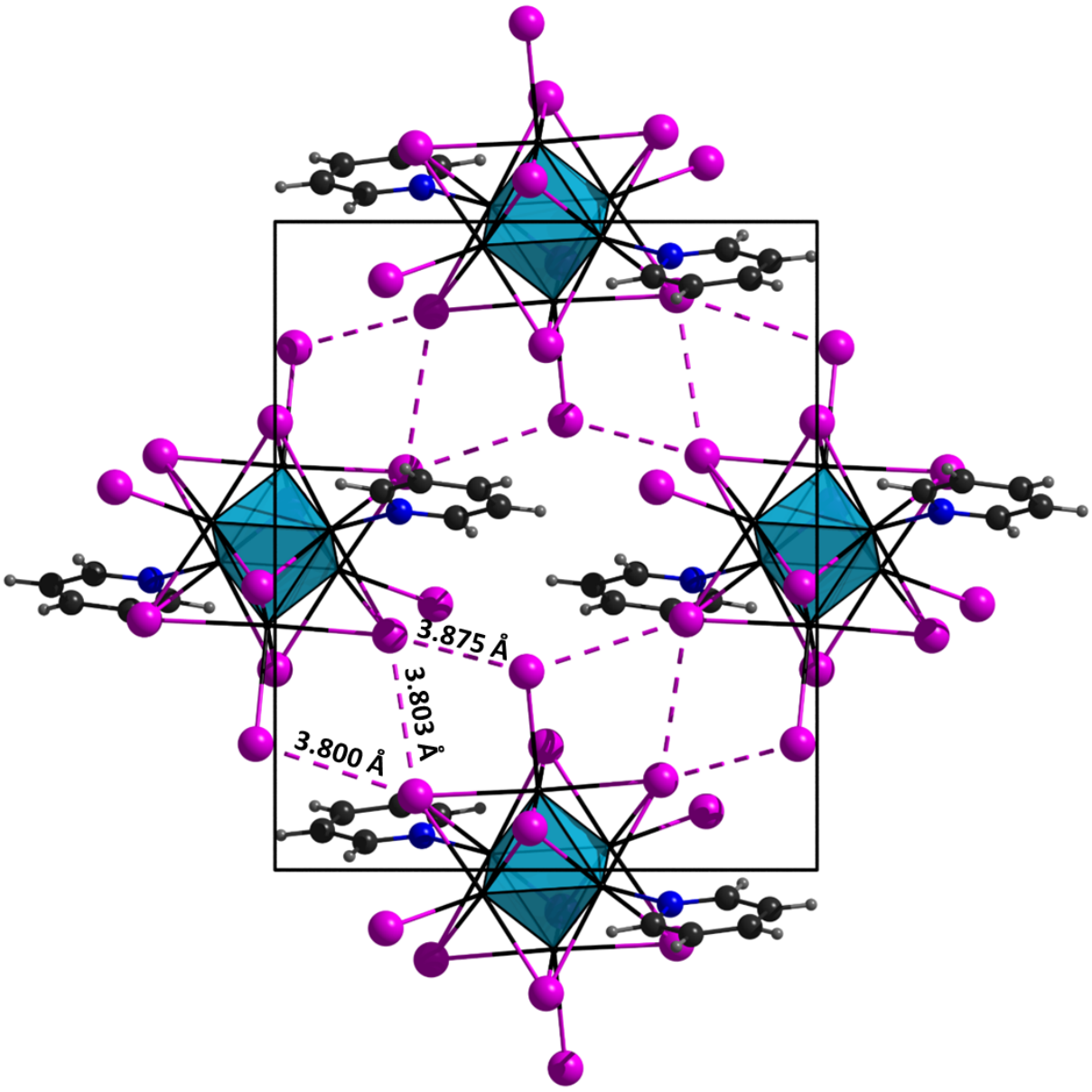

Figure S5. I^{i}-I^{a} and I^{i}-I^{i} interactions in $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$.

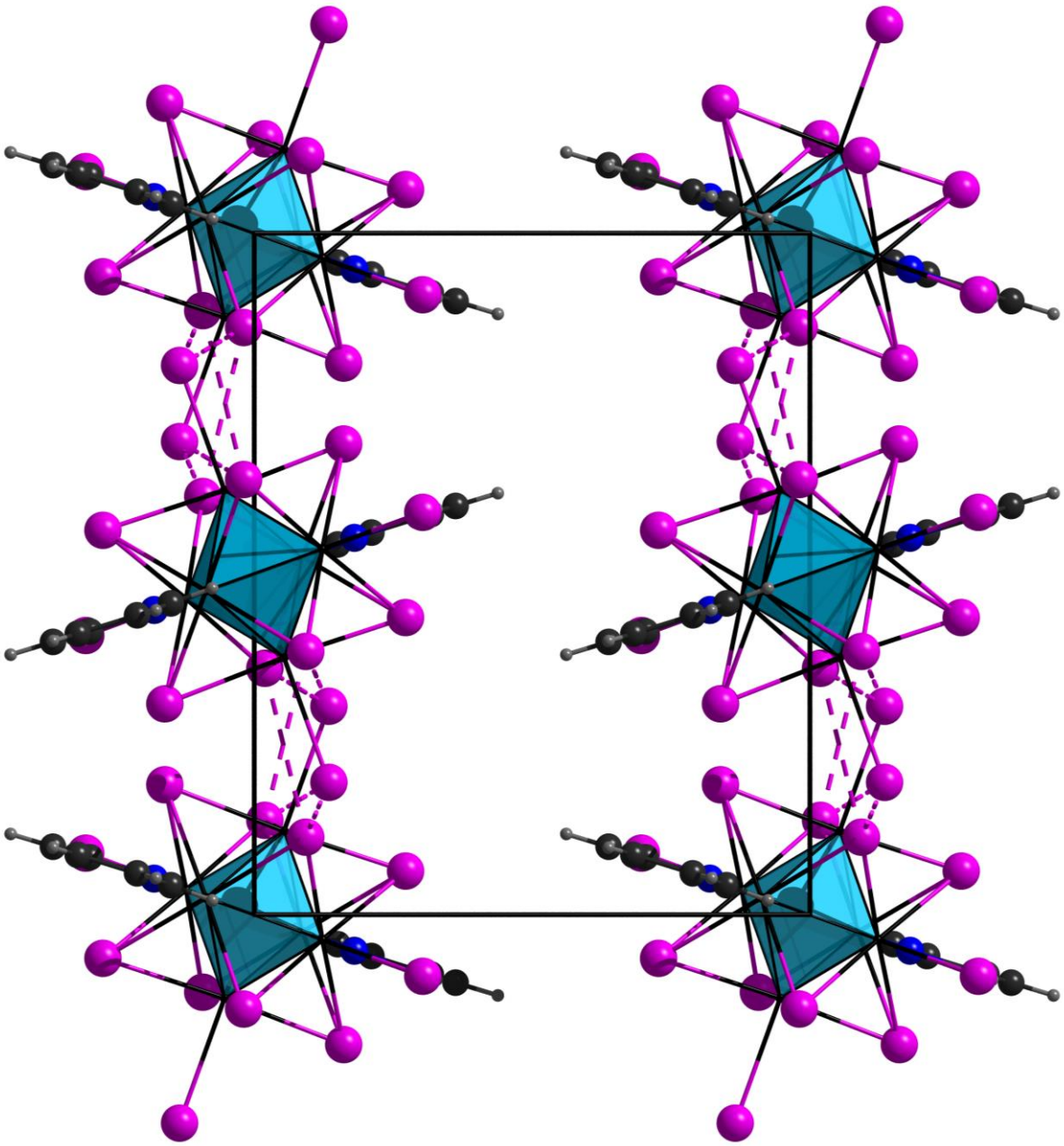

Figure S6. Layers in $(pyH)_{0.2}[\{Mo_6I_8\}(py)_{1.8}I_{4.2}]\cdot 1.8py$.