Electronic Supplementary Information for Dalton Transactions

Convenient Syntheses and Structural Characterizations of Mono-substituted Alkylimido Hexamolybdates: $[Mo_6O_{18}(NR)]^{2-}$ (R = Me, Et, n-Pr, i-Pr, n-Bu, t-Bu, Cy, Hex, Ode) †

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Table S1 Summary of crystallographic data for compounds 5 and 7I.

	5	**7I**
Formula	$C_{36}H_{81}Mo_6N_3O_{18}$	$C_{38}H_{83}Mo_6N_3O_{18}$
F.W..	1419.68	1445.71
Crys. Sys.	Orthorhombic	Triclinic
Space group	Pbca	P-1
a (Å)	16.8504(8)	12.5288(4)
b (Å)	20.0036(10)	19.4569(6)
c (Å)	31.6503(15)	23.1302(7)
α (°)	90	93.7700(10)
β (°)	90	103.1410(10)
γ (°)	90	91.4990(10)
V (Å^3)	10668.3(9)	5474.0(3)
Z	8	4
$\rho_{calc.}$ Mg/m^3	1.768	1.754
μ (mm^{-1})	1.433	1.398
Refl. collected	48987	44067
Unique refl. ($R_{int.}$)	9378(0.0327)	18581(0.0302)
R_1	0.0509	0.0559
wR_2	0.1351	0.1483
GOF	1.127	1.136

$R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $Rw = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}$ with $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$ **5** : a = 0.0449, b = 46.6940; **7I** : a = 0.0434, b = 21.3101.

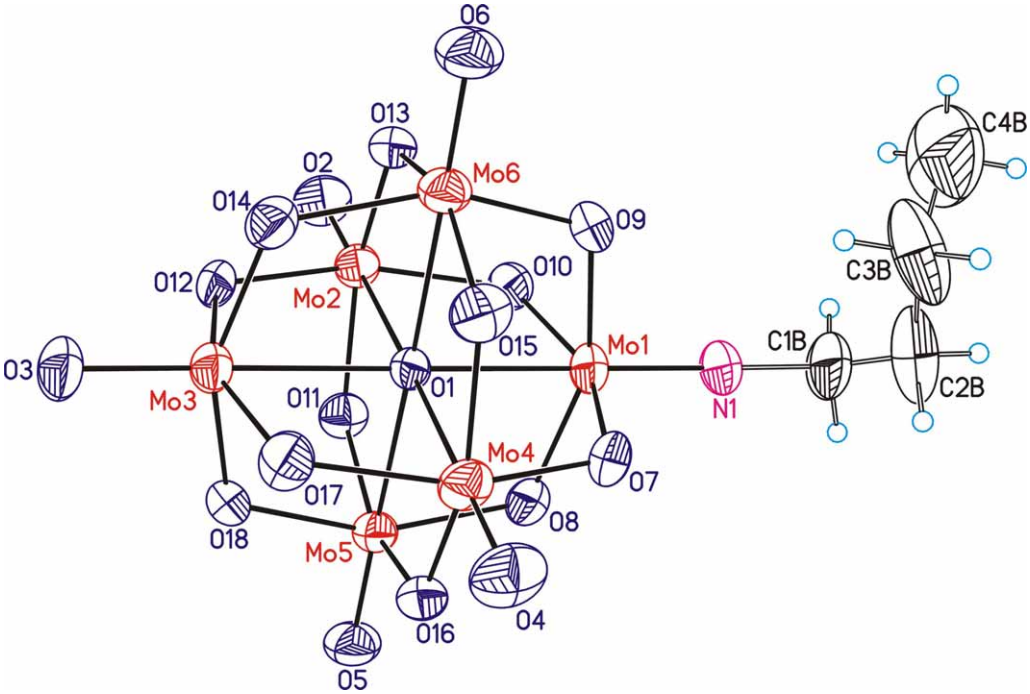

Figure S1. ORTEP drawing of the $[Mo_6O_{18}(=NR)]^{2-}$ anion of **5**

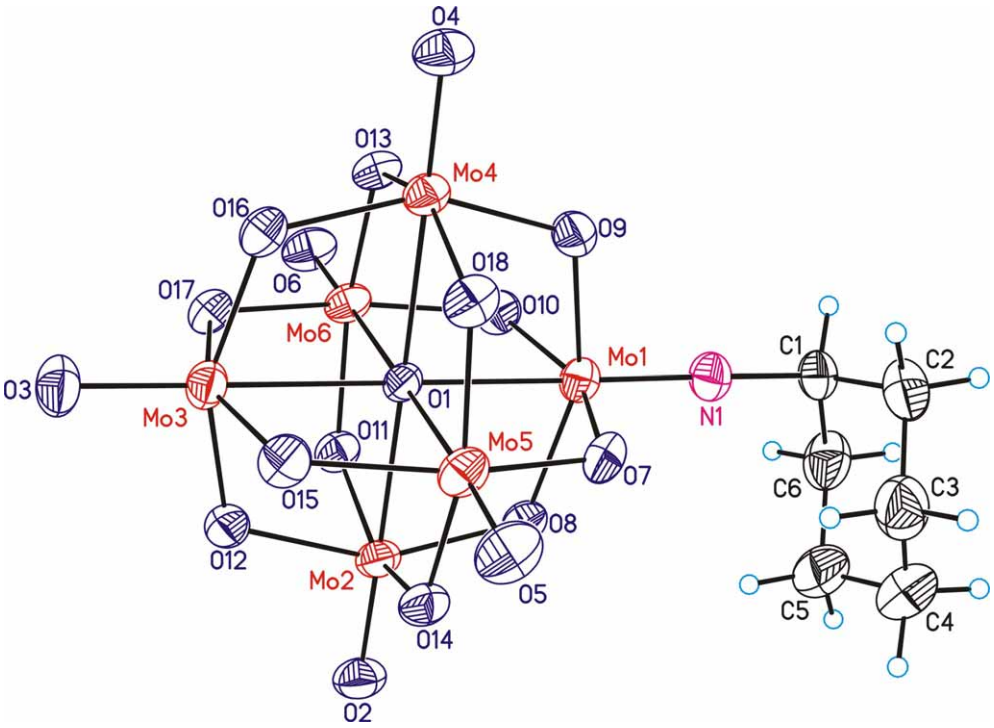

Figure S2. ORTEP drawing of the $[Mo_6O_{18}(=NR)]^{2-}$ anion of **7I**

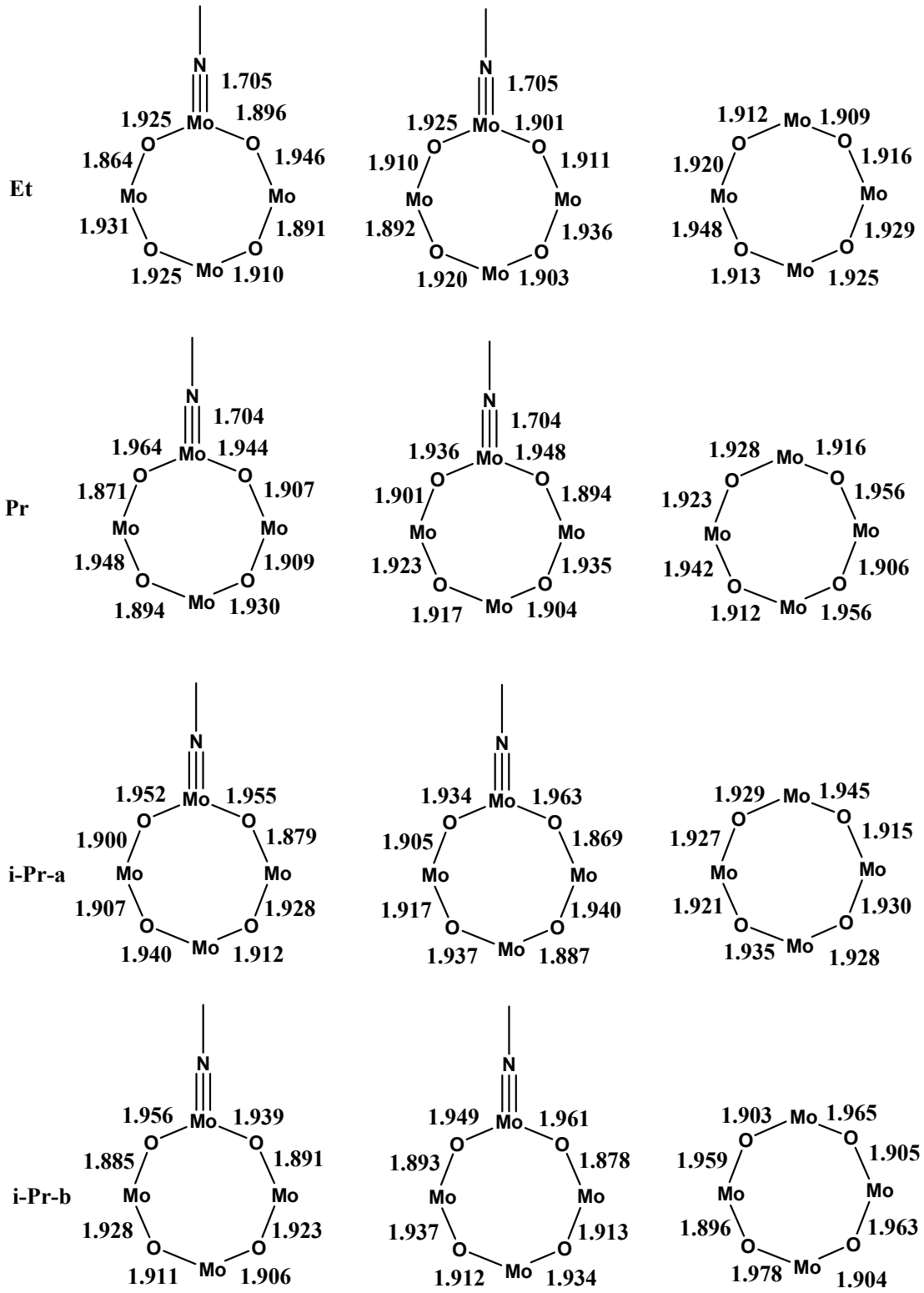

Figure S3. Bond length in the $Mo_4(O_b)_4$ belts in compounds **2**, 3, **4a** and **4b**

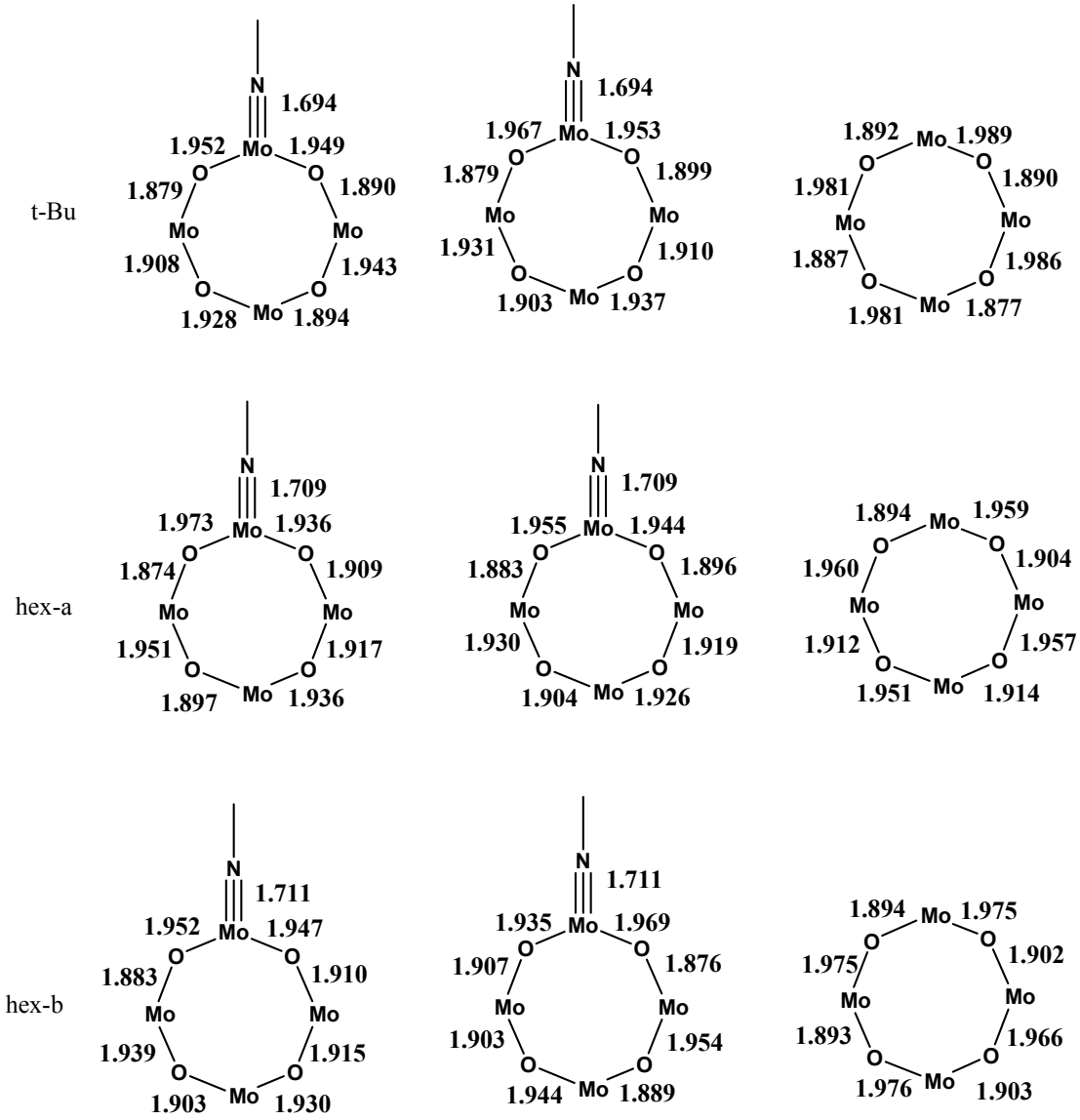

Figure S4. Bond length in the $Mo_4(O_b)_4$ belts in compounds **6**, **8a** and **8b.**