

A New Class of Functionalized Polyoxometalates: Synthesis, Structure and Preliminary Antitumor Activity Studies of Three Arylimido Substituted Hexamolybdate Bearing a Strong Electron-withdrawing Nitro Group, $(\text{Bu}_4\text{N})_2[\text{Mo}_6\text{O}_{18}(\equiv\text{NAr})]$ (Ar = 3-NO₂-C₆H₄, 2-CH₃-4-NO₂-C₆H₃, 2-CH₃-5-NO₂-C₆H₃)

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Table S1. Selected Bond lengths/Å and angles/° for Compounds 1, 2 and 3

Compound 1		Compound 2		Compound 3	
Mo(1)-N(1)	1.707(10)	Mo(1)-N(1)	1.714(12)	Mo(1)-N(1)	1.737(3)
Mo(1)-O(3)	1.901(7)	Mo(1)-O(2)	1.857(12)	Mo(1)-O(17)	1.903(2)
Mo(1)-O(18)	1.966(8)	Mo(1)-O(4)	1.943(9)	Mo(1)-O(2)	1.907(2)
Mo(1)-O(2)	1.964(7)	Mo(1)-O(1)	1.956(9)	Mo(1)-O(3)	1.979(2)
Mo(1)-O(4)	1.969(7)	Mo(1)-O(3)	1.991(10)	Mo(1)-O(1)	1.986(2)
Mo(1)-O(1)	2.242(6)	Mo(1)-O(18)	2.210(7)	Mo(1)-O(18)	2.2046(19)
Mo(2)-O(5)	1.678(7)	Mo(2)-O(6)	1.675(9)	Mo(2)-O(4)	1.681(3)
Mo(2)-O(7)	1.904(7)	Mo(2)-O(3)	1.841(9)	Mo(2)-O(1)	1.857(2)
Mo(2)-O(8)	1.923(7)	Mo(2)-O(8)	1.906(7)	Mo(2)-O(7)	1.893(3)
Mo(2)-O(3)	1.935(8)	Mo(2)-O(7)	1.938(8)	Mo(2)-O(6)	1.964(2)
Mo(2)-O(6)	1.973(6)	Mo(2)-O(5)	1.957(7)	Mo(2)-O(5)	1.969(2)
Mo(2)-O(1)	2.339(6)	Mo(2)-O(18)	2.330(7)	Mo(2)-O(18)	2.3259(19)
Mo(3)-O(9)	1.683(6)	Mo(3)-O(9)	1.681(7)	Mo(3)-O(8)	1.680(3)
Mo(3)-O(6)	1.896(6)	Mo(3)-O(10)	1.889(8)	Mo(3)-O(3)	1.869(2)
Mo(3)-O(2)	1.919(6)	Mo(3)-O(1)	1.900(9)	Mo(3)-O(6)	1.900(2)
Mo(3)-O(10)	1.944(6)	Mo(3)-O(11)	1.919(8)	Mo(3)-O(9)	1.955(2)
Mo(3)-O(11)	1.977(6)	Mo(3)-O(8)	1.955(8)	Mo(3)-O(10)	1.960(2)
Mo(3)-O(1)	2.354(5)	Mo(3)-O(18)	2.318(6)	Mo(3)-O(18)	2.331(2)
Mo(4)-O(12)	1.661(7)	Mo(4)-O(12)	1.693(8)	Mo(4)-O(11)	1.686(3)
Mo(4)-O(13)	1.895(6)	Mo(4)-O(5)	1.908(8)	Mo(4)-O(13)	1.884(3)
Mo(4)-O(14)	1.922(7)	Mo(4)-O(4)	1.890(10)	Mo(4)-O(12)	1.902(2)
Mo(4)-O(10)	1.919(6)	Mo(4)-O(13)	1.896(9)	Mo(4)-O(17)	1.946(2)
Mo(4)-O(7)	1.959(7)	Mo(4)-O(14)	1.960(9)	Mo(4)-O(7)	1.972(3)
Mo(4)-O(1)	2.370(6)	Mo(4)-O(18)	2.326(6)	Mo(4)-O(18)	2.324(2)
Mo(5)-O(15)	1.701(7)	Mo(5)-O(15)	1.673(10)	Mo(5)-O(14)	1.689(2)
Mo(5)-O(4)	1.882(7)	Mo(5)-O(7)	1.871(8)	Mo(5)-O(15)	1.895(2)
Mo(5)-O(11)	1.907(6)	Mo(5)-O(11)	1.918(7)	Mo(5)-O(10)	1.899(2)
Mo(5)-O(13)	1.945(7)	Mo(5)-O(13)	1.928(8)	Mo(5)-O(2)	1.930(2)
Mo(5)-O(16)	1.975(6)	Mo(5)-O(16)	1.964(9)	Mo(5)-O(12)	1.956(2)
Mo(5)-O(1)	2.337(5)	Mo(5)-O(18)	2.368(7)	Mo(5)-O(18)	2.3281(19)
Mo(6)-O(17)	1.687(7)	Mo(6)-O(17)	1.670(10)	Mo(6)-O(16)	1.679(3)
Mo(6)-O(16)	1.909(7)	Mo(6)-O(16)	1.872(9)	Mo(6)-O(5)	1.883(2)
Mo(6)-O(18)	1.911(8)	Mo(6)-O(14)	1.893(8)	Mo(6)-O(9)	1.889(2)
Mo(6)-O(14)	1.940(8)	Mo(6)-O(2)	1.944(11)	Mo(6)-O(15)	1.939(2)
C(1)-N(1)-Mo(1)	167.1(10)	Mo(6)-O(10)	1.962(7)	Mo(6)-O(13)	1.954(3)
		Mo(6)-O(18)	2.313(7)	Mo(6)-O(18)	2.3745(19)
		C(1)-N(1)-Mo(1)	152.5(15)	C(1)-N(1)-Mo(1)	169.1(3)

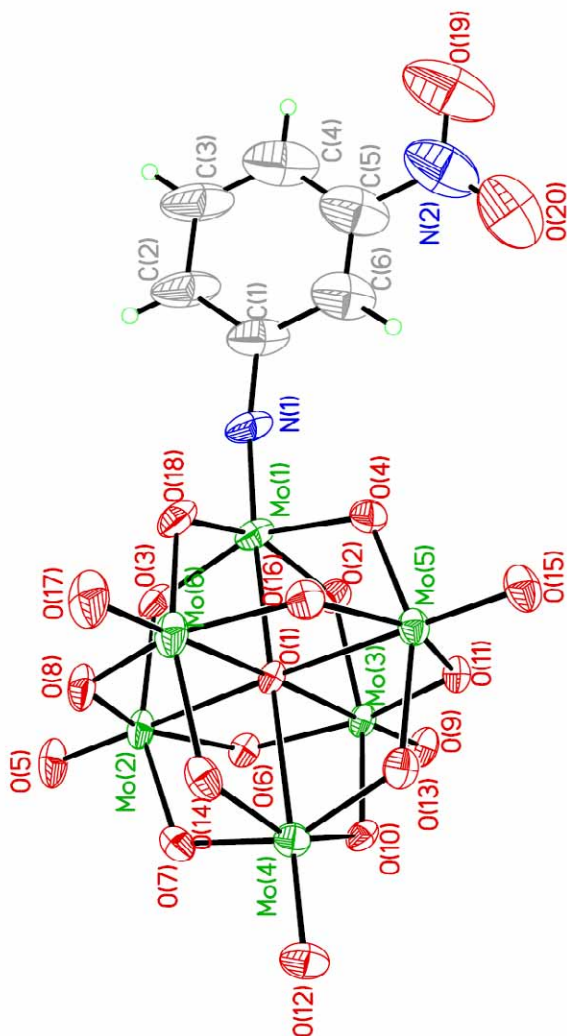


Figure S1. ORTEP viewing of the nitro-functionalized arylimido hexamolybdate ion **1**

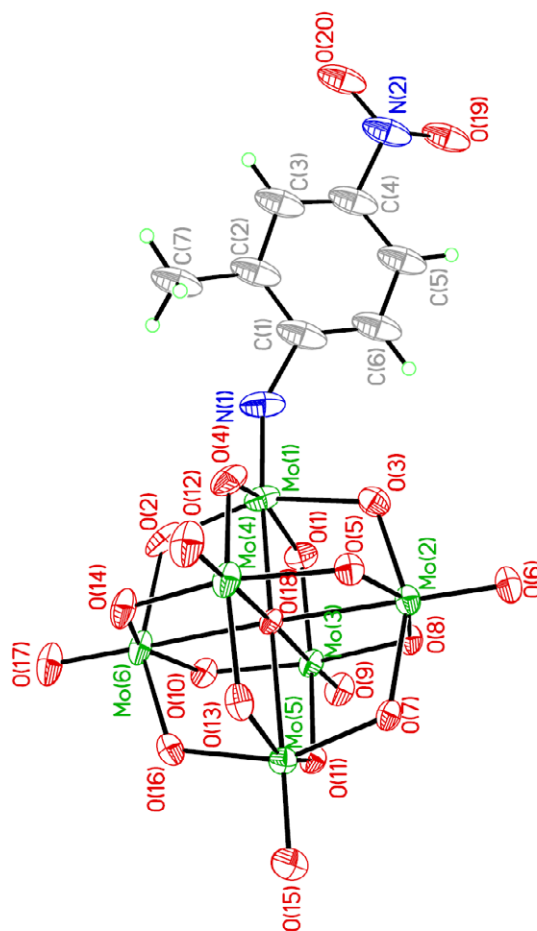


Figure S2. ORTEP viewing of the nitro-functionalized arylimido hexamolybdate ion 2

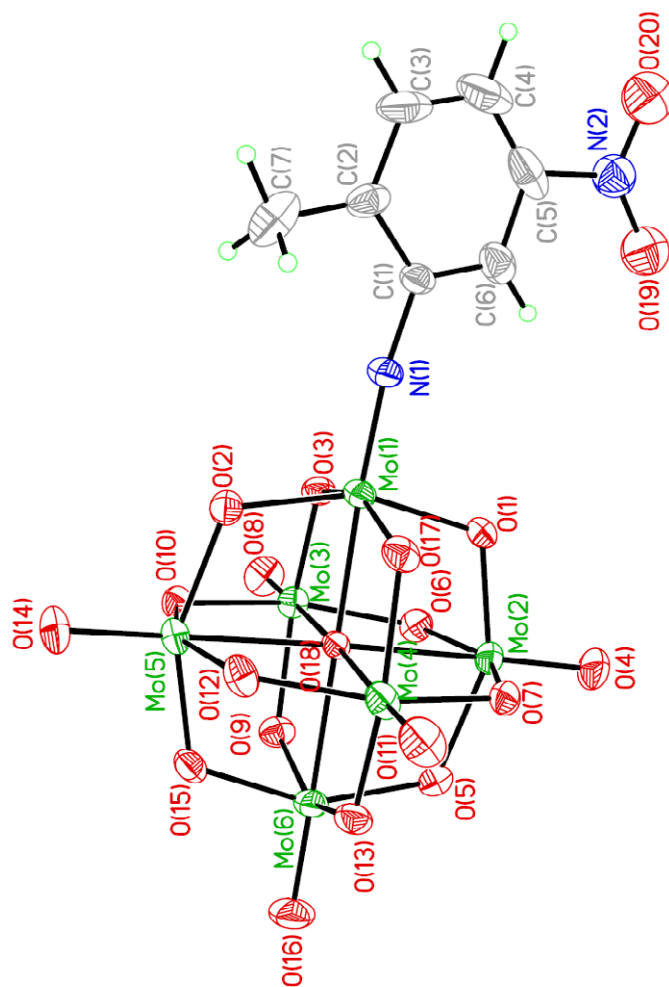


Figure S3. ORTEP viewing of the nitro-functionalized arylimido hexamolybdate ion **3**