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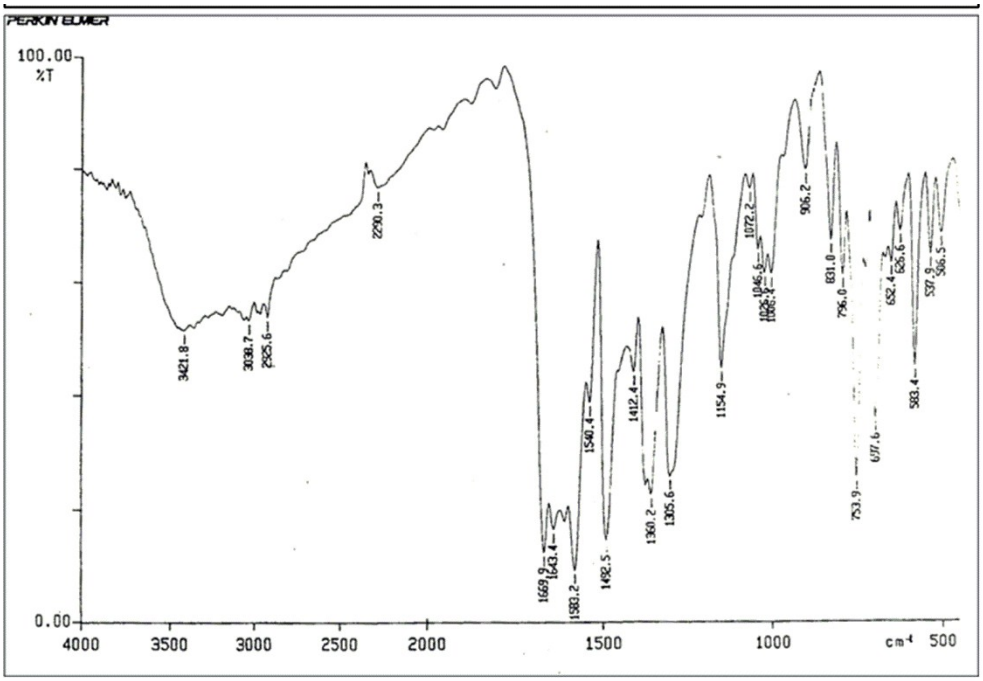

Fig S1: FT-IR spectrum of the Schiff base ligand, (dha-aapH) (**I**)

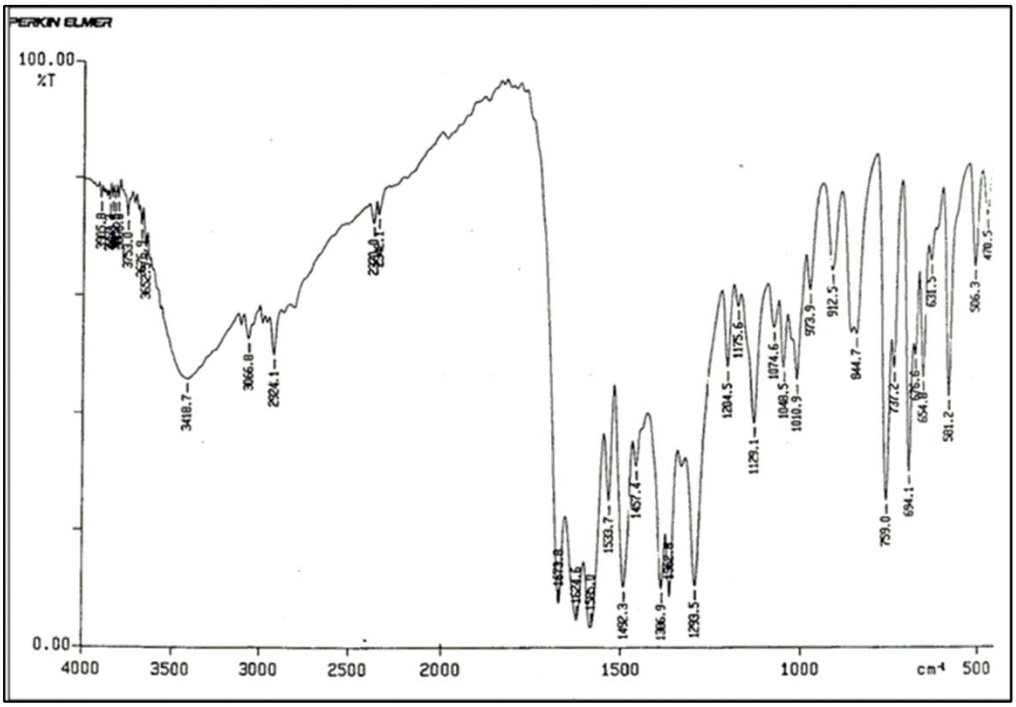

Fig S2: FT- IR. Spectrum of the Schiff base ligand, (amphp-aapH) (**II**)

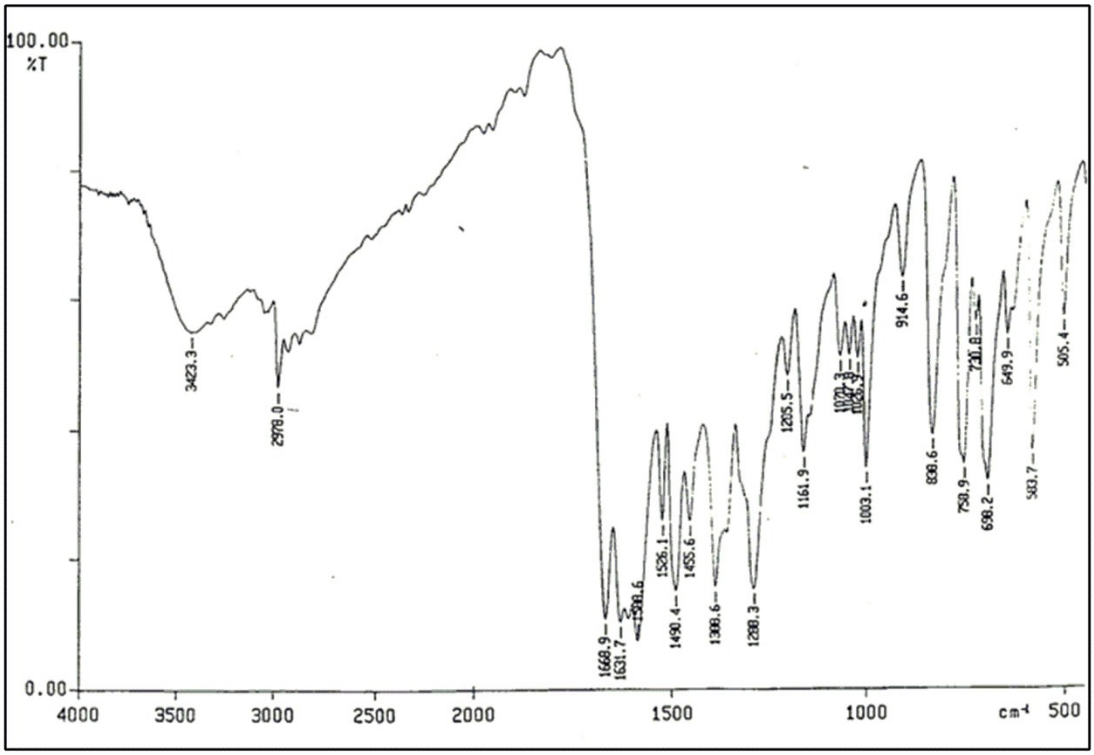

Fig S3: FT-IR. Spectrum of the Schiff base ligand, (mphpp-aapH) (**III**)

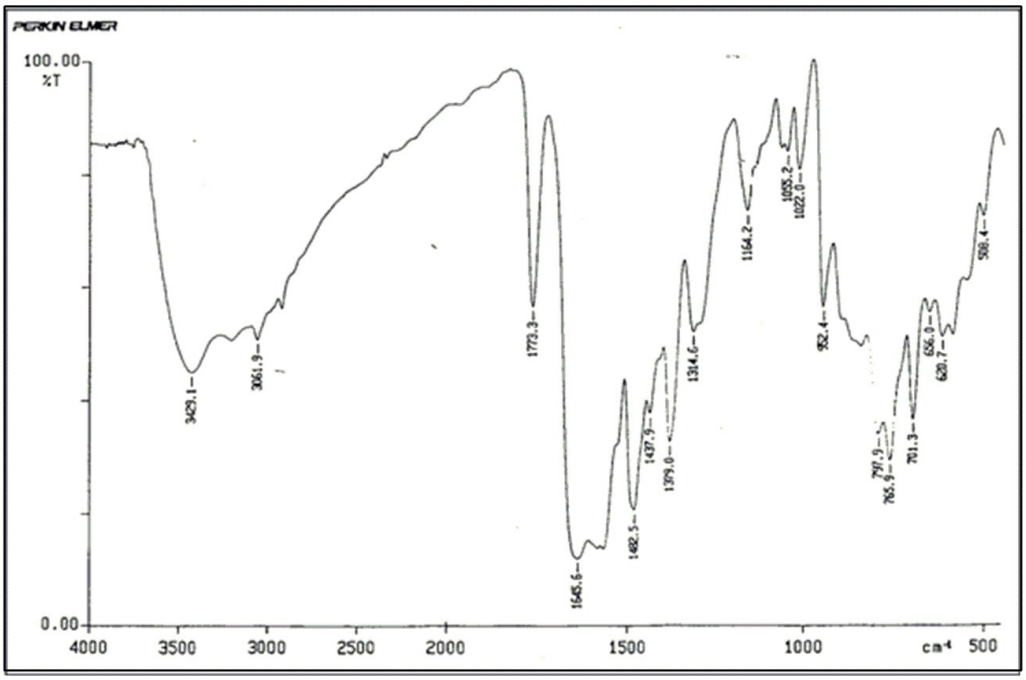

Fig S4: FT-IR spectrum of $[Mo(NO)_2(dha\text{-}aap)(OH)]$ (**1**) complex

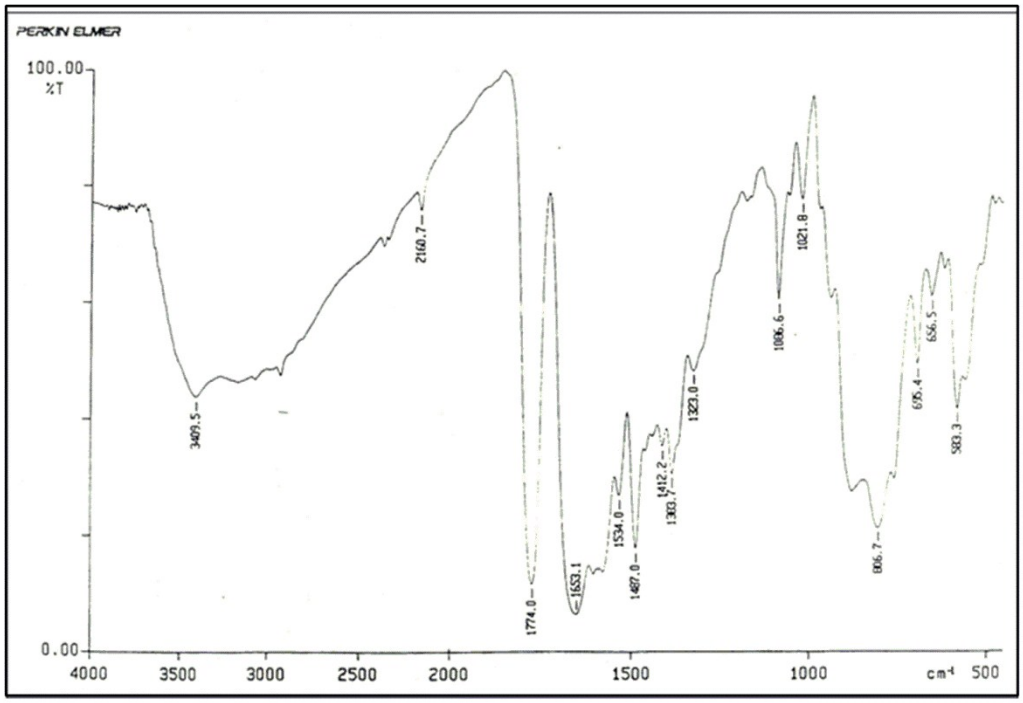

Fig S5: FT-IR spectrum of $[Mo(NO)_2(amphp\text{-}aap)(OH)]$ (**2**) complex

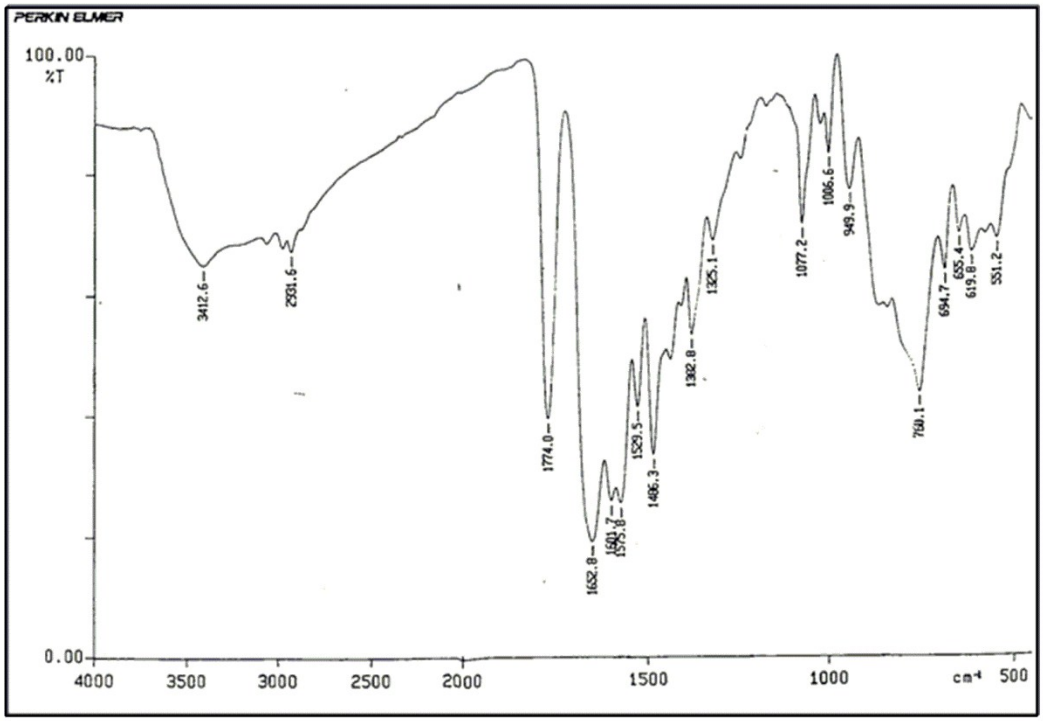

Fig S6: FT-IR spectrum of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**) complex

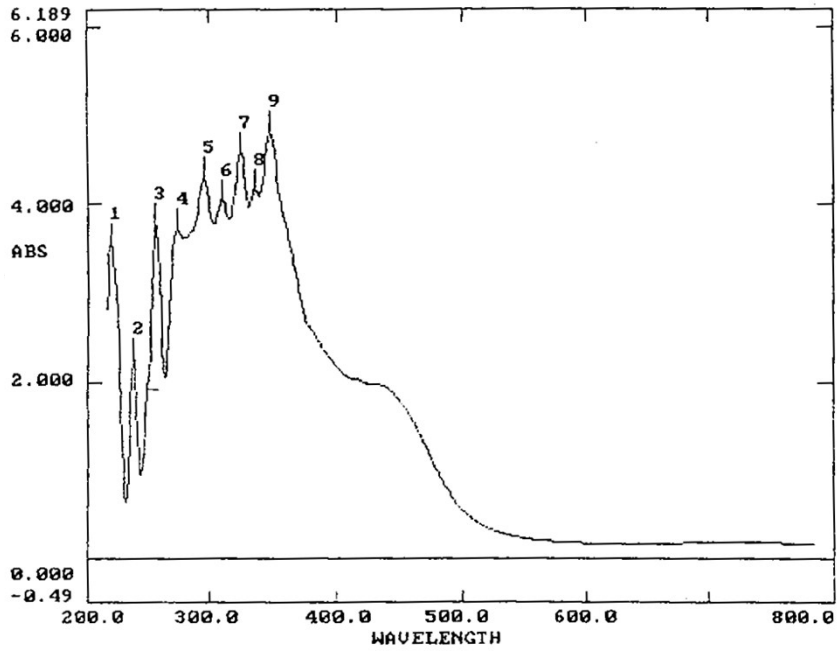

Fig S7: UV-Visible electronic spectrum of complex **1**

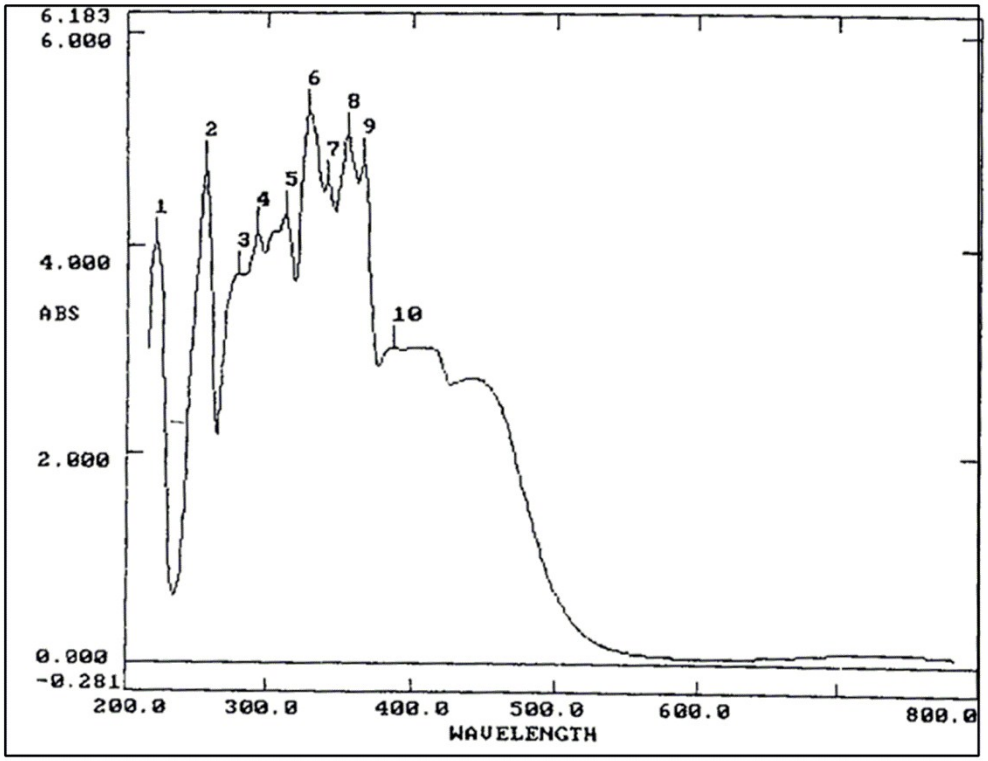

Fig S8: UV-Visible electronic spectrum of complex **2**

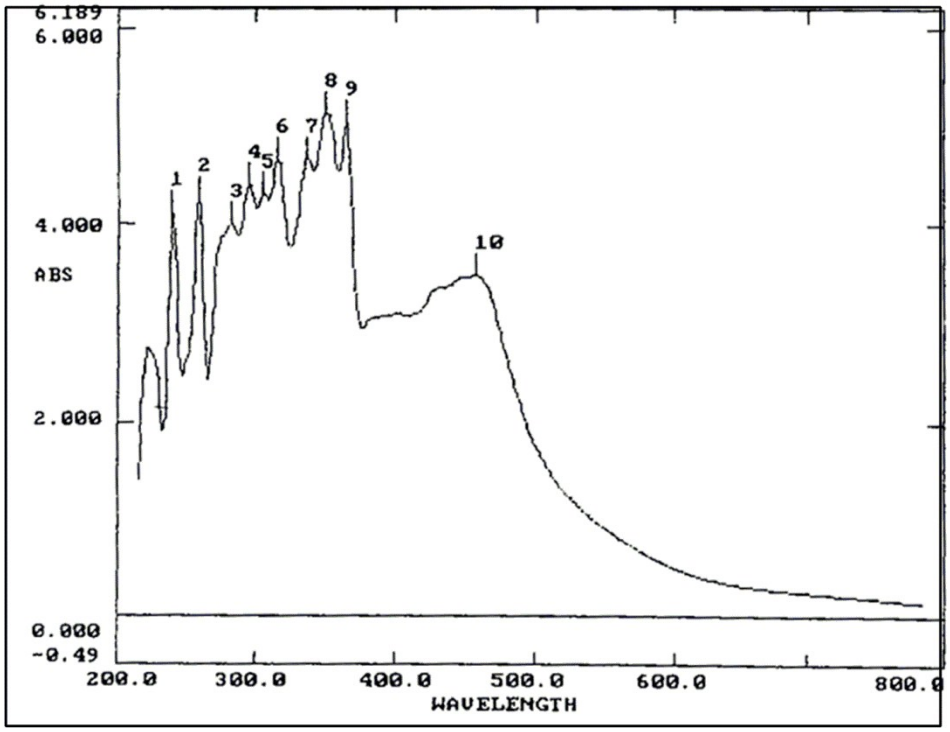

Fig S9: UV-Visible electronic spectrum of complex **3**

Table S1

Thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**) involving three decomposition steps

Temp.	1/T (K) x10^3	% (Res.)	W_t	Weight lost	Temp.	1/T (K) x10^3	% (Res.)	W_t	Weight lost	Temp.	1/T (K) x10^3	% (Res.)	W_t	Weight lost
200	2.114	96	2.01	0.084	370	1.555	80.56	1.687	0.407	600	1.145	25.38	0.531	1.563
210	2.07	95	1.989	0.105	380	1.531	79.75	1.67	0.424	610	1.132	24.56	0.514	1.58
220	2.028	94.5	1.979	0.115	390	1.508	79.34	1.661	0.433	620	1.12	23.58	0.494	1.6
230	1.988	93.2	1.952	0.142	400	1.485	77.7	1.627	0.467	630	1.107	22.1	0.463	1.631
240	1.949	92.8	1.943	0.151	410	1.464	76.88	1.61	0.484	640	1.095	20.46	0.428	1.666
250	1.912	91.8	1.922	0.172	420	1.443	76.22	1.596	0.498	650	1.083	19.64	0.411	1.683
260	1.876	89.34	1.871	0.223	430	1.422	73.76	1.544	0.55	660	1.072	18	0.377	1.717
270	1.841	87.7	1.836	0.258	440	1.402	70	1.466	0.628	670	1.06	17.18	0.36	1.734

Table S2

Freeman and Carroll Ist step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp. (T)	1/T (K)	Weight lost	Time (minute)	$W_r = W_f - W$	$\left[\frac{dw/dt}{W_r}\right]$	$ln\left[\frac{dw/dt}{W_r}\right]$
200	0.00211	0.084	10.78	1.756	0.0044	-5.4261
210	0.00207	0.105	11.48	1.735	0.0053	-5.2400
220	0.00202	0.115	12.18	1.725	0.0055	-5.2030
230	0.00198	0.142	12.88	1.698	0.0065	-5.0359
240	0.00194	0.151	13.58	1.689	0.0066	-5.0207
250	0.00191	0.172	14.28	1.668	0.0072	-4.9337
260	0.00188	0.223	14.98	1.617	0.0092	-4.6885
270	0.00184	0.258	15.68	1.582	0.0104	-4.5659

Table S3

Freeman and Carroll second step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$

Temp. (T)	1/T (K)	Weight lost	Time (minute)	$W_r = W_f - W$	$\left[\frac{dw/dt}{W_r}\right]$	$ln\left[\frac{dw/dt}{W_r}\right]$
370	0.00155	0.407	22.11	1.433	0.01284	-4.3547
380	0.00153	0.424	22.81	1.416	0.01313	-4.3330
390	0.00151	0.433	23.51	1.407	0.01309	-4.3359
400	0.00148	0.467	24.21	1.373	0.01405	-4.2652
410	0.00146	0.484	24.91	1.356	0.01433	-4.2455
420	0.00144	0.498	25.61	1.342	0.01449	-4.2343
430	0.00142	0.550	26.31	1.290	0.01620	-4.1224
440	0.00140	0.628	27.01	1.212	0.01918	-3.9537

Table S4

Freeman and Carroll third step thermal decomposition data of [Mo(NO)$_2$(mphpp-aap)(OH)] (**3**)

Temp. (T)	1/T (K)	Weight lost	Time (minute)	$W_r = W_f - W$	$\left[\frac{dw/dt}{W_r}\right]$	$ln\left[\frac{dw/dt}{W_r}\right]$
600	0.001145	1.563	37.63	0.277	0.1499	-1.8974
610	0.001132	1.580	38.33	0.26	0.1585	-1.8417
620	0.001120	1.600	39.03	0.24	0.1705	-1.7687
630	0.001107	1.631	39.73	0.209	0.1964	-1.6275
640	0.001095	1.666	40.43	0.174	0.2368	-1.4440
650	0.001083	1.683	41.13	0.157	0.2606	-1.3446
660	0.001071	1.717	41.83	0.123	0.3337	-1.0975
670	0.001060	1.734	42.53	0.106	0.3846	-0.9554

Table S5

Coats Redfern first step thermal decomposition data of [Mo(NO)$_2$(mphpp-aap)(OH)] (**3**)

Temp. (T)	1/T (K)	%(Res.)	W_t	$y = \frac{W_t - W_\infty}{W_0 - W_\infty}$	T^2	$-ln\left[\frac{(1-y)}{T^2}\right]$	$ln\left[-ln\left[\frac{(1-y)}{T^2}\right]\right]$
200	0.002114	96.00	2.010	0.9543	223729	15.4038	2.7346
210	0.002070	95.00	1.989	0.9429	233289	15.2230	2.7228
220	0.002028	94.50	1.979	0.9375	243049	15.1736	2.7195
230	0.001988	93.20	1.952	0.9228	253009	15.0025	2.7082
240	0.001949	92.80	1.943	0.9179	263169	14.9803	2.7067
250	0.001912	91.80	1.922	0.9065	273519	14.8889	2.7006
260	0.001876	89.34	1.871	0.8788	284089	14.6673	2.6856
270	0.001841	87.70	1.836	0.8598	294849	14.5589	2.6782

Table S6

Coats Redfern second step thermal decomposition data of [Mo(NO)$_2$(mphpp-aap)(OH)] (**3**)

Temp.	1/T (K)	% (Res.)	W_t	$y = \frac{W_t - W_\infty}{W_0 - W_\infty}$	T^2	$-\ln\left[\frac{(1-y)}{T^2}\right]$	$\ln\left[-\ln\left[\frac{(1-y)}{T^2}\right]\right]$
370	0.001555	80.56	1.687	0.7788	413449	14.4410	2.6702
380	0.001531	79.75	1.670	0.7696	426409	14.4310	2.6694
390	0.001508	79.34	1.661	0.7647	439569	14.4404	2.6700
400	0.001485	77.70	1.627	0.7462	452929	14.3947	2.6669
410	0.001464	76.88	1.610	0.7369	466489	14.3882	2.6665
420	0.001443	76.22	1.596	0.7293	480429	14.3891	2.6665
430	0.001422	73.76	1.544	0.7011	494209	14.3183	2.6615

Table S7

Coats Redfern first third thermal decomposition data of [Mo(NO)$_2$(mphpp-aap)(OH)] (**3**)

Temp.	1/T (K)	% (Res.)	W_t	$y = \frac{W_t - W_\infty}{W_0 - W_\infty}$	T^2	$-\ln\left[\frac{(1-y)}{T^2}\right]$	$\ln\left[-\ln\left[\frac{(1-y)}{T^2}\right]\right]$
600	0.001145	25.38	0.531	0.1505	762129	13.7070	2.6179
610	0.001132	24.56	0.514	0.1413	779689	13.7189	2.6188
620	0.001120	23.58	0.494	0.1304	797449	13.7289	2.6195
630	0.001107	22.1	0.463	0.1136	815409	13.7320	2.6197
640	0.001095	20.46	0.428	0.0946	833569	13.7328	2.6198
650	0.001083	19.64	0.411	0.0853	851929	13.7443	2.6206
660	0.001072	18.00	0.377	0.0668	870489	13.7459	2.6207
670	0.001060	17.18	0.360	0.0576	889249	13.7574	2.6215

Table S8

Broido first step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp. (T)	1/T (K) x10^3	%(Res.)	W_t	$y = \frac{W_t - W_0}{W_\infty - W_0}$	$\frac{1}{y}$	$ln\left[ln\left(\frac{1}{y}\right)\right]$
200	2.114	96.00	2.010	0.9543	1.0479	-3.0619
210	2.070	95.00	1.989	0.9429	1.060	-2.8421
220	2.028	94.50	1.979	0.9375	1.067	-2.7364
230	1.988	93.20	1.952	0.9228	1.084	-2.5182
240	1.949	92.80	1.943	0.9179	1.090	-2.4511
250	1.912	91.80	1.922	0.9065	1.103	-2.3228
260	1.876	89.34	1.871	0.8788	1.138	-2.0456
270	1.841	87.70	1.836	0.8598	1.163	-1.8904

Table S9

Broido second step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp.	1/T (K) x10^3	% (Res.)	W_t	$y = \frac{W_t - W_0}{W_\infty - W_0}$	$\frac{1}{y}$	$ln\left[ln\left(\frac{1}{y}\right)\right]$
370	1.555	80.56	1.687	0.7788	1.2840	-1.3863
380	1.531	79.75	1.670	0.7696	1.2994	-1.3398
390	1.508	79.34	1.661	0.7647	1.3077	-1.3158
400	1.485	77.70	1.627	0.7462	1.3401	-1.2284
410	1.464	76.88	1.610	0.7369	1.3570	-1.1865
420	1.443	76.22	1.596	0.7293	1.3712	-1.1530
430	1.422	73.76	1.544	0.7011	1.4263	-1.0354

Table S10

Broido third step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp.	1/T (K) x10^3	% (Res.)	W_t	$y = \frac{W_t - W_0}{W_\infty - W_0}$	$\frac{1}{y}$	$ln\left[ln\left(\frac{1}{y}\right)\right]$
600	1.145	25.38	0.531	0.1505	6.6440	0.6385
610	1.132	24.56	0.514	0.1413	7.0771	0.6713
620	1.120	23.58	0.494	0.1304	7.6687	0.7115
630	1.107	22.1	0.463	0.1136	8.8028	0.7771
640	1.095	20.46	0.428	0.0946	10.5702	0.8578
650	1.083	19.64	0.411	0.0853	11.7233	0.9008
660	1.072	18.00	0.377	0.0668	14.9700	0.9955
670	1.060	17.18	0.360	0.0576	17.3611	1.0488

Table S11

Horowitz-Metzger first Step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp. (T)	Kelvin Temp.	$\theta = T\text{-}T_m$	w_t	$\frac{w_\infty}{w_t}$	$log\left[log\left(\frac{w_\infty}{w_t}\right)\right]$	$W_r = W_\infty\text{-}W$
200	473	-57	0.084	21.905	0.1273	1.716
210	483	-47	0.105	17.524	0.0947	1.695
220	493	-37	0.115	16.000	0.0807	1.685
230	503	-27	0.142	12.958	0.0463	1.658
240	513	-17	0.151	12.185	0.0358	1.649
250	523	-7	0.172	10.698	0.0125	1.628
260	533	3	0.223	8.2511	-0.038	1.577
270	543	13	0.258	7.1318	-0.069	1.542

Table S12.

Horowitz-Metzger second Step thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (**3**)

Temp. (T)	$\theta = T-T_m$ (K)	W_t	$\frac{w_\infty}{w_t}$	$log\left[log\left(\frac{w_\infty}{w_t}\right)\right]$	$W_r = W_\infty - W_t$
370	-67	0.407	4.5209	-0.1836	1.433
380	-57	0.424	4.3396	-0.1955	1.416
390	-47	0.433	4.2494	-0.2018	1.407
400	-37	0.467	3.9400	-0.2251	1.373
410	-27	0.484	3.8016	-0.2366	1.356
420	-17	0.498	3.6948	-0.2460	1.342
430	-7	0.550	3.4545	-0.2689	1.290

Table S13

Horowitz-Metzger 3rd thermal decomposition data of $[Mo(NO)_2(mphpp\text{-}aap)(OH)]$ (3)

Temp. (T)	$\theta = T-T_m$ (K)	W_t	$\frac{w_\infty}{w_t}$	$log\left[log\left(\frac{w_\infty}{w_t}\right)\right]$	$W_r = W_\infty - W_t$
600	34	1.563	1.1772	-1.1496	0.277
610	24	1.580	1.1645	-1.1795	0.26
620	14	1.600	1.1500	-1.2168	0.24
630	4	1.631	1.1281	-1.2811	0.209
640	-6	1.666	1.1044	-1.3652	0.174
650	-16	1.683	1.0933	-1.4119	0.157
660	-26	1.717	1.0716	-1.5224	0.123
670	-36	1.734	1.0611	-1.5891	0.106