**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-aap)(OH)] (1) complex
Fig S5: FT-IR spectrum of [Mo(NO)$_2$(amphp-aap)(OH)] (2) complex

Fig S6: FT-IR spectrum of [Mo(NO)$_2$(mphpp-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-aap)(OH)] (3) involving three decomposition steps

| Temp. (K) | 1/T (K) x10$^3$ | % (Res.) | W$_t$ | Temp. (K) | 1/T (K) x10$^3$ | % (Res.) | W$_t$ | Temp. (K) | 1/T (K) x10$^3$ | % (Res.) | W$_t$ |
|-----------|-----------------|--------|------|-----------|-----------------|--------|------|-----------|-----------------|--------|------|
| 200       | 2.114           | 96     | 2.01 | 0.084     | 370             | 1.555  | 80.56 | 1.687     | 0.407           | 600     | 1.145 |
| 210       | 2.07            | 95     | 1.989| 0.105     | 380             | 1.531  | 79.75 | 1.67      | 0.424           | 610     | 1.132 |
| 220       | 2.028           | 94.5   | 1.979| 0.115     | 390             | 1.508  | 79.34 | 1.661     | 0.433           | 620     | 1.12  |
| 230       | 1.988           | 93.2   | 1.952| 0.142     | 400             | 1.485  | 77.7  | 1.627     | 0.467           | 630     | 1.107 |
| 240       | 1.949           | 92.8   | 1.943| 0.151     | 410             | 1.464  | 76.88 | 1.61      | 0.484           | 640     | 1.095 |
| 250       | 1.912           | 91.8   | 1.922| 0.172     | 420             | 1.443  | 76.22 | 1.596     | 0.498           | 650     | 1.083 |
| 260       | 1.876           | 89.34  | 1.871| 0.223     | 430             | 1.422  | 73.76 | 1.544     | 0.55            | 660     | 1.072 |
| 270       | 1.841           | 87.7   | 1.836| 0.258     | 440             | 1.402  | 70    | 1.466     | 0.628           | 670     | 1.06  |
Table S2

Freeman and Carroll 1st step thermal decomposition data of [Mo(NO)2(mphpp-aap)(OH)]

| Temp. (T) | 1/T (K) | Weight lost | Time (minute) | Wf-Wr | [dw/dt] | ln [dw/dt] |
|-----------|---------|-------------|---------------|-------|---------|------------|
| 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 2nd step thermal decomposition data of [Mo(NO)2(mphpp-aap)(OH)]

| Temp. (T) | 1/T (K) | Weight lost | Time (minute) | Wf-Wr | [dw/dt] | ln [dw/dt] |
|-----------|---------|-------------|---------------|-------|---------|------------|
| 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) | \( W_t = W_t - W \) | \( \frac{dw}{dt} \) | \( ln \left( \frac{dw}{dt} \right) \) |
|-----------|---------|-------------|---------------|-----------------|-----------------|-----------------|
| 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.) | Wi | \( y = \frac{W_t - W_\infty}{W_0 - W_\infty} \) | \( T^2 \) | \( -\ln \left( \frac{1 - y}{T^2} \right) \) | \( \ln \left[ -\ln \left( \frac{1 - y}{T^2} \right) \right] \) |
|-----------|---------|----------|----|-----------------|---------|-----------------|-----------------|
| 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)\textsubscript{2}(mphpp-aap)(OH)] \textsuperscript{(3)}

| Temp. | 1/T (K)   | % (Res.) | W\textsubscript{t} | $y = \frac{W_t - W_\infty}{W_0 - W_\infty}$ | T\textsuperscript{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)\textsubscript{2}(mphpp-aap)(OH)] \textsuperscript{(3)}

| Temp. | 1/T (K)   | % (Res.) | W\textsubscript{t} | $y = \frac{W_t - W_\infty}{W_0 - W_\infty}$ | T\textsuperscript{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-aap)(OH)] (3)

| Temp. (T) | 1/T (K) x10$^3$ | % (Res.) | $W_t$ | $\frac{W_t - W_0}{W_\infty - W_0}$ | $\frac{1}{y}$ | $ln\left[ln\left(\frac{1}{y}\right)\right]$ |
|-----------|-----------------|-----------|-------|---------------------------------|---------------|---------------------------------|
| 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-aap)(OH)] (3)

| Temp. | 1/T (K) x10$^3$ | % (Res.) | $W_t$ | $\frac{W_t - W_0}{W_\infty - W_0}$ | $\frac{1}{y}$ | $ln\left[ln\left(\frac{1}{y}\right)\right]$ |
|-------|-----------------|-----------|-------|---------------------------------|---------------|---------------------------------|
| 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-aap)(OH)] (3)

| Temp. | 1/T (K) x10\(^3\) | % (Res.) | W\(_t\) | \(y = \frac{W_t - W_0}{W_\infty - W_0}\) | \(\frac{1}{y}\) | \(ln(ln(\frac{1}{y}))\) |
|-------|-----------------|---------|---------|-----------------|----------------|----------------|
| 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-aap)(OH)] (3)

| Temp. (T) | Kelvin Temp. | \(\theta = T - T_m\) | \(w_t\) | \(\frac{w_\infty}{w_t}\) | \(log\left[log(\frac{w_\infty}{w_t})\right]\) | \(W_r = W_\infty - W\) |
|-----------|--------------|----------------------|---------|-----------------|-----------------------|---------------------|
| 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-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-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            |