# Hydrogen bonds in crystals of HO-(N∩N')M(CO)$_3$L complexes: chains, dimers and an unexpected hexamer

**- Supplementary Material -**

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## Supplementary material

Figure S1. Solution IR spectra of **1a**-**1c**

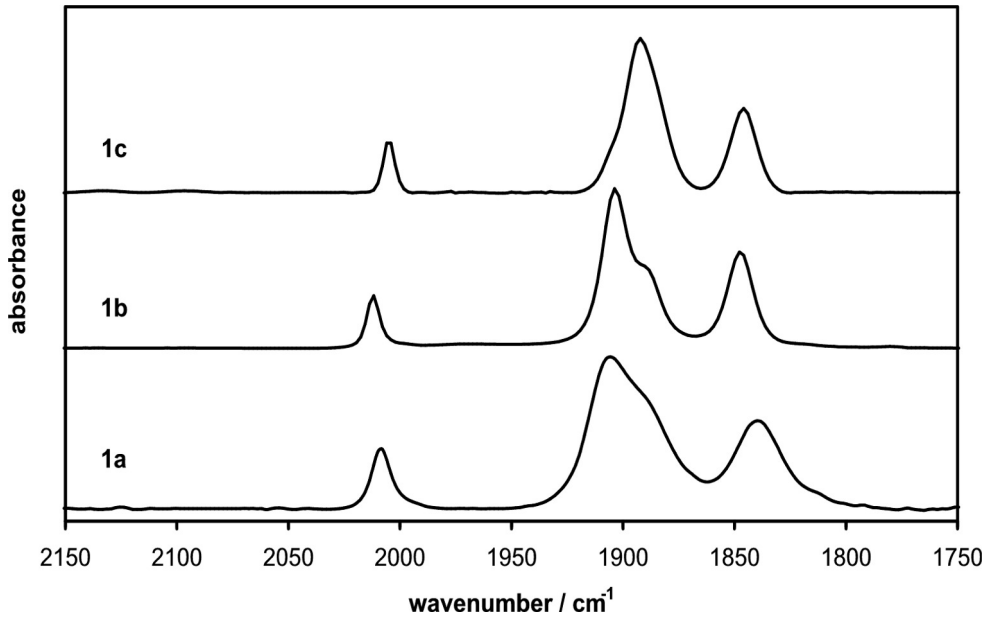


Figure S2. Solution IR spectra of **2a**-**2c**

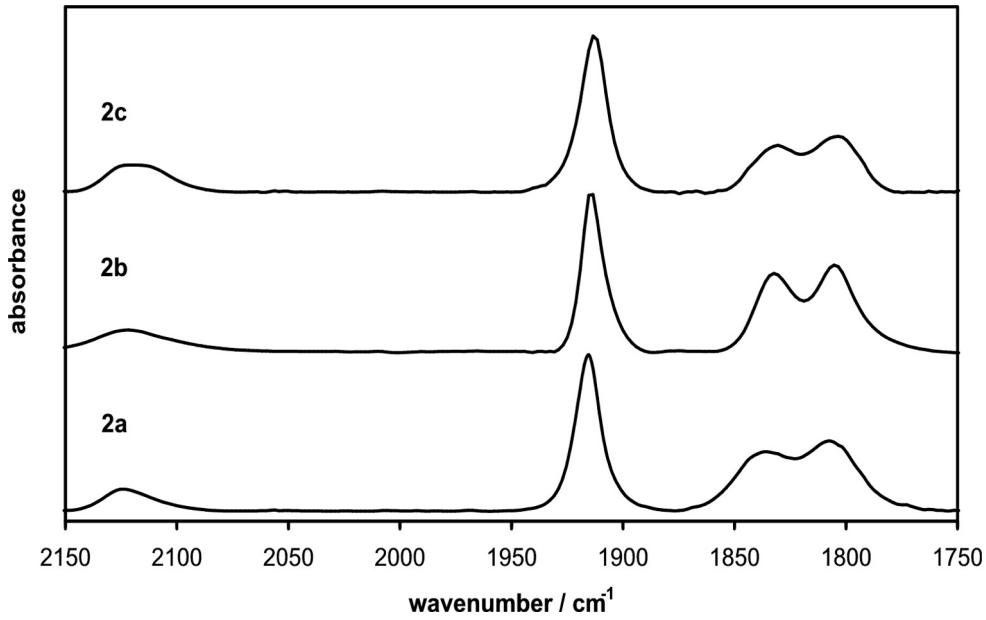
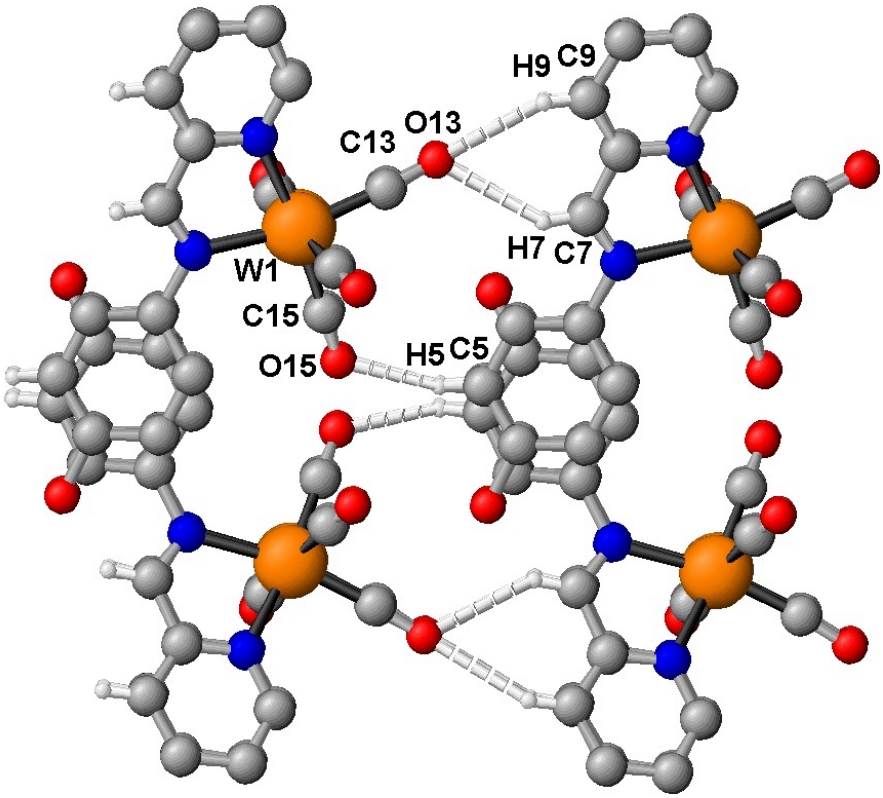
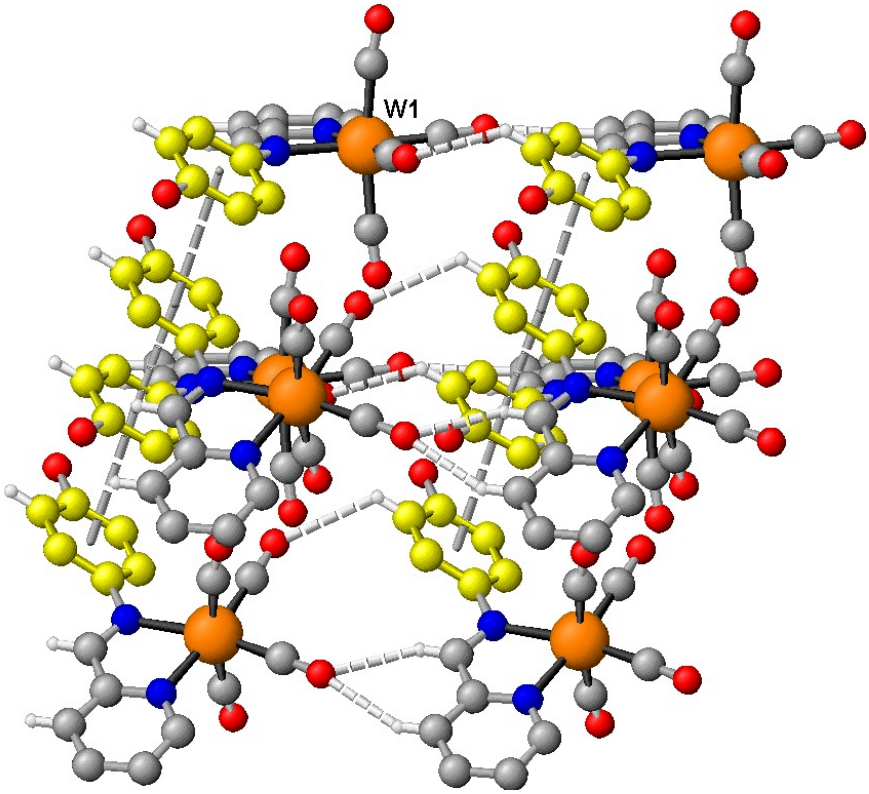



Figure S3. Packing of **1c** (top view) [a]




[a] Hydrogen bonds indicated by light dashed lines.

Figure S4. Packing of **1c** (side view) [a]




[a] Hydrogen bonds indicated by light dashed lines; π-π interactions by dark dashed lines. Phenol-C atoms colour-coded yellow.

Figure S5. Superimposed optimised structures of $HOLMo(CO)_3CNCH_3$ and $HOLMo(CO)_3CNCH_3 \cdot H_2O$.

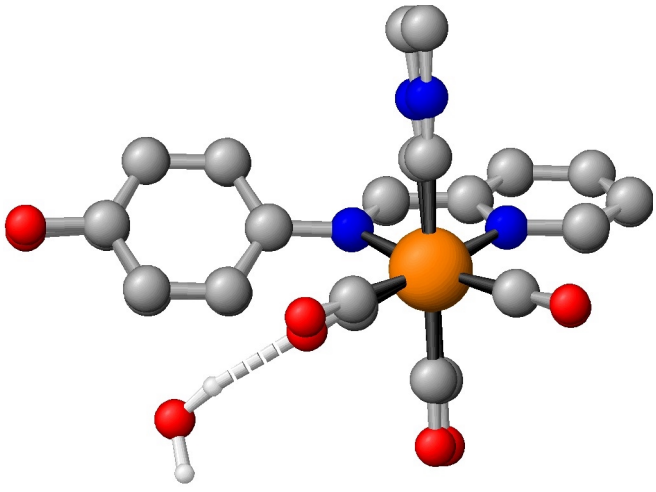


Table S6. DFT Optimised coordinates of $HOLMo(CO)_3CNCH_3$.

| Center Number | Atomic Number | X / Å | Y / Å | Z / Å |
|---|---|---|---|---|
| 1 | 7 | .837336 | -1.659045 | 2.801680 |
| 2 | 6 | .848949 | -1.336683 | 1.654353 |
| 3 | 6 | .817354 | -2.130649 | 4.148160 |
| 4 | 42 | .870084 | -.925497 | -.436553 |
| 5 | 1 | .348197 | -1.389891 | 4.806616 |
| 6 | 1 | 1.838353 | -2.317335 | 4.502181 |
| 7 | 1 | .248857 | -3.066222 | 4.213331 |
| 8 | 6 | -.475786 | -2.365233 | -.625213 |
| 9 | 7 | -.494457 | .837814 | -.130912 |
| 10 | 6 | 2.352254 | -2.218515 | -.589045 |
| 11 | 7 | 2.183667 | .862566 | -.149358 |
| 12 | 6 | .896009 | -.784361 | -2.448661 |
| 13 | 8 | -1.298748 | -3.225910 | -.728398 |
| 14 | 6 | -1.932210 | .780964 | -.077185 |
| 15 | 8 | 3.296188 | -2.952065 | -.662890 |
| 16 | 6 | .094998 | 1.997510 | .098864 |
| 17 | 6 | 1.539086 | 2.061872 | .085940 |
| 18 | 6 | 3.547397 | .864938 | -.194711 |
| 19 | 8 | .913412 | -.764676 | -3.638995 |
| 20 | 6 | -2.652100 | 1.439254 | .944509 |
| 21 | 6 | -2.639437 | .046961 | -1.055958 |
| 22 | 6 | 2.252548 | 3.266809 | .278173 |
| 23 | 6 | 4.308129 | 2.026223 | -.011076 |
| 24 | 1 | -.476758 | 2.911795 | .255860 |
| 25 | 1 | 4.020747 | -.090641 | -.385759 |
| 26 | 6 | -4.054691 | 1.374551 | .984878 |
| 27 | 6 | -4.036815 | -.005500 | -1.032476 |
| 28 | 6 | 3.651227 | 3.254271 | .230952 |
| 29 | 1 | -2.118578 | 1.967464 | 1.730763 |
| 30 | 1 | -2.086690 | -.465989 | -1.834758 |
| 31 | 1 | 1.704764 | 4.188349 | .455161 |
| 32 | 1 | 5.390721 | 1.967806 | -.060262 |
| 33 | 6 | -4.745748 | .657553 | -.011517 |
| 34 | 1 | -4.598836 | 1.867994 | 1.788858 |
| 35 | 1 | -4.590237 | -.559467 | -1.783409 |
| 36 | 1 | 4.219704 | 4.168586 | .373378 |
| 37 | 8 | -6.139284 | .552534 | -.042238 |
| 38 | 1 | -6.566774 | 1.026297 | .700153 |

Table S7. Selected harmonic frequencies [$cm^{-1}$], IR intensities and normal coordinates of $HOLMo(CO)_3CNCH_3$.

| Frequency<br>Intensity | | 1819.7823 $cm^{-1}$<br>1231.4200 | | | 1844.9488 $cm^{-1}$<br>1021.8420 | | | 1902.7450 $cm^{-1}$<br>1563.8938 | | | 2175.6876 $cm^{-1}$<br>1095.1303 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Center Number | Atomic Number | X | Y | Z | X | Y | Z | X | Y | Z | X | Y | Z |
| 1 | 7 | .00 | .00 | .00 | .00 | .00 | -.01 | .00 | .03 | -.09 | -.01 | -.19 | .64 |
| 2 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | -.02 | .06 | .01 | .18 | -.63 |
| 3 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .03 | -.09 |
| 4 | 42 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | -.01 | .00 | .00 | .00 | .00 |
| 5 | 1 | .00 | .00 | -.01 | .00 | .00 | .00 | .01 | -.04 | .05 | -.03 | .12 | -.14 |
| 6 | 1 | .00 | -.01 | -.01 | .00 | .00 | .00 | -.03 | -.02 | .06 | .07 | .05 | -.16 |
| 7 | 1 | .01 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .07 | -.03 | .00 | -.18 |
| 8 | 6 | .33 | .35 | .04 | -.33 | -.35 | -.04 | .31 | .33 | .04 | .03 | .03 | .01 |
| 9 | 7 | .00 | .02 | .00 | .00 | .00 | .00 | -.01 | -.03 | -.01 | .00 | -.01 | .00 |
| 10 | 6 | .51 | -.41 | -.04 | .23 | -.18 | -.02 | -.31 | .24 | .03 | -.03 | .03 | .00 |
| 11 | 7 | -.01 | -.01 | .00 | .00 | .01 | .00 | -.01 | -.02 | -.01 | .00 | -.01 | .00 |
| 12 | 6 | .00 | .00 | .07 | -.01 | .00 | .60 | -.01 | -.01 | .54 | .00 | .00 | .07 |
| 13 | 8 | -.23 | -.25 | -.03 | .23 | .24 | .03 | -.21 | -.22 | -.03 | -.02 | -.02 | .00 |
| 14 | 6 | .01 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 15 | 8 | -.36 | .28 | .03 | -.16 | .12 | .01 | .21 | -.16 | -.02 | .02 | -.02 | .00 |
| 16 | 6 | -.01 | -.01 | .00 | .00 | .00 | .00 | .03 | .03 | .01 | .01 | .01 | .00 |
| 17 | 6 | .01 | .01 | .00 | .00 | .00 | .00 | -.03 | .01 | .00 | -.01 | .00 | .00 |
| 18 | 6 | .01 | .00 | .00 | .00 | .00 | .00 | .01 | .01 | .00 | .01 | .00 | .00 |
| 19 | 8 | .00 | .00 | -.05 | .01 | .01 | -.42 | .01 | .01 | -.38 | .00 | .00 | -.04 |
| 20 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 21 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 22 | 6 | -.01 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .00 | .00 | .00 | .00 |
| 23 | 6 | -.01 | .01 | .00 | .00 | .00 | .00 | .00 | -.02 | .00 | .00 | -.01 | .00 |
| 24 | 1 | .01 | .00 | .00 | .00 | .00 | .01 | -.01 | .01 | .01 | .00 | .01 | -.01 |
| 25 | 1 | -.05 | -.03 | .00 | .00 | .00 | .01 | -.01 | .00 | .00 | -.01 | .00 | .00 |
| 26 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 27 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 28 | 6 | .01 | .00 | .00 | .00 | .00 | .00 | -.01 | .01 | .00 | .00 | .00 | .00 |
| 29 | 1 | .01 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | -.01 | .00 | .00 | -.01 |
| 30 | 1 | .00 | .02 | -.01 | -.02 | -.03 | .01 | .02 | .01 | .01 | .01 | .00 | .00 |
| 31 | 1 | .00 | .00 | .00 | .00 | .00 | .00 | -.01 | -.01 | .00 | .00 | .00 | .00 |
| 32 | 1 | -.01 | -.02 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .00 | .00 | .00 |
| 33 | 6 | .00 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .00 | .00 | .00 | .00 |
| 34 | 1 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 35 | 1 | -.01 | .01 | .00 | .00 | -.01 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 36 | 1 | -.01 | .00 | .00 | .00 | .00 | .00 | .01 | .00 | .00 | .00 | .00 | .00 |
| 37 | 8 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |
| 38 | 1 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 | .00 |

Table S8. DFT Optimised coordinates of $HOLMo(CO)_3CNCH_3 \cdot H_2O$.

| Center Number | Atomic Number | X / Å | Y / Å | Z / Å |
|---|---|---|---|---|
| 1 | 42 | 0.306437 | 0.163274 | -1.135552 |
| 2 | 7 | 0.296890 | 0.160353 | 1.130471 |
| 3 | 7 | 2.456309 | 0.136676 | -0.476776 |
| 4 | 6 | -0.876189 | 0.068417 | 1.960218 |
| 5 | 6 | -2.021577 | 0.834433 | 1.646722 |
| 6 | 6 | -3.178291 | 0.751056 | 2.428695 |
| 7 | 6 | -3.201667 | -0.112273 | 3.541381 |
| 8 | 6 | -2.073181 | -0.894972 | 3.863133 |
| 9 | 6 | -0.915551 | -0.801488 | 3.074649 |
| 10 | 6 | 1.481597 | 0.133688 | 1.709531 |
| 11 | 6 | 2.672627 | 0.142015 | 0.885869 |
| 12 | 6 | 3.975302 | 0.163700 | 1.432288 |
| 13 | 6 | 5.081772 | 0.176977 | 0.574072 |
| 14 | 6 | 4.856534 | 0.168080 | -0.820273 |
| 15 | 6 | 3.540722 | 0.149168 | -1.302115 |
| 16 | 6 | 0.700336 | 0.053587 | -3.065892 |
| 17 | 6 | 0.317459 | 2.173536 | -1.313424 |
| 18 | 6 | -1.618897 | 0.222971 | -1.498772 |
| 19 | 6 | 0.173449 | -1.965510 | -1.112268 |
| 20 | 8 | 0.997937 | -0.027287 | -4.222571 |
| 21 | 8 | 0.290925 | 3.352876 | -1.468481 |
| 22 | 8 | -2.805074 | 0.291830 | -1.697401 |
| 23 | 1 | -4.330443 | -0.787550 | 5.033119 |
| 24 | 1 | -2.008903 | 1.509284 | 0.800118 |
| 25 | 1 | -4.053609 | 1.329540 | 2.153063 |
| 26 | 1 | -2.100308 | -1.582463 | 4.707574 |
| 27 | 1 | -0.064299 | -1.438692 | 3.301734 |
| 28 | 1 | 1.590981 | 0.136014 | 2.793686 |
| 29 | 1 | 4.101357 | 0.174196 | 2.511362 |
| 30 | 1 | 6.091983 | 0.196371 | 0.972259 |
| 31 | 1 | 5.682631 | 0.178930 | -1.523927 |
| 32 | 1 | 3.333458 | 0.146878 | -2.365622 |
| 33 | 8 | -4.385553 | -0.161384 | 4.282382 |
| 34 | 7 | 0.041770 | -3.148242 | -1.164994 |
| 35 | 6 | -0.178680 | -4.553139 | -1.283724 |
| 36 | 1 | -0.234411 | -4.839703 | -2.340717 |
| 37 | 1 | 0.639727 | -5.110389 | -0.812728 |
| 38 | 1 | -1.120287 | -4.832518 | -0.796036 |
| 39 | 8 | -4.536842 | 2.002806 | -0.153261 |
| 40 | 1 | -4.116295 | 1.307657 | -0.707071 |
| 41 | 1 | -4.752450 | 2.781226 | -0.700448 |

Table S9. Selected harmonic frequencies [$cm^{-1}$], IR intensities and normal coordinates of $HOLMo(CO)_3CNCH_3 \cdot H_2O$.

| Frequency<br>Intensity | | 1788.8933 $cm^{-1}$<br>1347.6114 | | | 1839.2818 $cm^{-1}$<br>1032.7120 | | | 1899.6064 $cm^{-1}$<br>1612.6356 | | | 2180.5050 $cm^{-1}$<br>1035.6327 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Center Number | Atomic Number | X | Y | Z | X | Y | Z | X | Y | Z | X | Y | Z |
| 1 | 42 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| 2 | 7 | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 | 0.00 | -0.01 | -0.03 | 0.00 | 0.00 | 0.01 | 0.00 |
| 3 | 7 | -0.02 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 | 0.00 | 0.01 | 0.00 |
| 4 | 6 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 5 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 6 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 7 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 8 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 9 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 10 | 6 | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 | 0.03 | 0.03 | 0.00 | -0.01 | -0.01 | 0.00 |
| 11 | 6 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | -0.02 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 |
| 12 | 6 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 13 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| 14 | 6 | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 | 0.01 | 0.00 |
| 15 | 6 | 0.02 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.01 | 0.01 | 0.00 | -0.01 | 0.00 | 0.00 |
| 16 | 6 | 0.23 | -0.23 | 0.05 | 0.44 | -0.43 | 0.10 | -0.29 | 0.28 | -0.06 | 0.03 | -0.03 | 0.01 |
| 17 | 6 | 0.00 | -0.04 | -0.11 | 0.00 | 0.14 | 0.46 | -0.01 | 0.18 | 0.61 | 0.00 | -0.02 | -0.06 |
| 18 | 6 | 0.56 | 0.47 | -0.05 | -0.16 | -0.14 | 0.02 | 0.22 | 0.19 | -0.02 | -0.03 | -0.03 | 0.00 |
| 19 | 6 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.06 | -0.02 | 0.04 | 0.66 |
| 20 | 8 | -0.17 | 0.16 | -0.04 | -0.31 | 0.30 | -0.07 | 0.20 | -0.19 | 0.04 | -0.02 | 0.02 | 0.00 |
| 21 | 8 | 0.00 | 0.02 | 0.08 | 0.00 | -0.10 | -0.33 | 0.00 | -0.13 | -0.43 | 0.00 | 0.01 | 0.04 |
| 22 | 8 | -0.38 | -0.32 | 0.04 | 0.11 | 0.09 | -0.01 | -0.15 | -0.12 | 0.01 | 0.02 | 0.02 | 0.00 |
| 23 | 1 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 24 | 1 | 0.03 | 0.04 | -0.03 | -0.02 | -0.01 | 0.01 | 0.02 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| 25 | 1 | -0.02 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 26 | 1 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 27 | 1 | 0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| 28 | 1 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 |
| 29 | 1 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| 30 | 1 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 31 | 1 | -0.01 | -0.01 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| 32 | 1 | -0.06 | -0.02 | 0.01 | -0.03 | -0.01 | 0.01 | -0.01 | 0.00 | 0.01 | 0.01 | 0.00 | 0.00 |
| 33 | 8 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 34 | 7 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.09 | 0.03 | -0.04 | -0.67 |
| 35 | 6 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 | 0.00 | 0.10 |
| 36 | 1 | 0.01 | 0.01 | 0.01 | 0.01 | -0.01 | -0.01 | -0.02 | 0.03 | 0.06 | -0.04 | 0.06 | 0.17 |
| 37 | 1 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 | -0.01 | -0.02 | -0.02 | 0.06 | -0.04 | -0.06 | 0.17 |
| 38 | 1 | 0.01 | 0.01 | 0.02 | 0.00 | 0.00 | -0.01 | 0.02 | 0.00 | 0.06 | 0.06 | 0.00 | 0.17 |
| 39 | 8 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 40 | 1 | -0.03 | -0.05 | 0.08 | 0.00 | 0.00 | -0.02 | -0.02 | 0.01 | 0.03 | 0.00 | 0.00 | 0.01 |
| 41 | 1 | -0.03 | 0.01 | -0.02 | 0.00 | -0.01 | 0.01 | -0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Table S10. Selected Bond Lengths (Å) of $HOLMo(CO)_3CNCH_3$ and $HOLMo(CO)_3CNCH_3 \cdot H_2O$ (numbering identical to experimental structures for ease of comparison).

| | **$HOLMo(CO)_3CNCH_3$** | **$HOLMo(CO)_3CNCH_3 \cdot H_2O$** |
|---|---|---|
| Mo-N1 | 2.250 | 2.266 |
| Mo-N2 | 2.237 | 2.249 |
| Mo-C13 | 1.973 | 1.973 |
| Mo-C14 | 2.017 | 2.018 |
| Mo-C15 | 1.980 | 1.960 |
| Mo-C16 | 2.131 | 2.133 |
| C13-O13 | 1.198 | 1.197 |
| C14-O14 | 1.191 | 1.190 |
| C15-O15 | 1.195 | 1.205 |
| C16-N3 | 1.192 | 1.191 |
| N1-C7 | 1.321 | 1.319 |
| N2-C8 | 1.382 | 1.380 |
| C7-C8 | 1.446 | 1.448 |
| N1-C1 | 1.440 | 1.440 |
| O1-C4 | 1.398 | 1.398 |
| $O_w \cdots O15$ [a] | - | 2.883 |
| $O_w$-$H_b$ [a] | - | 0.983 |
| $O_w$-$H_t$ [a] | - | 0.976 |
| $H_b \cdots O15$ [a] | - | 1.932 |

[a] $O_w$ = water oxygen atom, $H_b$ = bridging water hydrogen atom, $H_t$ = terminal water hydrogen atom.

Table S11. Selected Bond Angles (°) of $HOLMo(CO)_3CNCH_3$ and $HOLMo(CO)_3CNCH_3 \cdot H_2O$ (numbering identical to experimental structures for ease of comparison).

| | **$HOLMo(CO)_3CNCH_3$** | **$HOLMo(CO)_3CNCH_3 \cdot H_2O$** |
|---|---|---|
| N1-Mo-N2 | 73.3 | 73.2 |
| N1-Mo-C13 | 168.4 | 168.3 |
| N1-Mo-C14 | 95.1 | 95.1 |
| N1-Mo-C15 | 99.8 | 100.4 |
| N1-Mo-C16 | 90.7 | 89.3 |
| N2-Mo-C13 | 97.1 | 95.5 |
| N2-Mo-C14 | 95.3 | 91.9 |
| N2-Mo-C15 | 173.0 | 173.6 |
| N2-Mo-C16 | 92.0 | 92.6 |
| C13-Mo-C14 | 87.7 | 88.2 |
| C13-Mo-C15 | 91.5 | 90.9 |
| C13-Mo-C16 | 87.5 | 91.2 |
| C14-Mo-C15 | 88.0 | 88.1 |
| C14-Mo-C16 | 172.9 | 174.5 |
| C15-Mo-C16 | 86.9 | 88.3 |
| $O_w$-$H_b \cdots O15$ [a] | - | 162.0 |
| $H_b$-$O_w$-$H_t$ [a] | - | 110.0 |
| C15-O15$\cdots H_b$ [a] | - | 127.9 |
| C7-N1-C1-C2 | -137.6 | -141.8 |
| C7-C8-N2-C12 | -179.0 | -179.8 |

[a] $O_w$ = water oxygen atom, $H_b$ = bridging water hydrogen atom, $H_t$ = terminal water hydrogen atom.