**Supplementary**

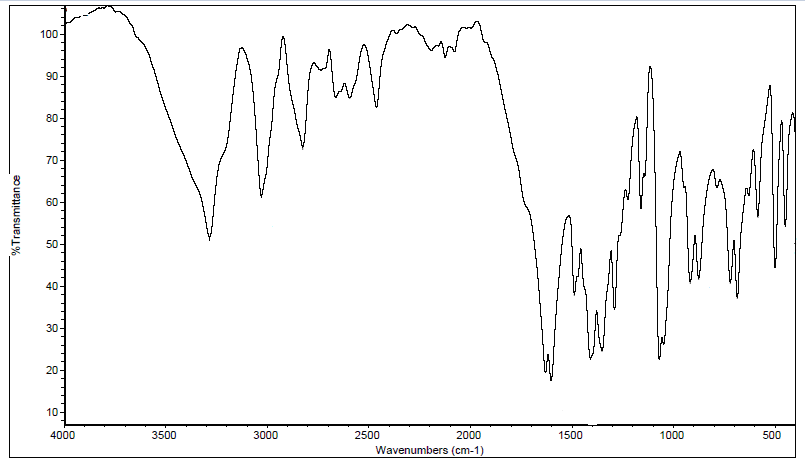


Figure S1:IR spectrum of tricine in KBr.

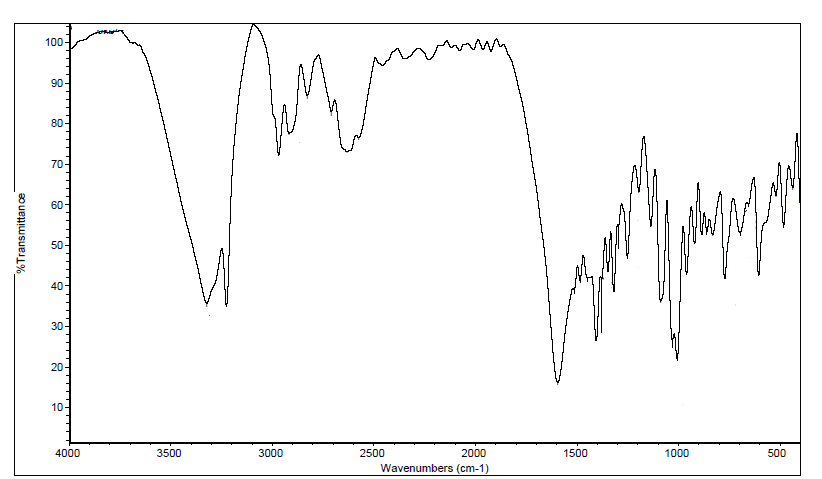


Figure S2:IR spectrum of [Ni(tric)2Cl2].3H2O in KBr.

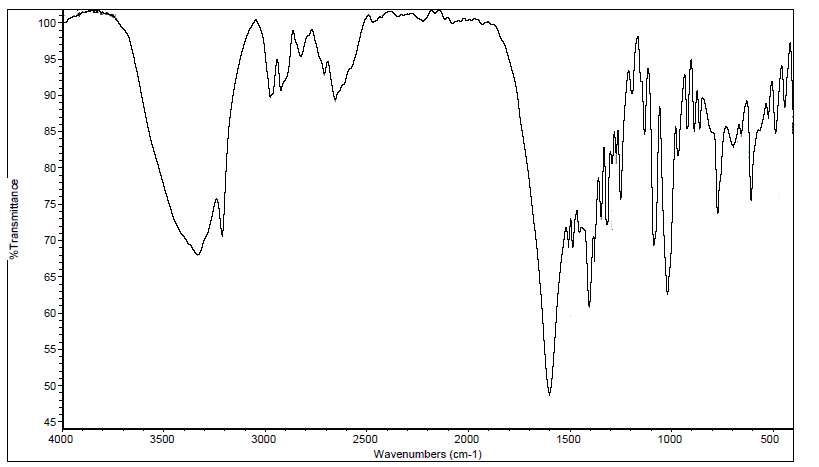


Figure S3:IR spectrum of[Co(tric)2Cl2].2H2O in KBr.

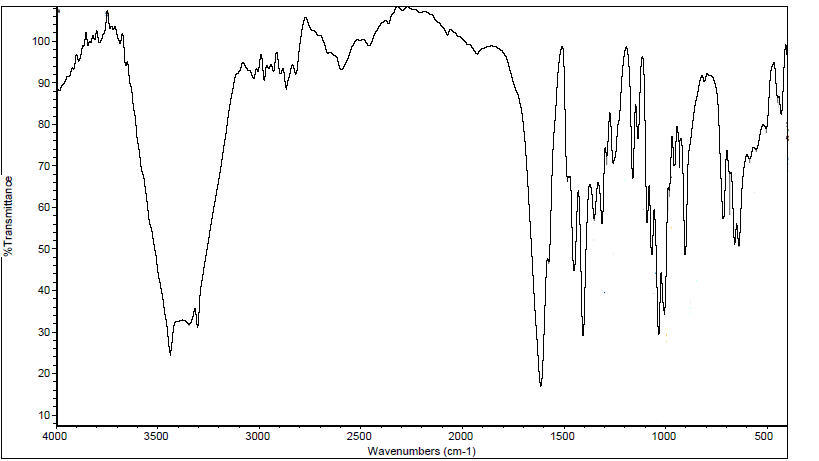


Figure S4: IR spectrum of[Zn(tric)2Cl2].EtOH in KBr.

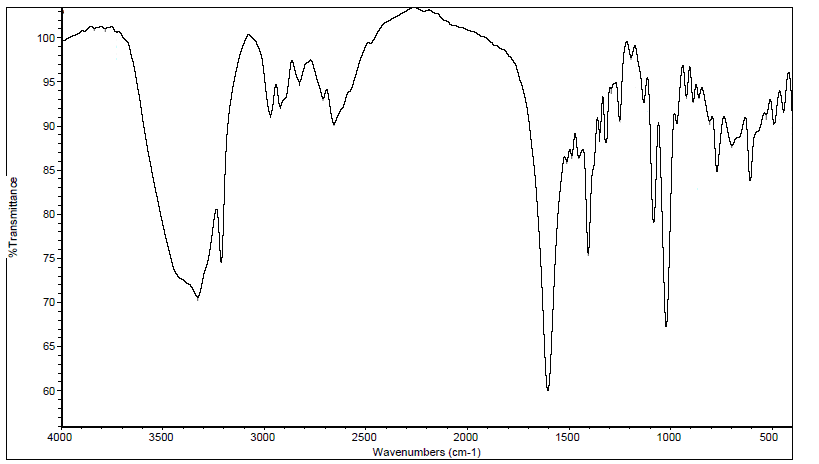


Figure S5: IR spectrum of[Cd(tric)2(Ac)2].H2O in KBr.

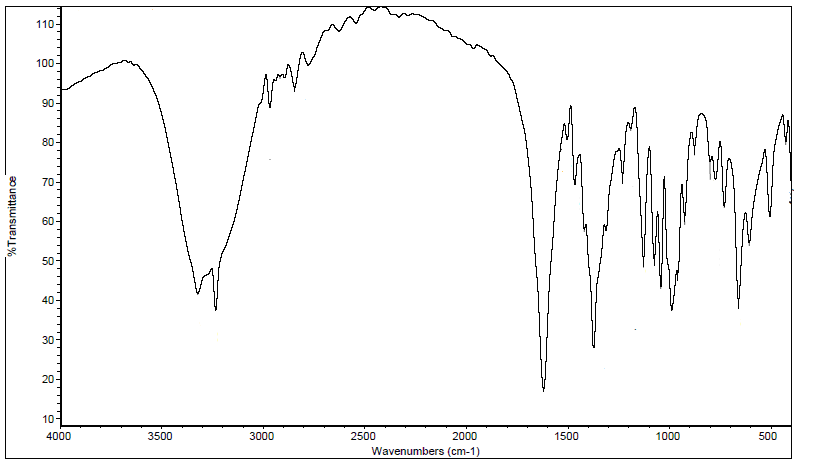


Figure S6: IR spectrum of [Ni(tric-H)2].2H2O in KBr.

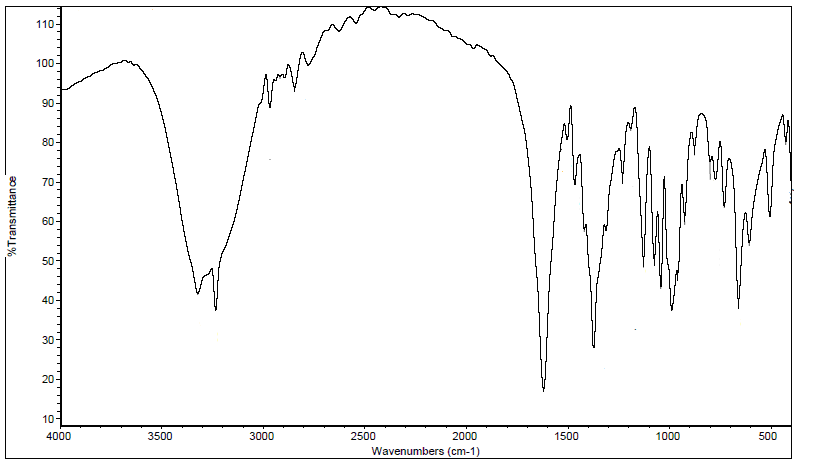


Figure S7: IR spectrum of [Cu(tric)2]Cl2.3H2O in KBr.

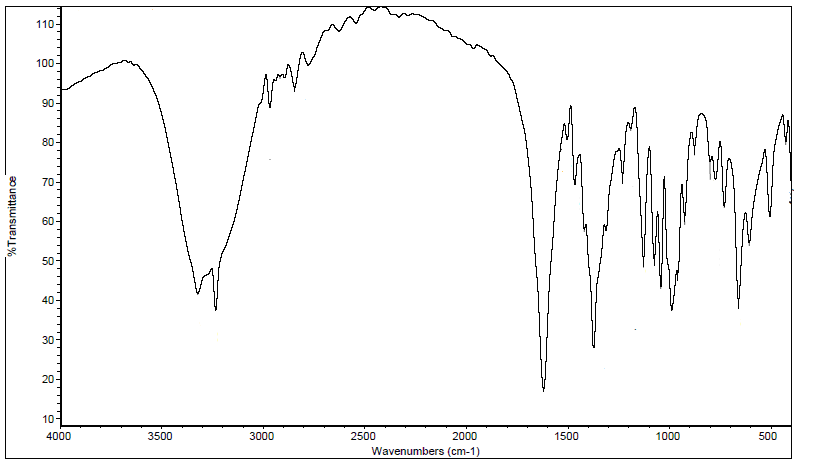


Figure S8: IR spectrum of [Co(tric-H)2].0.5H2O in KBr.

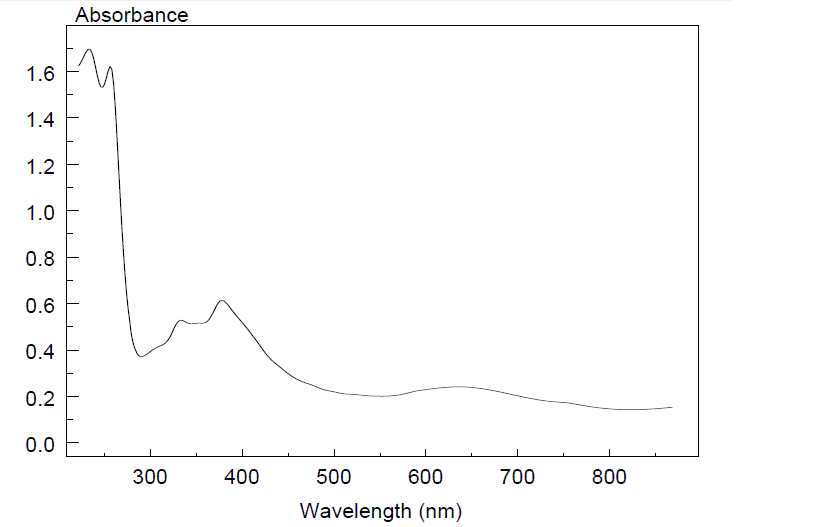


Figure S9: Electronic spectrum of [Ni(tric)2Cl2].3H2O.

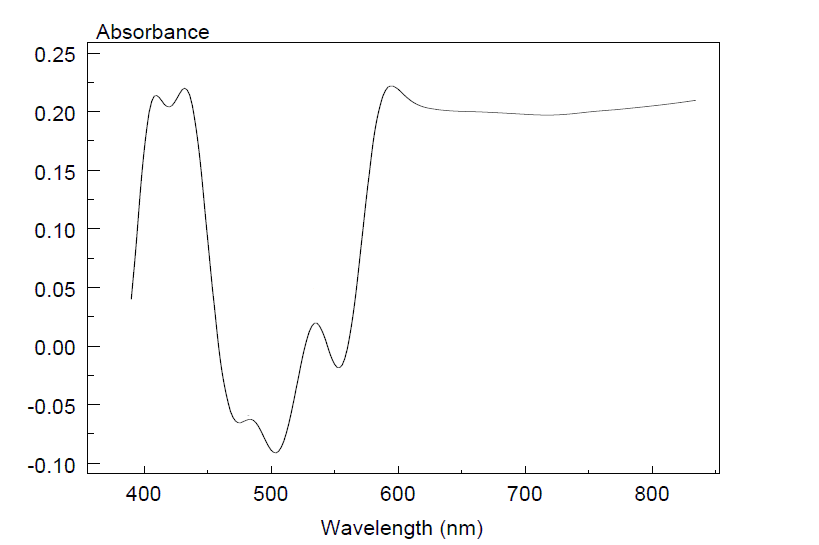


Figure S10: Electronic spectrum of [Co(tric-H)2].0.5H2O.

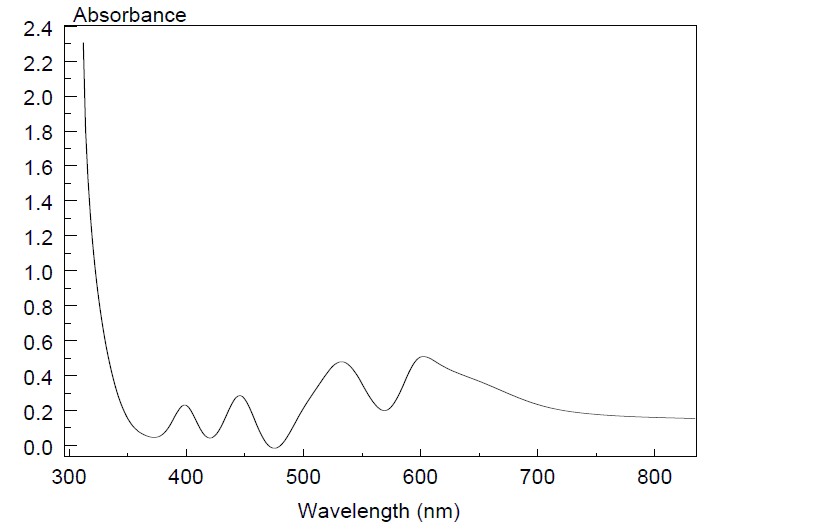


Figure S11: Electronic spectrum of [Co(tric)2Cl2].2H2O.

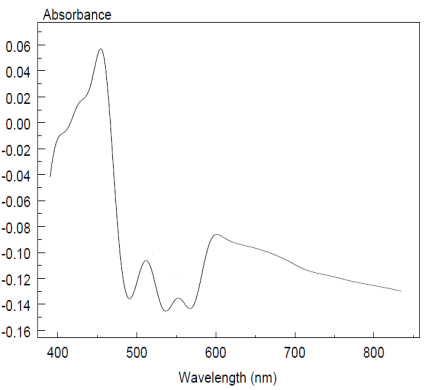


Figure S12: Electronic spectrum of [Ni(tric-H)2].2H2O.

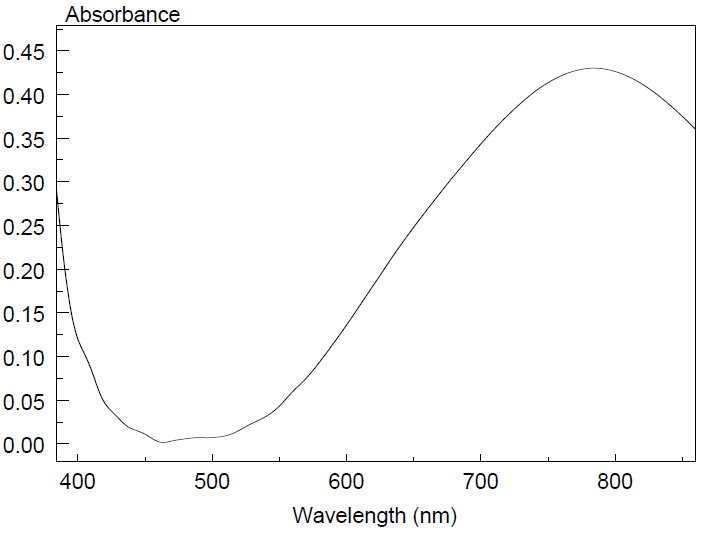


Figure S13: Electronic spectrum of [Cu(tric)2]Cl2.3H2O.

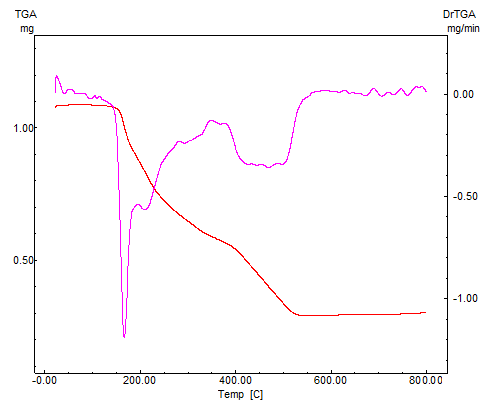


Figure S14: Thermal analysis curves (TGA, DTG) of [Cu(tric)2]Cl2.3H2O.

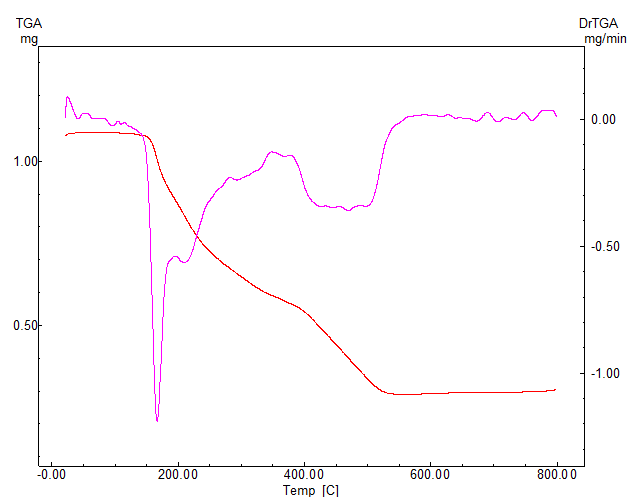


Figure S15:TGA curves of [Cu(tric)2]Cl2.3H2O.

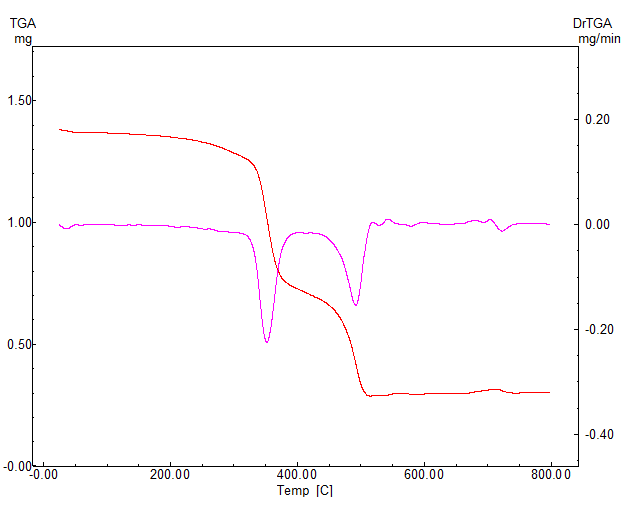


Figure S16:TGA curves of Co(tric)2Cl2].2H2O.

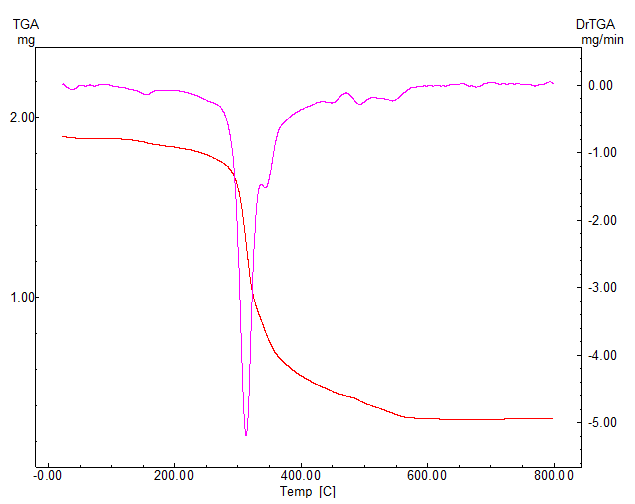


Figure S17: TGA curves of [Ni(tric)2(Cl)2].3H2O.

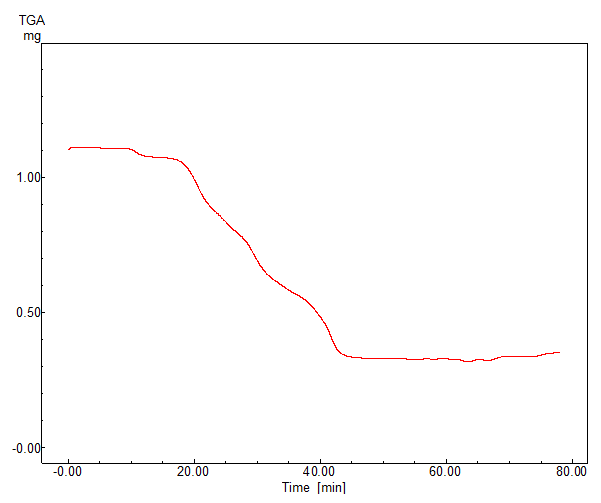
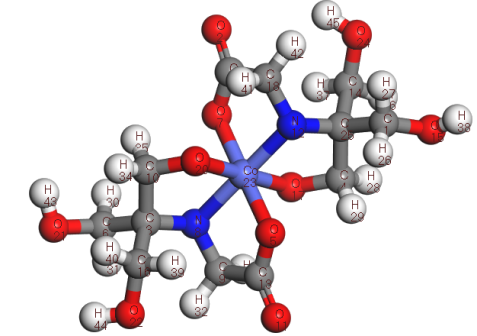
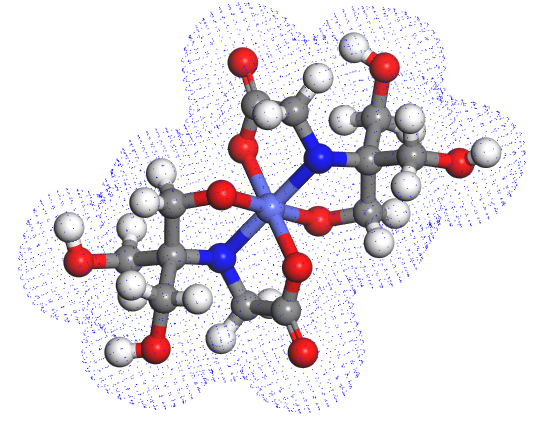


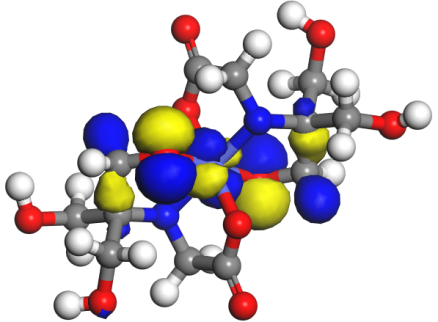
Figure S18:TGA curves of [Cd(tric)2(Ac)2].H2O.



Molecular modeling of [Co(tric-H)2].0.5H2O.

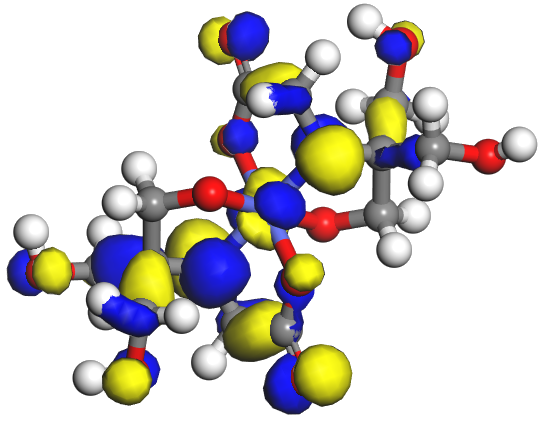


Electron density of [Co(tric-H)2]. 0.5H2O



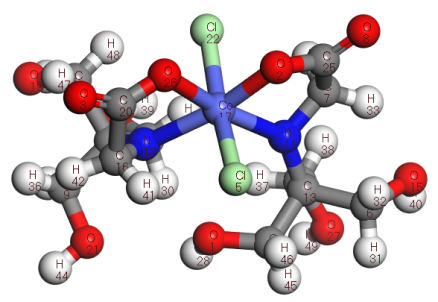
ELUMO = -5.195 eV

ΔE = -0.308 eV



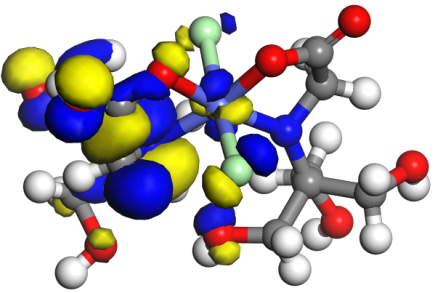
EHOMO = -5.503 eV

Scheme S1: Molecular modeling of [Co(tric-H)2]. 0.5H2O.



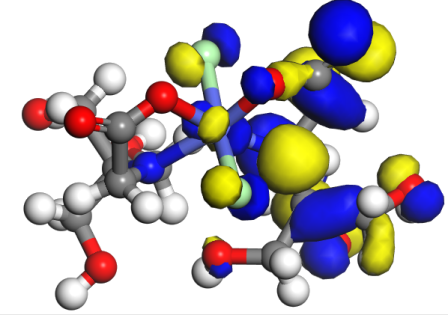


Electron density of [Co(tric)2Cl2].2H2O.



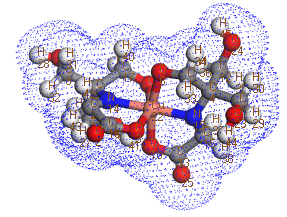
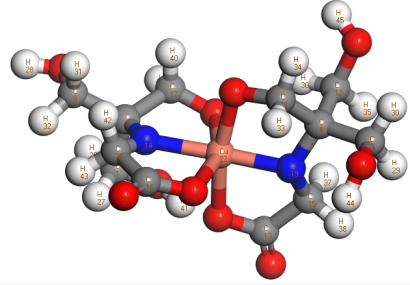
ELUMO = -5.150

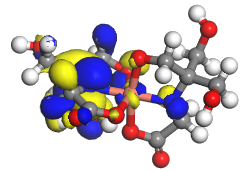
ΔE = -0.573 eV



EHOMO = -5.723 eV

Scheme S2:Molecular modeling of [Co(tric)2Cl2].2H2O.

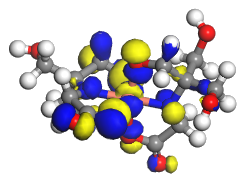


 (a) (b)

ELUMO = -4.958eV

(d)

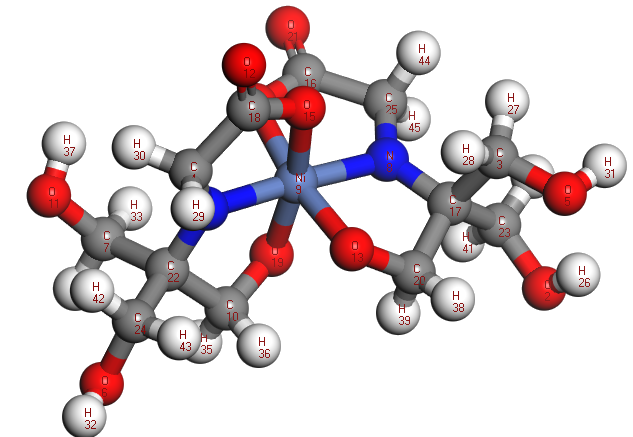
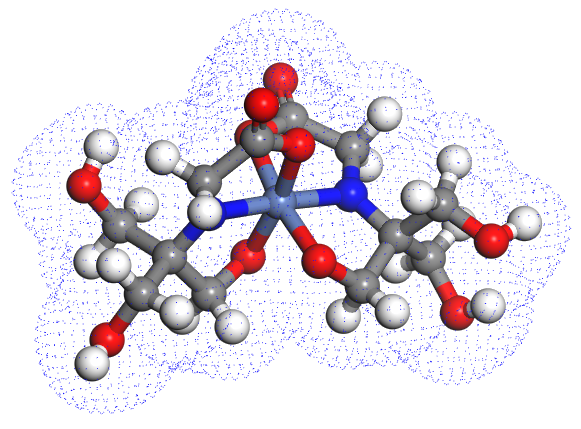
ΔE = -0.32eV



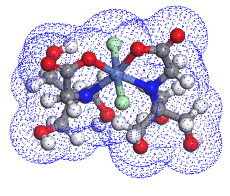
E HOMO = -5.278eV

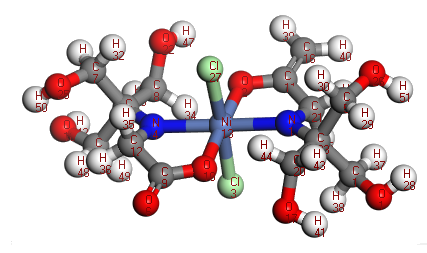
(c)

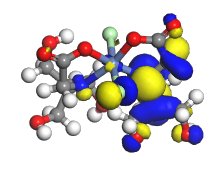
Scheme S3: Molecular modeling of (a) [Cu(tric)2]Cl2.3H2O, (b) electron density,(c) HOMO and (d) LUMO.



1. (b)



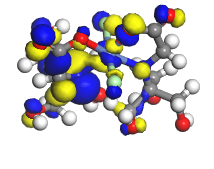


1. (b)

ELUMO = -5,328 eV

(d)

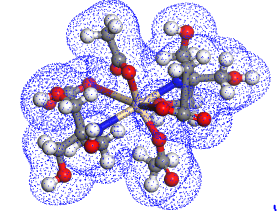
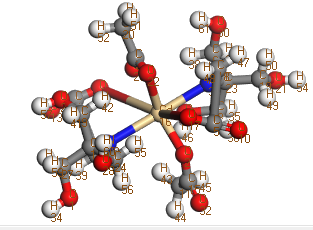
Δ E = -0.105 eV



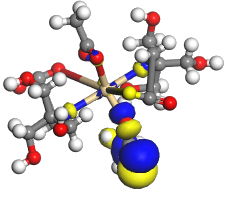
EHOMO = -5.433eV

(c)

Scheme S4: Molecular modeling of (a) [Ni(tric)2Cl2].3H2O,(b) electron density,(c) HOMO and (d) LUMO.



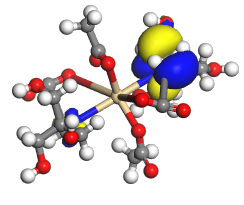
1. (b)



ELUMO = -1.942eV

(d)

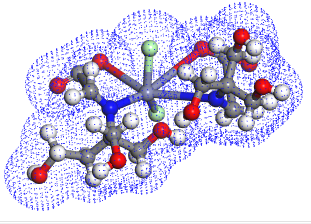
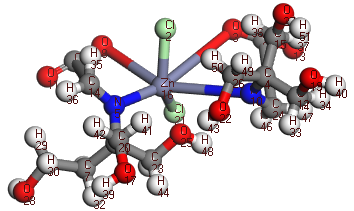
ΔE=-3.425eV

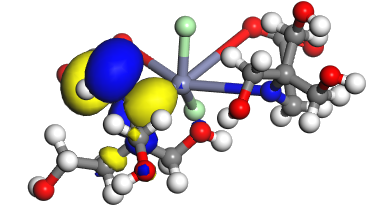


EHOMO = -5.367eV

(c)

Scheme S5: Molecular modeling of (a) [Cd(tric)2(Ac)2].H2O, (b) electron density, (c) HOMO and (d) LUMO.

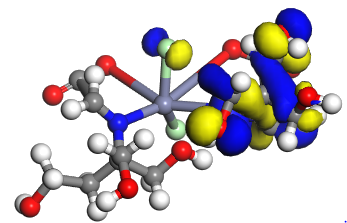


1.  (B)

ELUMO = -2.530 eV

(D)

ΔE = -3.397 eV

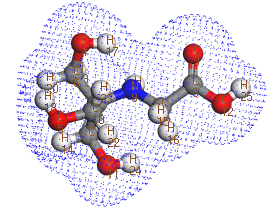
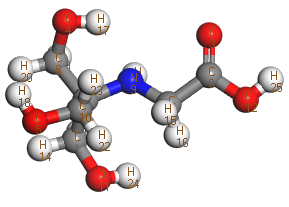


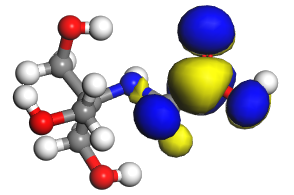
EHOMO = -5.927 eV

(C)

Scheme S6: Molecular modeling of (a) [Zn(tric)2Cl2].EtOH, (b) electron density, (c) HOMO and (d) LUMO.

.

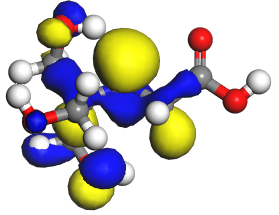


 (a) (b)

ELUMO = -0.678 eV

(d)

ΔE = -4.502 eV



EHOMO = -5.180 eV

(c)

Scheme 7: Molecular modeling of tricine (a), electron density (b), HOMO (c) and LUMO (d).

Table S1: Thermal analysis (DTA, DTG) of the complexes.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound, No. | Decomposition Step | Temperature  range  ﹾ)C) | Remove species | Wt. Loss | |
| % (Calcd.) | % (Found) |
| [Co(tric)2(Cl)2].2H2O | 1st | 25-135 | 2H2O+CH2 | 9.55 | 8.632 |
| 2nd +3rd | 135-340.44,  340.44-800 | C9H22N2O6 + 2HCl | 62.036 | 62.199 |
| Residue | 800-1000 | CoNCO4 | 28.412 | 29.1 |
| [Cu(tric)2]Cl2.3H2O | 1st | 10-179.47 | 3H2O + 2HCl + 2NH3 + COOH | 37.68 | 37.43 |
| 2nd | 179.47-432.2 | C9H17O4 | 34.6 | 35.289 |
| Residue | 432.2-1000 | CuC2O4 | 27.72 | 27.281 |
| [Ni(tric)2(Cl)2].3H2O | 1st | 20-268.75 | 3H2O | 9.97 | 9.236 |
| 2nd | 268.75-378.85 | C10H26N2O8Cl2 | 68.86 | 69.309 |
| Residue | 378.85-1000 | NiC2O2 | 21.165 | 21.455 |
| [Ni(tric-H)2].2H2O | 1st | 15-314.51 | 2H2O + C10H24NO8 | 71.461 | 71.254 |
| 2nd | 314.51-570 | NCO | 9.315 | 9.582 |
| Residue | 570-1000 | NiCO | 19.222 | 19.164 |
| [Cd(tric)2(Ac)2].H2O | 1st | 18-300 | C5N2O4H18 + H2O | 31.0162 | 31.273 |
| 2nd | 300-582 | C8H15O7 | 39.250 | 39.818 |
| Residue | 582-1000 | CdC3O2 | 29.733 | 28.909 |

Table S2: Bond lengths (Å) of tricine using DFT-method from DMOL3calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length | Bond | Length |
| O(24)-H(45) | 0.973 | C(25)-C(4) | 1.558 |
| O(22)-H(44) | 0.974 | O(5)-Co(23) | 1.972 |
| O(21)-H(43) | 0.974 | C(1)-O(15) | 1.439 |
| C(18)-H(42) | 1.094 | O(17)-Co(23) | 1.875 |
| C(18)-H(41) | 1.101 | C(10)-O(20) | 1.414 |
| C(16)-H(40) | 1.098 | C(13)-O(11) | 1.234 |
| C(16)-H(39) | 1.096 | C(25)-C(1) | 1.558 |
| O(15)-H(38) | 0.973 | O(20)-Co(23) | 1.878 |
| C(14)-H(37) | 1.097 | N(12)-Co(23) | 1.92 |
| C(14)-H(36) | 1.097 | C(18)-N(12) | 1.426 |
| C(10)-H(35) | 1.108 | C(3)-C(10) | 1.557 |
| C(10)-H(34) | 1.103 | C(19)-O(2) | 1.234 |
| C(9)-H(33) | 1.102 | Co(23)-O(7) | 1.978 |
| C(9)-H(32) | 1.093 | N(8)-C(9) | 1.427 |
| C(6)-H(31) | 1.098 | C(6)-O(21) | 1.429 |
| C(6)-H(30) | 1.098 | C(19)-C(18) | 1.593 |
| C(4)-H(29) | 1.107 | C(4)-O(17) | 1.414 |
| C(4)-H(28) | 1.101 | N(8)-Co(23) | 1.922 |
| C(1)-H(27) | 1.1 | O(5)-C(13) | 1.306 |
| C(1)-H(26) | 1.103 | C(14)-O(24) | 1.429 |
| N(12)-C(25) | 1.472 | C(13)-C(9) | 1.592 |
| C(25)-C(14) | 1.586 | N(8)-C(3) | 1.458 |
| C(3)-C(16) | 1.59 | O(7)-C(19) | 1.305 |
| C(3)-C(6) | 1.582 | C(16)-O(22) | 1.424 |

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Angle | Bond | Angle |
| N(12)-C(25)-C(14) | 114.818 | O(11)-C(13)-O(5) | 125.853 |
| N(12)-C(25)-C(4) | 103.728 | O(11)-C(13)-C(9) | 120.029 |
| N(12)-C(25)-C(1) | 109.286 | O(5)-C(13)-C(9) | 114.116 |
| C(14)-C(25)-C(4) | 106.259 | C(25)-N(12)-Co(23) | 115.54 |
| C(14)-C(25)-C(1) | 110.005 | C(25)-N(12)-C(18) | 121.022 |
| C(4)-C(25)-C(1) | 112.651 | Co(23)-N(12)-C(18) | 109.086 |
| H(45)-O(24)-C(14) | 108.387 | H(35)-C(10)-H(34) | 107.568 |
| O(5)-Co(23)-O(17) | 87.77 | H(35)-C(10)-O(20) | 110.767 |
| O(5)-Co(23)-O(20) | 92.259 | H(35)-C(10)-C(3) | 109.219 |
| O(5)-Co(23)-N(12) | 98.292 | H(34)-C(10)-O(20) | 109.095 |
| O(5)-Co(23)-O(7) | 179.527 | H(34)-C(10)-C(3) | 111.862 |
| O(5)-Co(23)-N(8) | 81.273 | O(20)-C(10)-C(3) | 108.343 |
| O(17)-Co(23)-O(20) | 179.947 | H(33)-C(9)-H(32) | 110.727 |
| O(17)-Co(23)-N(12) | 83.456 | H(33)-C(9)-N(8) | 110.493 |
| O(17)-Co(23)-O(7) | 91.909 | H(33)-C(9)-C(13) | 104.184 |
| O(17)-Co(23)-N(8) | 96.809 | H(32)-C(9)-N(8) | 115.17 |
| O(20)-Co(23)-N(12) | 96.495 | H(32)-C(9)-C(13) | 110.798 |
| O(20)-Co(23)-O(7) | 88.062 | N(8)-C(9)-C(13) | 104.757 |
| O(20)-Co(23)-N(8) | 83.24 | C(9)-N(8)-Co(23) | 109.765 |
| N(12)-Co(23)-O(7) | 81.323 | C(9)-N(8)-C(3) | 120.854 |
| N(12)-Co(23)-N(8) | 179.477 | Co(23)-N(8)-C(3) | 115.672 |
| O(7)-Co(23)-N(8) | 99.113 | Co(23)-O(7)-C(19) | 112.972 |
| H(44)-O(22)-C(16) | 107.825 | H(31)-C(6)-H(30) | 109.454 |
| H(43)-O(21)-C(6) | 108.192 | H(31)-C(6)-C(3) | 108.693 |
| C(10)-O(20)-Co(23) | 109.693 | H(31)-C(6)-O(21) | 106.532 |
| O(2)-C(19)-C(18) | 120.261 | H(30)-C(6)-C(3) | 108.367 |
| O(2)-C(19)-O(7) | 126.168 | H(30)-C(6)-O(21) | 111.73 |
| C(18)-C(19)-O(7) | 113.567 | C(3)-C(6)-O(21) | 111.997 |
| H(42)-C(18)-H(41) | 110.346 | Co(23)-O(5)-C(13) | 112.675 |
| H(42)-C(18)-N(12) | 115.746 | H(29)-C(4)-H(28) | 107.531 |
| H(42)-C(18)-C(19) | 111.639 | H(29)-C(4)-C(25) | 109.138 |
| H(41)-C(18)-N(12) | 110.155 | H(29)-C(4)-O(17) | 110.963 |
| H(41)-C(18)-C(19) | 103.868 | H(28)-C(4)-C(25) | 111.856 |
| N(12)-C(18)-C(19) | 104.3 | H(28)-C(4)-O(17) | 108.992 |
| Co(23)-O(17)-C(4) | 110.067 | C(25)-C(4)-O(17) | 108.379 |
| H(40)-C(16)-H(39) | 108.916 | C(16)-C(3)-C(6) | 109.354 |
| H(40)-C(16)-C(3) | 105.212 | C(16)-C(3)-C(10) | 107.013 |
| H(40)-C(16)-O(22) | 110.651 | C(16)-C(3)-N(8) | 114.415 |
| H(39)-C(16)-C(3) | 108.216 | C(6)-C(3)-C(10) | 112.661 |
| H(39)-C(16)-O(22) | 107.411 | C(6)-C(3)-N(8) | 109.332 |
| C(3)-C(16)-O(22) | 116.252 | C(10)-C(3)-N(8) | 104.042 |
| H(38)-O(15)-C(1) | 106.659 | H(27)-C(1)-H(26) | 109.068 |

Table S3: Bond lengths (Å) of [Co(tric)2Cl2].2H2O using DFT-method from DMOL3calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length | Bond | Length |
| O(27)-H(49) | 0.973 | C(20)-C(16) | 1.642 |
| C(24)-H(48) | 1.096 | O(2)-C(25) | 1.305 |
| C(24)-H(47) | 1.094 | C(13)-C(10) | 1.575 |
| C(23)-H(46) | 1.096 | C(6)-O(15) | 1.427 |
| C(23)-H(45) | 1.098 | N(11)-Co(17) | 2.004 |
| O(21)-H(44) | 0.973 | O(26)-C(20) | 1.281 |
| O(19)-H(43) | 0.983 | N(11)-C(7) | 1.442 |
| C(16)-H(42) | 1.091 | C(10)-O(27) | 1.439 |
| C(16)-H(41) | 1.116 | Co(17)-Cl(5) | 2.313 |
| O(15)-H(40) | 0.977 | N(18)-C(12) | 1.433 |
| O(14)-H(39) | 0.973 | C(12)-C(24) | 1.684 |
| C(10)-H(38) | 1.099 | C(24)-O(19) | 1.391 |
| C(10)-H(37) | 1.094 | C(13)-C(6) | 1.597 |
| C(9)-H(36) | 1.099 | N(11)-C(13) | 1.471 |
| C(9)-H(35) | 1.101 | C(25)-C(7) | 1.549 |
| C(7)-H(34) | 1.109 | C(9)-O(21) | 1.431 |
| C(7)-H(33) | 1.095 | C(12)-C(9) | 1.566 |
| C(6)-H(32) | 1.097 | C(20)-O(3) | 1.227 |
| C(6)-H(31) | 1.1 | C(12)-C(4) | 1.546 |
| C(4)-H(30) | 1.099 | C(25)-O(8) | 1.238 |
| C(4)-H(29) | 1.093 | C(13)-C(23) | 1.557 |
| O(1)-H(28) | 0.972 | Co(17)-Cl(22) | 2.304 |
| N(18)-Co(17) | 2.096 | C(16)-N(18) | 1.391 |
| O(26)-Co(17) | 1.975 | C(4)-O(14) | 1.444 |
| O(2)-Co(17) | 1.941 | C(23)-O(1) | 1.426 |

Table S4: Bond angles (°) of [Co(tric)2Cl2].2H2O using DFT-method from DMOL3calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Angle | Bond | Angle |
| H(49)-O(27)-C(10) | 107.405 | C(10)-C(13)-N(11) | 107.333 |
| Co(17)-O(26)-C(20) | 114.468 | C(10)-C(13)-C(23) | 110.705 |
| O(2)-C(25)-C(7) | 114.852 | C(6)-C(13)-N(11) | 112.178 |
| O(2)-C(25)-O(8) | 124.412 | C(6)-C(13)-C(23) | 103.403 |
| C(7)-C(25)-O(8) | 120.72 | N(11)-C(13)-C(23) | 114.405 |
| H(48)-C(24)-H(47) | 112.377 | N(18)-C(12)-C(24) | 106.009 |
| H(48)-C(24)-C(12) | 103.962 | N(18)-C(12)-C(9) | 115.038 |
| H(48)-C(24)-O(19) | 114.014 | N(18)-C(12)-C(4) | 112.236 |
| H(47)-C(24)-C(12) | 106.823 | C(24)-C(12)-C(9) | 104.343 |
| H(47)-C(24)-O(19) | 107.81 | C(24)-C(12)-C(4) | 107.85 |
| C(12)-C(24)-O(19) | 111.648 | C(9)-C(12)-C(4) | 110.693 |
| H(46)-C(23)-H(45) | 108.91 | Co(17)-N(11)-C(7) | 105.713 |
| H(46)-C(23)-C(13) | 107.941 | Co(17)-N(11)-C(13) | 137.971 |
| H(46)-C(23)-O(1) | 106.774 | C(7)-N(11)-C(13) | 116.09 |
| H(45)-C(23)-C(13) | 106.233 | H(38)-C(10)-H(37) | 108.87 |
| H(45)-C(23)-O(1) | 110.318 | H(38)-C(10)-C(13) | 108.941 |
| C(13)-C(23)-O(1) | 116.48 | H(38)-C(10)-O(27) | 109.943 |
| H(44)-O(21)-C(9) | 106.118 | H(37)-C(10)-C(13) | 109.487 |
| C(16)-C(20)-O(26) | 112.841 | H(37)-C(10)-O(27) | 110.726 |
| C(16)-C(20)-O(3) | 116.544 | C(13)-C(10)-O(27) | 108.847 |
| O(26)-C(20)-O(3) | 130.612 | H(36)-C(9)-H(35) | 107.241 |
| H(43)-O(19)-C(24) | 106.149 | H(36)-C(9)-O(21) | 111.301 |
| Co(17)-N(18)-C(12) | 137.244 | H(36)-C(9)-C(12) | 111.395 |
| Co(17)-N(18)-C(16) | 102.656 | H(35)-C(9)-O(21) | 110.969 |
| C(12)-N(18)-C(16) | 116.821 | H(35)-C(9)-C(12) | 105.469 |
| N(18)-Co(17)-O(26) | 80.109 | O(21)-C(9)-C(12) | 110.278 |
| N(18)-Co(17)-O(2) | 166.821 | H(34)-C(7)-H(33) | 107.953 |
| N(18)-Co(17)-N(11) | 110.215 | H(34)-C(7)-N(11) | 109.124 |
| N(18)-Co(17)-Cl(5) | 95.382 | H(34)-C(7)-C(25) | 103.551 |
| N(18)-Co(17)-Cl(22) | 90.897 | H(33)-C(7)-N(11) | 114.731 |
| O(26)-Co(17)-O(2) | 86.741 | H(33)-C(7)-C(25) | 112.312 |
| O(26)-Co(17)-N(11) | 169.61 | N(11)-C(7)-C(25) | 108.542 |
| O(26)-Co(17)-Cl(5) | 88.278 | H(32)-C(6)-H(31) | 108.079 |
| O(26)-Co(17)-Cl(22) | 88.107 | H(32)-C(6)-O(15) | 106.974 |
| O(2)-Co(17)-N(11) | 82.951 | H(32)-C(6)-C(13) | 108.727 |
| O(2)-Co(17)-Cl(5) | 85.039 | H(31)-C(6)-O(15) | 109.802 |
| O(2)-Co(17)-Cl(22) | 87.761 | H(31)-C(6)-C(13) | 105.967 |
| N(11)-Co(17)-Cl(5) | 89.532 | O(15)-C(6)-C(13) | 117.015 |
| N(11)-Co(17)-Cl(22) | 92.776 | H(30)-C(4)-H(29) | 110.16 |
| Cl(5)-Co(17)-Cl(22) | 172.115 | H(30)-C(4)-C(12) | 107.422 |
| H(42)-C(16)-H(41) | 113.087 | H(30)-C(4)-O(14) | 109.196 |
| H(42)-C(16)-C(20) | 110.527 | H(29)-C(4)-C(12) | 109.798 |
| H(42)-C(16)-N(18) | 118.296 | H(29)-C(4)-O(14) | 110.485 |
| H(41)-C(16)-N(18) | 109.176 | Co(17)-O(2)-C(25) | 113.811 |

Table S5: Bond lengths (Å) of [Cu(tric)2]Cl2.3H2O using DFT-method from DMOL3calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length(Å) | Bond | Length(Å) |
| O(24)-H(45) | 0.97 | C(4)-C(7) | 1.589 |
| O(23)-H(44) | 0.972 | C(4)-C(11) | 1.549 |
| C(21)-H(43) | 1.105 | C(11)-O(6) | 1.406 |
| C(21)-H(42) | 1.108 | N(19)-C(4) | 1.461 |
| O(18)-H(41) | 1 | C(16)-O(2) | 1.255 |
| C(17)-H(40) | 1.11 | O(3)-Cu(22) | 2.237 |
| C(17)-H(39) | 1.102 | C(20)-C(9) | 1.542 |
| C(15)-H(38) | 1.103 | N(19)-Cu(22) | 1.918 |
| C(15)-H(37) | 1.105 | C(20)-C(17) | 1.614 |
| C(12)-H(36) | 1.097 | C(21)-N(14) | 1.435 |
| C(12)-H(35) | 1.101 | C(1)-O(18) | 1.346 |
| C(11)-H(34) | 1.106 | C(16)-C(21) | 1.544 |
| C(11)-H(33) | 1.102 | C(13)-O(25) | 1.236 |
| C(9)-H(32) | 1.099 | O(6)-Cu(22) | 1.913 |
| C(9)-H(31) | 1.102 | C(20)-C(1) | 1.792 |
| C(7)-H(30) | 1.096 | C(13)-C(15) | 1.544 |
| C(7)-H(29) | 1.1 | O(10)-Cu(22) | 2.015 |
| O(5)-H(28) | 0.971 | N(14)-C(20) | 1.352 |
| C(1)-H(27) | 1.097 | O(10)-C(13) | 1.321 |
| C(1)-H(26) | 1.093 | O(8)-Cu(22) | 2.154 |
| N(14)-Cu(22) | 2 | C(12)-O(24) | 1.435 |
| C(15)-N(19) | 1.452 | C(17)-O(8) | 1.349 |
| C(4)-C(12) | 1.571 | O(3)-C(16) | 1.281 |
| C(9)-O(5) | 1.43 | C(7)-O(23) | 1.421 |

Table S6:Bond angles (°) of [Cu(tric)2]Cl2.3H2O using DFT-method from DMOL3calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Angle | Degree(°) | Angle | Degree(°) | Angle | Degree(°) |
| H(45)-O(24)-C(12) | 107.274 | C(15)-N(19)-Cu(22) | 110.1 | H(34)-C(11)-H(33) | 108.38 |
| H(44)-O(23)-C(7) | 107.774 | C(4)-N(19)-Cu(22) | 111.597 | H(34)-C(11)-C(4) | 111.689 |
| N(14)-Cu(22)-O(3) | 78.439 | H(41)-O(18)-C(1) | 111.206 | H(34)-C(11)-O(6) | 107.303 |
| N(14)-Cu(22)-N(19) | 175.925 | H(40)-C(17)-H(39) | 108.797 | H(33)-C(11)-C(4) | 108.087 |
| N(14)-Cu(22)-O(6) | 93.485 | H(40)-C(17)-C(20) | 101.092 | H(33)-C(11)-O(6) | 111.947 |
| N(14)-Cu(22)-O(10) | 96.349 | H(40)-C(17)-O(8) | 113.132 | C(4)-C(11)-O(6) | 109.468 |
| N(14)-Cu(22)-O(8) | 80.029 | H(39)-C(17)-C(20) | 109.548 | Cu(22)-O(10)-C(13) | 111.882 |
| O(3)-Cu(22)-N(19) | 97.519 | H(39)-C(17)-O(8) | 111.415 | H(32)-C(9)-H(31) | 107.672 |
| O(3)-Cu(22)-O(6) | 92.302 | C(20)-C(17)-O(8) | 112.35 | H(32)-C(9)-O(5) | 111.276 |
| O(3)-Cu(22)-O(10) | 93.608 | O(2)-C(16)-C(21) | 118.132 | H(32)-C(9)-C(20) | 110.103 |
| O(3)-Cu(22)-O(8) | 158.415 | O(2)-C(16)-O(3) | 124.633 | H(31)-C(9)-O(5) | 111.469 |
| N(19)-Cu(22)-O(6) | 86.114 | C(21)-C(16)-O(3) | 117.235 | H(31)-C(9)-C(20) | 108.167 |
| N(19)-Cu(22)-O(10) | 84.361 | H(38)-C(15)-H(37) | 105.805 | O(5)-C(9)-C(20) | 108.113 |
| N(19)-Cu(22)-O(8) | 104.025 | H(38)-C(15)-N(19) | 109.831 | Cu(22)-O(8)-C(17) | 108.833 |
| O(6)-Cu(22)-O(10) | 169.371 | H(38)-C(15)-C(13) | 108.583 | H(30)-C(7)-H(29) | 108.813 |
| O(6)-Cu(22)-O(8) | 90.486 | H(37)-C(15)-N(19) | 114.864 | H(30)-C(7)-C(4) | 106.806 |
| O(10)-Cu(22)-O(8) | 87.262 | H(37)-C(15)-C(13) | 107.054 | H(30)-C(7)-O(23) | 106.545 |
| H(43)-C(21)-H(42) | 105.57 | N(19)-C(15)-C(13) | 110.439 | H(29)-C(7)-C(4) | 108.822 |
| H(43)-C(21)-N(14) | 111.465 | Cu(22)-N(14)-C(21) | 117.306 | H(29)-C(7)-O(23) | 111.922 |
| H(43)-C(21)-C(16) | 108.736 | Cu(22)-N(14)-C(20) | 118.651 | C(4)-C(7)-O(23) | 113.689 |
| H(42)-C(21)-N(14) | 110.122 | C(21)-N(14)-C(20) | 123.932 | C(11)-O(6)-Cu(22) | 107.119 |
| H(42)-C(21)-C(16) | 108.257 | O(25)-C(13)-C(15) | 122.404 | H(28)-O(5)-C(9) | 106.737 |
| N(14)-C(21)-C(16) | 112.413 | O(25)-C(13)-O(10) | 122.064 | C(12)-C(4)-C(7) | 107.444 |
| C(9)-C(20)-C(17) | 117.697 | C(15)-C(13)-O(10) | 115.263 | C(12)-C(4)-C(11) | 111.465 |
| C(9)-C(20)-C(1) | 104.649 | H(36)-C(12)-H(35) | 109.266 | C(12)-C(4)-N(19) | 113.885 |
| C(9)-C(20)-N(14) | 117.588 | H(36)-C(12)-C(4) | 107.815 | C(7)-C(4)-C(11) | 112.783 |
| C(17)-C(20)-C(1) | 100.397 | H(36)-C(12)-O(24) | 111.273 | C(7)-C(4)-N(19) | 109.955 |
| C(17)-C(20)-N(14) | 107.407 | H(35)-C(12)-C(4) | 108.883 | C(11)-C(4)-N(19) | 101.363 |
| C(1)-C(20)-N(14) | 107.126 | H(35)-C(12)-O(24) | 109.003 | Cu(22)-O(3)-C(16) | 113.028 |
| C(15)-N(19)-C(4) | 121.272 | C(4)-C(12)-O(24) | 110.558 | H(27)-C(1)-H(26) | 114.644 |

Table S7: Bond lengths (Å) of [Ni(tric-H)2].2H2O using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond | Length | Bond | Length | Bond | Length |
| C(25)-H(45) | 1.104 | C(18)-O(12) | 1.238 | C(7)-O(11) | 1.419 |
| C(25)-H(44) | 1.106 | O(11)-H(37) | 0.973 | O(6)-H(32) | 0.973 |
| C(24)-H(43) | 1.102 | C(10)-H(36) | 1.104 | C(24)-O(6) | 1.437 |
| C(24)-H(42) | 1.104 | C(10)-H(35) | 1.103 | O(5)-H(31) | 0.973 |
| C(23)-H(41) | 1.097 | C(22)-C(10) | 1.571 | C(4)-H(30) | 1.104 |
| C(23)-H(40) | 1.102 | C(10)-O(19) | 1.411 | C(4)-H(29) | 1.105 |
| C(22)-C(24) | 1.55 | O(19)-Ni(9) | 1.899 | C(18)-C(4) | 1.537 |
| C(20)-H(39) | 1.103 | Ni(9)-O(15) | 1.939 | C(3)-H(28) | 1.097 |
| C(20)-H(38) | 1.103 | Ni(9)-O(14) | 1.947 | C(3)-H(27) | 1.098 |
| C(17)-C(23) | 1.576 | O(13)-Ni(9) | 1.899 | C(17)-C(3) | 1.592 |
| C(17)-C(20) | 1.561 | C(25)-N(8) | 1.437 | C(3)-O(5) | 1.432 |
| C(16)-C(25) | 1.539 | N(8)-C(17) | 1.436 | O(2)-H(26) | 0.976 |
| C(16)-O(21) | 1.239 | N(8)-Ni(9) | 1.874 | C(23)-O(2) | 1.428 |
| O(15)-C(18) | 1.319 | C(7)-H(34) | 1.096 | N(1)-C(22) | 1.431 |
| O(14)-C(16) | 1.317 | C(7)-H(33) | 1.095 | N(1)-Ni(9) | 1.877 |
| C(20)-O(13) | 1.417 | C(22)-C(7) | 1.605 | C(4)-N(1) | 1.435 |

Table S8: Bond angles (°) of [Ni(tric-H)2].2H2O using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Angle | Degree | Angle | Degree | Angle | Degree |
| H(45)-C(25)-H(44) | 106.078 | O(15)-C(18)-O(12) | 122.523 | O(14)-Ni(9)-O(13) | 170.012 |
| H(45)-C(25)-C(16) | 110.388 | O(15)-C(18)-C(4) | 115.719 | O(14)-Ni(9)-N(8) | 85.38 |
| H(45)-C(25)-N(8) | 111.829 | O(12)-C(18)-C(4) | 121.747 | O(14)-Ni(9)-N(1) | 97.127 |
| H(44)-C(25)-C(16) | 108.129 | C(23)-C(17)-C(20) | 113.246 | O(13)-Ni(9)-N(8) | 84.937 |
| H(44)-C(25)-N(8) | 111.52 | C(23)-C(17)-N(8) | 111.372 | O(13)-Ni(9)-N(1) | 92.617 |
| C(16)-C(25)-N(8) | 108.822 | C(23)-C(17)-C(3) | 110.154 | N(8)-Ni(9)-N(1) | 177.092 |
| H(43)-C(24)-H(42) | 108.521 | C(20)-C(17)-N(8) | 103.735 | C(25)-N(8)-C(17) | 127.617 |
| H(43)-C(24)-C(22) | 108.368 | C(20)-C(17)-C(3) | 110.196 | C(25)-N(8)-Ni(9) | 115.602 |
| H(43)-C(24)-O(6) | 111.05 | N(8)-C(17)-C(3) | 107.857 | C(17)-N(8)-Ni(9) | 116.766 |
| H(42)-C(24)-C(22) | 109.735 | C(25)-C(16)-O(21) | 121.177 | H(34)-C(7)-H(33) | 110.749 |
| H(42)-C(24)-O(6) | 110.986 | C(25)-C(16)-O(14) | 116.131 | H(34)-C(7)-C(22) | 105.102 |
| C(22)-C(24)-O(6) | 108.139 | O(21)-C(16)-O(14) | 122.673 | H(34)-C(7)-O(11) | 107.322 |
| H(41)-C(23)-H(40) | 108.869 | C(18)-O(15)-Ni(9) | 114.23 | H(33)-C(7)-C(22) | 107.512 |
| H(41)-C(23)-C(17) | 108.725 | C(16)-O(14)-Ni(9) | 113.813 | H(33)-C(7)-O(11) | 112.233 |
| H(41)-C(23)-O(2) | 106.099 | C(20)-O(13)-Ni(9) | 107.8 | C(22)-C(7)-O(11) | 113.708 |
| H(40)-C(23)-C(17) | 109.335 | H(37)-O(11)-C(7) | 108.133 | H(32)-O(6)-C(24) | 106.179 |
| H(40)-C(23)-O(2) | 111.508 | H(36)-C(10)-H(35) | 108.598 | H(31)-O(5)-C(3) | 107.69 |
| C(17)-C(23)-O(2) | 112.178 | H(36)-C(10)-C(22) | 106.778 | H(30)-C(4)-H(29) | 105.999 |
| C(24)-C(22)-C(10) | 113.585 | H(36)-C(10)-O(19) | 112.462 | H(30)-C(4)-C(18) | 110.742 |
| C(24)-C(22)-C(7) | 110.584 | H(35)-C(10)-C(22) | 111.299 | H(30)-C(4)-N(1) | 111.311 |
| C(24)-C(22)-N(1) | 111.586 | H(35)-C(10)-O(19) | 107.506 | H(29)-C(4)-C(18) | 108.261 |
| C(10)-C(22)-C(7) | 107.101 | C(22)-C(10)-O(19) | 110.234 | H(29)-C(4)-N(1) | 111.521 |
| C(10)-C(22)-N(1) | 103.851 | O(19)-Ni(9)-O(15) | 170.481 | C(18)-C(4)-N(1) | 108.951 |
| C(7)-C(22)-N(1) | 109.838 | O(19)-Ni(9)-O(14) | 89.985 | H(28)-C(3)-C(17) | 107.203 |
| H(39)-C(20)-H(38) | 108.3 | O(19)-Ni(9)-O(13) | 92.957 | H(28)-C(3)-O(5) | 109.105 |
| H(39)-C(20)-C(17) | 108.177 | O(19)-Ni(9)-N(8) | 92.979 | H(27)-C(3)-C(17) | 109.098 |
| H(39)-C(20)-O(13) | 112.476 | O(19)-Ni(9)-N(1) | 85.566 | H(27)-C(3)-O(5) | 110.499 |
| H(38)-C(20)-C(17) | 111.363 | O(15)-Ni(9)-O(14) | 88.595 | C(17)-C(3)-O(5) | 110.793 |
| H(38)-C(20)-O(13) | 106.951 | O(15)-Ni(9)-O(13) | 90.035 | H(26)-O(2)-C(23) | 106.758 |
| C(17)-C(20)-O(13) | 109.602 | O(15)-Ni(9)-N(8) | 96.286 | C(22)-N(1)-Ni(9) | 116.441 |
| C(10)-O(19)-Ni(9) | 107.7 | O(15)-Ni(9)-N(1) | 85.273 | Ni(9)-N(1)-C(4) | 115.379 |

Table S9: Bond lengths (Å) of [Ni(tric)2Cl2].3H2O using DFT-method from DMOL3calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
| C(23)-H(49) | 1.091 | C(17)-H(43) | 1.096 | C(10)-H(34) | 1.098 |
| C(23)-H(48) | 1.105 | C(26)-C(17) | 1.567 | C(26)-C(10) | 1.668 |
| C(23)-N(27) | 1.439 | O(16)-H(42) | 0.984 | C(9)-H(33) | 1.093 |
| N(27)-Ni(22) | 2.212 | C(17)-O(16) | 1.424 | C(9)-H(32) | 1.099 |
| Ni(22)-Cl(25) | 2.274 | C(15)-H(41) | 1.096 | C(9)-O(20) | 1.407 |
| Ni(22)-O(24) | 1.921 | C(15)-H(40) | 1.092 | O(8)-H(31) | 0.984 |
| N(21)-C(26) | 1.414 | C(14)-H(39) | 1.102 | C(10)-O(8) | 1.396 |
| N(21)-Ni(22) | 2.029 | C(14)-H(38) | 1.107 | C(7)-C(14) | 1.523 |
| O(20)-H(47) | 0.974 | N(21)-C(14) | 1.45 | C(7)-O(13) | 1.244 |
| C(18)-H(46) | 1.095 | C(12)-H(37) | 1.095 | O(11)-C(7) | 1.302 |
| C(18)-H(45) | 1.098 | C(12)-H(36) | 1.103 | N(27)-C(6) | 1.445 |
| C(26)-C(18) | 1.603 | O(11)-Ni(22) | 1.977 | C(6)-C(15) | 1.569 |
| C(17)-H(44) | 1.092 | C(10)-H(35) | 1.091 | C(6)-C(12) | 1.604 |
| O(5)-H(30) | 0.982 | C(18)-O(4) | 1.417 | C(2)-C(23) | 1.564 |
| C(12)-O(5) | 1.417 | O(3)-H(28) | 0.972 | C(2)-O(19) | 1.234 |
| O(4)-H(29) | 0.975 | C(15)-O(3) | 1.443 | Ni(22)-Cl(1) | 2.311 |

Table S10: Bond angles (°) of [Ni(tric)2Cl2].3H2O using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Angle | Degree | Angle | Degree | Angle | Degree |
| C(23)-N(27)-Ni(22) | 100.293 | C(26)-N(21)-Ni(22) | 132.462 | H(37)-C(12)-O(5) | 106.261 |
| C(23)-N(27)-C(6) | 113.297 | C(26)-N(21)-C(14) | 116.669 | H(36)-C(12)-C(6) | 105.772 |
| Ni(22)-N(27)-C(6) | 135.498 | Ni(22)-N(21)-C(14) | 110.654 | H(36)-C(12)-O(5) | 111.409 |
| N(21)-C(26)-C(18) | 114.406 | H(47)-O(20)-C(9) | 108.477 | C(6)-C(12)-O(5) | 114.993 |
| N(21)-C(26)-C(17) | 112.409 | H(46)-C(18)-H(45) | 109.721 | Ni(22)-O(11)-C(7) | 116.593 |
| N(21)-C(26)-C(10) | 104.148 | H(46)-C(18)-C(26) | 107.848 | H(35)-C(10)-H(34) | 110.533 |
| C(18)-C(26)-C(17) | 109.467 | H(46)-C(18)-O(4) | 106.725 | H(35)-C(10)-C(26) | 107.312 |
| C(18)-C(26)-C(10) | 105.459 | H(45)-C(18)-C(26) | 109.114 | H(35)-C(10)-O(8) | 112.278 |
| C(17)-C(26)-C(10) | 110.583 | H(45)-C(18)-O(4) | 110.762 | H(34)-C(10)-C(26) | 104.002 |
| Ni(22)-O(24)-C(2) | 116.955 | C(26)-C(18)-O(4) | 112.582 | H(34)-C(10)-O(8) | 108.839 |
| H(49)-C(23)-H(48) | 110.274 | H(44)-C(17)-H(43) | 109.543 | C(26)-C(10)-O(8) | 113.566 |
| H(49)-C(23)-N(27) | 114.461 | H(44)-C(17)-C(26) | 108.611 | H(33)-C(9)-H(32) | 110.769 |
| H(49)-C(23)-C(2) | 107.92 | H(44)-C(17)-O(16) | 106.552 | H(33)-C(9)-O(20) | 112.044 |
| H(48)-C(23)-N(27) | 109.04 | H(43)-C(17)-C(26) | 108.653 | H(33)-C(9)-C(6) | 105.975 |
| H(48)-C(23)-C(2) | 102.622 | H(43)-C(17)-O(16) | 111.259 | H(32)-C(9)-O(20) | 107.163 |
| N(27)-C(23)-C(2) | 111.876 | C(26)-C(17)-O(16) | 112.156 | H(32)-C(9)-C(6) | 102.934 |
| N(27)-Ni(22)-Cl(25) | 90.02 | H(42)-O(16)-C(17) | 106.233 | O(20)-C(9)-C(6) | 117.568 |
| N(27)-Ni(22)-O(24) | 82.391 | H(41)-C(15)-H(40) | 108.233 | H(31)-O(8)-C(10) | 105.394 |
| N(27)-Ni(22)-N(21) | 110.6 | H(41)-C(15)-C(6) | 107.566 | C(14)-C(7)-O(13) | 121.377 |
| N(27)-Ni(22)-O(11) | 166.107 | H(41)-C(15)-O(3) | 108.663 | C(14)-C(7)-O(11) | 115.91 |
| N(27)-Ni(22)-Cl(1) | 94.292 | H(40)-C(15)-C(6) | 108.697 | O(13)-C(7)-O(11) | 122.713 |
| Cl(25)-Ni(22)-O(24) | 92.094 | H(40)-C(15)-O(3) | 107.714 | N(27)-C(6)-C(15) | 116.458 |
| Cl(25)-Ni(22)-N(21) | 96.049 | C(6)-C(15)-O(3) | 115.758 | N(27)-C(6)-C(12) | 113.948 |
| Cl(25)-Ni(22)-O(11) | 86.77 | H(39)-C(14)-H(38) | 106.277 | N(27)-C(6)-C(9) | 109.045 |
| Cl(25)-Ni(22)-Cl(1) | 175.63 | H(39)-C(14)-N(21) | 111.722 | C(15)-C(6)-C(12) | 108.332 |
| O(24)-Ni(22)-N(21) | 164.584 | H(39)-C(14)-C(7) | 108.396 | C(15)-C(6)-C(9) | 102.782 |
| O(24)-Ni(22)-O(11) | 84.221 | H(38)-C(14)-N(21) | 110.417 | C(12)-C(6)-C(9) | 105.107 |
| O(24)-Ni(22)-Cl(1) | 89.189 | H(38)-C(14)-C(7) | 107.161 | H(30)-O(5)-C(12) | 108.974 |
| N(21)-Ni(22)-O(11) | 83.196 | N(21)-C(14)-C(7) | 112.568 | H(29)-O(4)-C(18) | 108.188 |
| N(21)-Ni(22)-Cl(1) | 81.773 | H(37)-C(12)-H(36) | 108.017 | H(28)-O(3)-C(15) | 108.048 |
| O(11)-Ni(22)-Cl(1) | 89.204 | H(37)-C(12)-C(6) | 110.251 | O(24)-C(2)-C(23) | 114.814 |
| C(23)-N(27)-Ni(22) | 100.293 | C(26)-N(21)-Ni(22) | 132.462 | H(37)-C(12)-O(5) | 106.261 |
| C(23)-N(27)-C(6) | 113.297 | C(26)-N(21)-C(14) | 116.669 | H(36)-C(12)-C(6) | 105.772 |
| Ni(22)-N(27)-C(6) | 135.498 | Ni(22)-N(21)-C(14) | 110.654 | H(36)-C(12)-O(5) | 111.409 |
| N(21)-C(26)-C(18) | 114.406 | H(47)-O(20)-C(9) | 108.477 | C(6)-C(12)-O(5) | 114.993 |
| N(21)-C(26)-C(17) | 112.409 | H(46)-C(18)-H(45) | 109.721 | Ni(22)-O(11)-C(7) | 116.593 |
| N(21)-C(26)-C(10) | 104.148 | H(46)-C(18)-C(26) | 107.848 | H(35)-C(10)-H(34) | 110.533 |
| C(18)-C(26)-C(17) | 109.467 | H(46)-C(18)-O(4) | 106.725 | H(35)-C(10)-C(26) | 107.312 |
| C(18)-C(26)-C(10) | 105.459 | H(45)-C(18)-C(26) | 109.114 | H(35)-C(10)-O(8) | 112.278 |
| C(17)-C(26)-C(10) | 110.583 | H(45)-C(18)-O(4) | 110.762 | H(34)-C(10)-C(26) | 104.002 |
| Ni(22)-O(24)-C(2) | 116.955 | C(26)-C(18)-O(4) | 112.582 | H(34)-C(10)-O(8) | 108.839 |
| H(49)-C(23)-H(48) | 110.274 | H(44)-C(17)-H(43) | 109.543 | C(26)-C(10)-O(8) | 113.566 |
| H(49)-C(23)-N(27) | 114.461 | H(44)-C(17)-C(26) | 108.611 | H(33)-C(9)-H(32) | 110.769 |
| H(49)-C(23)-C(2) | 107.92 | H(44)-C(17)-O(16) | 106.552 | H(33)-C(9)-O(20) | 112.044 |
| H(48)-C(23)-N(27) | 109.04 | H(43)-C(17)-C(26) | 108.653 | H(33)-C(9)-C(6) | 105.975 |
| H(48)-C(23)-C(2) | 102.622 | H(43)-C(17)-O(16) | 111.259 | H(32)-C(9)-O(20) | 107.163 |
| N(27)-C(23)-C(2) | 111.876 | C(26)-C(17)-O(16) | 112.156 | H(32)-C(9)-C(6) | 102.934 |
| N(27)-Ni(22)-Cl(25) | 90.02 | H(42)-O(16)-C(17) | 106.233 | O(20)-C(9)-C(6) | 117.568 |
| N(27)-Ni(22)-O(24) | 82.391 | H(41)-C(15)-H(40) | 108.233 | H(31)-O(8)-C(10) | 105.394 |
| N(27)-Ni(22)-N(21) | 110.6 | H(41)-C(15)-C(6) | 107.566 | C(14)-C(7)-O(13) | 121.377 |
| N(27)-Ni(22)-O(11) | 166.107 | H(41)-C(15)-O(3) | 108.663 | C(14)-C(7)-O(11) | 115.91 |
| N(27)-Ni(22)-Cl(1) | 94.292 | H(40)-C(15)-C(6) | 108.697 | O(13)-C(7)-O(11) | 122.713 |
| Cl(25)-Ni(22)-O(24) | 92.094 | H(40)-C(15)-O(3) | 107.714 | N(27)-C(6)-C(15) | 116.458 |
| Cl(25)-Ni(22)-N(21) | 96.049 | C(6)-C(15)-O(3) | 115.758 | N(27)-C(6)-C(12) | 113.948 |
| Cl(25)-Ni(22)-O(11) | 86.77 | H(39)-C(14)-H(38) | 106.277 | N(27)-C(6)-C(9) | 109.045 |
| Cl(25)-Ni(22)-Cl(1) | 175.63 | H(39)-C(14)-N(21) | 111.722 | C(15)-C(6)-C(12) | 108.332 |
| O(24)-Ni(22)-N(21) | 164.584 | H(39)-C(14)-C(7) | 108.396 | C(15)-C(6)-C(9) | 102.782 |
| O(24)-Ni(22)-O(11) | 84.221 | H(38)-C(14)-N(21) | 110.417 | C(12)-C(6)-C(9) | 105.107 |
| O(24)-Ni(22)-Cl(1) | 89.189 | H(38)-C(14)-C(7) | 107.161 | H(30)-O(5)-C(12) | 108.974 |
| N(21)-Ni(22)-O(11) | 83.196 | N(21)-C(14)-C(7) | 112.568 | H(29)-O(4)-C(18) | 108.188 |
| N(21)-Ni(22)-Cl(1) | 81.773 | H(37)-C(12)-H(36) | 108.017 | H(28)-O(3)-C(15) | 108.048 |
| O(11)-Ni(22)-Cl(1) | 89.204 | H(37)-C(12)-C(6) | 110.251 | O(24)-C(2)-C(23) | 114.814 |
| C(23)-N(27)-Ni(22) | 100.293 | C(26)-N(21)-Ni(22) | 132.462 | H(37)-C(12)-O(5) | 106.261 |
| C(23)-N(27)-C(6) | 113.297 | C(26)-N(21)-C(14) | 116.669 | H(36)-C(12)-C(6) | 105.772 |
| Ni(22)-N(27)-C(6) | 135.498 | Ni(22)-N(21)-C(14) | 110.654 | H(36)-C(12)-O(5) | 111.409 |
| N(21)-C(26)-C(18) | 114.406 | H(47)-O(20)-C(9) | 108.477 | C(6)-C(12)-O(5) | 114.993 |
| N(21)-C(26)-C(17) | 112.409 | H(46)-C(18)-H(45) | 109.721 | Ni(22)-O(11)-C(7) | 116.593 |
| N(21)-C(26)-C(10) | 104.148 | H(46)-C(18)-C(26) | 107.848 | H(35)-C(10)-H(34) | 110.533 |
| C(18)-C(26)-C(17) | 109.467 | H(46)-C(18)-O(4) | 106.725 | H(35)-C(10)-C(26) | 107.312 |
| C(18)-C(26)-C(10) | 105.459 | H(45)-C(18)-C(26) | 109.114 | H(35)-C(10)-O(8) | 112.278 |
| C(17)-C(26)-C(10) | 110.583 | H(45)-C(18)-O(4) | 110.762 | H(34)-C(10)-C(26) | 104.002 |
| Ni(22)-O(24)-C(2) | 116.955 | C(26)-C(18)-O(4) | 112.582 | H(34)-C(10)-O(8) | 108.839 |
| H(49)-C(23)-H(48) | 110.274 | H(44)-C(17)-H(43) | 109.543 | C(26)-C(10)-O(8) | 113.566 |
| H(49)-C(23)-N(27) | 114.461 | H(44)-C(17)-C(26) | 108.611 | H(33)-C(9)-H(32) | 110.769 |
| H(49)-C(23)-C(2) | 107.92 | H(44)-C(17)-O(16) | 106.552 | H(33)-C(9)-O(20) | 112.044 |
| H(48)-C(23)-N(27) | 109.04 | H(43)-C(17)-C(26) | 108.653 | H(33)-C(9)-C(6) | 105.975 |
| H(48)-C(23)-C(2) | 102.622 | H(43)-C(17)-O(16) | 111.259 | H(32)-C(9)-O(20) | 107.163 |
| N(27)-C(23)-C(2) | 111.876 | C(26)-C(17)-O(16) | 112.156 | H(32)-C(9)-C(6) | 102.934 |
| N(27)-Ni(22)-Cl(25) | 90.02 | H(42)-O(16)-C(17) | 106.233 | O(20)-C(9)-C(6) | 117.568 |
| N(27)-Ni(22)-O(24) | 82.391 | H(41)-C(15)-H(40) | 108.233 | H(31)-O(8)-C(10) | 105.394 |
| N(27)-Ni(22)-N(21) | 110.6 | H(41)-C(15)-C(6) | 107.566 | C(14)-C(7)-O(13) | 121.377 |

Table S11: Bond lengths (Å) of [Cd(tric)2(Ac)2].H2O using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond | Length(Å) | Bond | Length(Å) | Bond | Length(Å) |
| O(30)-H(61) | 0.972 | C(9)-H(41) | 1.099 | C(7)-C(20) | 1.518 |
| O(28)-H(60) | 0.973 | C(8)-H(40) | 1.094 | C(8)-N(29) | 1.282 |
| C(27)-H(59) | 1.1 | C(8)-H(39) | 1.096 | C(18)-N(31) | 1.283 |
| C(27)-H(58) | 1.101 | C(6)-H(38) | 1.096 | C(14)-C(9) | 1.559 |
| O(25)-H(57) | 0.972 | C(6)-H(37) | 1.099 | C(23)-C(6) | 1.562 |
| C(24)-H(56) | 1.093 | C(3)-H(36) | 1.1 | C(14)-C(24) | 1.563 |
| C(24)-H(55) | 1.098 | C(3)-H(35) | 1.096 | C(5)-C(18) | 3.968 |
| O(21)-H(54) | 0.973 | O(1)-H(34) | 0.973 | O(17)-C(5) | 1.179 |
| C(20)-H(53) | 1.097 | N(31)-C(23) | 1.482 | O(17)-Cd(16) | 4.523 |
| C(20)-H(52) | 1.1 | C(4)-C(8) | 3.654 | C(7)-O(26) | 1.286 |
| C(20)-H(51) | 1.094 | O(2)-C(15) | 1.309 | C(23)-C(19) | 1.552 |
| C(19)-H(50) | 1.1 | O(22)-C(7) | 1.281 | C(4)-O(13) | 1.18 |
| C(19)-H(49) | 1.103 | C(15)-O(32) | 1.255 | C(6)-O(30) | 1.437 |
| C(18)-H(48) | 1.093 | C(15)-C(11) | 1.534 | N(29)-C(14) | 1.496 |
| C(18)-H(47) | 1.094 | C(27)-O(1) | 1.443 | C(23)-C(3) | 1.546 |
| O(12)-H(46) | 0.973 | C(14)-C(27) | 1.544 | C(3)-O(12) | 1.455 |
| C(11)-H(45) | 1.101 | Cd(16)-O(22) | 2.477 | C(5)-O(10) | 1.18 |
| C(11)-H(44) | 1.095 | C(19)-O(21) | 1.443 | C(9)-O(25) | 1.44 |
| C(11)-H(43) | 1.095 | C(24)-O(28) | 1.44 | O(33)-Cd(16) | 4.464 |
| C(9)-H(42) | 1.093 | O(33)-C(4) | 1.179 | Cd(16)-O(2) | 2.238 |

Table S12: Bond angles (°) of [Cd(tric)2(Ac)2].H2O using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Angle | Degree(°) | Angle | Degree(°) | Angle | Degree(°) |
| C(4)-O(33)-Cd(16) | 113.759 | H(50)-C(19)-C(23) | 109.626 | H(45)-C(11)-C(15) | 109.047 |
| C(23)-N(31)-C(18) | 121.443 | H(49)-C(19)-O(21) | 110.608 | H(44)-C(11)-H(43) | 109.057 |
| C(23)-N(31)-Cd(16) | 119.843 | H(49)-C(19)-C(23) | 108.558 | H(44)-C(11)-C(15) | 110.491 |
| C(18)-N(31)-Cd(16) | 118.515 | O(21)-C(19)-C(23) | 109.731 | H(43)-C(11)-C(15) | 112.807 |
| H(61)-O(30)-C(6) | 107.26 | H(48)-C(18)-H(47) | 117.686 | H(42)-C(9)-H(41) | 108.44 |
| C(8)-N(29)-C(14) | 120.095 | H(48)-C(18)-N(31) | 117.655 | H(42)-C(9)-C(14) | 108.634 |
| C(8)-N(29)-Cd(16) | 115.836 | H(48)-C(18)-C(5) | 43.107 | H(42)-C(9)-O(25) | 106.385 |
| C(14)-N(29)-Cd(16) | 123.943 | H(47)-C(18)-N(31) | 124.655 | H(41)-C(9)-C(14) | 108.649 |
| H(60)-O(28)-C(24) | 107.679 | H(47)-C(18)-C(5) | 111.219 | H(41)-C(9)-O(25) | 110.358 |
| H(59)-C(27)-H(58) | 107.753 | N(31)-C(18)-C(5) | 108.865 | C(14)-C(9)-O(25) | 114.209 |
| H(59)-C(27)-O(1) | 110.186 | C(5)-O(17)-Cd(16) | 92.398 | H(40)-C(8)-H(39) | 116.722 |
| H(59)-C(27)-C(14) | 106.619 | O(22)-Cd(16)-O(17) | 56.817 | H(40)-C(8)-C(4) | 56.883 |
| H(58)-C(27)-O(1) | 110.446 | O(22)-Cd(16)-O(33) | 101.785 | H(40)-C(8)-N(29) | 118.729 |
| H(58)-C(27)-C(14) | 109.971 | O(22)-Cd(16)-O(2) | 118.597 | H(39)-C(8)-C(4) | 94.457 |
| O(1)-C(27)-C(14) | 111.72 | O(22)-Cd(16)-N(31) | 81.377 | H(39)-C(8)-N(29) | 124.546 |
| H(57)-O(25)-C(9) | 107.624 | O(22)-Cd(16)-N(29) | 96.115 | C(4)-C(8)-N(29) | 115.756 |
| H(56)-C(24)-H(55) | 107.888 | O(17)-Cd(16)-O(33) | 155.741 | O(22)-C(7)-C(20) | 119.688 |
| H(56)-C(24)-O(28) | 106.194 | O(17)-Cd(16)-O(2) | 61.842 | O(22)-C(7)-O(26) | 122.284 |
| H(56)-C(24)-C(14) | 108.635 | O(17)-Cd(16)-N(31) | 80.146 | C(20)-C(7)-O(26) | 118.008 |
| H(55)-C(24)-O(28) | 110.703 | O(17)-Cd(16)-N(29) | 97.266 | H(38)-C(6)-H(37) | 108.412 |
| H(55)-C(24)-C(14) | 109.349 | O(33)-Cd(16)-O(2) | 136.956 | H(38)-C(6)-C(23) | 109.755 |
| O(28)-C(24)-C(14) | 113.848 | O(33)-Cd(16)-N(31) | 109.899 | H(38)-C(6)-O(30) | 110.638 |
| N(31)-C(23)-C(6) | 109.055 | O(33)-Cd(16)-N(29) | 71.982 | H(37)-C(6)-C(23) | 107.417 |
| N(31)-C(23)-C(19) | 111.41 | O(2)-Cd(16)-N(31) | 91.292 | H(37)-C(6)-O(30) | 107.288 |
| N(31)-C(23)-C(3) | 107.116 | O(2)-Cd(16)-N(29) | 88.622 | C(23)-C(6)-O(30) | 113.146 |
| C(6)-C(23)-C(19) | 111.293 | N(31)-Cd(16)-N(29) | 177.093 | C(18)-C(5)-O(17) | 95.079 |
| C(6)-C(23)-C(3) | 108.693 | O(2)-C(15)-O(32) | 122.115 | C(18)-C(5)-O(10) | 84.745 |
| C(19)-C(23)-C(3) | 109.149 | O(2)-C(15)-C(11) | 119.069 | O(17)-C(5)-O(10) | 179.636 |
| C(7)-O(22)-Cd(16) | 88.125 | O(32)-C(15)-C(11) | 118.773 | C(8)-C(4)-O(33) | 94.068 |
| H(54)-O(21)-C(19) | 106.184 | C(27)-C(14)-C(9) | 107.928 | C(8)-C(4)-O(13) | 85.64 |
| H(53)-C(20)-H(52) | 107.329 | C(27)-C(14)-C(24) | 110.849 | O(33)-C(4)-O(13) | 179.704 |
| H(53)-C(20)-H(51) | 110.297 | C(27)-C(14)-N(29) | 116.495 | H(36)-C(3)-H(35) | 108.885 |
| H(53)-C(20)-C(7) | 110.929 | C(9)-C(14)-C(24) | 109.137 | H(36)-C(3)-C(23) | 109.283 |
| H(52)-C(20)-H(51) | 108.293 | C(9)-C(14)-N(29) | 106.664 | H(36)-C(3)-O(12) | 110.109 |
| H(52)-C(20)-C(7) | 108.513 | C(24)-C(14)-N(29) | 105.533 | H(35)-C(3)-C(23) | 109.842 |
| H(51)-C(20)-C(7) | 111.34 | H(46)-O(12)-C(3) | 106.39 | H(35)-C(3)-O(12) | 109.37 |
| H(50)-C(19)-H(49) | 108.539 | H(50)-C(19)-C(23) | 109.626 | C(23)-C(3)-O(12) | 109.34 |
| H(50)-C(19)-O(21) | 109.752 | H(49)-C(19)-O(21) | 110.608 | C(15)-O(2)-Cd(16) | 131.913 |

Table S13: Bond lengths (Å) of [Zn(tric)2Cl2].EtOH using DFT-method from DMOL3 calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length (Å) | Bond | Length (Å) |
| O(28)-H(52) | 0.974 | C(4)-C(15) | 1.564 |
| O(27)-H(51) | 0.981 | Zn(16)-O(3) | 3.89 |
| C(26)-H(50) | 1.102 | N(10)-C(4) | 1.488 |
| C(26)-H(49) | 1.095 | Zn(16)-Cl(2) | 2.226 |
| O(25)-H(48) | 0.975 | C(9)-C(14) | 3.499 |
| C(24)-H(47) | 1.102 | C(15)-O(27) | 1.436 |
| C(24)-H(46) | 1.099 | C(18)-C(20) | 1.569 |
| C(23)-H(45) | 1.099 | C(18)-C(23) | 1.543 |
| C(23)-H(44) | 1.095 | C(1)-O(28) | 1.444 |
| O(22)-H(43) | 0.978 | C(20)-O(17) | 1.431 |
| C(20)-H(42) | 1.101 | O(8)-C(9) | 1.178 |
| C(20)-H(41) | 1.099 | Zn(16)-N(10) | 3.529 |
| O(19)-H(40) | 0.972 | C(9)-O(11) | 1.179 |
| O(17)-H(39) | 0.973 | N(5)-C(14) | 1.284 |
| C(15)-H(38) | 1.098 | Zn(16)-N(5) | 2.167 |
| C(15)-H(37) | 1.105 | C(4)-C(12) | 1.546 |
| C(14)-H(36) | 1.094 | C(4)-C(26) | 1.552 |
| C(14)-H(35) | 1.095 | O(3)-C(6) | 1.178 |
| C(12)-H(34) | 1.097 | C(6)-C(24) | 3.544 |
| C(12)-H(33) | 1.102 | Zn(16)-Cl(21) | 2.258 |
| C(7)-H(32) | 1.101 | C(6)-O(13) | 1.182 |
| C(7)-H(31) | 1.1 | C(18)-C(7) | 1.557 |
| C(1)-H(30) | 1.098 | C(26)-O(22) | 1.443 |
| C(1)-H(29) | 1.1 | C(12)-O(19) | 1.455 |
| Zn(16)-O(8) | 3.446 | C(23)-O(25) | 1.46 |

Table S14: Bond angles (0) of [Zn(tric)2Cl2].EtOH using DFT-method from DMOL3 calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Angle | Degree (°) | Angle | Degree (°) |
| H(52)-O(28)-C(1) | 106.924 | N(5)-Zn(16)-Cl(21) | 116.42 |
| H(51)-O(27)-C(15) | 104.754 | H(38)-C(15)-H(37) | 108.17 |
| H(50)-C(26)-H(49) | 108.508 | H(38)-C(15)-C(4) | 108.693 |
| H(50)-C(26)-C(4) | 107.79 | H(38)-C(15)-O(27) | 106.9 |
| H(50)-C(26)-O(22) | 110.407 | H(37)-C(15)-C(4) | 107.592 |
| H(49)-C(26)-C(4) | 110.119 | H(37)-C(15)-O(27) | 111.043 |
| H(49)-C(26)-O(22) | 106.181 | C(4)-C(15)-O(27) | 114.277 |
| C(4)-C(26)-O(22) | 113.74 | H(36)-C(14)-H(35) | 117.972 |
| H(48)-O(25)-C(23) | 107.928 | H(36)-C(14)-C(9) | 120.267 |
| H(47)-C(24)-H(46) | 116.133 | H(36)-C(14)-N(5) | 123.986 |
| H(47)-C(24)-C(6) | 101.058 | H(35)-C(14)-C(9) | 56.398 |
| H(47)-C(24)-N(10) | 125.99 | H(35)-C(14)-N(5) | 118.043 |
| H(46)-C(24)-C(6) | 68.345 | C(9)-C(14)-N(5) | 90.894 |
| H(46)-C(24)-N(10) | 117.775 | H(34)-C(12)-H(33) | 109.017 |
| C(6)-C(24)-N(10) | 95.384 | H(34)-C(12)-C(4) | 110.405 |
| H(45)-C(23)-H(44) | 109.938 | H(34)-C(12)-O(19) | 109.017 |
| H(45)-C(23)-C(18) | 110.638 | H(33)-C(12)-C(4) | 108.983 |
| H(45)-C(23)-O(25) | 108.767 | H(33)-C(12)-O(19) | 110.059 |
| H(44)-C(23)-C(18) | 109.696 | C(4)-C(12)-O(19) | 109.352 |
| H(44)-C(23)-O(25) | 109.501 | C(4)-N(10)-Zn(16) | 125.631 |
| C(18)-C(23)-O(25) | 108.267 | C(4)-N(10)-C(24) | 120.704 |
| H(43)-O(22)-C(26) | 105.862 | Zn(16)-N(10)-C(24) | 112.813 |
| H(42)-C(20)-H(41) | 107.829 | C(14)-C(9)-O(8) | 97.664 |
| H(42)-C(20)-C(18) | 109.97 | C(14)-C(9)-O(11) | 81.741 |
| H(42)-C(20)-O(17) | 110.824 | O(8)-C(9)-O(11) | 179.395 |
| H(41)-C(20)-C(18) | 108.652 | Zn(16)-O(8)-C(9) | 104.351 |
| H(41)-C(20)-O(17) | 106.057 | H(32)-C(7)-H(31) | 106.251 |
| C(18)-C(20)-O(17) | 113.275 | H(32)-C(7)-C(18) | 106.601 |
| H(40)-O(19)-C(12) | 106.874 | H(32)-C(7)-C(1) | 107 |
| C(20)-C(18)-C(23) | 110.008 | H(31)-C(7)-C(18) | 107.994 |
| C(20)-C(18)-C(7) | 113.589 | H(31)-C(7)-C(1) | 109.418 |
| C(20)-C(18)-N(5) | 106.799 | C(18)-C(7)-C(1) | 118.873 |
| C(23)-C(18)-C(7) | 105.982 | O(3)-C(6)-C(24) | 103.536 |
| C(23)-C(18)-N(5) | 106.313 | O(3)-C(6)-O(13) | 179.888 |
| C(7)-C(18)-N(5) | 113.909 | C(24)-C(6)-O(13) | 76.353 |
| H(39)-O(17)-C(20) | 108.082 | C(14)-N(5)-Zn(16) | 120.455 |
| O(8)-Zn(16)-O(3) | 83.612 | C(14)-N(5)-C(18) | 121.356 |
| O(8)-Zn(16)-Cl(2) | 78.231 | Zn(16)-N(5)-C(18) | 116.888 |
| O(8)-Zn(16)-N(10) | 148.547 | C(15)-C(4)-N(10) | 105.378 |
| O(8)-Zn(16)-N(5) | 85.559 | C(15)-C(4)-C(12) | 111.463 |
| O(8)-Zn(16)-Cl(21) | 76.438 | C(15)-C(4)-C(26) | 109.26 |
| O(3)-Zn(16)-Cl(2) | 64.925 | N(10)-C(4)-C(12) | 112.42 |
| O(3)-Zn(16)-N(10) | 65.077 | N(10)-C(4)-C(26) | 106.537 |
| O(3)-Zn(16)-N(5) | 165.762 | C(12)-C(4)-C(26) | 111.479 |
| O(3)-Zn(16)-Cl(21) | 69.81 | Zn(16)-O(3)-C(6) | 122.321 |
| Cl(2)-Zn(16)-N(10) | 85.472 | H(30)-C(1)-H(29) | 107.802 |
| Cl(2)-Zn(16)-N(5) | 103.786 | H(30)-C(1)-O(28) | 105.291 |
| Cl(2)-Zn(16)-Cl(21) | 129.865 | H(30)-C(1)-C(7) | 111.312 |
| N(10)-Zn(16)-N(5) | 124.716 | H(29)-C(1)-O(28) | 109.562 |
| N(10)-Zn(16)-Cl(21) | 94.458 | H(29)-C(1)-C(7) | 112.068 |

Table S15: Bond lengths (Å) of tricine using DFT-method from DMOL3 calculations.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length (Å) | Bond | Length (Å) |
| O(11)-H(24) | 0.97 | N(9)-C(2) | 1.462 |
| C(10)-H(23) | 1.102 | C(2)-C(8) | 1.526 |
| C(10)-H(22) | 1.096 | C(7)-C(10) | 1.555 |
| N(9)-H(21) | 1.022 | N(9)-C(7) | 1.494 |
| C(6)-H(20) | 1.098 | C(7)-C(6) | 1.553 |
| C(6)-H(19) | 1.104 | C(8)-O(12) | 1.364 |
| O(5)-H(18) | 0.971 | C(1)-O(11) | 1.443 |
| O(4)-H(17) | 0.982 | C(10)-O(5) | 1.439 |
| C(2)-H(16) | 1.1 | C(6)-O(4) | 1.438 |
| C(2)-H(15) | 1.096 | C(8)-O(3) | 1.224 |
| C(1)-H(14) | 1.099 | C(7)-C(1) | 1.555 |
| C(1)-H(13) | 1.101 | N(9)-C(2) | 1.462 |

Table S16: Bond angles (°) of tricin using DFT-method from DMOL3 calculations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Angle | Degree(°) | Angle | Degree(°) | Angle | Degree(°) |
| H(25)-O(12)-C(8) | 107.009 | O(12)-C(8)-O(3) | 123.598 | H(18)-O(5)-C(10) | 107.095 |
| H(24)-O(11)-C(1) | 107.241 | C(10)-C(7)-N(9) | 109.201 | H(17)-O(4)-C(6) | 102.316 |
| H(23)-C(10)-H(22) | 108.611 | C(10)-C(7)-C(6) | 111.086 | H(16)-C(2)-H(15) | 105.99 |
| H(23)-C(10)-C(7) | 109.58 | C(10)-C(7)-C(1) | 110.405 | H(16)-C(2)-N(9) | 115.801 |
| H(23)-C(10)-O(5) | 111.076 | N(9)-C(7)-C(6) | 103.232 | H(16)-C(2)-C(8) | 107.315 |
| H(22)-C(10)-C(7) | 109.046 | N(9)-C(7)-C(1) | 114.877 | H(15)-C(2)-N(9) | 110.279 |
| H(22)-C(10)-O(5) | 105.146 | C(6)-C(7)-C(1) | 107.831 | H(15)-C(2)-C(8) | 106.076 |
| C(7)-C(10)-O(5) | 113.192 | H(20)-C(6)-H(19) | 107.145 | N(9)-C(2)-C(8) | 110.829 |
| H(21)-N(9)-C(2) | 109.095 | H(20)-C(6)-C(7) | 111.208 | H(14)-C(1)-H(13) | 107.914 |
| H(21)-N(9)-C(7) | 108.304 | H(20)-C(6)-O(4) | 108.16 | H(14)-C(1)-O(11) | 105.725 |
| C(2)-N(9)-C(7) | 120.411 | H(19)-C(6)-C(7) | 108.469 | H(14)-C(1)-C(7) | 108.551 |
| C(2)-C(8)-O(12) | 110.123 | H(19)-C(6)-O(4) | 110.179 | H(13)-C(1)-O(11) | 110.758 |