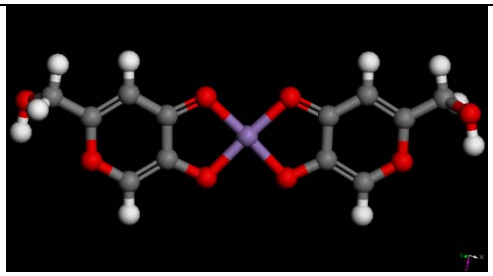
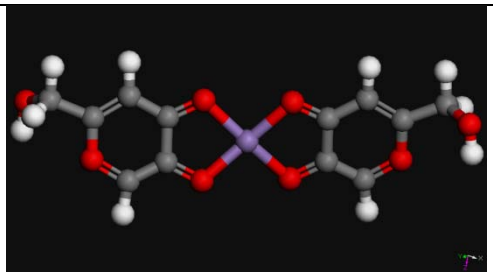
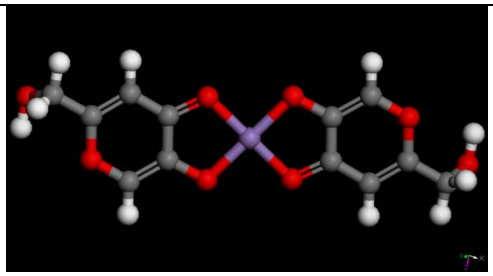
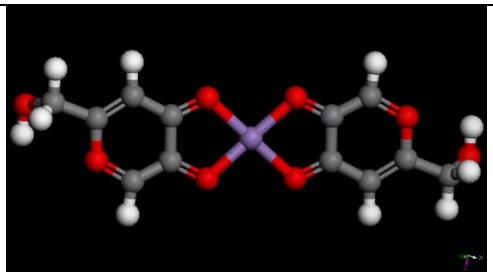
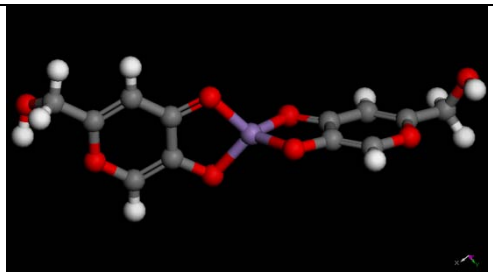
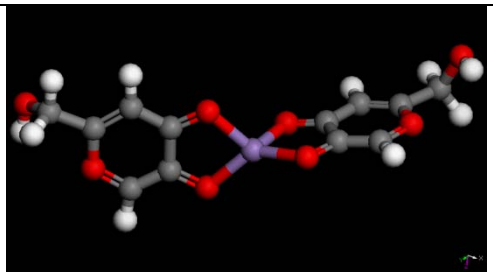
## Supporting Information

**Table A1:** Optimized geometries and total energies (kcalmol$^{-1}$) of the metal kojate complexes:

**(a) Mn(II)**

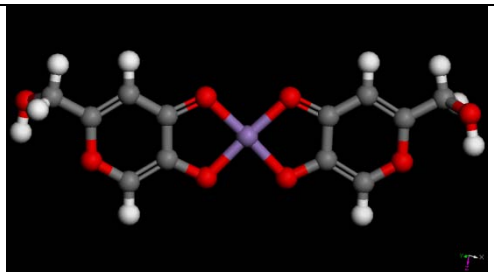
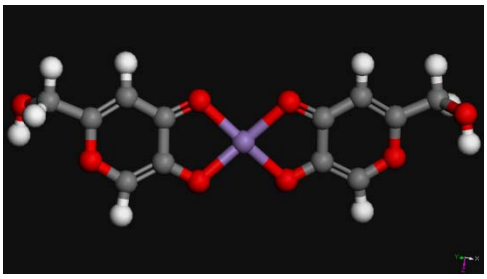
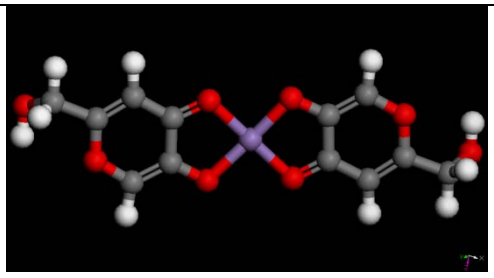
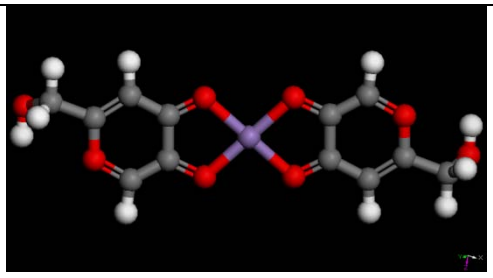
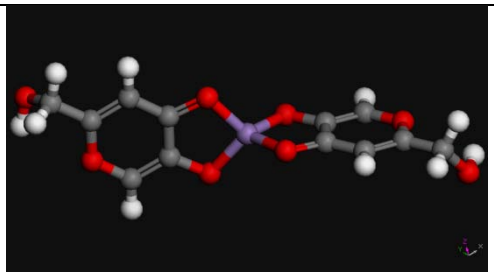
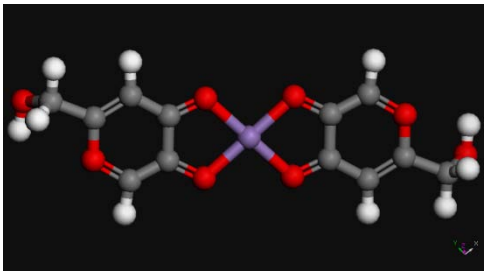
*(i) doublet*

| **Mn(II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-744315.9) |
| *Trans* square planar |  |  (-744316.1) |
| Tetrahedral |  |  (-744316.8) |

Colour Code: H-white, C-grey, O-red, Mn-purple

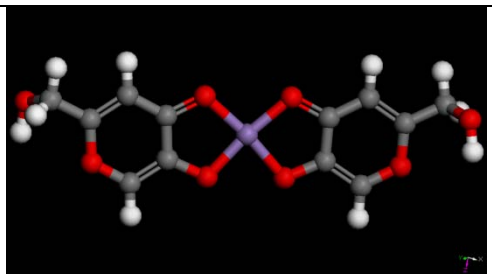
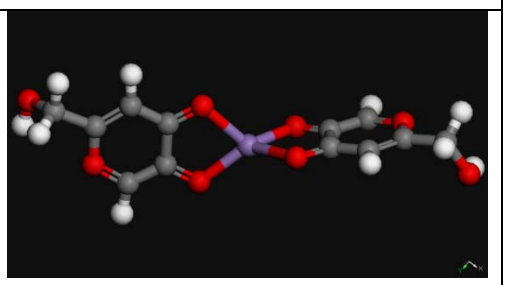
*(ii) Quartet*

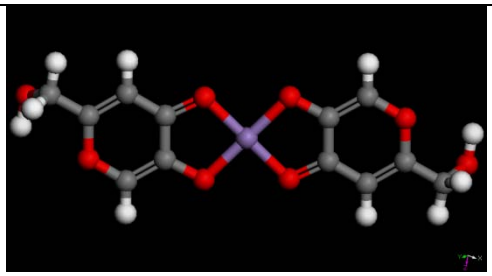
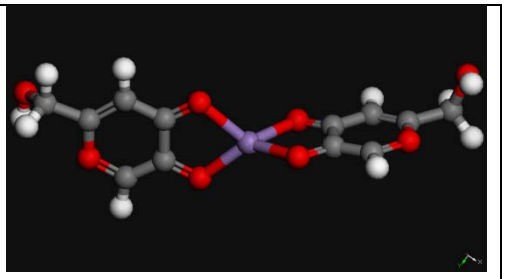
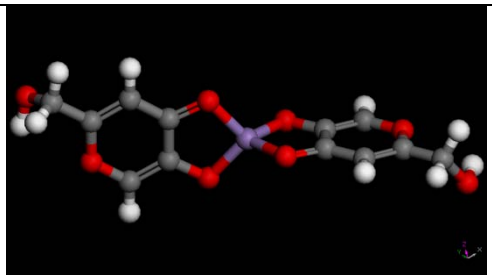
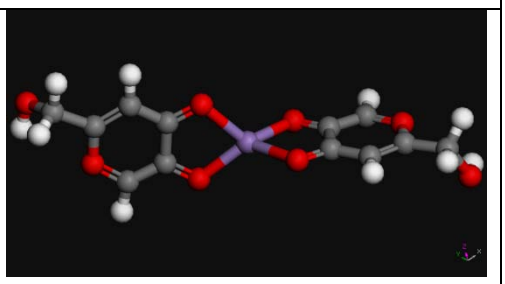
| **Mn (II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|

| | | |
|---|---|---|
| *Cis* square planar |  |  (-744337.7) |
| *Trans* square planar |  |  (-744330.6) |
| Tetrahedral |  |  (-744331.1) |

Colour Code: H-white, C-grey, O-red, Mn-purple

*(iii) Sextet*

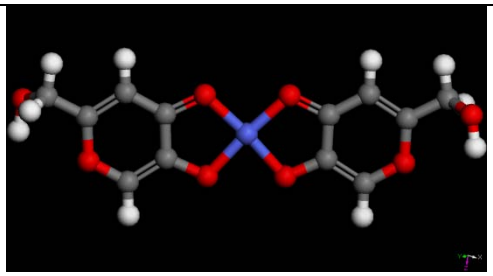
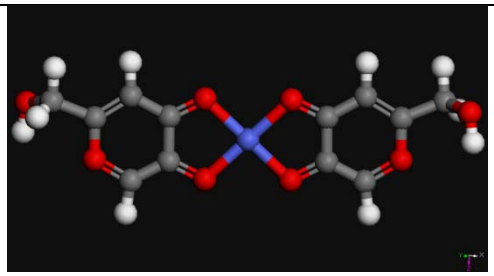
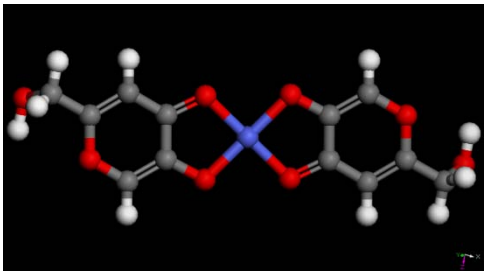
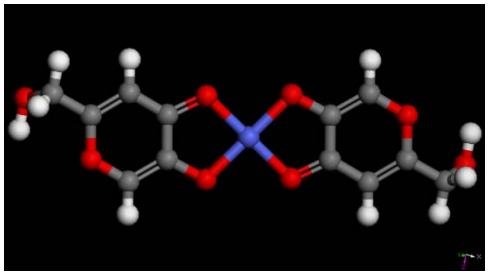
| **Mn(II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-744335.6) |

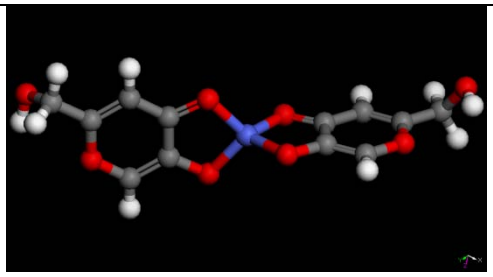
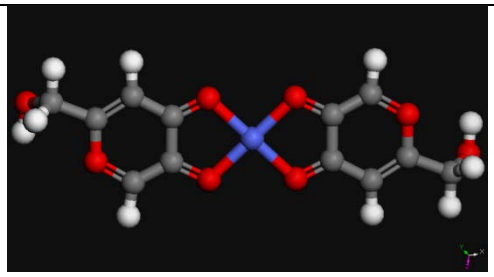
| | | |
|---|---|---|
| *Trans* square planar |  |  (-744335.7) |
| Tetrahedral |  |  (-744335.7) |

Colour Code: H-white, C-grey, O-red, Mn-purple

**(b ) Co(II)**

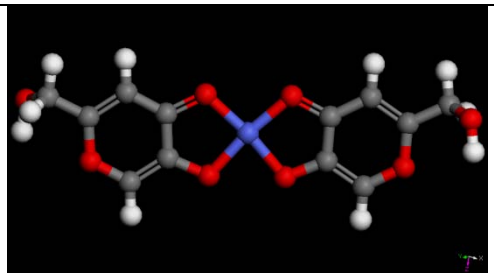
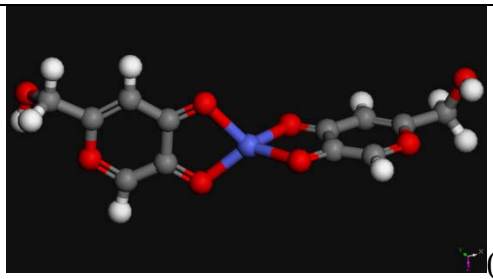
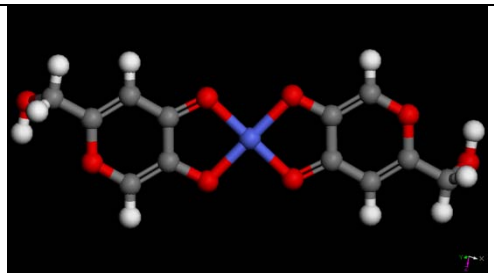
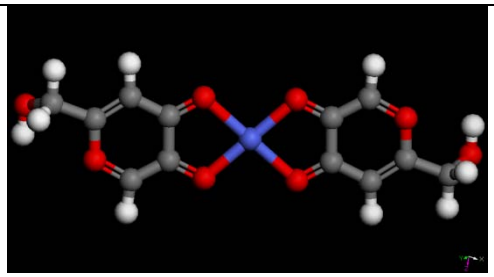
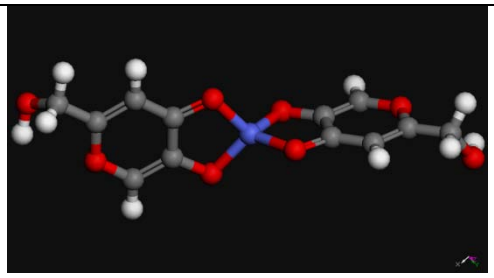
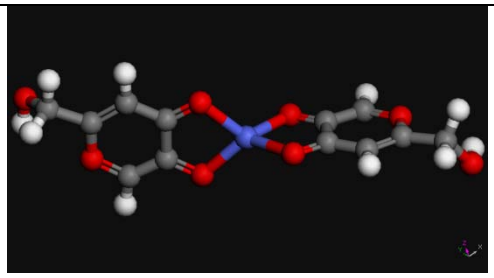
*(i) Doublet*

| **Co(II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-772585.4) |
| *Trans* square planar |  |  (-772591.2) |
| | | |
| Tetrahedral | | |

| | | |
|---|---|---|
| |  |  (-772591.2) |

Colour Code: H-white, C-grey, O-red, Co-dark blue

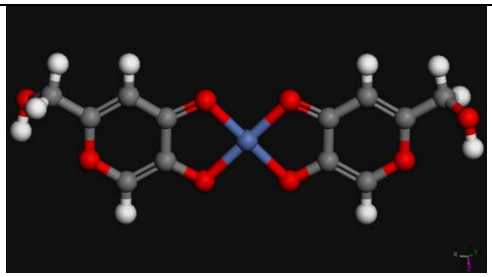
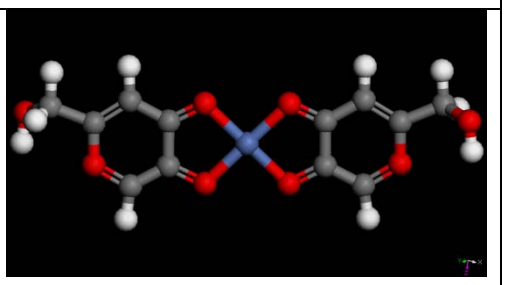
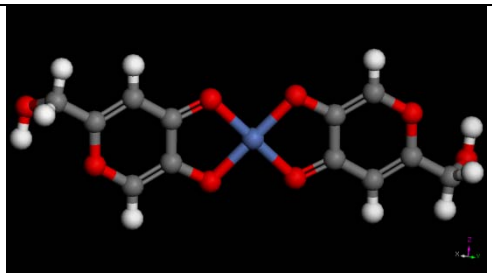
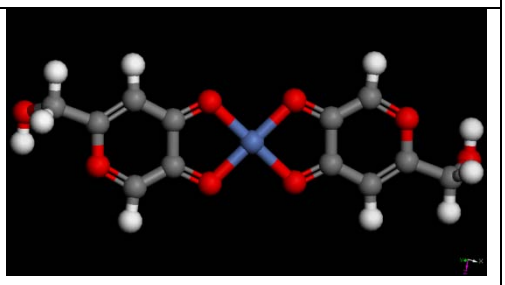
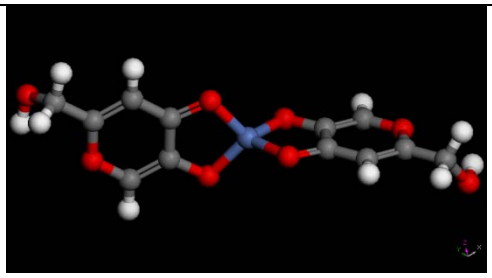
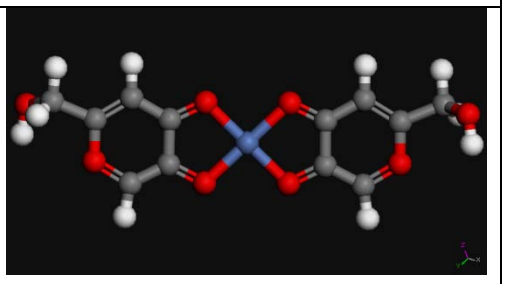
*(ii) Quartet*

| **Co(II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-772585.4) |
| *Trans* square planar |  |  (-772579.9) |
| Tetrahedral |  |  (-772584.4) |

Colour Code: H-white, C-grey, O-red, Co-dark blue

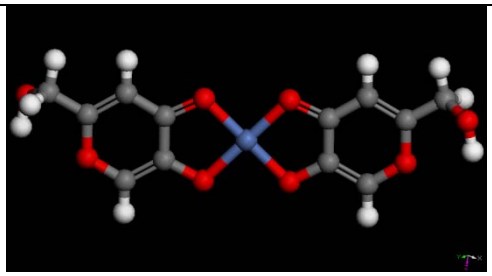
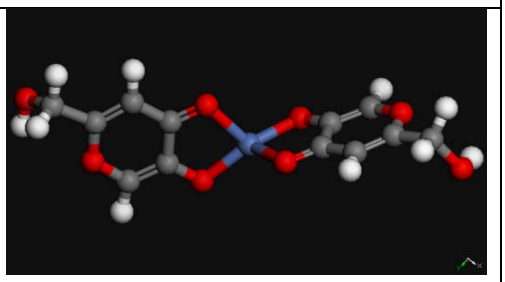
**(c) Ni(II)**

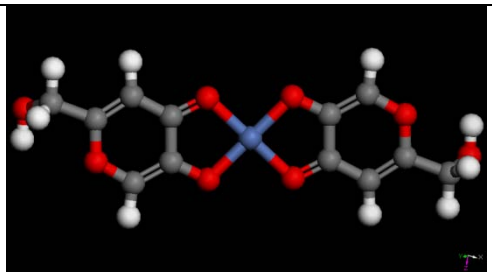
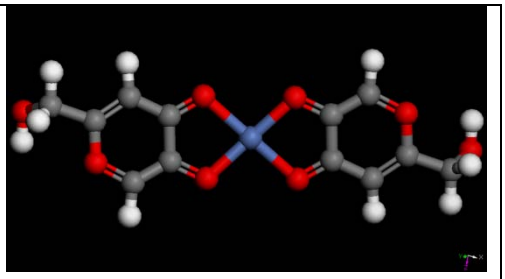
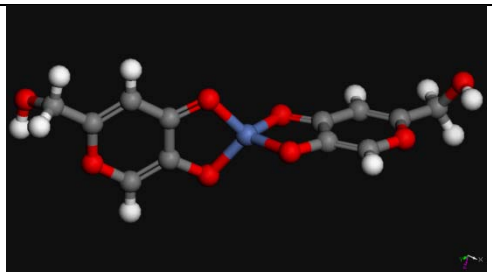
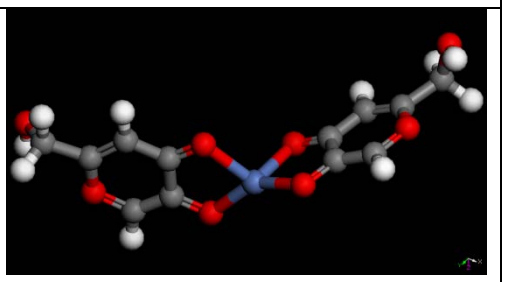
*(i) Singlet*

| **Ni(II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-789321.1) |
| *Trans* square planar |  |  (-789320.7) |
| Tetrahedral |  |  (-789320.2) |

Colour Code: H-white, C-grey, O-red, Ni-navy blue

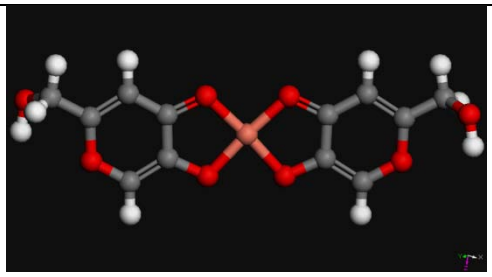
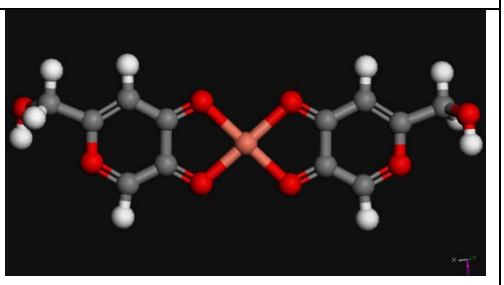
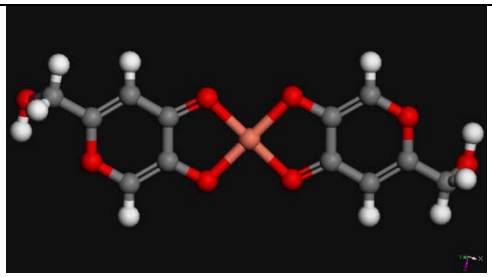
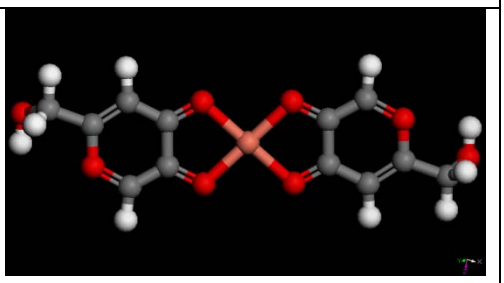
*(ii) Triplet*

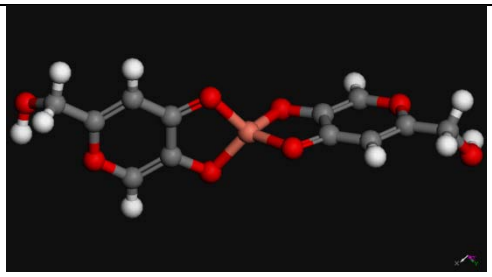
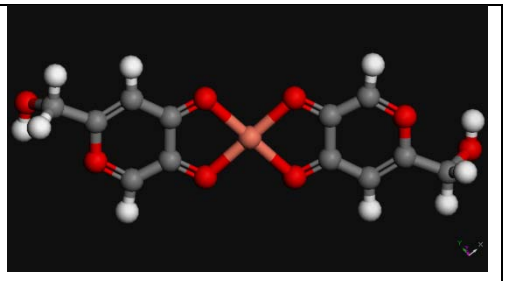
| **Ni (II)** | **Initial geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-789310.4) |

| | | |
|---|---|---|
| *Trans* square planar |  |  (-789308.7) |
| Tetrahedral |  |  (-789310.7) |

Colour Code: H-white, C-grey, O-red, Ni-navy blue

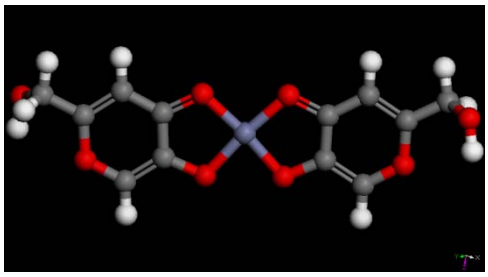
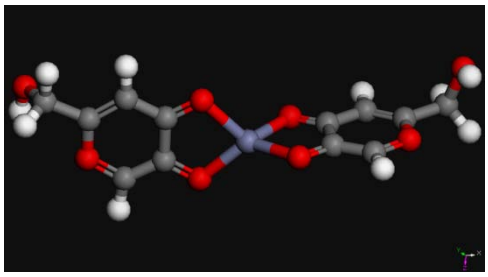
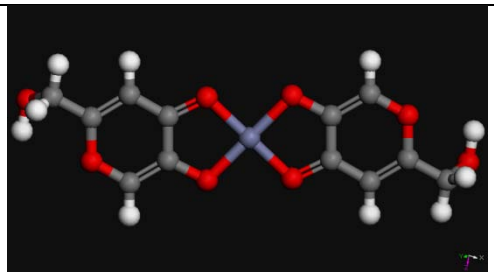
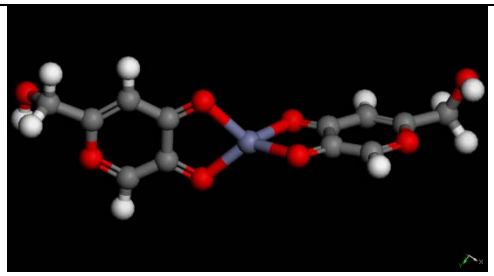
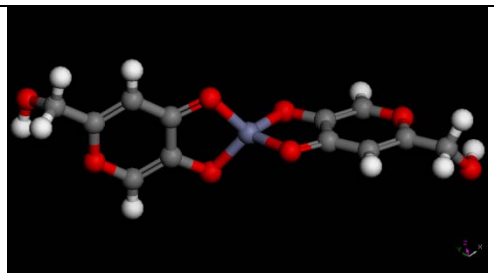
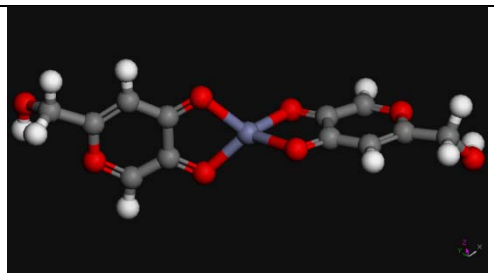
(d) Cu(II) doublet

| **Cu(II)** | **Initial Geometry** | **Final optimized geometry** |
|---|---|---|
| *Cis* square planar |  |  (-807490.0) |
| *Trans* square planar |  |  (-807489.9) |
| Tetrahedral | | |

| | | |
|---|---|---|
| |  |  <br>(-807489.9) |

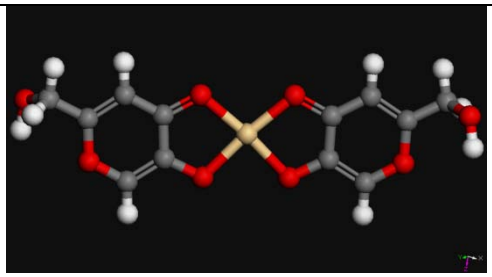
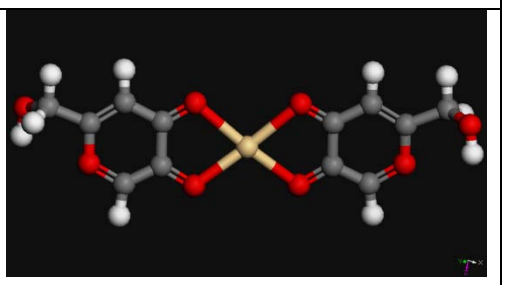
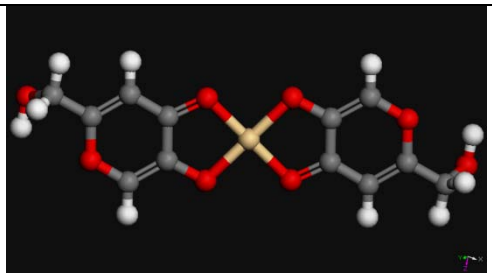
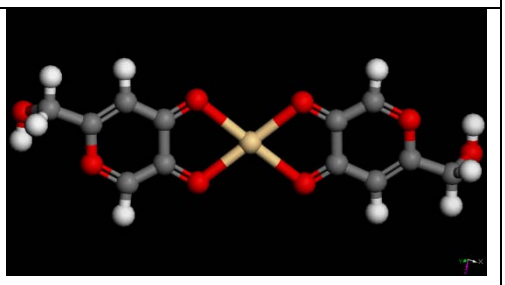
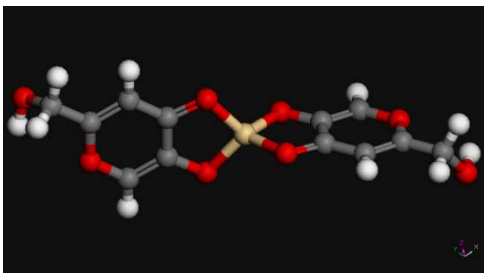
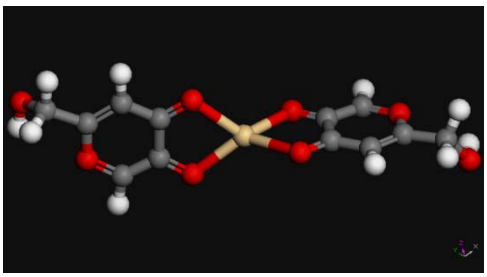
Colour Code: H-white, C-grey, O-red, Cu-reddish orange

**(e) Zn(II) singlet**

| Zn(II) | Initial geometry | Final optimized geometry |
|---|---|---|
| *Cis* square planar |  |  <br>(-827523.1) |
| *Trans* square planar |  |  <br>(-827523.2) |
| Tetrahedral |  |  <br>(-827523.1) |

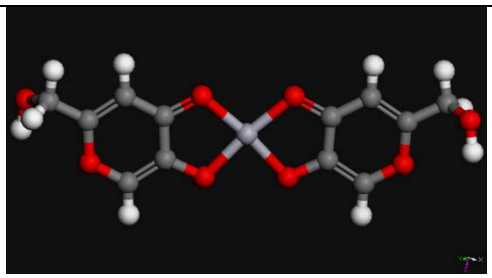
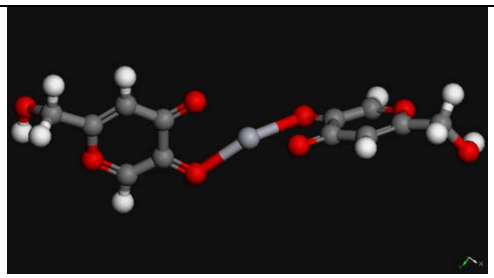
Colour Code: H-white, C-grey, O-red, Zn-Dark Blue

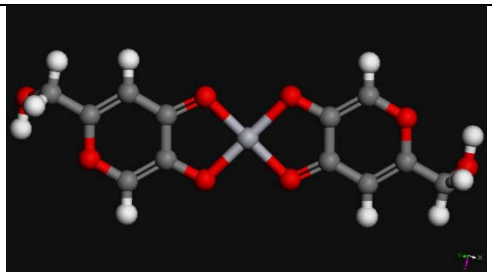
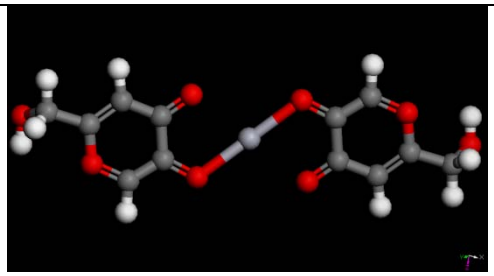
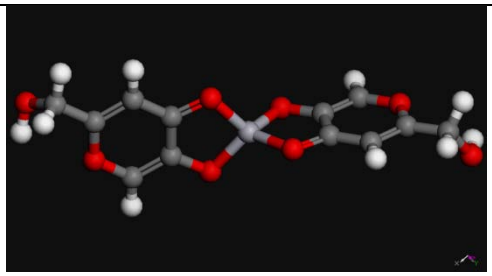
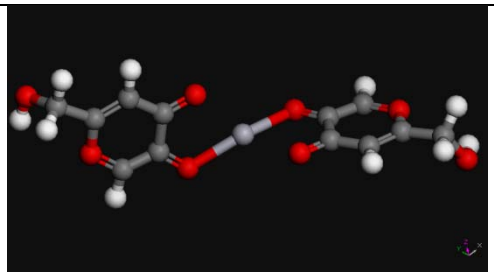
**(f) Cd(II) singlet**

| Cd(II) | Initial geometry | Final optimized geometry |
|---|---|---|
| *Cis* square planar |  |  (-724219.9) |
| *Trans* square planar |  |  (-724220.1) |
| Tetrahedral |  |  (-724222.4) |

Colour Code: H-white, C-grey, O-red, Cd-Dark yellow

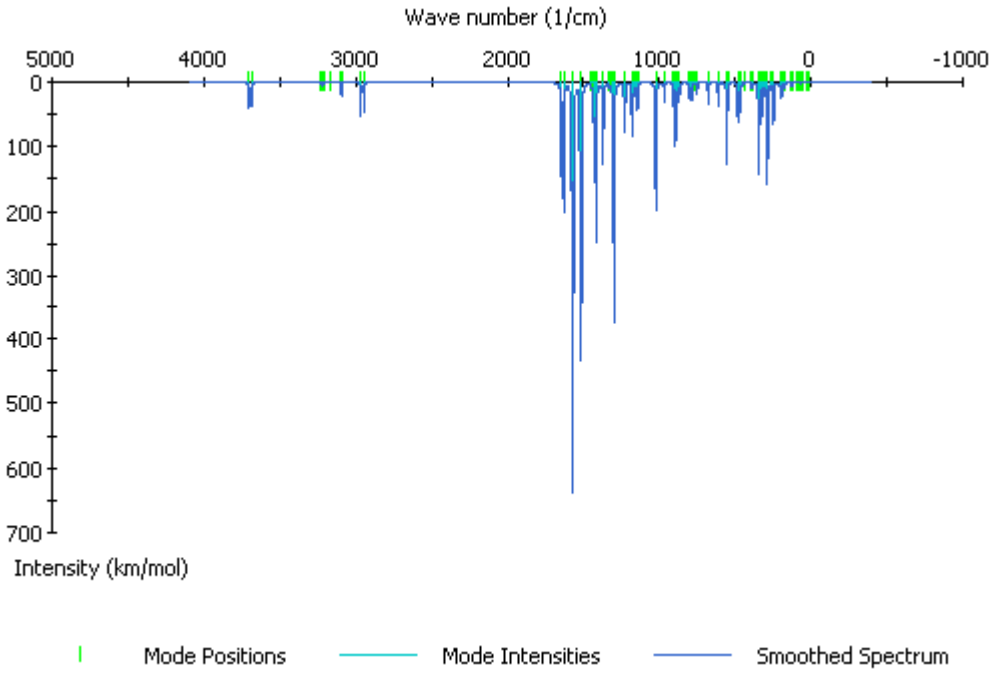
(g) Hg(II) singlet

| Hg(II) | Initial geometry | Final optimized geometry |
|---|---|---|
| *Cis* square planar |  |  (-811261.4) |

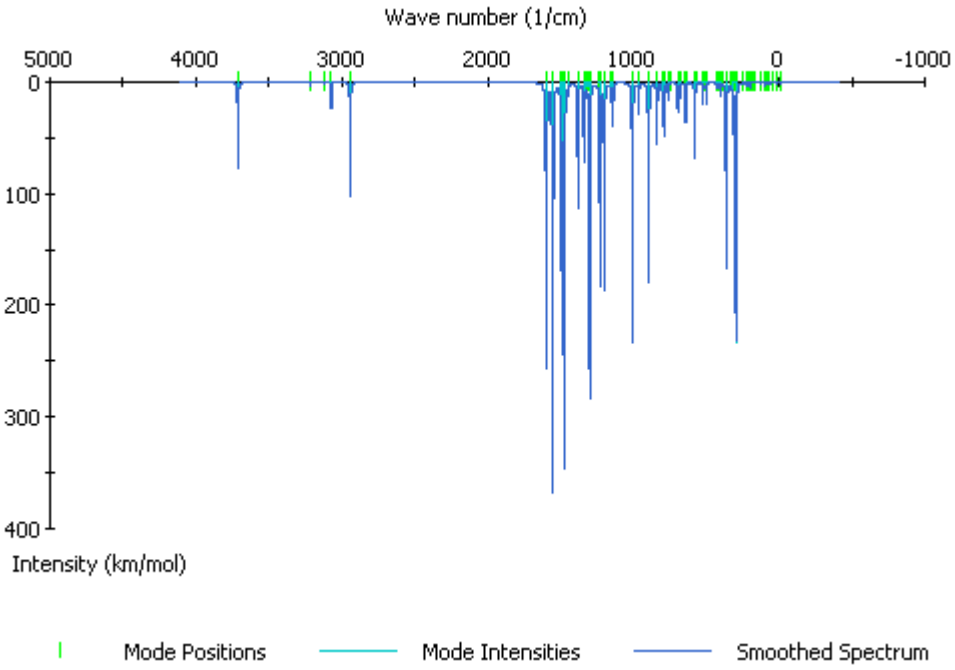
| | | |
|---|---|---|
| Trans-square planar |  |  (-811254.5) |
| Tetrahedral |  |  (-811261.7) |

Colour Code: H-white, C-grey, O-red, Hg-light grey

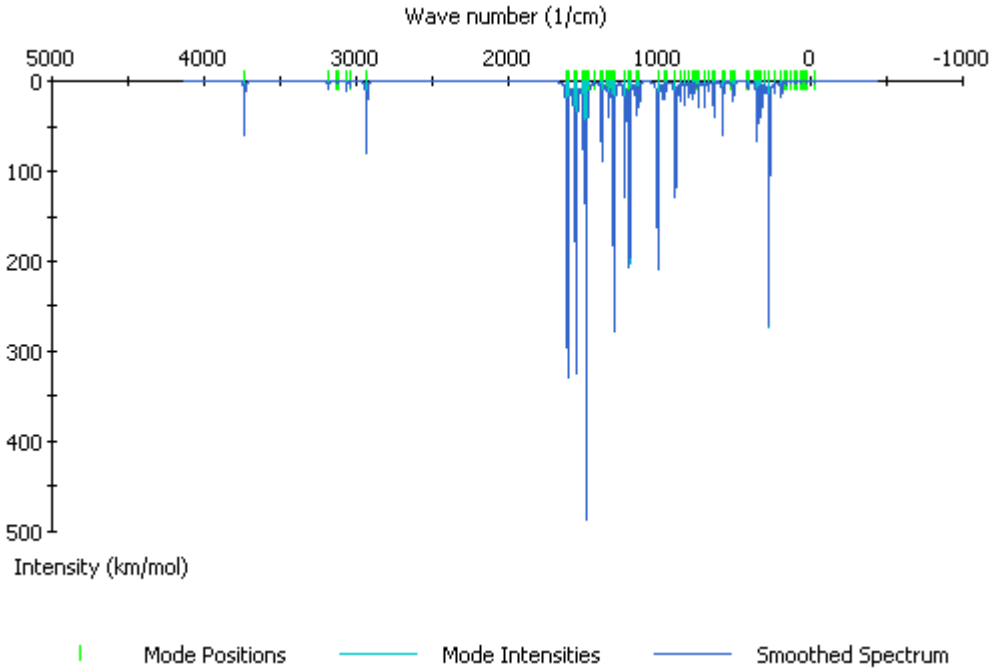
**Mn(II)**



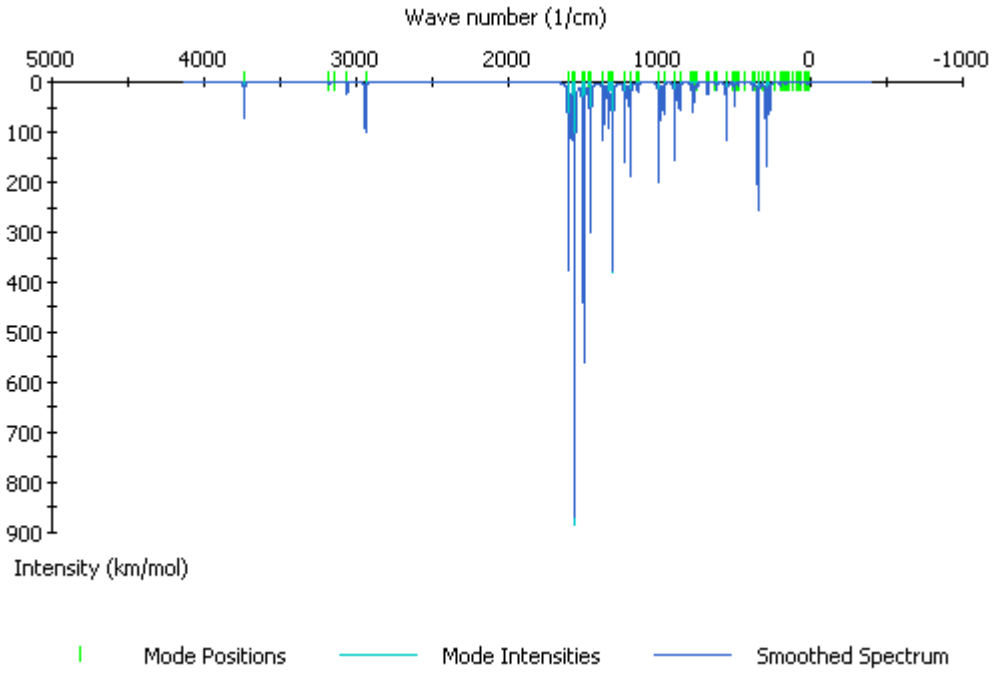

**Co(II)**


Wave number (1/cm)
5000
4000
3000
2000
1000
0
-1000
0
100
200
300
400
Intensity (km/mol)
Mode Positions
Mode Intensities
Smoothed Spectrum

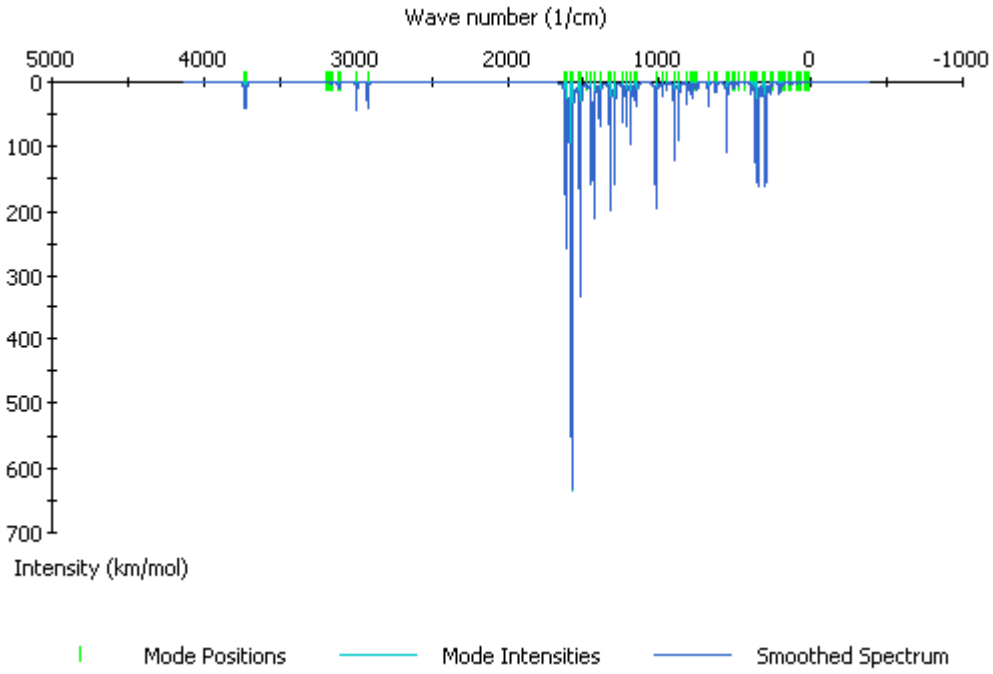
**Ni(II)**


Wave number (1/cm)
5000
4000
3000
2000
1000
0
-1000
0
100
200
300
400
500
Intensity (km/mol)
Mode Positions
Mode Intensities
Smoothed Spectrum

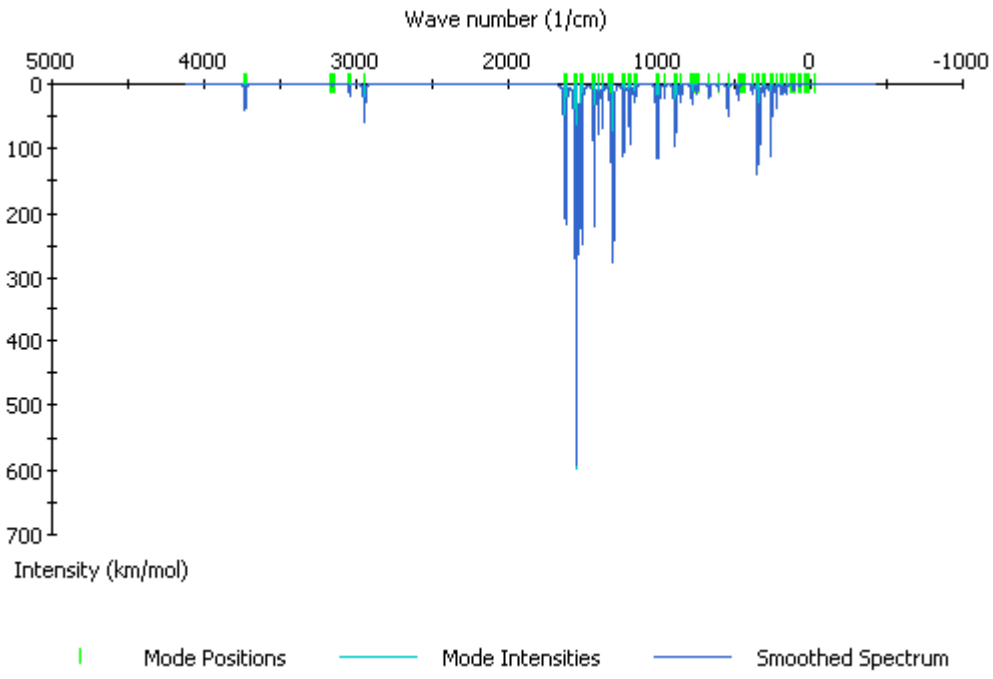
**Cu(II)**


Wave number (1/cm)
5000
4000
3000
2000
1000
0
-1000
0
100
200
300
400
500
600
700
800
900
Intensity (km/mol)
Mode Positions
Mode Intensities
Smoothed Spectrum

**Zn(II)**


Wave number (1/cm)
5000
4000
3000
2000
1000
0
-1000
0
100
200
300
400
500
600
700
Intensity (km/mol)
Mode Positions
Mode Intensities
Smoothed Spectrum

**Cd(II)**




**Hg(II)**

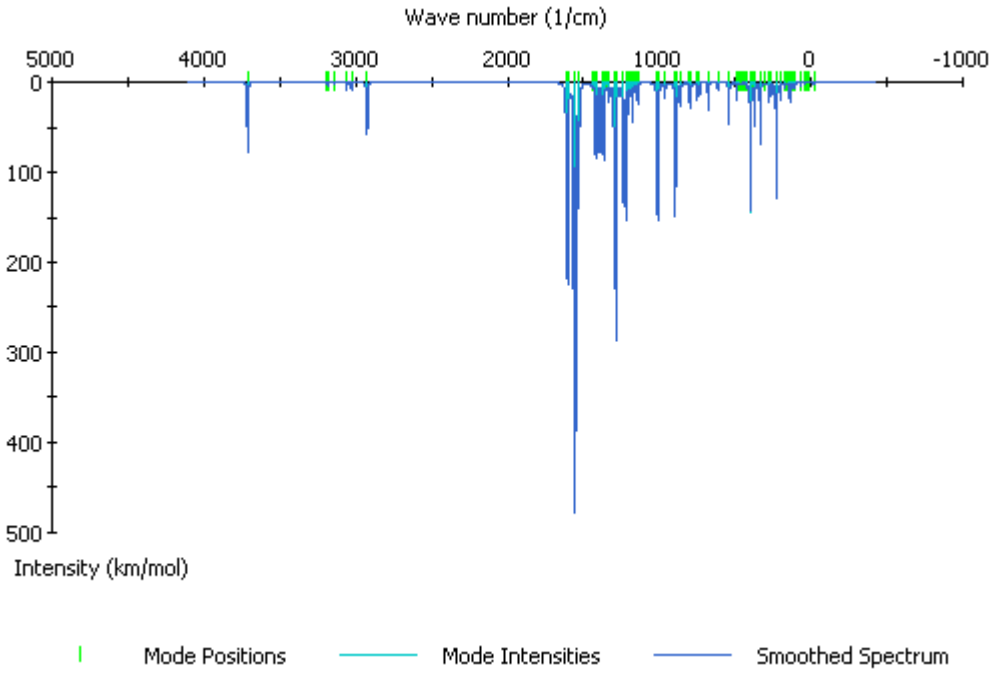



**Table A2:** Calculated zero-point corrected energies (kcal/mol) of the complexes

| Metal ion | Energy of the complex | Energy of the metal ion |
|---|---|---|
| Mn(II) | -744204.0 | -75878.5 |
| Co(II) | -772462.0 | -104048.1 |
| Ni(II) | -789188.6 | -120763.0 |
| Cu(II) | -807358.3 | -138953.0 |

| | | |
|---|---|---|
| Zn(II) | -827391.0 | -159024.5 |
| Cd(II) | -724091.5 | -55783.8 |
| Hg(II) | -811131.2 | -142793.8 |

**Table A3:** Calculated ESP charges on the various atoms in the complexes

| Atom | Mn(II) | Co(II) | Ni(II) | Cu(II) | Zn(II) | Cd(II) | Hg(II) |
|---|---|---|---|---|---|---|---|
| $C_1$ | -0.553 | -0.529 | -0.547 | -0.549 | -0.519 | -0.479 | -0.524 |
| $C_2$ | 0.278 | 0.272 | 0.291 | 0.289 | 0.270 | 0.246 | 0.277 |
| $C_3$ | -0.150 | -0.131 | -0.175 | -0.134 | -0.137 | -0.088 | -0.139 |
| $C_4$ | 0.176 | 0.151 | 0.180 | 0.139 | 0.173 | 0.138 | 0.177 |
| $C_5$ | 0.551 | 0.523 | 0.534 | 0.541 | 0.510 | 0.513 | 0.518 |
| $O_6$ | -0.546 | -0.454 | -0.400 | -0.452 | -0.516 | -0.578 | -0.494 |
| $O_7$ | -0.558 | -0.451 | -0.397 | -0.444 | -0.543 | -0.591 | -0.501 |
| $C_8$ | -0.006 | -0.024 | -0.046 | -0.037 | -0.029 | -0.024 | -0.016 |
| $O_9$ | -0.162 | -0.161 | -0.150 | -0.162 | -0.162 | -0.179 | -0.167 |
| $H_{10}$ | 0.241 | 0.235 | 0.236 | 0.237 | 0.237 | 0.228 | 0.232 |
| $H_{11}$ | 0.198 | 0.195 | 0.207 | 0.196 | 0.197 | 0.189 | 0.196 |
| $H_{12}$ | 0.139 | 0.145 | 0.152 | 0.149 | 0.144 | 0.141 | 0.14 |
| $H_{13}$ | 0.060 | 0.066 | 0.070 | 0.069 | 0.068 | 0.072 | 0.064 |
| $O_{14}$ | -0.530 | -0.524 | -0.515 | -0.519 | -0.519 | -0.522 | -0.526 |
| $H_{15}$ | 0.385 | 0.382 | 0.379 | 0.381 | 0.382 | 0.383 | 0.382 |
| $M_{16}$ | 0.95 | 0.609 | 0.365 | 0.592 | 0.889 | 1.099 | 0.759 |
| $C_{17}$ | -0.545 | -0.529 | -0.571 | -0.545 | -0.521 | -0.490 | -0.519 |
| $C_{18}$ | 0.277 | 0.272 | 0.306 | 0.287 | 0.273 | 0.260 | 0.282 |
| $C_{19}$ | -0.157 | -0.131 | -0.160 | -0.138 | -0.141 | -0.092 | -0.145 |
| $C_{20}$ | 0.181 | 0.151 | 0.152 | 0.147 | 0.176 | 0.128 | 0.177 |
| $C_{21}$ | 0.545 | 0.523 | 0.559 | 0.534 | 0.510 | 0.525 | 0.518 |
| $O_{22}$ | -0.545 | -0.454 | -0.400 | -0.449 | -0.518 | -0.578 | -0.495 |
| $O_{23}$ | -0.558 | -0.451 | -0.392 | -0.448 | -0.543 | -0.586 | -0.499 |
| $C_{24}$ | -0.017 | -0.024 | -0.053 | -0.035 | -0.03 | -0.031 | -0.030 |
| $O_{25}$ | -0.157 | -0.161 | -0.158 | -0.160 | -0.162 | -0.179 | -0.165 |
| $H_{26}$ | 0.238 | 0.235 | 0.239 | 0.237 | 0.237 | 0.225 | 0.227 |
| $H_{27}$ | 0.200 | 0.195 | 0.204 | 0.196 | 0.199 | 0.191 | 0.199 |
| $H_{28}$ | 0.143 | 0.145 | 0.155 | 0.148 | 0.144 | 0.144 | 0.145 |
| $H_{29}$ | 0.064 | 0.066 | 0.074 | 0.069 | 0.069 | 0.073 | 0.069 |
| $O_{30}$ | -0.527 | -0.524 | -0.516 | -0.520 | -0.519 | -0.520 | -0.523 |
| $H_{31}$ | 0.383 | 0.382 | 0.379 | 0.381 | 0.382 | 0.380 | 0.381 |

**Table A4:** Calculated Mayer bond orders

| Bond | Mn(II) | Co(II) | Ni(II) | Cu(II) | Zn(II) | Cd(II) | Hg(II) |
|---|---|---|---|---|---|---|---|
| $C_1$-$C_2$ | 1.479 | 1.468 | 1.451 | 1.451 | 1.448 | 1.457 | 1.489 |
| $C_3$-$C_4$ | 1.428 | 1.411 | 1.392 | 1.390 | 1.389 | 1.400 | 1.440 |
| $C_1$-$C_5$ | 1.218 | 1.221 | 1.207 | 1.203 | 1.193 | 1.193 | 1.184 |
| $C_4$-$C_5$ | 1.067 | 1.063 | 1.054 | 1.045 | 1.034 | 1.038 | 1.043 |
| $C_5$-$O_6$ | 1.426 | 1.349 | 1.365 | 1.386 | 1.428 | 1.465 | 1.538 |
| $C_4$-$O_7$ | 1.253 | 1.232 | 1.249 | 1.252 | 1.268 | 1.286 | 1.230 |
| $C_2$-$C_8$ | 0.977 | 0.975 | 0.957 | 0.959 | 0.953 | 0.959 | 0.973 |
| $C_2$-$O_9$ | 1.097 | 1.086 | 1.095 | 1.100 | 1.100 | 1.097 | 1.083 |
| $C_3$-$O_9$ | 1.028 | 1.033 | 1.033 | 1.034 | 1.035 | 1.031 | 1.026 |
| $C_1$-$H_{10}$ | 0.964 | 0.966 | 0.968 | 0.969 | 0.972 | 0.971 | 0.969 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $C_3$-$H_{11}$ | 0.972 | 0.976 | 0.978 | 0.979 | 0.982 | 0.980 | 0.979 |
| $C_8$-$H_{12}$ | 0.967 | 0.969 | 0.971 | 0.970 | 0.971 | 0.971 | 0.970 |
| $C_8$-$H_{13}$ | 0.950 | 0.953 | 0.953 | 0.954 | 0.956 | 0.954 | 0.953 |
| $C_8$-$O_{14}$ | 0.988 | 0.982 | 0.984 | 0.981 | 0.978 | 0.982 | 0.982 |
| $O_{14}$-$H_{15}$ | 0.951 | 0.951 | 0.950 | 0.951 | 0.951 | 0.951 | 0.952 |
| $C_{17}$-$C_{18}$ | 1.480 | 1.468 | 1.453 | 1.451 | 1.448 | 1.457 | 1.489 |
| $C_{19}$-$C_{20}$ | 1.429 | 1.411 | 1.393 | 1.390 | 1.389 | 1.401 | 1.440 |
| $C_{17}$-$C_{21}$ | 1.217 | 1.221 | 1.206 | 1.203 | 1.193 | 1.194 | 1.185 |
| $C_{20}$-$C_{21}$ | 1.067 | 1.063 | 1.054 | 1.044 | 1.034 | 1.037 | 1.043 |
| $C_{21}$-$O_{22}$ | 1.428 | 1.349 | 1.360 | 1.386 | 1.428 | 1.464 | 1.534 |
| $C_{20}$-$O_{23}$ | 1.251 | 1.232 | 1.252 | 1.253 | 1.268 | 1.288 | 1.232 |
| $C_{18}$-$C_{24}$ | 0.977 | 0.975 | 0.958 | 0.959 | 0.953 | 0.957 | 0.972 |
| $C_{18}$-$O_{24}$ | 1.097 | 1.086 | 1.095 | 1.100 | 1.099 | 1.098 | 1.084 |
| $C_{19}$-$O_{24}$ | 1.027 | 1.033 | 1.029 | 1.033 | 1.035 | 1.028 | 1.025 |
| $C_{17}$-$H_{25}$ | 0.964 | 0.966 | 0.968 | 0.969 | 0.971 | 0.970 | 0.968 |
| $C_{19}$-$H_{27}$ | 0.972 | 0.976 | 0.978 | 0.979 | 0.982 | 0.980 | 0.979 |
| $C_{24}$-$H_{28}$ | 0.967 | 0.969 | 0.970 | 0.970 | 0.971 | 0.970 | 0.970 |
| $C_{24}$-$H_{29}$ | 0.949 | 0.953 | 0.951 | 0.954 | 0.956 | 0.951 | 0.953 |
| $C_{24}$-$O_{30}$ | 0.989 | 0.982 | 0.986 | 0.981 | 0.979 | 0.986 | 0.984 |
| $O_{30}$-$H_{31}$ | 0.951 | 0.951 | 0.950 | 0.951 | 0.951 | 0.949 | 0.951 |
| $O_6$-$M_{16}$ | 0.421 | 0.625 | 0.597 | 0.562 | 0.463 | 0.366 | 0.314 |
| $O_7$-$M_{16}$ | 0.555 | 0.687 | 0.653 | 0.647 | 0.573 | 0.479 | 0.564 |
| $O_{22}$-$M_{16}$ | 0.419 | 0.625 | 0.607 | 0.563 | 0.463 | 0.367 | 0.317 |
| $O_{23}$-$M_{16}$ | 0.557 | 0.687 | 0.647 | 0.645 | 0.573 | 0.478 | 0.561 |

**Table A5:** Calculated bond lengths of the various bonds in the complexes

| Bond | Mn(II) | Co(II) | Ni(II) | Cu(II) | Zn(II) | Cd(II) | Hg(II) |
|---|---|---|---|---|---|---|---|
| **$C_1$-$C_2$** | 1.371 | 1.371 | 1.372 | 1.372 | 1.371 | 1.368 | 1.365 |
| **$C_1$-$H_{10}$** | 1.090 | 1.089 | 1.090 | 1.090 | 1.090 | 1.090 | 1.089 |
| **$C_1$-$C_5$** | 1.424 | 1.418 | 1.418 | 1.421 | 1.423 | 1.426 | 1.432 |
| **$C_2$-$C_8$** | 1.501 | 1.498 | 1.499 | 1.500 | 1.500 | 1.500 | 1.498 |
| **$C_2$-$O_9$** | 1.351 | 1.354 | 1.352 | 1.351 | 1.351 | 1.351 | 1.354 |
| **$C_3$-$O_9$** | 1.370 | 1.368 | 1.369 | 1.368 | 1.367 | 1.368 | 1.367 |
| **$C_3$-$H_{11}$** | 1.086 | 1.086 | 1.086 | 1.087 | 1.087 | 1.087 | 1.086 |
| **$C_3$-$C_4$** | 1.382 | 1.379 | 1.378 | 1.381 | 1.382 | 1.384 | 1.377 |
| **$C_4$-$C_5$** | 1.466 | 1.450 | 1.450 | 1.456 | 1.467 | 1.474 | 1.474 |
| **$C_4$-$O_7$** | 1.308 | 1.312 | 1.313 | 1.308 | 1.308 | 1.306 | 1.312 |
| **$C_5$-$O_6$** | 1.281 | 1.289 | 1.291 | 1.284 | 1.281 | 1.277 | 1.265 |
| **$O_6$-$M_{16}$** | 2.124 | 1.914 | 1.884 | 1.987 | 2.053 | 2.285 | 2.445 |
| **$O_7$-$M_{16}$** | 2.028 | 1.900 | 1.866 | 1.946 | 1.979 | 2.190 | 2.201 |
| **$C_8$-$H_{12}$** | 1.095 | 1.096 | 1.096 | 1.096 | 1.097 | 1.097 | 1.096 |
| **$C_8$-$H_{13}$** | 1.104 | 1.105 | 1.107 | 1.106 | 1.106 | 1.106 | 1.105 |
| **$C_8$-$O_{14}$** | 1.431 | 1.431 | 1.430 | 1.431 | 1.432 | 1.430 | 1.431 |
| **$O_{14}$-$H_{15}$** | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 |
| **$C_{17}$-$C_{21}$** | 1.424 | 1.418 | 1.417 | 1.421 | 1.423 | 1.428 | 1.431 |
| **$C_{17}$-$H_{26}$** | 1.089 | 1.089 | 1.090 | 1.090 | 1.091 | 1.090 | 1.089 |
| **$C_{17}$-$C_{18}$** | 1.371 | 1.371 | 1.370 | 1.372 | 1.371 | 1.368 | 1.364 |
| **$C_{18}$-$C_{24}$** | 1.501 | 1.498 | 1.501 | 1.500 | 1.500 | 1.501 | 1.499 |
| **$C_{18}$-$O_{25}$** | 1.351 | 1.354 | 1.352 | 1.351 | 1.351 | 1.349 | 1.353 |
| **$C_{19}$-$O_{25}$** | 1.370 | 1.368 | 1.371 | 1.368 | 1.368 | 1.368 | 1.368 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **$C_{19}$-$H_{27}$** | 1.086 | 1.086 | 1.086 | 1.087 | 1.087 | 1.087 | 1.086 |
| **$C_{19}$-$C_{20}$** | 1.381 | 1.379 | 1.380 | 1.381 | 1.383 | 1.384 | 1.378 |
| **$C_{20}$-$C_{21}$** | 1.465 | 1.450 | 1.445 | 1.456 | 1.467 | 1.475 | 1.474 |
| **$C_{20}$-$O_{23}$** | 1.309 | 1.312 | 1.315 | 1.308 | 1.308 | 1.305 | 1.311 |
| **$C_{21}$-$O_{22}$** | 1.280 | 1.289 | 1.290 | 1.284 | 1.281 | 1.277 | 1.265 |
| **$O_{22}$-$M_{16}$** | 2.125 | 1.914 | 1.873 | 1.987 | 2.053 | 2.286 | 2.437 |
| **$O_{23}$-$M_{16}$** | 2.027 | 1.900 | 1.874 | 1.946 | 1.979 | 2.191 | 2.205 |
| **$C_{24}$-$H_{28}$** | 1.095 | 1.06 | 1.097 | 1.096 | 1.097 | 1.097 | 1.096 |
| **$C_{24}$-$H_{29}$** | 1.105 | 1.105 | 1.108 | 1.106 | 1.106 | 1.107 | 1.105 |
| **$C_{24}$-$O_{30}$** | 1.430 | 1.431 | 1.429 | 1.431 | 1.431 | 1.428 | 1.430 |
| **$O_{30}$-$H_{31}$** | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 | 0.973 |

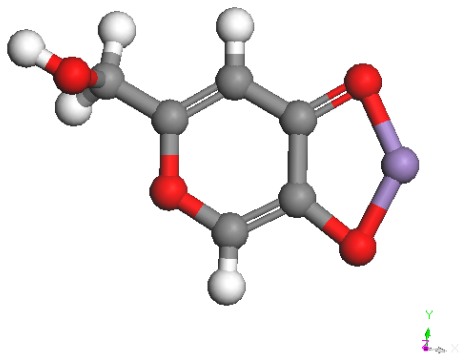
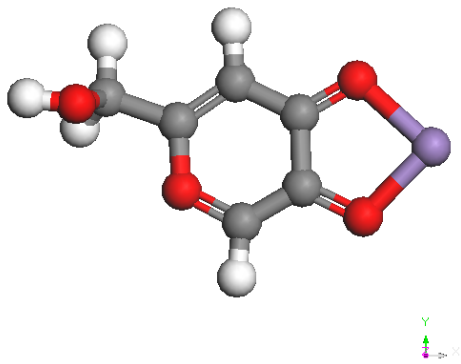
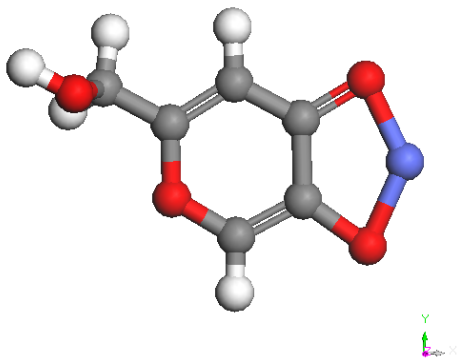
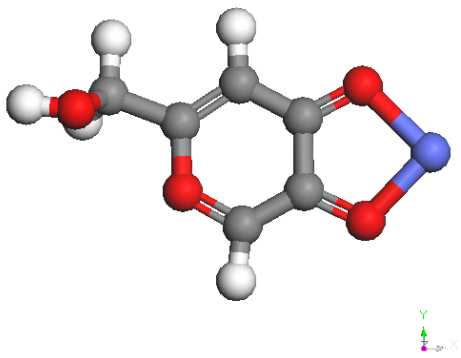
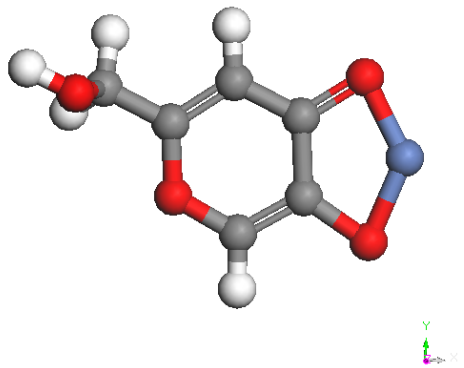
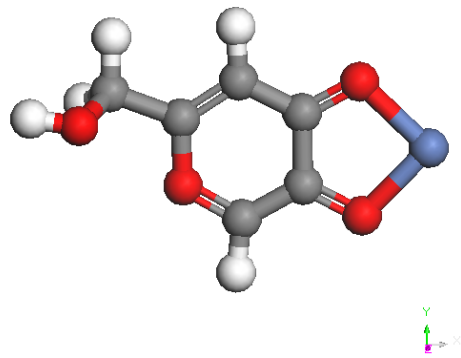
**Table A6:** Calculated vibrational frequencies ($cm^{-1}$) and intensities (km/mol) for the complexes

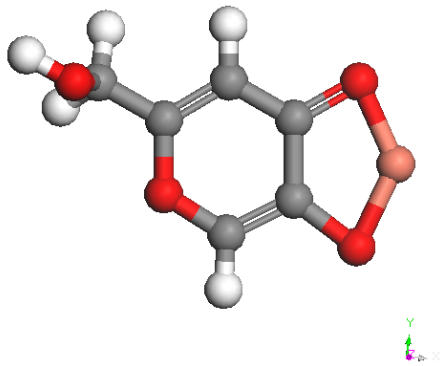
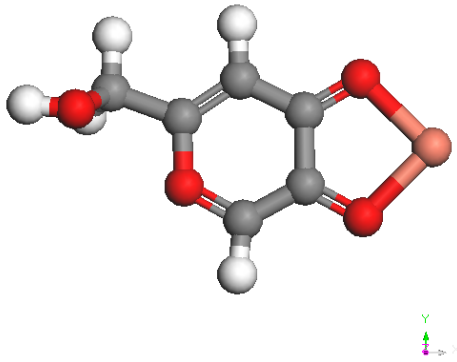
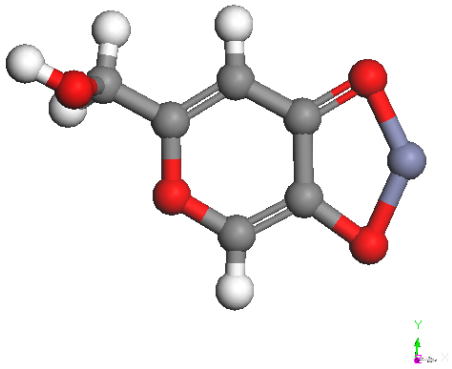
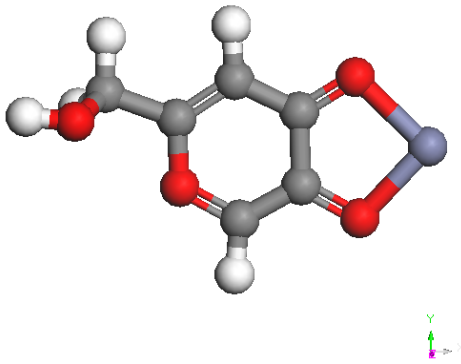
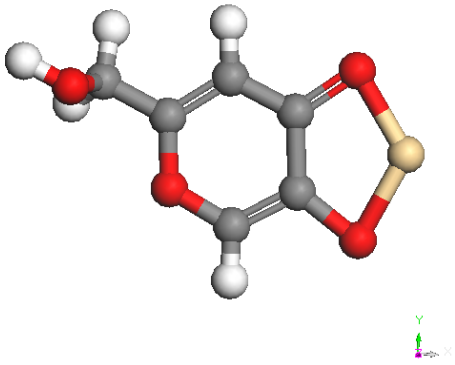
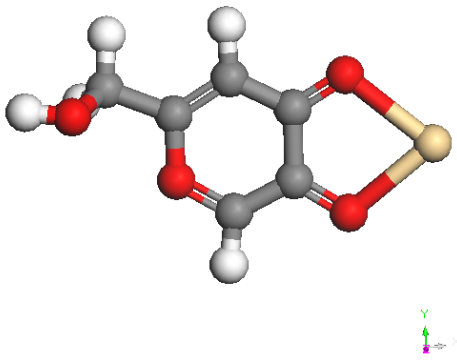
| **Mn(II)** | | **Co(II)** | | **Ni(II)** | | **Cu(II)** | | **Zn(II)** | | **Cd(II)** | | **Hg(II)** | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ | $\bar{\nu}$ | $I$ |
| 14 | 0 | -9 | 2 | -22 | 3 | 15 | 0 | 21 | 1 | -20 | 1 | -19 | 2 |
| 25 | 0 | 18 | 1 | 24 | 1 | 23 | 3 | 29 | 0 | 14 | 1 | 11 | 0 |
| 51 | 0 | 38 | 0 | 45 | 1 | 41 | 0 | 48 | 0 | 25 | 0 | 24 | 1 |
| 65 | 1 | 48 | 0 | 56 | 1 | 45 | 0 | 64 | 3 | 42 | 1 | 41 | 0 |
| 66 | 2 | 66 | 2 | 74 | 2 | 65 | 4 | 73 | 1 | 46 | 0 | 41 | 2 |
| 85 | 1 | 91 | 1 | 90 | 2 | 79 | 1 | 84 | 1 | 75 | 2 | 68 | 3 |
| 96 | 1 | 98 | 3 | 105 | 3 | 97 | 1 | 97 | 2 | 84 | 1 | 72 | 1 |
| 121 | 6 | 125 | 1 | 130 | 3 | 118 | 1 | 128 | 2 | 114 | 7 | 106 | 6 |
| 129 | 4 | 169 | 0 | 163 | 4 | 151 | 0 | 131 | 2 | 118 | 4 | 111 | 5 |
| 140 | 1 | 174 | 1 | 171 | 0 | 166 | 2 | 149 | 2 | 130 | 1 | 121 | 5 |
| 170 | 6 | 200 | 5 | 194 | 17 | 175 | 3 | 174 | 0 | 157 | 3 | 137 | 20 |
| 174 | 3 | 206 | 1 | 204 | 6 | 181 | 0 | 183 | 4 | 160 | 13 | 143 | 14 |
| 192 | 20 | 224 | 3 | 240 | 1 | 203 | 7 | 201 | 16 | 181 | 13 | 162 | 1 |
| 201 | 24 | 252 | 0 | 243 | 10 | 239 | 1 | 214 | 17 | 194 | 15 | 176 | 7 |
| 246 | 63 | 296 | 236 | 275 | 276 | 273 | 63 | 259 | 6 | 229 | 38 | 202 | 18 |
| 262 | 8 | 299 | 1 | 303 | 9 | 293 | 4 | 272 | 16 | 259 | 33 | 228 | 129 |
| 287 | 158 | 318 | 43 | 309 | 1 | 296 | 167 | 299 | 163 | 265 | 108 | 260 | 14 |
| 303 | 16 | 326 | 1 | 327 | 397 | 317 | 3 | 311 | 15 | 303 | 16 | 280 | 22 |
| 320 | 51 | 357 | 1 | 349 | 41 | 325 | 0 | 325 | 19 | 312 | 10 | 305 | 1 |
| 337 | 53 | 364 | 165 | 357 | 64 | 350 | 256 | 352 | 159 | 340 | 118 | 334 | 69 |
| 346 | 138 | 383 | 0 | 371 | 5 | 373 | 2 | 367 | 120 | 353 | 140 | 372 | 49 |
| 389 | 8 | 404 | 11 | 408 | 7 | 383 | 0 | 387 | 7 | 386 | 14 | 390 | 5 |
| 396 | 7 | 411 | 2 | 410 | 2 | 386 | 16 | 395 | 17 | 390 | 6 | 398 | 145 |
| 433 | 1 | 425 | 1 | 414 | 6 | 431 | 0 | 440 | 1 | 434 | 1 | 424 | 5 |
| 435 | 1 | 431 | 5 | 422 | 5 | 433 | 2 | 440 | 1 | 446 | 0 | 442 | 0 |
| 458 | 4 | 499 | 18 | 503 | 14 | 476 | 7 | 478 | 4 | 465 | 1 | 456 | 1 |
| 470 | 44 | 508 | 2 | 512 | 2 | 494 | 1 | 482 | 5 | 475 | 1 | 464 | 1 |
| 478 | 3 | 521 | 19 | 518 | 22 | 505 | 49 | 497 | 0 | 477 | 4 | 472 | 2 |
| 483 | 60 | 527 | 1 | 535 | 1 | 511 | 1 | 510 | 8 | 481 | 23 | 490 | 19 |
| 548 | 17 | 568 | 2 | 575 | 6 | 557 | 4 | 546 | 8 | 544 | 22 | 541 | 11 |
| 554 | 125 | 578 | 69 | 582 | 59 | 557 | 115 | 555 | 109 | 548 | 45 | 542 | 37 |
| 606 | 4 | 640 | 37 | 640 | 39 | 621 | 16 | 621 | 8 | 607 | 3 | 608 | 4 |
| 612 | 36 | 651 | 0 | 652 | 2 | 631 | 3 | 629 | 16 | 611 | 7 | 615 | 7 |
| 677 | 19 | 675 | 15 | 674 | 11 | 679 | 21 | 675 | 19 | 669 | 18 | 677 | 19 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 678 | 15 | 694 | 27 | 701 | 30 | 683 | 14 | 677 | 24 | 673 | 18 | 678 | 15 |
| 749 | 10 | 747 | 0 | 736 | 1 | 749 | 11 | 748 | 10 | 743 | 4 | 734 | 14 |
| 750 | 8 | 747 | 0 | 740 | 29 | 750 | 1 | 752 | 10 | 749 | 8 | 745 | 6 |
| 760 | 2 | 762 | 16 | 753 | 2 | 763 | 5 | 758 | 2 | 749 | 6 | 747 | 4 |
| 764 | 1 | 764 | 0 | 763 | 11 | 763 | 1 | 763 | 1 | 765 | 3 | 752 | 15 |
| 782 | 24 | 790 | 0 | 765 | 4 | 775 | 0 | 777 | 24 | 776 | 22 | 753 | 3 |
| 792 | 6 | 790 | 47 | 785 | 19 | 775 | 59 | 795 | 12 | 784 | 26 | 792 | 5 |
| 793 | 20 | 800 | 11 | 803 | 11 | 794 | 7 | 798 | 11 | 790 | 13 | 795 | 25 |
| 801 | 22 | 802 | 11 | 805 | 7 | 797 | 12 | 816 | 32 | 793 | 8 | 804 | 21 |
| 867 | 27 | 837 | 0 | 833 | 26 | 866 | 0 | 871 | 20 | 854 | 27 | 858 | 25 |
| 885 | 66 | 837 | 57 | 864 | 21 | 866 | 53 | 872 | 68 | 882 | 24 | 880 | 22 |
| 892 | 91 | 895 | 142 | 893 | 108 | 897 | 112 | 900 | 55 | 894 | 80 | 893 | 89 |
| 910 | 34 | 896 | 46 | 897 | 72 | 898 | 51 | 901 | 66 | 900 | 88 | 894 | 59 |
| 967 | 19 | 962 | 22 | 954 | 9 | 971 | 57 | 952 | 12 | 965 | 13 | 961 | 14 |
| 967 | 13 | 962 | 6 | 971 | 19 | 971 | 4 | 980 | 21 | 966 | 10 | 967 | 10 |
| 1021 | 126 | 1006 | 234 | 1008 | 155 | 1001 | 200 | 1022 | 120 | 1002 | 115 | 1010 | 122 |
| 1024 | 104 | 1006 | 0 | 1011 | 96 | 1002 | 0 | 1023 | 91 | 1020 | 112 | 1014 | 113 |
| 1140 | 25 | 1138 | 35 | 1131 | 25 | 1139 | 16 | 1146 | 17 | 1153 | 14 | 1142 | 23 |
| 1143 | 18 | 1139 | 5 | 1138 | 15 | 1140 | 3 | 1148 | 21 | 1157 | 14 | 1156 | 6 |
| 1144 | 17 | 1157 | 16 | 1153 | 34 | 1147 | 14 | 1158 | 11 | 1164 | 8 | 1159 | 6 |
| 1158 | 16 | 1157 | 0 | 1154 | 3 | 1148 | 0 | 1160 | 18 | 1167 | 20 | 1178 | 41 |
| 1174 | 74 | 1199 | 187 | 1195 | 203 | 1191 | 184 | 1187 | 67 | 1193 | 87 | 1188 | 8 |
| 1181 | 72 | 1201 | 3 | 1198 | 5 | 1193 | 6 | 1190 | 62 | 1199 | 48 | 1198 | 32 |
| 1225 | 68 | 1229 | 182 | 1226 | 103 | 1227 | 163 | 1215 | 66 | 1231 | 50 | 1221 | 153 |
| 1231 | 55 | 1231 | 1 | 1229 | 55 | 1230 | 2 | 1238 | 60 | 1236 | 97 | 1241 | 128 |
| 1299 | 374 | 1299 | 283 | 1299 | 276 | 1307 | 384 | 1294 | 160 | 1302 | 279 | 1287 | 275 |
| 1305 | 79 | 1303 | 5 | 1305 | 65 | 1314 | 10 | 1321 | 192 | 1313 | 139 | 1296 | 185 |
| 1314 | 1 | 1324 | 4 | 1325 | 6 | 1325 | 19 | 1327 | 29 | 1322 | 2 | 1329 | 19 |
| 1321 | 0 | 1324 | 6 | 1331 | 33 | 1325 | 2 | 1328 | 5 | 1329 | 12 | 1334 | 3 |
| 1328 | 3 | 1339 | 70 | 1337 | 26 | 1337 | 88 | 1336 | 2 | 1332 | 11 | 1342 | 2 |
| 1331 | 4 | 1340 | 1 | 1351 | 5 | 1338 | 0 | 1337 | 4 | 1334 | 1 | 1344 | 4 |
| 1369 | 100 | 1380 | 113 | 1375 | 79 | 1369 | 114 | 1387 | 55 | 1375 | 66 | 1364 | 84 |
| 1369 | 27 | 1381 | 0 | 1381 | 54 | 1369 | 0 | 1392 | 56 | 1398 | 75 | 1380 | 77 |
| 1417 | 240 | 1446 | 8 | 1429 | 3 | 1452 | 294 | 1430 | 209 | 1426 | 207 | 1407 | 80 |
| 1430 | 145 | 1446 | 1 | 1464 | 6 | 1458 | 16 | 1446 | 153 | 1432 | 86 | 1422 | 79 |
| 1446 | 3 | 1473 | 345 | 1481 | 480 | 1462 | 10 | 1448 | 1 | 1440 | 3 | 1439 | 3 |
| 1453 | 3 | 1479 | 24 | 1489 | 68 | 1462 | 0 | 1473 | 5 | 1442 | 2 | 1446 | 3 |
| 1513 | 427 | 1490 | 237 | 1494 | 95 | 1498 | 558 | 1521 | 323 | 1511 | 237 | 1526 | 42 |
| 1523 | 135 | 1497 | 17 | 1505 | 63 | 1508 | 42 | 1527 | 105 | 1517 | 92 | 1533 | 125 |
| 1567 | 625 | 1551 | 368 | 1546 | 321 | 1558 | 887 | 1577 | 640 | 1541 | 600 | 1552 | 472 |
| 1577 | 166 | 1556 | 30 | 1558 | 164 | 1570 | 42 | 1588 | 192 | 1559 | 258 | 1565 | 220 |
| 1630 | 200 | 1595 | 246 | 1603 | 324 | 1595 | 371 | 1614 | 223 | 1613 | 207 | 1602 | 206 |
| 1646 | 139 | 1600 | 76 | 1609 | 68 | 1602 | 61 | 1618 | 117 | 1625 | 204 | 1611 | 201 |
| 2946 | 47 | 2941 | 102 | 2927 | 49 | 2936 | 90 | 2921 | 42 | 2939 | 54 | 2924 | 44 |
| 2967 | 52 | 2941 | 0 | 2929 | 49 | 2936 | 8 | 2993 | 44 | 2946 | 50 | 2928 | 46 |
| 3093 | 11 | 3071 | 1 | 3040 | 7 | 3056 | 1 | 3106 | 10 | 3038 | 15 | 3027 | 9 |
| 3095 | 15 | 3071 | 24 | 3060 | 11 | 3056 | 24 | 3118 | 10 | 3044 | 11 | 3058 | 9 |
| 3168 | 1 | 3119 | 2 | 3118 | 1 | 3144 | 0 | 3159 | 2 | 3135 | 1 | 3144 | 1 |
| 3209 | 1 | 3119 | 1 | 3133 | 1 | 3145 | 0 | 3165 | 1 | 3154 | 2 | 3178 | 2 |
| 3216 | 5 | 3214 | 0 | 3179 | 8 | 3175 | 4 | 3181 | 1 | 3155 | 1 | 3185 | 3 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3235 | 3 | 3214 | 3 | 3185 | 6 | 3175 | 1 | 3189 | 1 | 3173 | 1 | 3188 | 1 |
| 3688 | 38 | 3712 | 38 | 3732 | 29 | 3733 | 31 | 3721 | 40 | 3723 | 35 | 3712 | 42 |
| 3702 | 40 | 3712 | 39 | 3732 | 32 | 3733 | 42 | 3734 | 41 | 3732 | 36 | 3713 | 39 |

**Table A7:** Optimized geometries and total energies (kcal/mol) of the metal kojate 1:1 complexes

| **Metal ion** | **Initial geometry** | **Final geometry** |
|---|---|---|
| Mn(II) |  |  **(-410223.4)** |
| Co(II) |  |  **(-438471.9)** |
| Ni(II) |  |  **(-455229.1)** |

| | | |
|---|---|---|
| Cu(II) |  |  **(-473386.7)** |
| Zn(II) |  |  **(-493412.2)** |
| Cd(II) |  |  **(-390125.1)** |

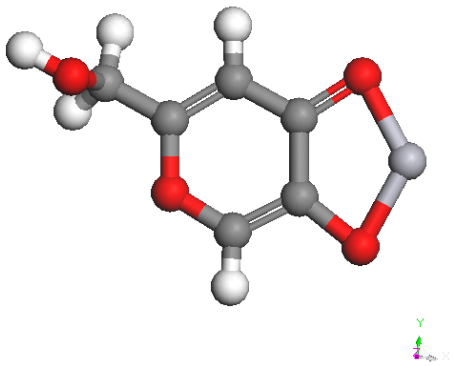
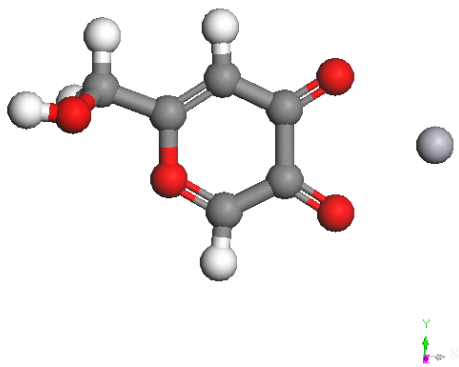
| | | |
|---|---|---|
| Hg(II) |  |  **(-477179.9)** |

**Table A8:** Calculated zero-point corrected energies (kcal/mol) of the complexes and the corresponding metal ions

| Metal ion | Energy of the complex | Energy of the metal ion |
|---|---|---|
| Mn(II) | -410157.3 | -75882.3 |
| Co(II) | -438406.1 | -104070.4 |
| Ni(II) | -455163.7 | -120785.0 |
| Cu(II) | -473321.3 | -138969.5 |
| Zn(II) | -493346.5 | -159028.4 |
| Cd(II) | -390060.2 | -55786.7 |
| Hg(II) | -477115.7 | -142797.6 |

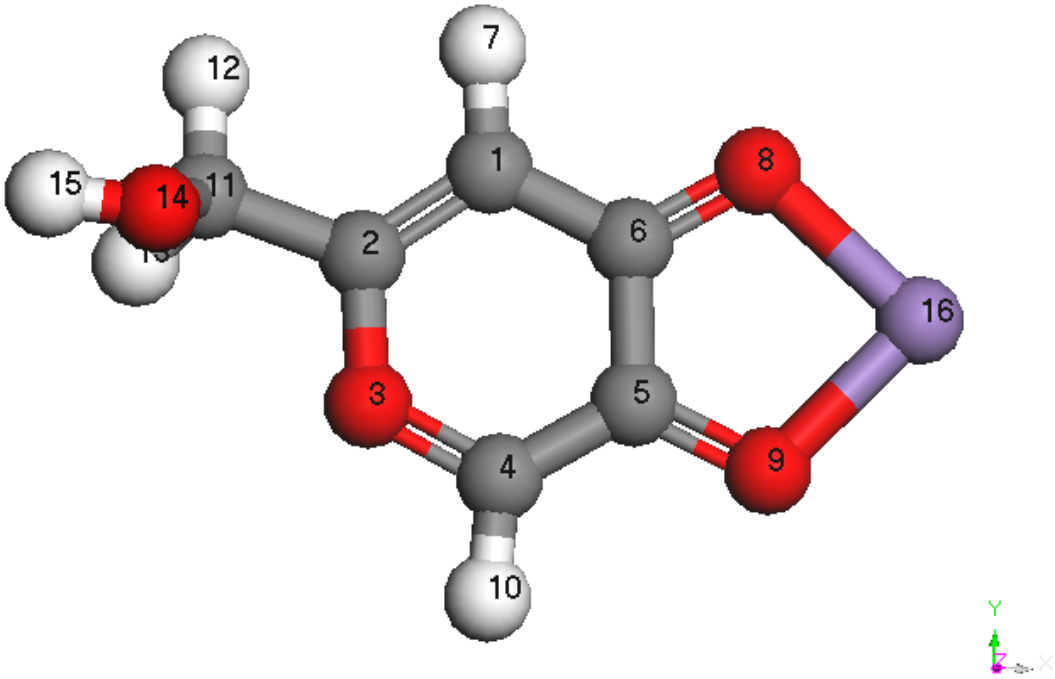



**Figure 1**Metal kojate complex with the atom numbering