

Title:

Synthesis and molecular structure of oxydiacetate complexes of nickel(II) and cobalt(II). Theoretical analysis of the planar and non planar conformations of oxydiacetate ligand and oxydiacetic acid

Authors

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Cartesian Coordinates of computed models.

1) oxydiacetic acid, shown in Figure 2 (symmetry C_2)

C,0.7725732117,0.5184454954,0.918354152
C,-0.0575894414,-0.1452814507,2.0089597486
H,1.4587187314,1.227054019,1.3906746231
H,1.3874050061,-0.2458681895,0.4253285631
O,-0.0000001353,1.2578759779,0.0000000739
O,-1.2647714784,-0.2383804932,2.0382017232
O,0.7486947335,-0.6571206039,2.970149183
C,-0.7725733232,0.518445437,-0.9183540911
C,0.0575894726,-0.1452812024,-2.0089597657
H,-1.4587189954,1.2270538685,-1.390674479
H,-1.3874049532,-0.2458684379,-0.425328592
O,1.2647715297,-0.2383799817,-2.0382017512
O,-0.7486945921,-0.6571204161,-2.9701492602
H,0.1796932303,-1.0876685933,3.6311013829
H,-0.1796929963,-1.0876682055,-3.6311015106

2) oxydiacetic acid, shown in Figure 2 (symmetry C_{2v})

C,0.,2.3864659925,0.16169009
C,0.,1.1659124335,-0.7416004448
H,-0.8865774911,1.2246415531,-1.394078492
H,0.8865774911,1.2246415531,-1.394078492
O,0.,0.,0.0406691455
C,0.,-1.1659124335,-0.7416004448
H,0.8865774911,-1.2246415531,-1.394078492
H,-0.8865774911,-1.2246415531,-1.394078492
C,0.,-2.3864659925,0.16169009
O,0.,2.3993538928,1.3663972229

O,0.,3.510708845,-0.6035478803
O,0.,-2.3993538928,1.3663972229
O,0.,-3.510708845,-0.6035478803
H,0.,4.2710861175,0.0021477902
H,0.,-4.2710861175,0.0021477902

3) oxydiacetic acid, shown in Figure 2 (symmetry C_s)

C,-0.2683120953,1.8670765346,0.0096835647
C,1.1052446949,1.199410512,-0.0239870578
H,1.4072578812,1.0688149584,-1.0719286208
H,1.8078085669,1.9110743426,0.4272422211
O,1.1932139975,0.,0.7067174737
O,-1.1968444935,1.5970863499,0.7272062048
O,-0.2860247452,2.8913544228,-0.8889825822
H,-1.1465641262,3.3356653649,-0.8021515176
C,-0.2683120953,-1.8670765346,0.0096835647
C,1.1052446949,-1.199410512,-0.0239870578
H,1.4072578812,-1.0688149584,-1.0719286208
H,1.8078085669,-1.9110743426,0.4272422211
O,-1.1968444935,-1.5970863499,0.7272062048
O,-0.2860247452,-2.8913544228,-0.8889825822
H,-1.1465641262,-3.3356653649,-0.8021515176

4) oxydiacetate dianion, shown in Figure 3.

C,0.,2.5504836304,0.1018532513
C,0.,1.1659948692,-0.6245534653
H,-0.8829219679,1.1587253469,-1.2912099637
H,0.8829219679,1.1587253469,-1.2912099637
O,0.,0.,0.1865942229

C,0.,-1.1659948692,-0.6245534653
H,0.8829219679,-1.1587253469,-1.2912099637
H,-0.8829219679,-1.1587253469,-1.2912099637
C,0.,-2.5504836304,0.1018532513
O,0.,2.6067170574,1.3525678581
O,0.,3.5129283775,-0.7310373181
O,0.,-2.6067170574,1.3525678581
O,0.,-3.5129283775,-0.7310373181

5) complex Ni(oda)(H₂O)₃, *mer* isomer, shown in Figure 4.

Ni,0.5521340879,0.5123490513,-0.0607239829
O,0.7857603236,0.1186966004,1.8694548488
O,-0.0827234017,0.6260328294,-1.9349700711
O,-1.2103629241,-0.4736514957,0.2121270866
O,-0.0094949613,-1.2636891052,3.4690332585
O,-1.5774166652,-0.3379925937,-3.3271963131
O,1.6126798698,-1.3012293583,-0.5661975287
O,2.382201615,1.5687336211,-0.3300371184
O,-0.3231983932,2.4236058143,0.4367660118
C,-0.0239433244,-0.7880601133,2.3399967127
C,-1.0938095199,-1.3431732613,1.3594816255
H,-0.7868103977,-2.3446523689,1.0341854944
H,-2.0582451941,-1.4125903327,1.8698917719
C,-1.6578576066,-1.0086163283,-1.0527079303
H,-2.7502293928,-0.9898305779,-1.0955104359
H,-1.3125415885,-2.0442081742,-1.1585774214
C,-1.0754515823,-0.1676356791,-2.2224079748
H,2.3612074813,-1.4318065705,0.0336577754
H,1.9674599386,-1.2196121086,-1.4635539957
H,2.6130380325,2.0167272018,0.4970459681
H,2.2567855952,2.2571524333,-0.9995998702

H,-0.6585227606,2.3359120595,1.3417043958

H,-1.0837467986,2.5714873078,-0.1442279838

6) complex Ni(oda)(H₂O)₃, *fac* isomer, shown in Figure 4.

Ni,0.000000254,0.7931777302,0.

O,1.1590969652,-1.0108394554,0.

C,0.8913658504,-1.7275204125,1.233849

H,0.6953866819,-2.7803443812,1.018595

H,1.7968628596,-1.6702895575,1.846538

C,-0.2869390582,-1.1564872239,2.051961

O,-0.8063918804,-0.0458131407,1.614539

O,-0.605622155,-1.7613611729,3.06752

O,0.9316244466,1.996600581,1.539266

O,-1.7636315543,1.9908260125,0.

H,-2.2128976153,1.6099450844,-0.773363

C,0.8913658504,-1.7275204125,-1.233849

H,0.6953866819,-2.7803443812,-1.018595

H,1.7968628596,-1.6702895575,-1.846538

C,-0.2869390582,-1.1564872239,-2.051961

O,-0.8063918804,-0.0458131407,-1.614539

O,-0.605622155,-1.7613611729,-3.06752

O,0.9316244466,1.996600581,-1.539266

H,-2.2128976153,1.6099450844,0.773363

H,0.478284382,1.5927366536,-2.30007

H,1.8770544491,2.0121534297,-1.735871

H,1.8770544491,2.0121534297,1.735871

H,0.478284382,1.5927366536,2.30007