Supporting Information

Dissolution and Reduction of Cobalt ions in Polyol Process Using Ethylene Glycol

- Identification of the Active Species and its Role -

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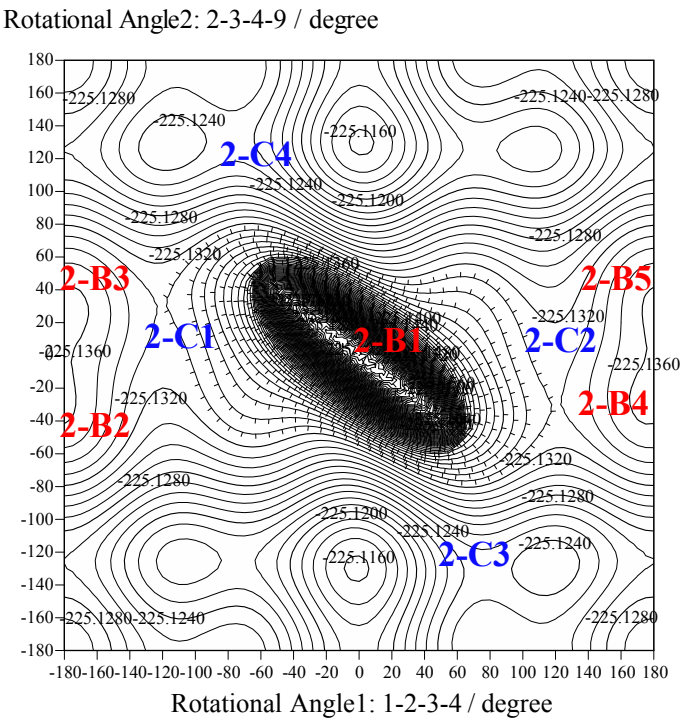
(a)



(b)

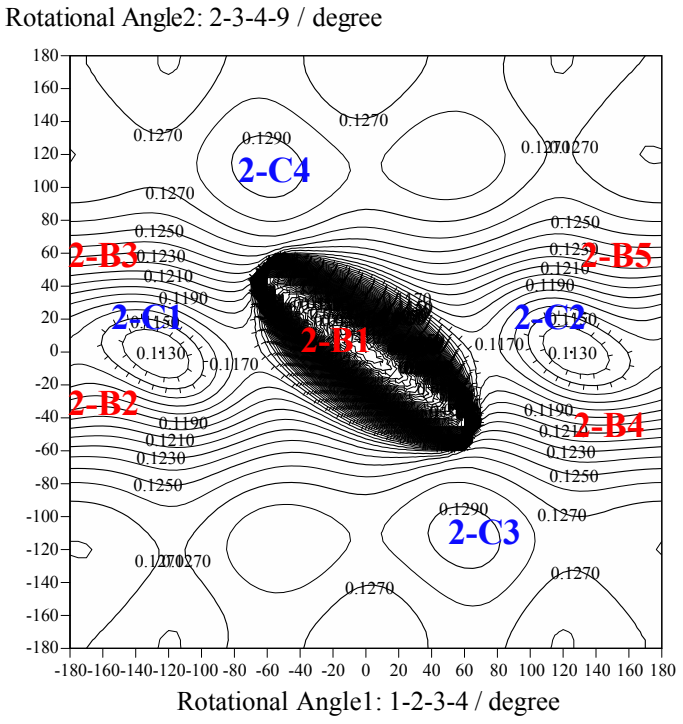
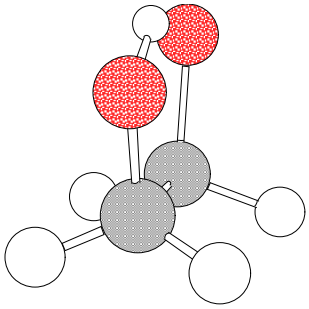


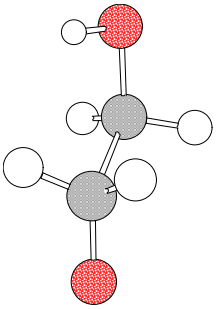
Figure S1. (a) SCF energy surface and (b) HOMO energy surface at each conformer for the ethylene glycol at mono-anion state.



2-B1

(Angle1, Angle2)=(0,0)

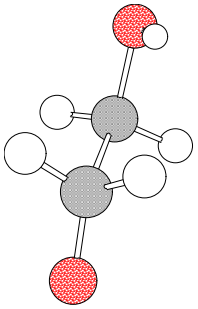
0.03897 a.u.



2-B2

(-180,25)

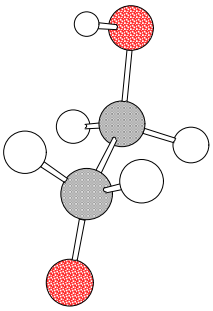
0.11743 a.u.



2-B3

(-175,25)

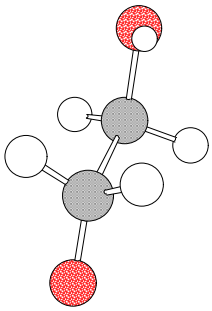
0.11729 a.u.



2-B4

(175,-25)

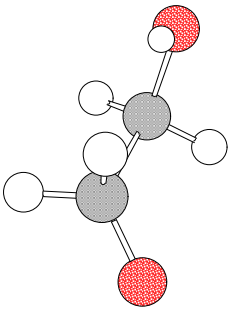
0.11720 a.u.



2-B5

(180,20)

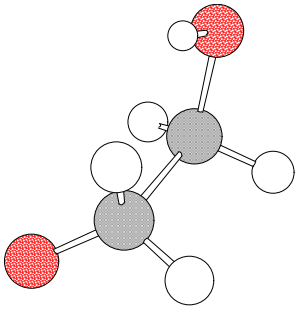
0.11684 a.u.



2-C1

(-125,0)

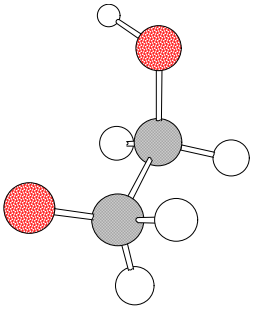
0.11300 a.u.



2-C2

(-125,0)

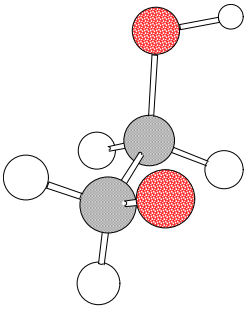
0.11300 a.u.



2-C3

(60,-110)

0.12943 a.u.



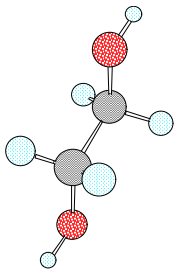
2-C4

(-60,110)

0.12943 a.u.

Figure S2. Characteristic conformers of the mono anion state derived from ethylene glycol, the rotational angles and theirs HOMO energies

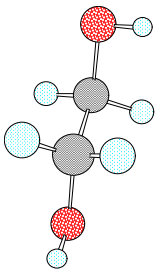
<The case of the starting structure: **3-D**>



3-D1

(180,180)

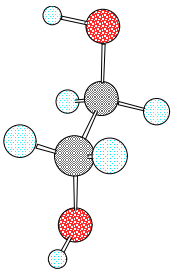
-0.35570 a.u.



3-D2

(180,65)

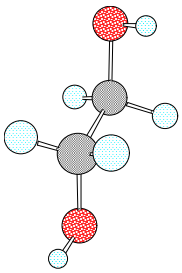
-0.35358 a.u.



3-D3

(180,-65)

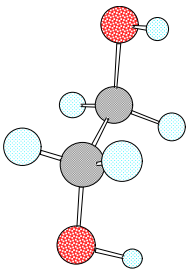
-0.35358 a.u.



3-D4

(65,180)

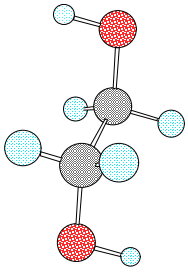
-0.35358 a.u.



3-D5

(60,60)

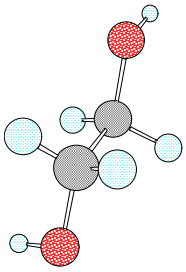
-0.33955 a.u.



3-D6

(65,-65)

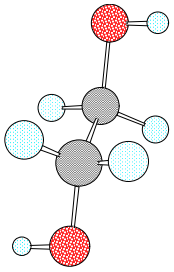
-0.33627 a.u.



3-D7

(-65,180)

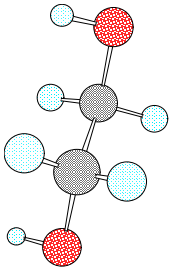
-0.35358 a.u.



3-D8

(-65,65)

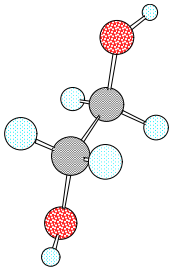
-0.33627 a.u.



3-D9

(-60,-60)

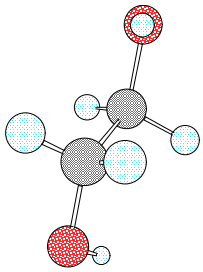
-0.33955 a.u.



3-D10

(165,165)

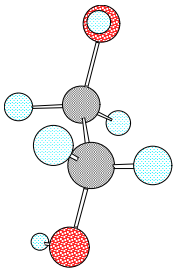
-0.35705 a.u.



3-D11

(15,20)

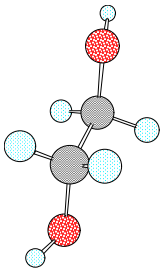
-0.36308 a.u.



3-D12

(-15,-20)

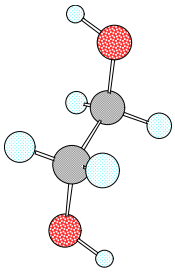
-0.36308 a.u.



3-D13

(60,60)

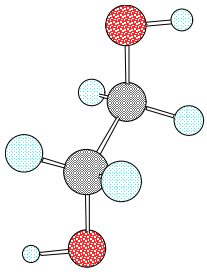
-0.33955 a.u.



3-D14

(65,-65)

-0.33627 a.u.



3-D15

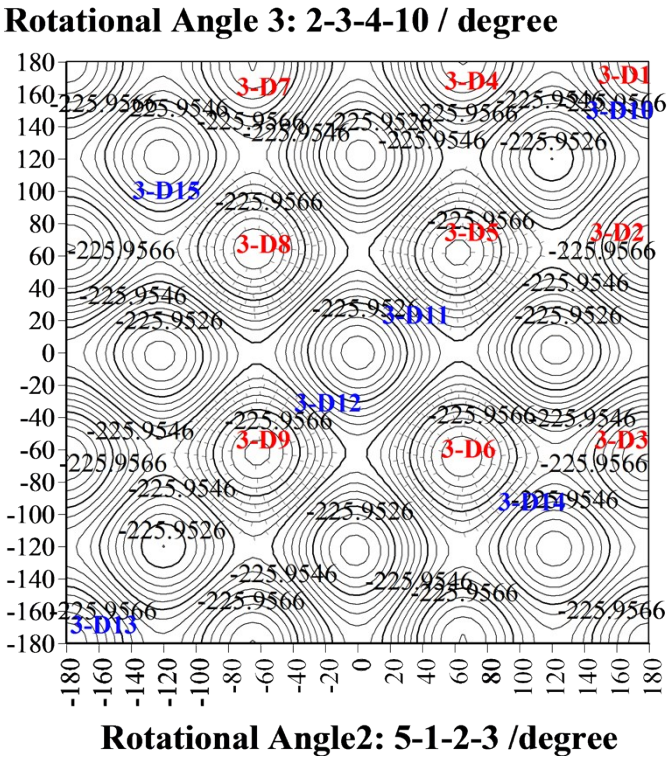
(-65,180)

-0.35358 a.u.

Figure S3. Stable conformers obtained using **3-D** as starting structure

<The case of the starting structure: **3-D**>

(a)



(b)

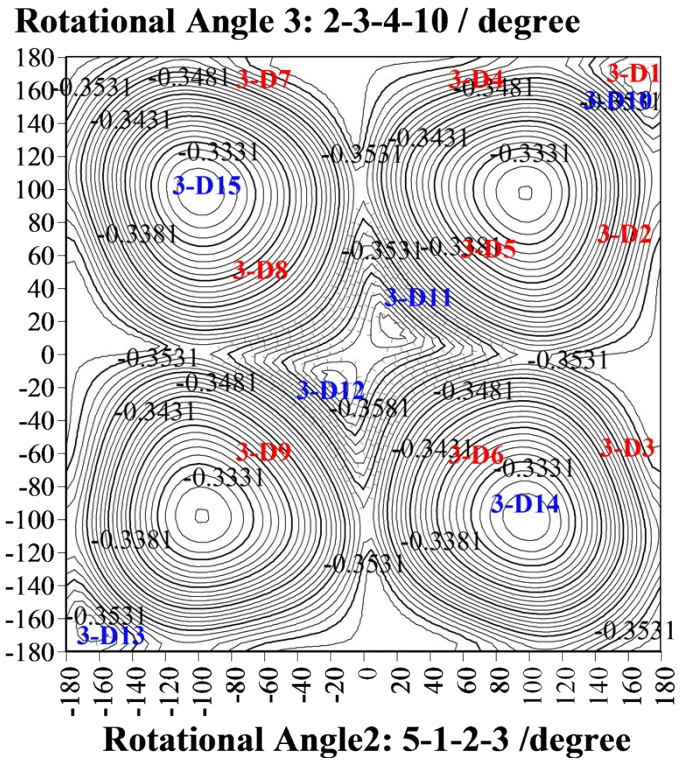
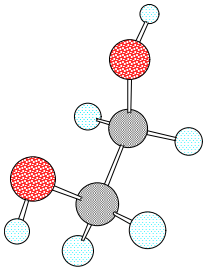


Figure S4. (a) SCF and (b) HOMO orbital energy surfaces for neutral state ethylene glycol obtained using **3-D** as starting structure

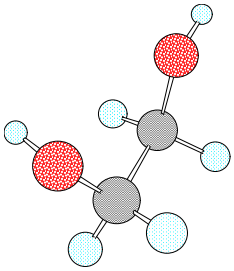
<The case of the starting structure: **3-E**>



3-E1

(180,180)

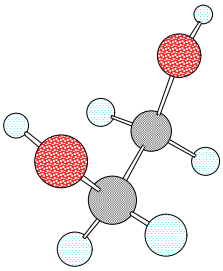
-0.34776 a.u.



3-E2

(180,55)

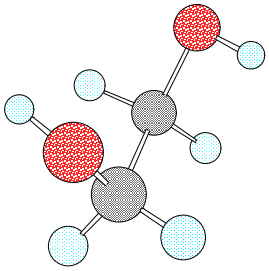
-0.34885 a.u.



3-E3

(55,180)

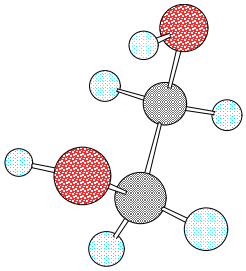
-0.34885 a.u.



3-E4

(55,55)

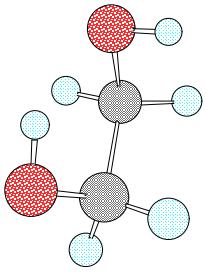
-0.33829 a.u.



3-E5

(75,-30)

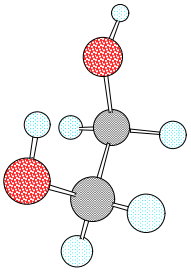
-0.34290 a.u.



3-E6

(-30,75)

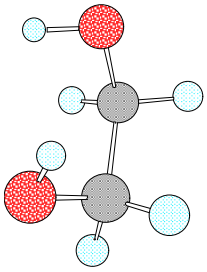
-0.34290 a.u.



3-E7

(-40,-175)

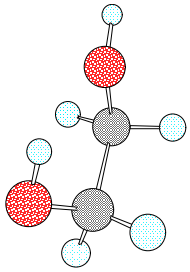
-0.34102 a.u.



3-E8

(-70,-70)

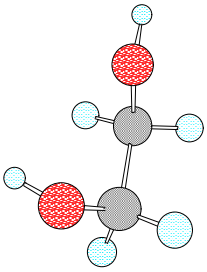
-0.33688 a.u.



3-E9

(-175,-40)

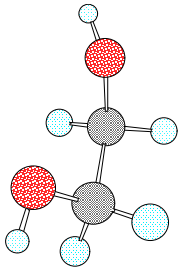
-0.34102 a.u.



3-E10

(180,50)

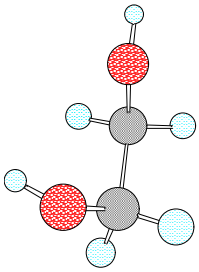
-0.34895 a.u.



3-E11

(165,-155)

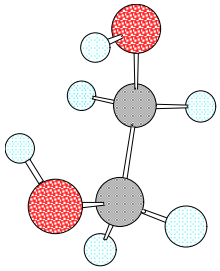
-0.35018a.u.



3-E12

(15,180)

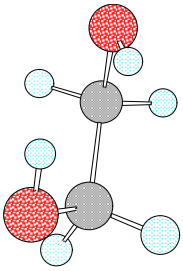
-0.34895 a.u.



3-E13

(15,-30)

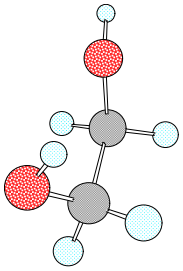
-0.36278 a.u.



3-E14

(-30,15)

-0.36278 a.u.



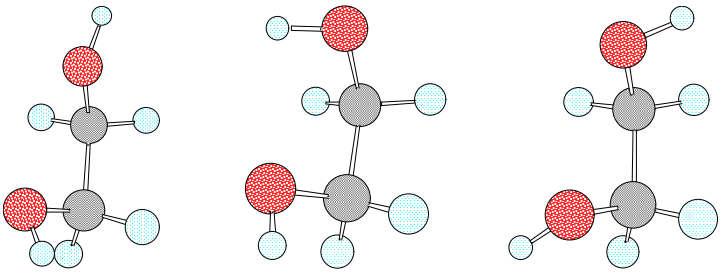
3-E15

(-75,-170)

-0.34403 a.u.

Figure S5. Stable conformers obtained using **3-E** as starting structure

<The case of the starting structure: **3-E**> (Continued)

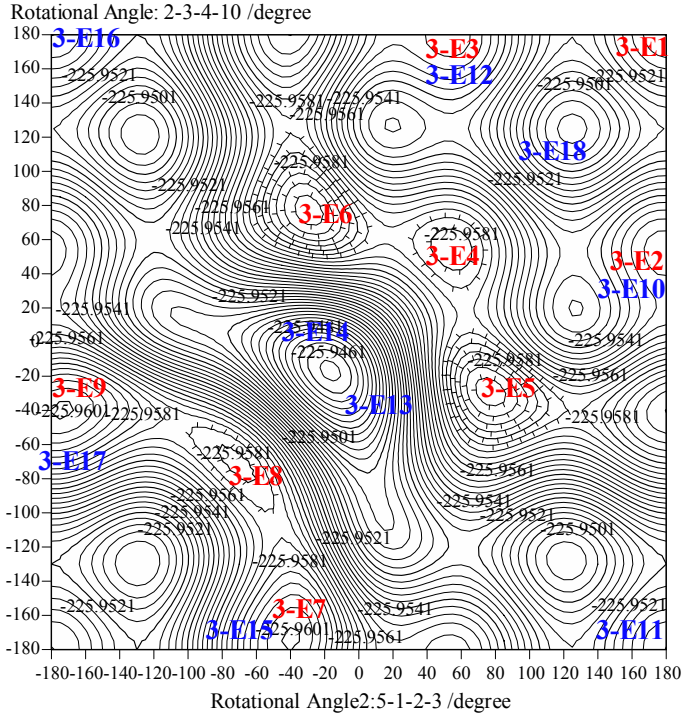


3-E16	**3-E17**	**3-E18**
(-155,165)	(-170,-75)	(105,105)
-0.35018 a.u.	-0.34403 a.u.	-0.32517 a.u.

Figure S5. Stable conformers obtained using **3-E** as starting structure (Continued)

<The case of the starting structure: **3-E**>

(a)



(b)

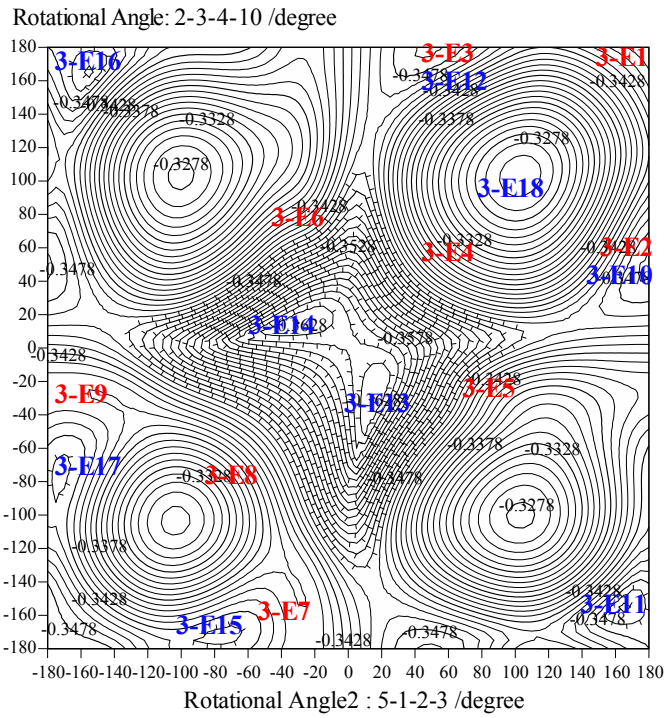
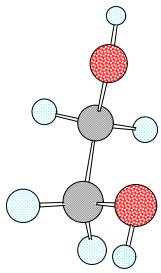


Figure S6. (a) SCF and (b) HOMO orbital energy surfaces for neutral state ethylene glycol obtained using **3-E** as starting structure

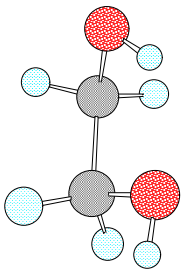
<The case of the starting structure: **3-F**>



3-F1

(180,180)

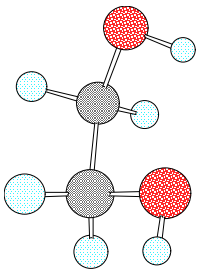
-0.34776 a.u.



3-F2

(175,40)

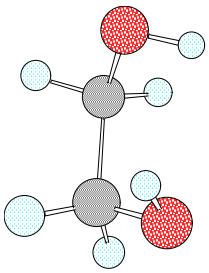
-0.34102 a.u.



3-F3

(180,55)

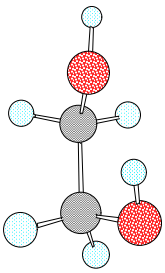
-0.34248 a.u.



3-F4

(70,70)

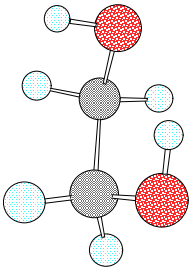
-0.33688 a.u.



3-F5

(40,175)

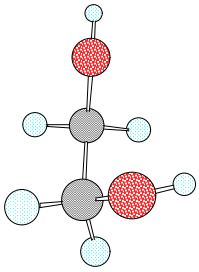
-0.34102 a.u.



3-F6

(30,-75)

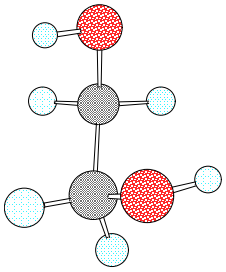
-0.34290 a.u.



3-F7

(-55,180)

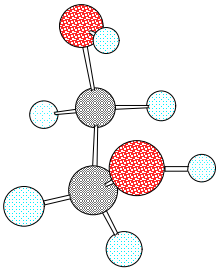
-0.34885 a.u.



3-F8

(-55,-55)

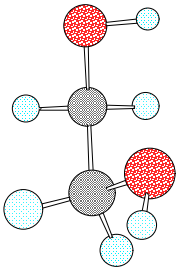
-0.33829 a.u.



3-F9

(-75,30)

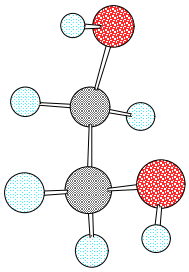
-0.34290 a.u.



3-F10

(170,75)

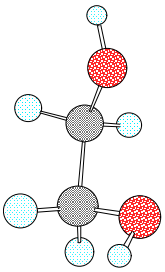
-0.34403 a.u.



3-F11

(180,-50)

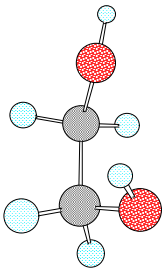
-0.34895 a.u.



3-F12

(155,-165)

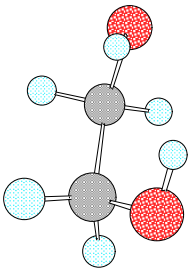
-0.35018 a.u.



3-F13

(75,170)

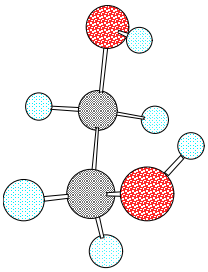
-0.34403 a.u.



3-F14

(30,-15)

-0.36278 a.u.



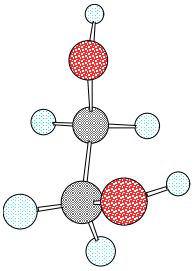
3-F15

(-15,30)

-0.36278 a.u.

Figure S7. Stable conformers obtained using **3-F** as starting structure

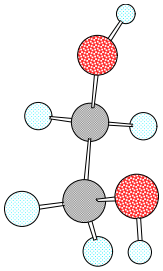
<The case of the starting structure: **3-F**> (Continued)



3-F16

(-50,180)

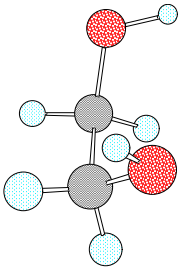
-0.34895 a.u.



3-F17

(-165,155)

-0.35018 a.u.



3-F18

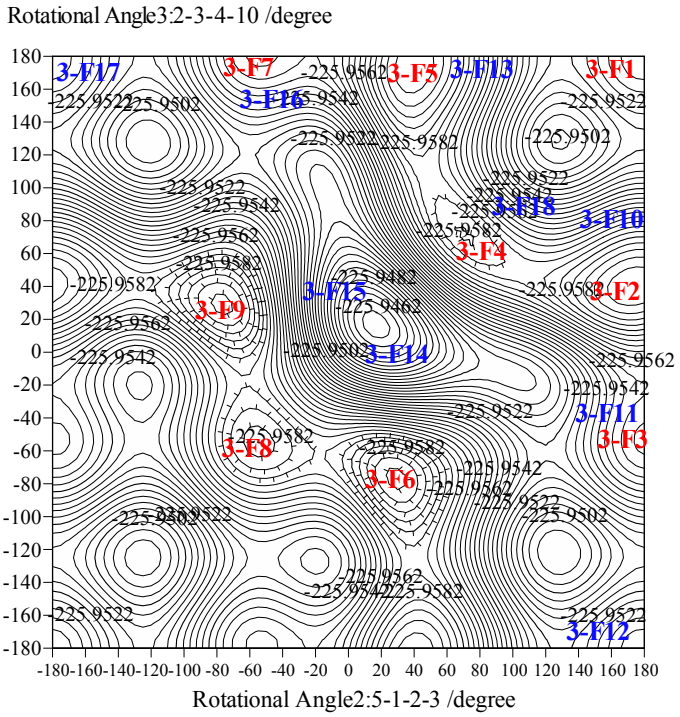
(105,105)

-0.32517 a.u.

Figure S7. Stable conformers obtained using **3-F** as starting structure (Continued)

<The case of the starting structure: **3-F**>

(a)



(b)

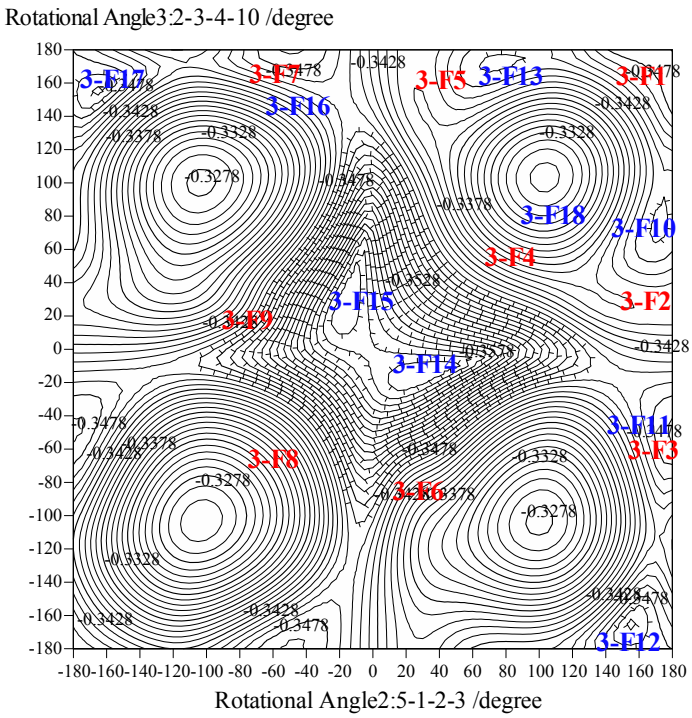


Figure S8. (a) SCF and (b) HOMO orbital energy surfaces for neutral state ethylene glycol obtained using **3-F** as starting structure

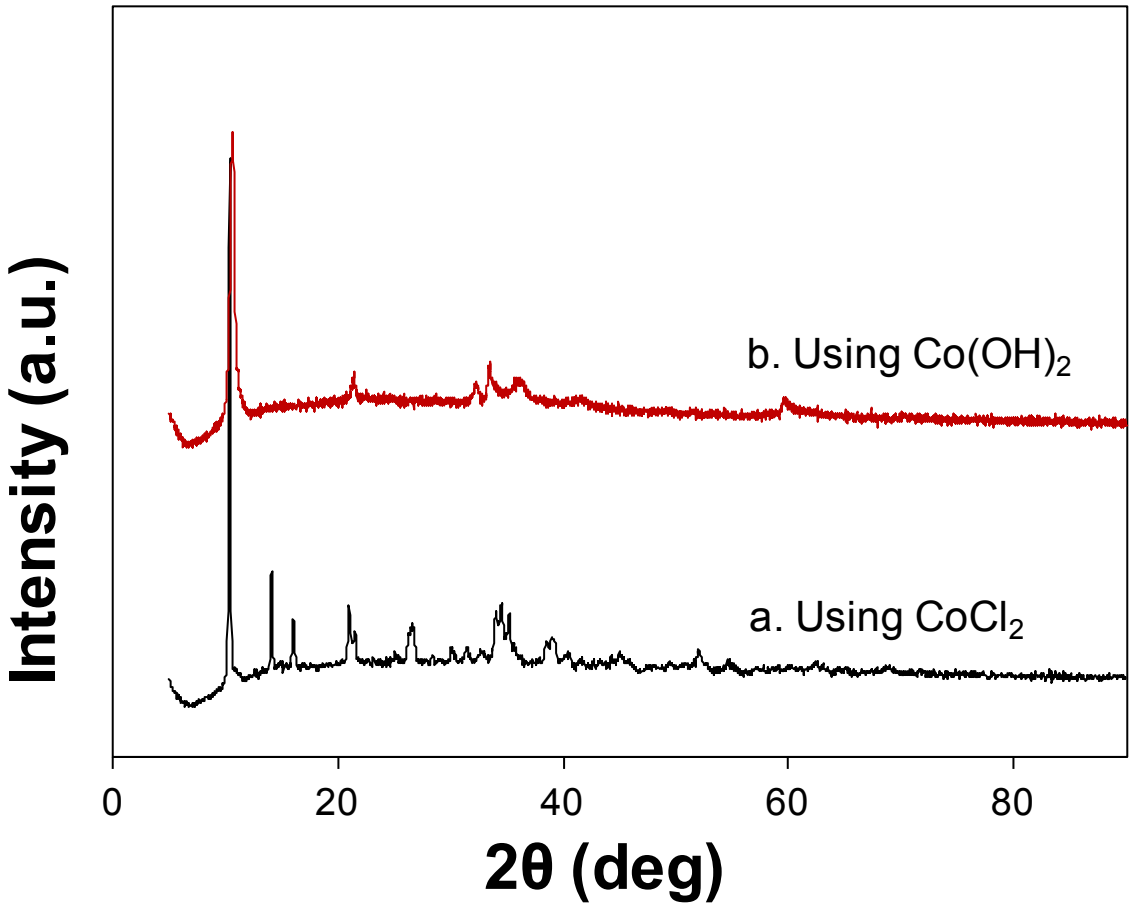
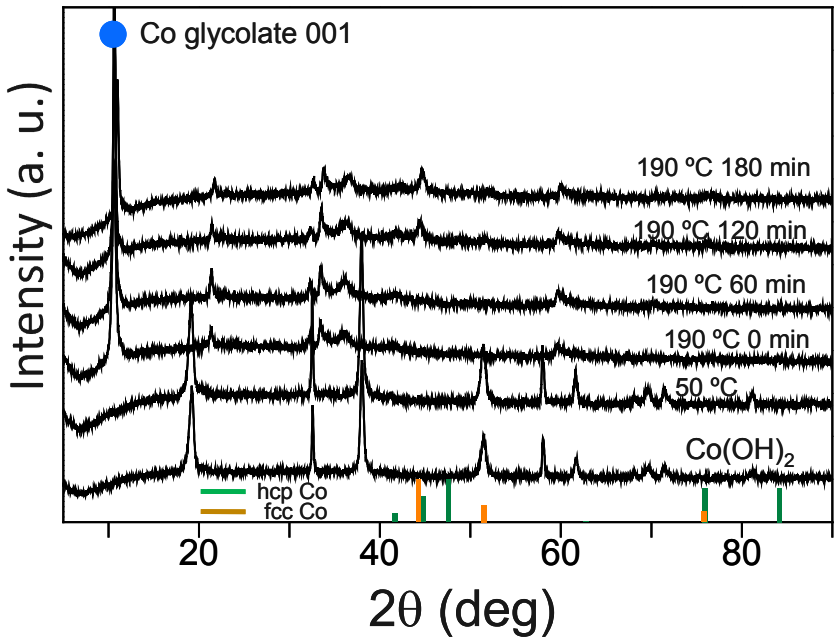


Figure S9. XRD patterns of glycolate prepared by using (a) $CoCl_2$ and metallic Na in ethylene glycol and (b) $CoCl_2$ and NaOH.

(a)



(b)

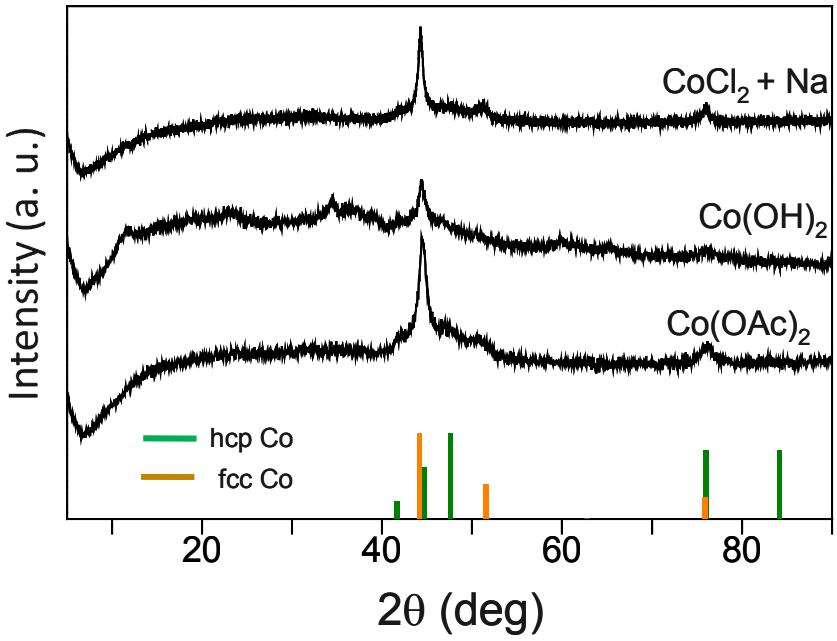
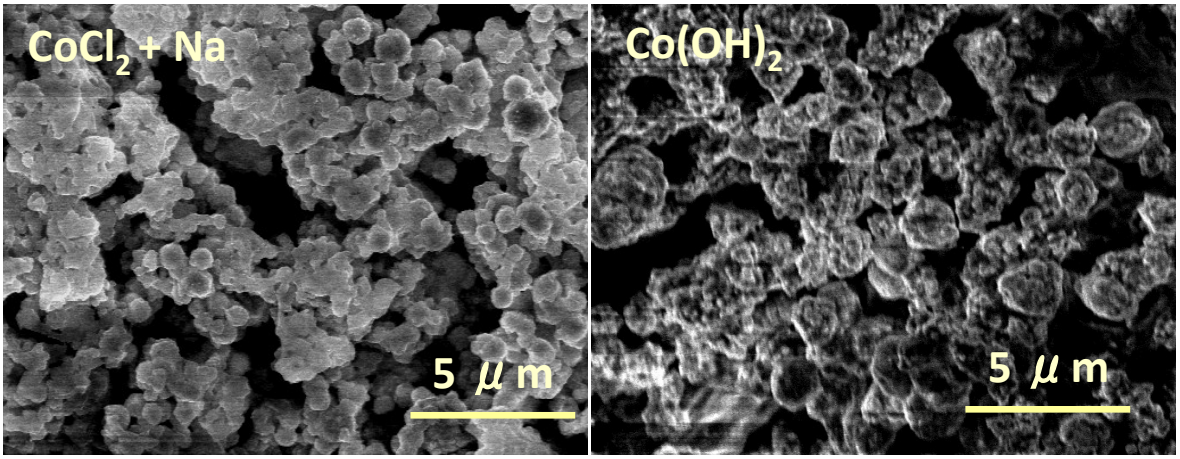


Figure S10. XRD patterns of (a) profiles obtained at different stages of the reduction reaction when $Co(OH)_2$ was heated in ethylene glycol and (b) Co nanoparticles obtained using different cobalt sources.

(a) (b)



(c)

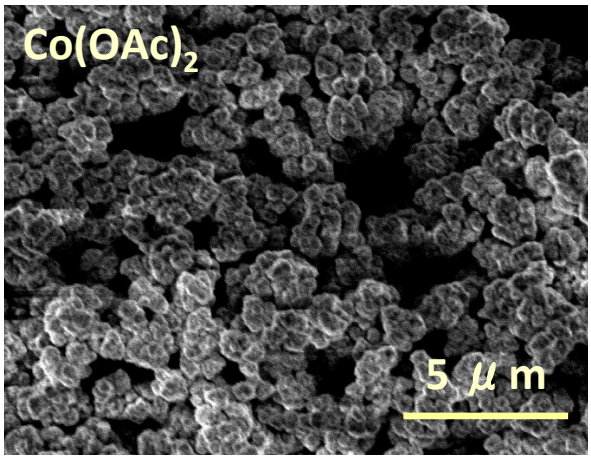


Figure S11. SEM images of metallic cobalt particles obtained using (a) $CoCl_2$, (b) $Co(OH)_2$, and (c) $Co(OAc)_2$ as metallic precursors in ethylene glycol.