

A New Role for Surfactants in the Formation of Cobalt Nanoparticles

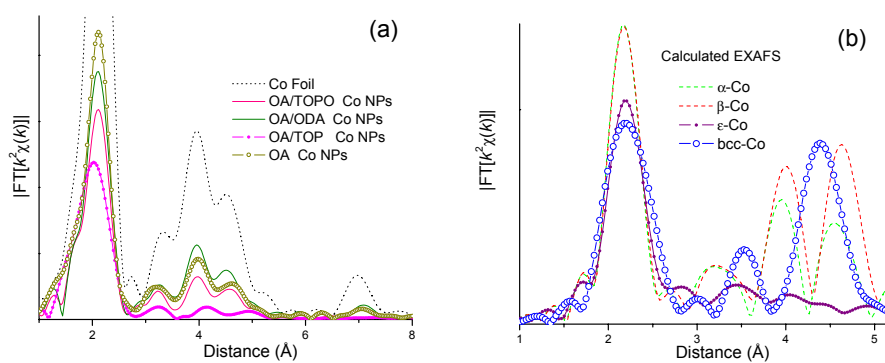
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Supporting Materials

- (1) **S1.** Table of EXAFS Fitting results for the Co NPs obtained using OA/ODA. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7 Å, k-weights=1,2,3.
- (2) **S2.** Experimental (a) and theoretical (b) FT EXAFS spectra of Co NPs
- (3) **S3.** Table of EXAFS Fitting results for the Co NPs obtained using OA. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7 Å, k-weights=1,2,3.
- (4) **S4.** Table of EXAFS Fitting results for the Co NPs obtained using OA/TOPO. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7 Å, k-weights=1,2,3.
- (5) **S5.** Table of EXAFS Fitting results for the Co NPs obtained using OA/TOP. k range: 3-12 Å⁻¹, R range: 1.5-5.4 Å, k-weights=1,2,3.
- (6) **S6.** FT-IR comparison of 7 min (red), 8 min (blue) spectra of the reaction mixture with the spectrum of the tricobalt intermediates (green) leading to cobalt nanoparticles.
- (7) **S7.** B3LYP optimized structure of [Co₃(μ-CO)₃(CO)₃CCH₃]. Blue, grey, red and white balls represent Co, C, O and hydrogen respectively. The calculated carbonyl vibration energies at 1812, 1856, 1975 and 2011 cm⁻¹ result from B3LYP method.
- (8) **S8.** B3LYP optimized structure of the suggested {Co(CO)[P(C₈H₁₅)]₃} intermediate Co complex showing the tetrahedral geometry around the Co atom (H atoms are removed for clarity)
- (9) **S9.** Table of the magnetic data from SQUID magnetometer
- (10) **S10.** Hysteresis loops - Magnetization vs Applied Magnetic field (300K and 10K)
- (11) **S11.** A summary of the influence of surfactants on the reaction mechanism and in turn on the properties of Co nanoparticles obtained.

Co-NPs (OA-ODA)	fcc fit	hcp fit
dr_1	-0.021+/-0.004	-0.018+/-0.005
Rmult	0.004 +/-0.002	0.003+/-0.003
N1	5.5+/-0.3	5.6+/-0.4
Nmult	0.46+/-0.02	0.47+/-0.03
E0_1	-0.6+/-0.6	-1.3+/-0.7
E0	2.7+/-0.8	2.6+/-1.5
ss1	0.0075+/-0.0004	0.0077+/-0.0006
χ^2_v	242	354
R-factor	0.013	0.014

S1: Table of EXAFS Fitting results for the Co NPs obtained using OA/ODA. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7Å, k-weights=1,2,3.



S2. Experimental (a) and theoretical (b) FT EXAFS spectra

Co NPs (OA)	fcc fit	hcp fit
dr_1	-0.023+/-0.005	-0.019+/-0.004
Rmult	0.007+/-0.003	0.005+/-0.004
N1	6.6+/-0.4	6.7+/-0.4
Nmult	0.55+/-0.03	0.56+/-0.03
E0_1	-1.5+/-0.7	-1.9+/-0.6
E0	3.8+/-0.8	3.5+/-1.4
ss1	0.0081+/-0.0005	0.0081+/-0.0006
χ^2_v	172	143
R-factor	0.015	0.012

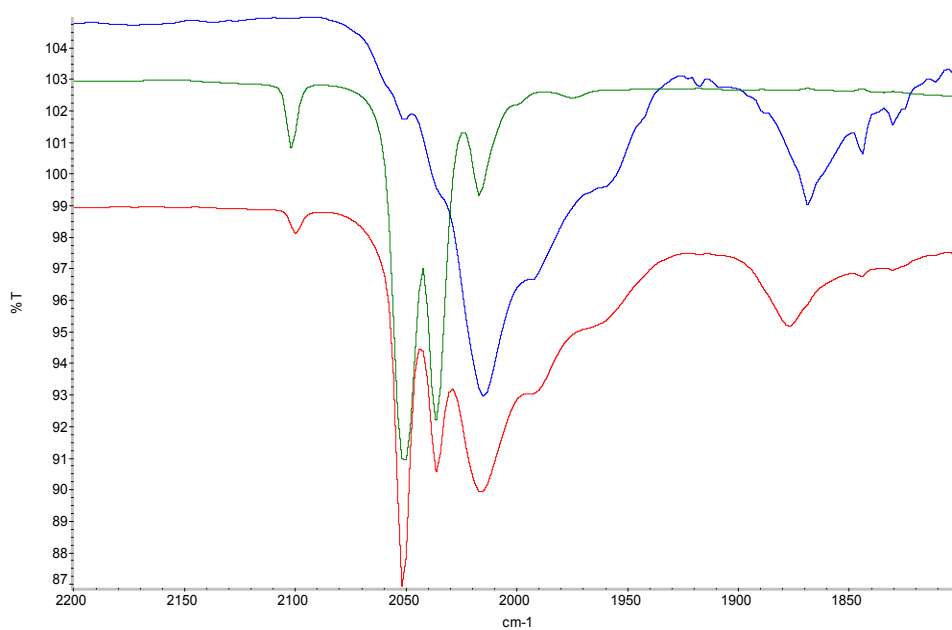
S3 - Table of EXAFS Fitting results for the Co NPs obtained using OA. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7Å, k-weights=1,2,3.

Co NPs (OA/TOPO)	fcc fit	hcp fit
dr_1	-0.019+/-0.004	-0.018 +/-0.005
Rmult	0.005+/-0.002	0.006+/-0.004
N1	5.8+/-0.3	5.8+/-0.4
Nmult	0.48+/-0.02	0.48+/-0.03
E0_1	-0.7+/-0.6	-1.6+/-0.7
E0	3.8+/-0.8	4.1+/-1.5
ss1	0.0095+/-0.0005	0.0095+/-0.0007
χ^2_v	117	209
R-factor	0.012	0.017

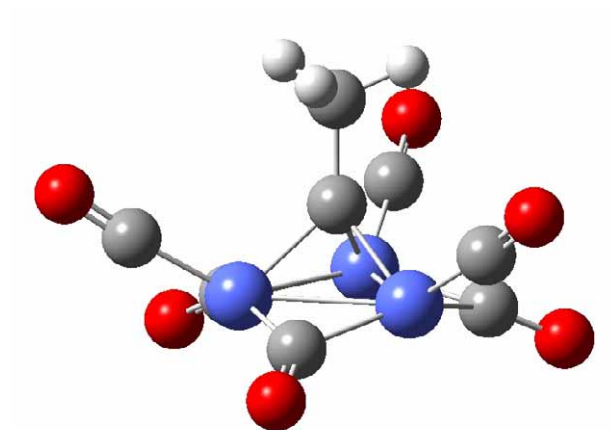
S4 -Table of EXAFS Fitting results for the Co NPs obtained using OA/TOPO. k range: 2.5-14 Å⁻¹, R range: 1.7-5.7Å, k-weights=1,2,3.

Co NPs (OA/TOP)	bcc fit	epsilon fit
dr_1	-0.006+/-0.017	-0.1 +/-0.01
Rmult	-0.025+/-0.026	-0.019+/-0.011
N1	8.6+/-2.0	8.8+/-1.6
Nmult	0.7+/-0.17	0.7+/-0.1
E0_1	-5.6+/-2.8	-5.5+/-1.9
E0	-6.9+/-6.8	-5.5+/-1.9
ss1	0.012+/-0.002	0.011+/-0.002
χ^2_v	1769	1648
R-factor	0.055	0.059

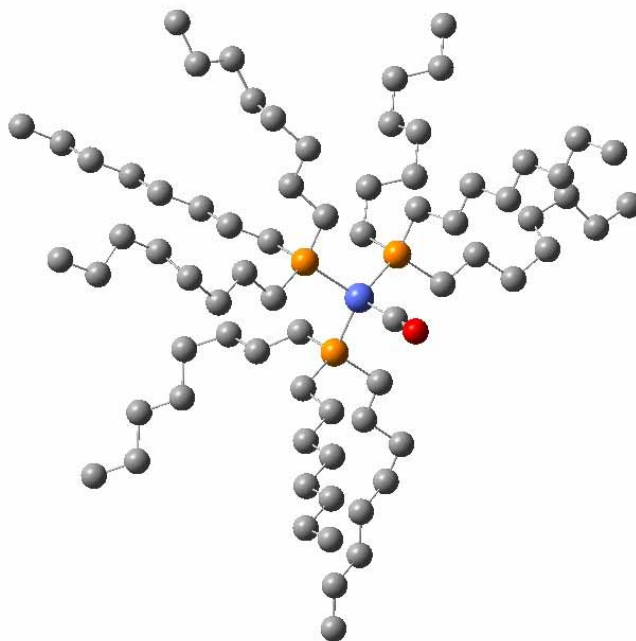
S5 : Table of EXAFS Fitting results for the Co NPs obtained using OA/TOP. k range: 3-12 Å⁻¹, R range: 1.5-5.4 Å, k-weights=1,2,3.



S6: FT-IR comparison of 7 min (red), 8 min (blue) spectra of the reaction mixture with the spectrum of the tricobalt intermediates (green) leading to cobalt nanoparticles.



S7: B3LYP optimized structure of $[\text{Co}_3(\mu\text{-CO})_3(\text{CO})_3\text{CCH}_3]$. Blue, grey, red and white balls represent Co, C, O and hydrogen respectively. The calculated carbonyl vibration energies at 1812, 1856, 1975 and 2011 cm^{-1} result from B3LYP method.

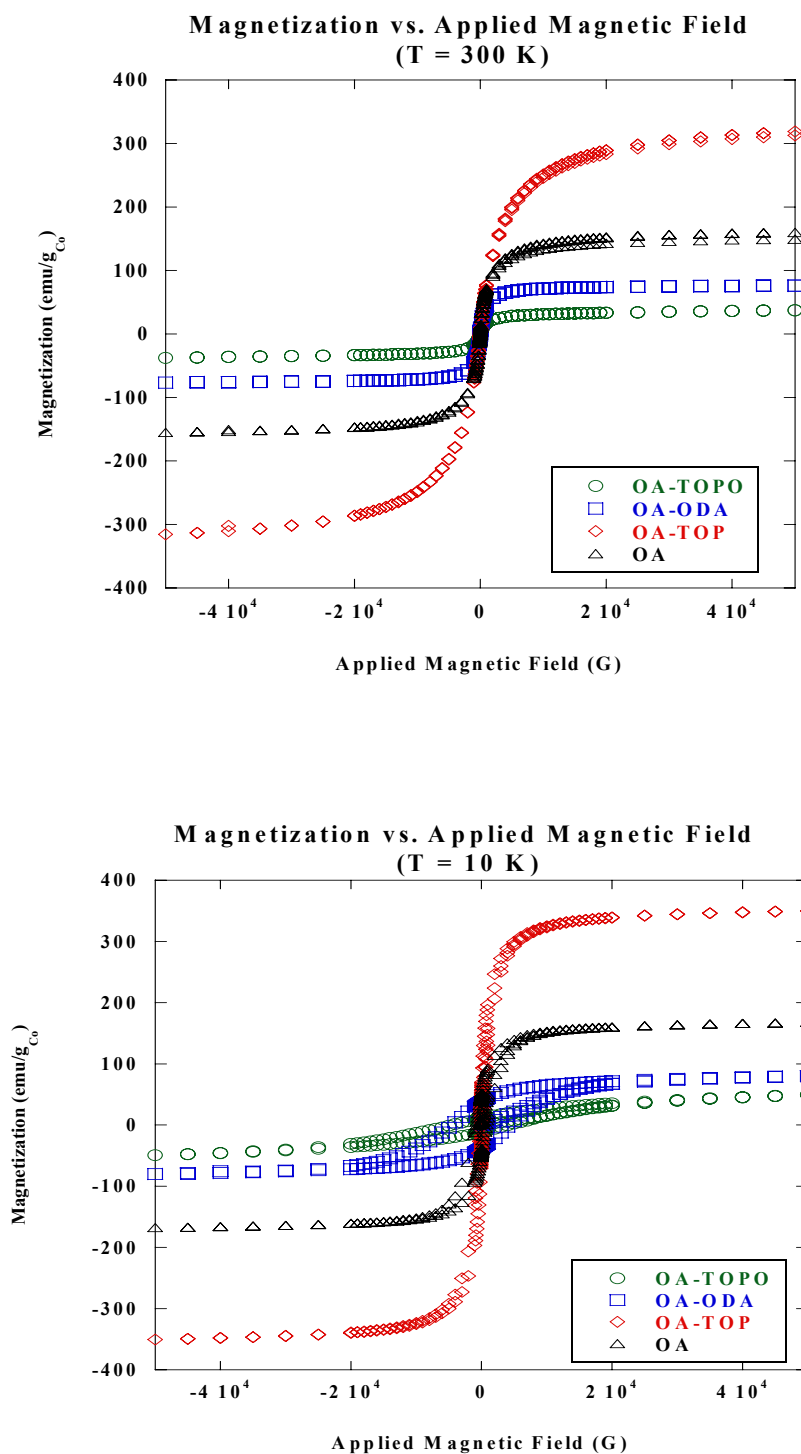


S8: B3LYP optimized structure of the suggested $\{\text{Co}(\text{CO})[\text{P}(\text{C}_8\text{H}_{15})_3]_3\}$ intermediate Co complex showing the tetrahedral geometry around the Co atom (H atoms are removed for clarity)

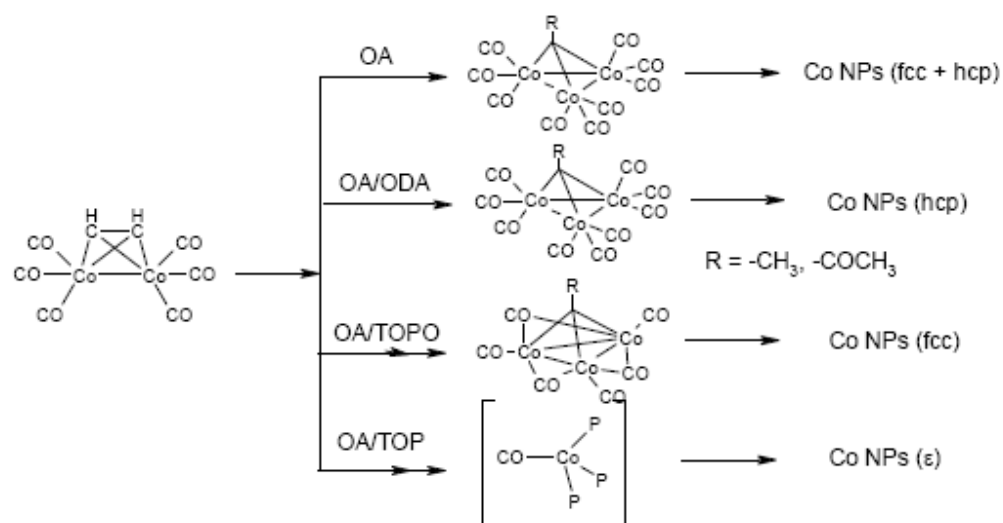
Co NPs	T _b (K)	M _s (emu/)	M _r (emu/)	M _r /M _s	H _c (G)	$\mu_H = \mu_B / \text{atom}$	T (K)
OA-TOPO		38	0.38	0.01	1300	0.39	300
OA-ODA		77	10	10	7.5	0.79	300
OA		153	0	0	0	1.61	300
OA-TOP		317	0	0	10	3.34	300
OA-TOPO	230	50	0.8	0.02	4600	0.51	10
OA-ODA	300	80	38	0.48	4600	0.82	10

OA	295	167	45	0.20	683	1.76	10
OA-TOP	37.8	351	45	0.16	179	3.7	10

S9. Table of the magnetic data from SQUID magnetometer



S10. Hysteresis loops (Magnetization vs Applied Magnetic field)



S11: A summary of the influence of surfactants on the reaction mechanism and in turn on the properties of Co nanoparticles obtained.