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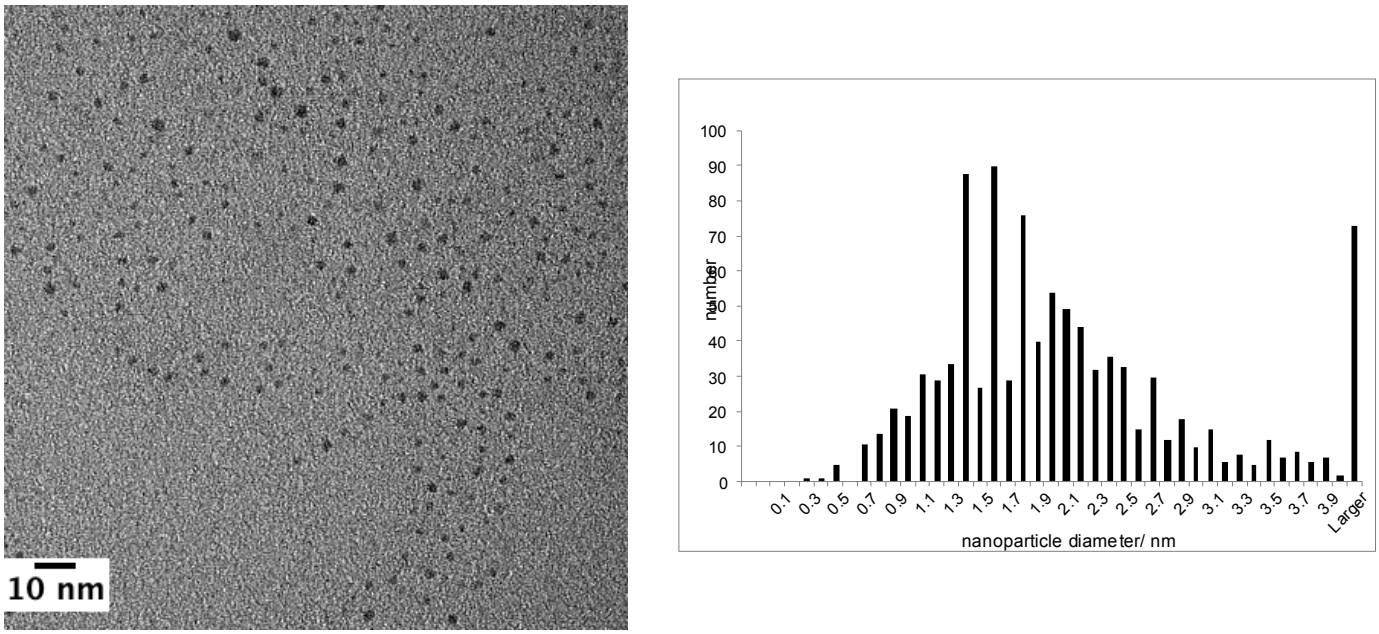


Figure S1. TEM image (left) and histogram (right) of as-synthesized Ag@BH_4 nanoparticles. Histogram reflects measurements of 999 nanoparticle diameters.

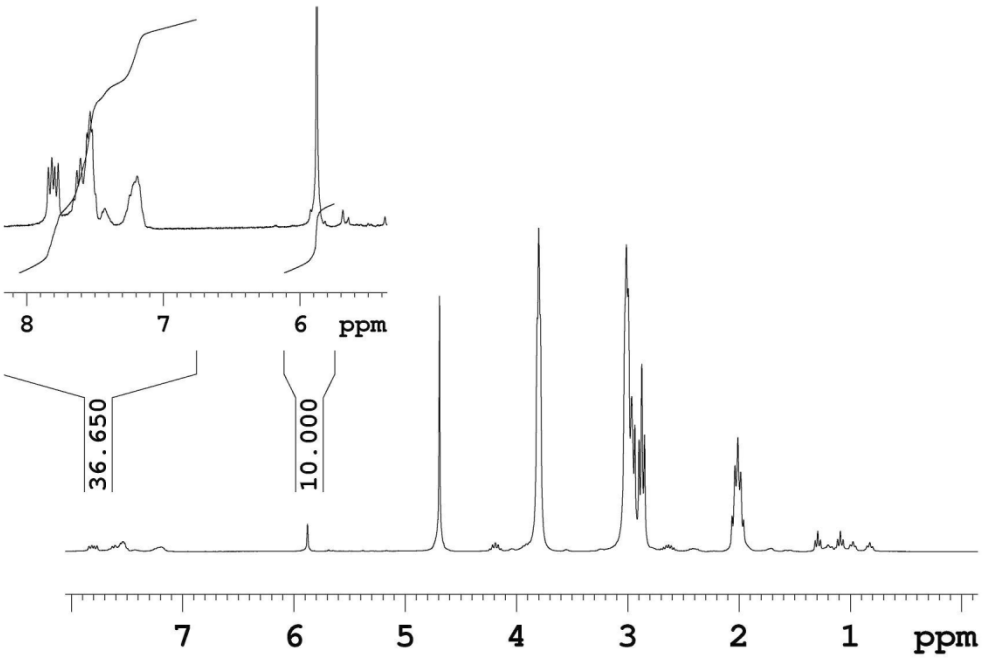


Figure S2. Demonstration by ^{1}H NMR of 6:1 DEPP to Cp_2MoCl_2 ratio in MOPS buffer before the addition of Ag@BH_4 nanoparticles at room temperature for Figure 1; time = 0. Phenyl protons of DEPP represent 5H and the cyclopentadienyl signals represent the 20H for the dimeric $Cp_2Mo(aq)^{2+}$ form.

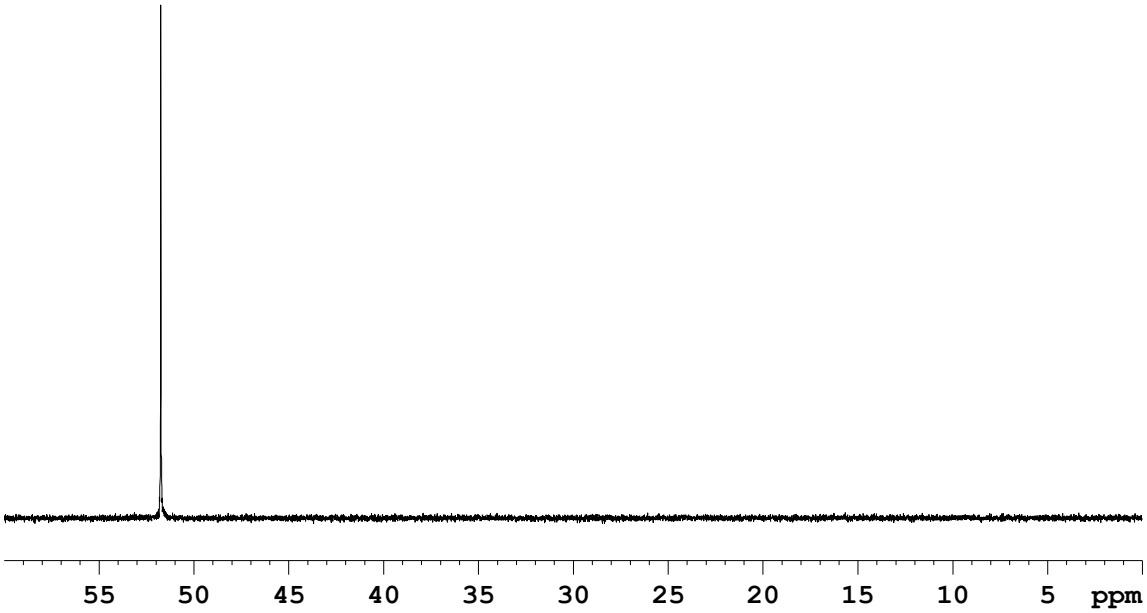


Figure S3. ^{31}P spectrum of DEPP + Ag@BH_4 NPs in MOPS buffer at 55 °C after 23 days, indicating that borohydride-capped nanoparticles do not degrade DEPP.

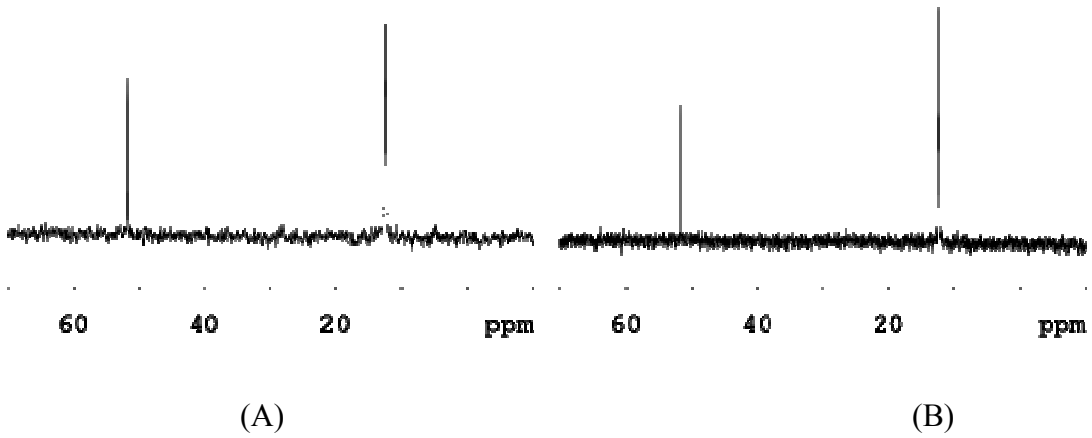


Figure S4. ^{31}P NMR spectra of DEPP in MOPS buffer with benzene phosphonic acid (pH 7 MOPS) as a flame-sealed capillary insert standard (A) at time = 0 and (B) after eight days 55 °C.

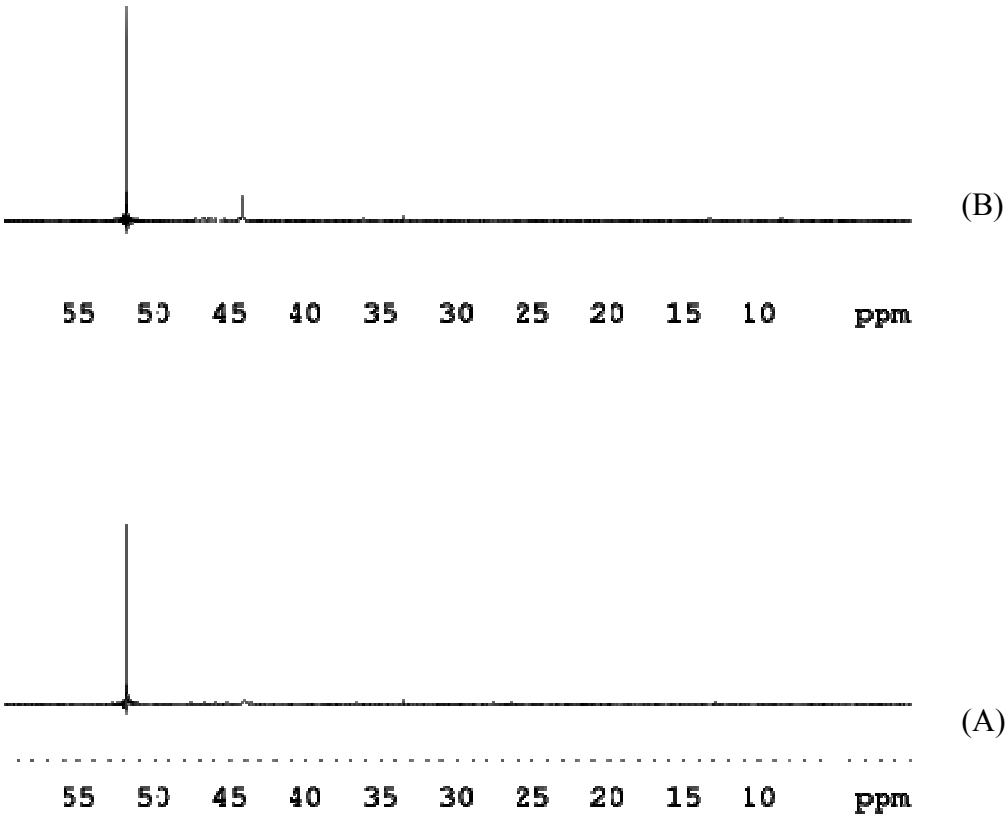


Figure S5. ^{31}P spectra of DEPP + $NaBH_4$ (2.0 mM) in MOPS buffer at 55 °C showing the absence of any effect by the BH_4^- capping agent at (A) time = 0 and (B) time = 24 days.

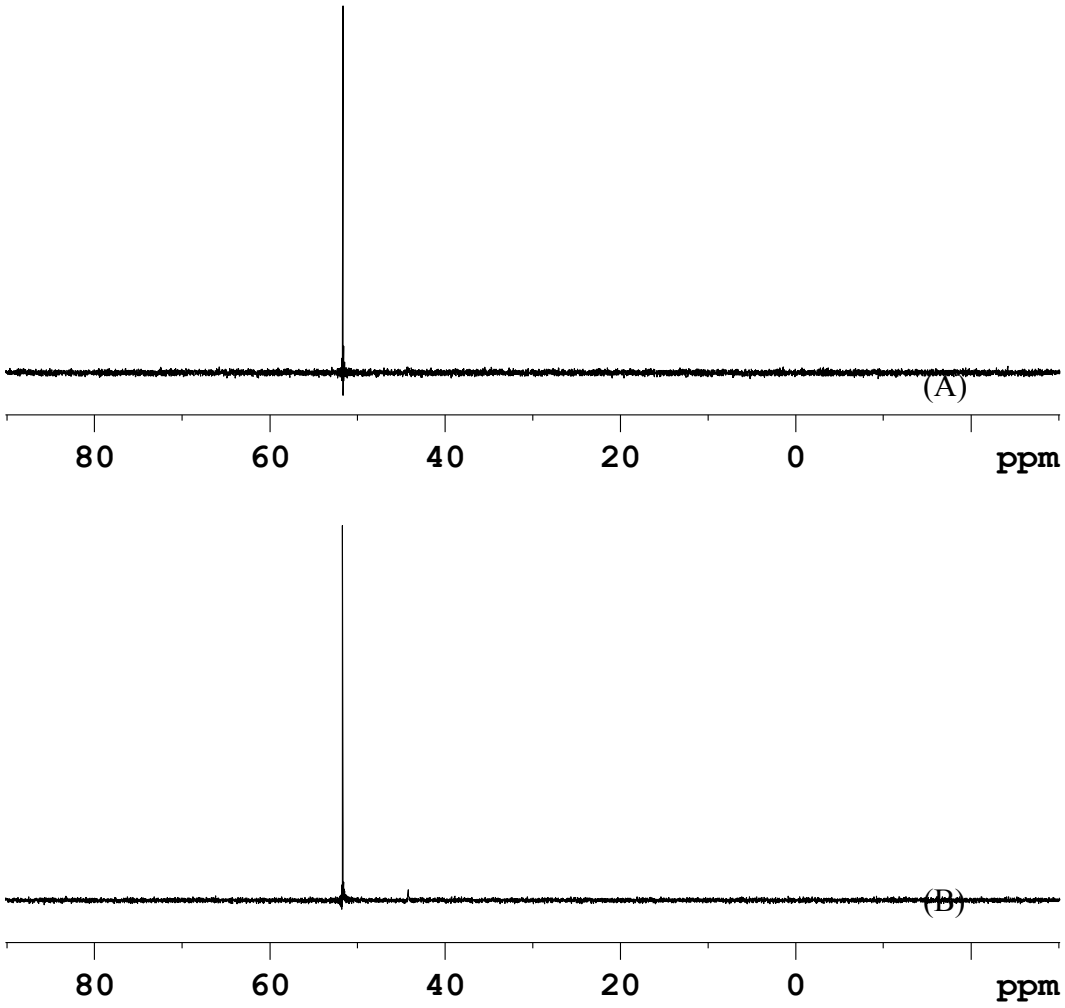


Figure S6. ^{31}P NMR spectrum of DEPP + NaI (60 mM) in MOPS (A) indicating residual iodide from the DEPP synthesis does not hydrolyze the phosphonothioate for up to 8 days (B) at 55 °C.

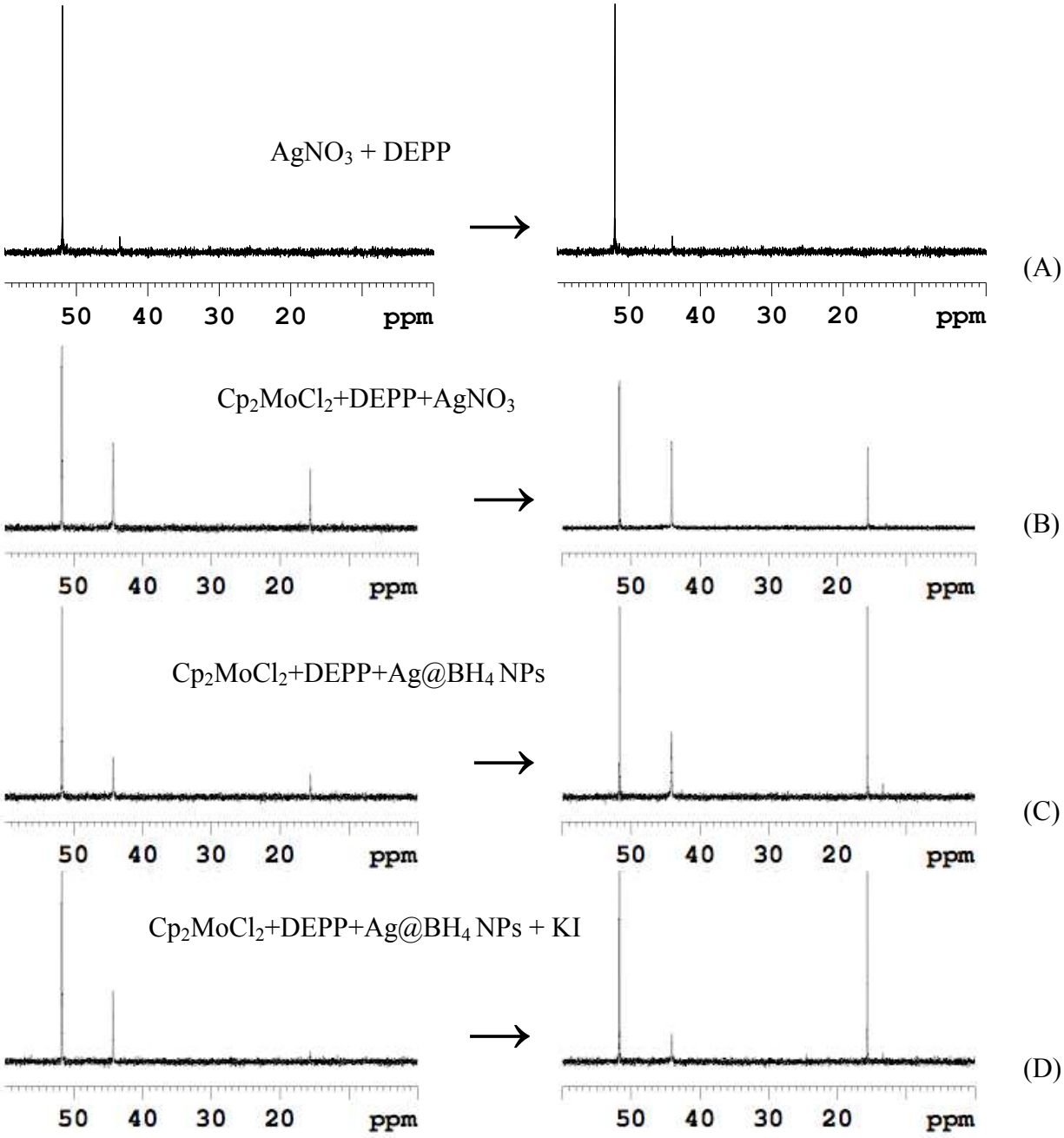


Figure S7. ^{31}P NMR analysis of a series of controls to see the effect of free $Ag^{+}(aq)$ ions on DEPP hydrolysis in MOPS (pH 7 buffer, 55 °C). Silver at 0.25 mM concentration is shown to not degrade DEPP (56 mM) at 55 °C, three days (A); a similar observation is seen with 0.50 mM of $AgNO_3$. The scans (B), (C), and (D) were taken after one day (left) and after eight days (right). Each of (B), (C) and (D) contained Cp_2MoCl_2 (23.98 mM) and DEPP (117.8 mM). Additionally, (B) had 0.25 mM $AgNO_3$ (no $Ag@BH_4$ NPs), (C) included $Ag@BH_4$ NPs, (D) included $Ag@BH_4$ NPs and KI (1 mL of a 10 mM solution). The signal at 44 ppm is found at high concentrations of DEPP, which is poorly soluble in water; the additional peak is due to a second phase of the phosphonothioate.

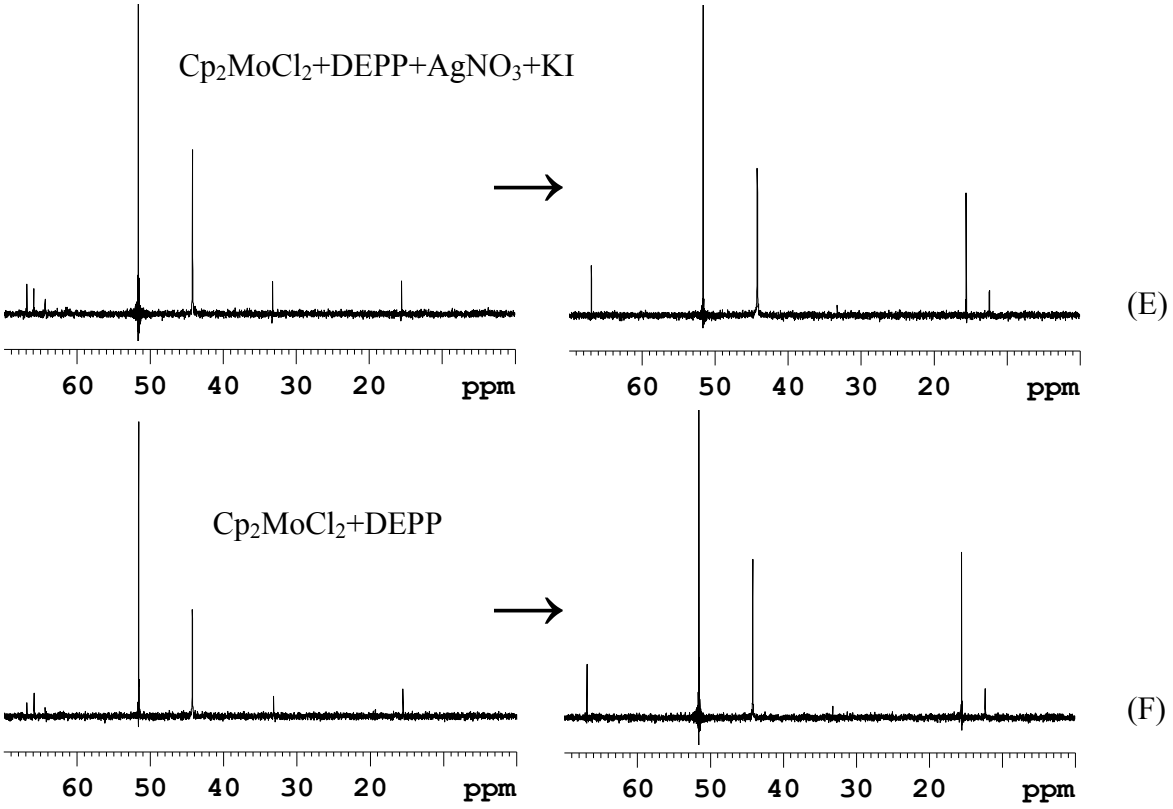


Figure S7(continued). A continuation of the controls in S7A to S7D above. Sets (E) and (F) were Cp_2MoCl_2 (10.0 mM) and DEPP (56.0 mM) hydrolysis reactions; the right spectra were taken after 5 days, while the leftmost spectra show the initial conditions. In addition to DEPP and Cp_2MoCl_2, tube (D) contained 1.0 mM $AgNO_3$ and 1.0 mM KI in equal volumes.

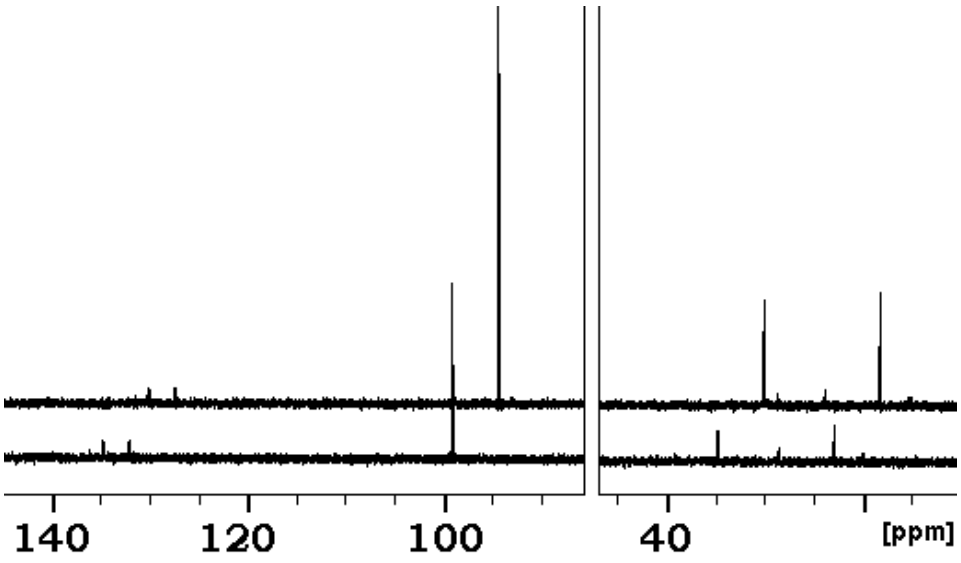
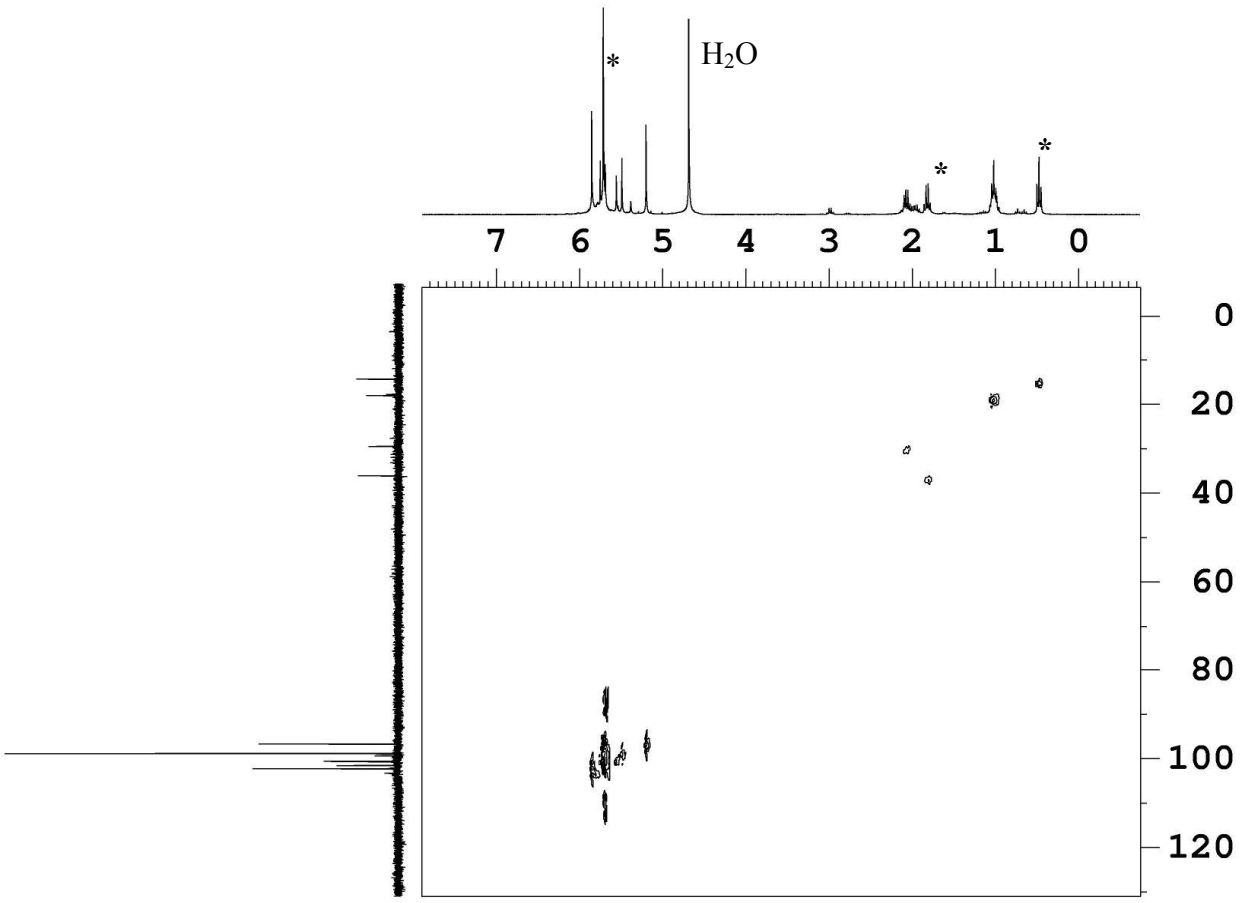


Figure S8. ^{13}C NMR spectra of authentic addition of compound **1** to DEPP + Cp_2MoCl_2 reaction (no Ag@BH_4 NPs). (A) $CDCl_3$ extraction of DEPP + Cp_2MoCl_2 (pH 7) reaction that removed the MOPS buffer and extracted mainly the signals the aliphatic and cyclopentadienyl signals. (B) addition of compound **1** to the $CDCl_3$ extraction. No other additional ^{13}C NMR signals appeared.



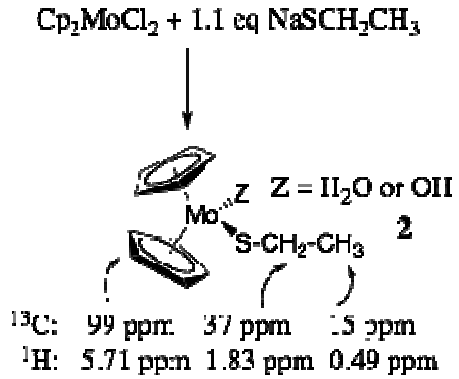
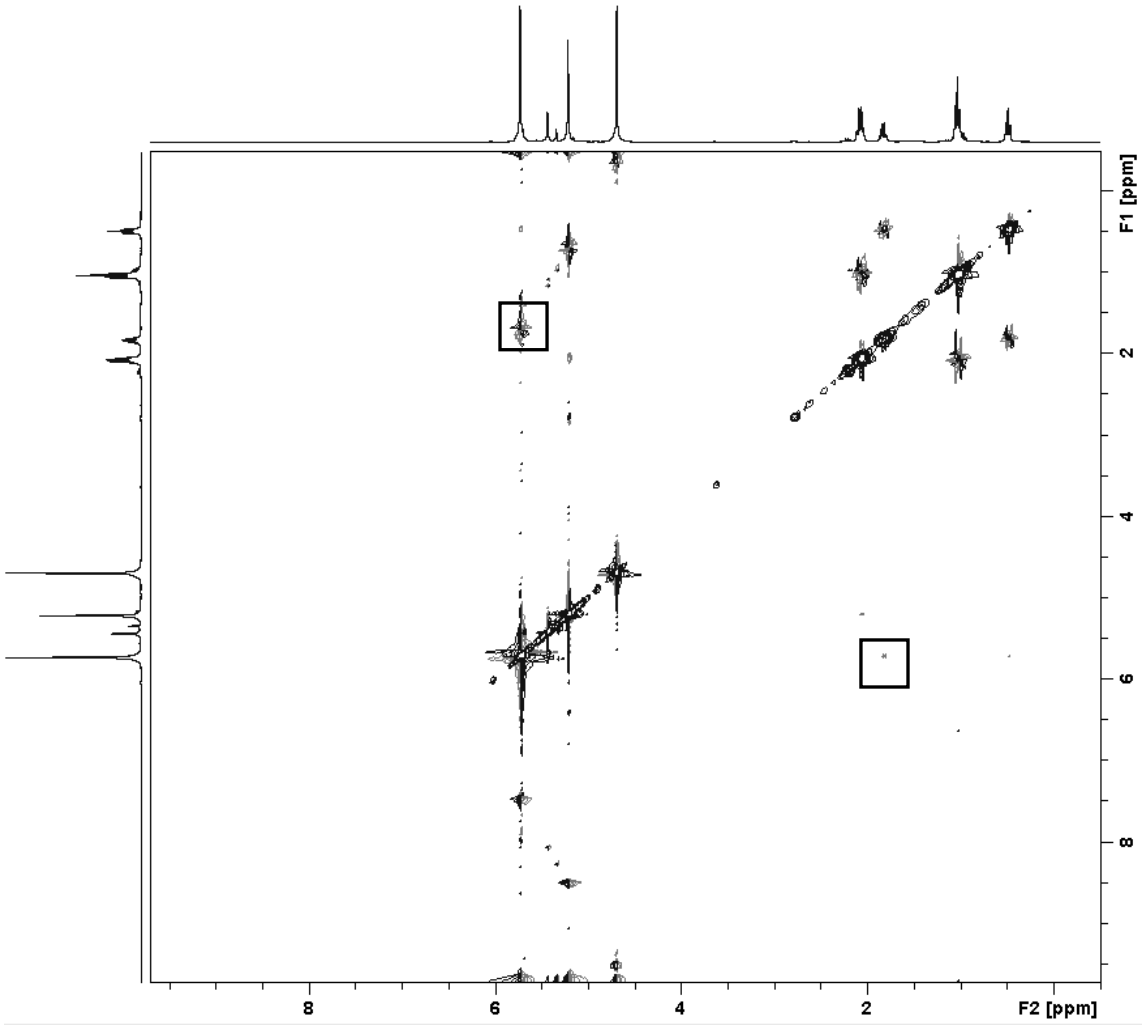
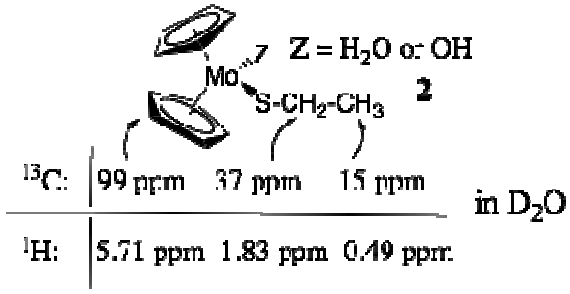


Figure S9. HSQC (in D_2O) of **2**(*) prepared from direct addition of 1.1 equivalent sodium ethanethiolate to molybdocene dichloride (50 mg, 0.16 mmole). Other ^1H cyclopentadienyl signal (5.2 ppm) and aliphatic (quartet at 2.20 ppm and triplet/multiplet at 1.1 ppm) are due to **1** that were not extracted out by $CDCl_3$. Supporting information that follow are the 2-D NOESY (S9), COSY (S10) and ^1H NMR that support this spectral assignment for **2**, and identify it as the monothiolated molybdocene with ^{13}C cyclopentadienyl signal at 99 ppm.





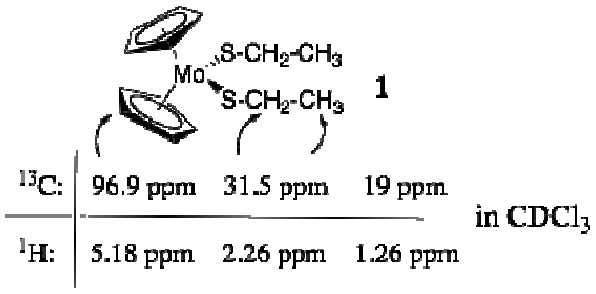


Figure S10. 2D NOESY of **2** prepared from direct addition of 1.1 equivalent of sodium ethanethiolate to molybdocene dichloride in D_2O. Cross peak (in box) correlates the Cp signal at 5.71 ppm with the quartet at 1.83 ppm. The 5.71 ppm Cp ^{1}H signal is connected to the 99 ppm ^{13}C signal (S8).

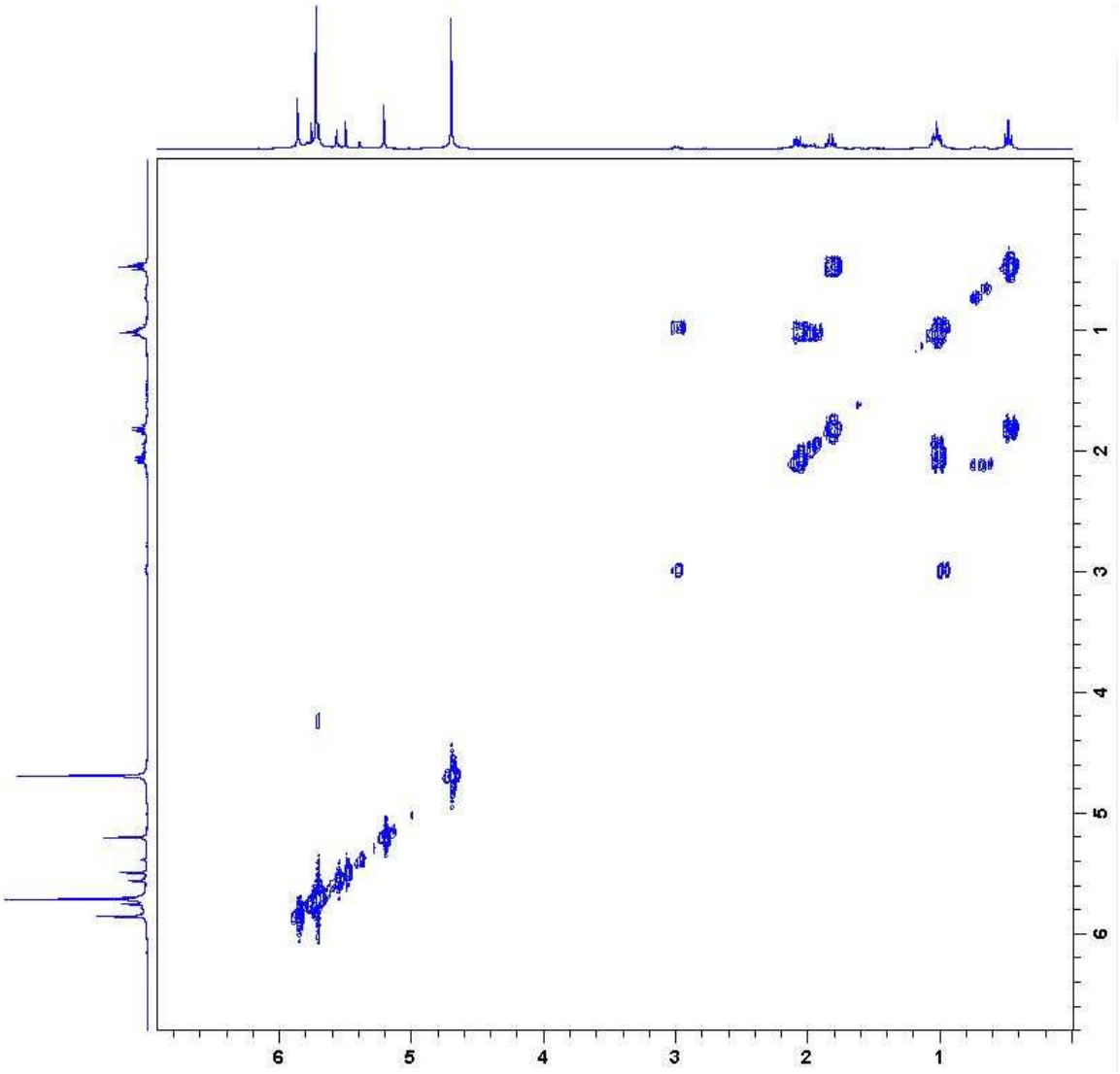


Figure S11. COSY of **2** prepared from direct addition of 1.1 equivalent of sodium ethanethiolate to molybdocene dichloride in D_2O. After correlating the 5.71 ppm ^1H Cp signal with the quartet at 1.83 ppm in S9, this COSY shows the quartet at 1.83 ppm is coupled to the triplet at 0.49 ppm.

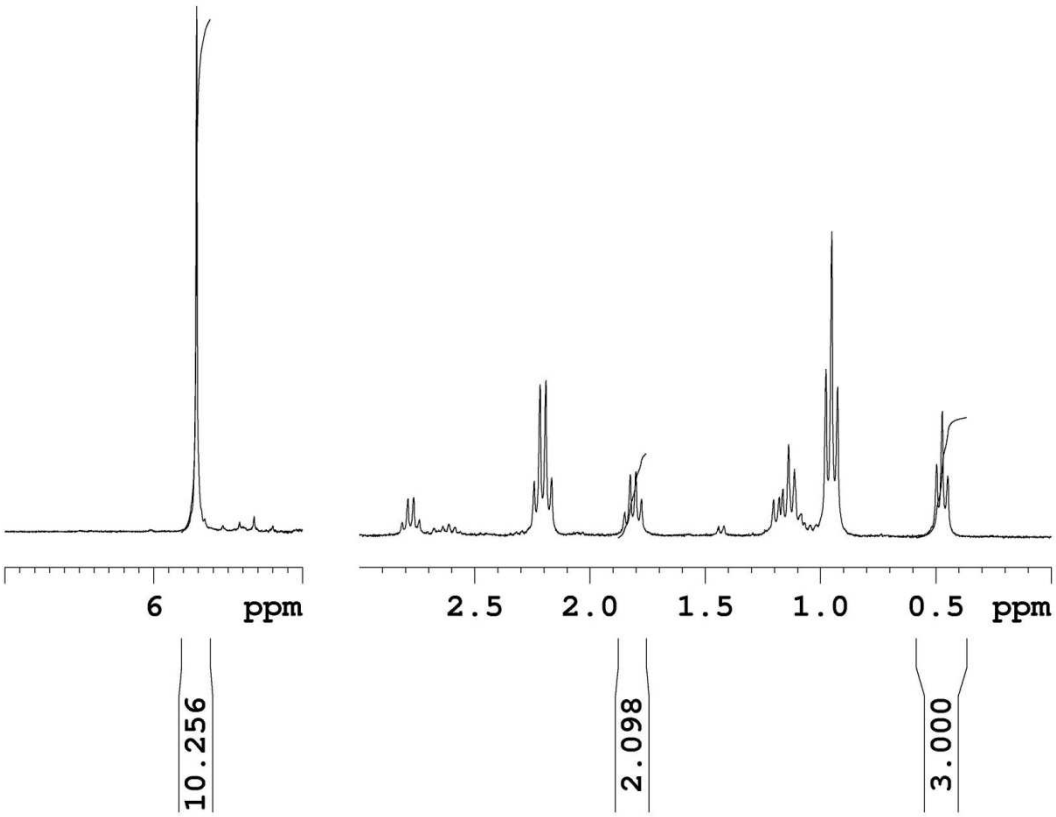


Figure S12. ^{1}H NMR spectrum of **2**, as above. Integrals indicative of monothiolate.

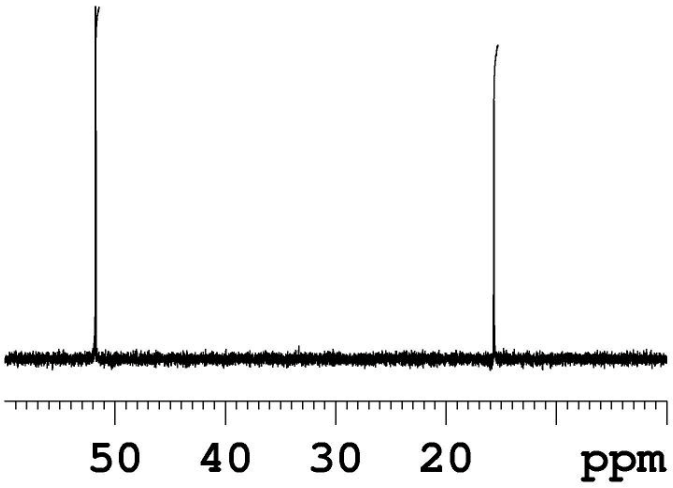


Figure S13. DEPP is degraded by **2** that is formed in eqn 5.

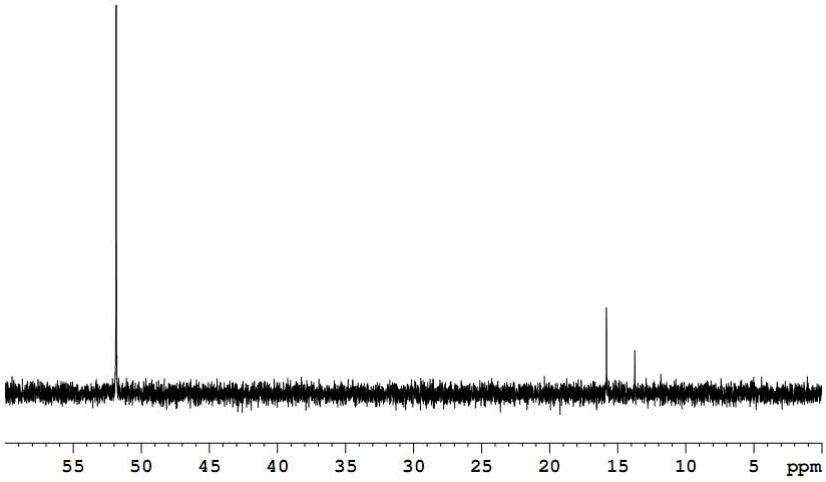


Figure S14. ^{31}P NMR of the "reverse reaction" of **1** + DEPP + Ag@BH_4 NPs (eqn 6c) after 3 days (55 °C). Ag@BH_4 NPs and compound **1** individually have no effect on DEPP (eqn 6a and 6b). The appearance of the 15 ppm ^{31}P signal (*O*-EPP phosphonate product) suggest the Ag@BH_4 NPs in conjunction with **1** can hydrolyze DEPP. Further incubation for additional time did not increase the amount of *O*-EPP phosphonate product.

Table 1. Crystal data and structure refinement for compound **3**.

Identification code	lkuo3	
Empirical formula	C12 H16 Mo S2	
Formula weight	320.31	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.0401(8) Å	a= 90°.
	b = 13.2467(16) Å	b= 91.223(2)°.
	c = 12.9711(15) Å	g = 90°.
Volume	1209.4(2) $Å^3$	
Z	4	
Density (calculated)	1.759 Mg/m^3	
Absorption coefficient	1.393 mm^{-1}	
F(000)	648	
Crystal size	0.16 x 0.06 x 0.04 mm^3	
Theta range for data collection	2.20 to 27.00°.	
Index ranges	-8<=h<=8, -16<=k<=16, -16<=l<=16	
Reflections collected	13320	
Independent reflections	2630 [R(int) = 0.0263]	
Completeness to theta = 27.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9464 and 0.8078	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2630 / 0 / 200	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0205, wR2 = 0.0446	
R indices (all data)	R1 = 0.0251, wR2 = 0.0475	
Largest diff. peak and hole	0.364 and -0.280 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for lkuo3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2629(1)	7544(1)	523(1)	15(1)
S(1)	5370(1)	6842(1)	-404(1)	22(1)
S(2)	5426(1)	8284(1)	1427(1)	22(1)
C(1)	4405(3)	6127(2)	-1488(2)	26(1)
C(2)	4571(4)	9178(2)	2369(2)	32(1)
C(3)	169(3)	6887(2)	1487(2)	26(1)
C(4)	487(3)	6181(2)	688(2)	26(1)
C(5)	2313(3)	5794(2)	828(2)	23(1)
C(6)	3161(3)	6274(2)	1692(2)	22(1)
C(7)	1817(3)	6947(2)	2116(2)	24(1)
C(8)	-18(3)	8279(2)	-184(2)	26(1)
C(9)	1212(3)	8056(2)	-1001(2)	30(1)
C(10)	2815(3)	8689(2)	-868(2)	29(1)
C(11)	2580(3)	9275(2)	7(2)	30(1)
C(12)	853(3)	9014(2)	460(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for lkuo3.

Mo(1)-C(8)	2.278(2)
Mo(1)-C(6)	2.290(2)
Mo(1)-C(7)	2.296(2)
Mo(1)-C(9)	2.297(2)
Mo(1)-C(12)	2.314(2)
Mo(1)-C(3)	2.327(2)
Mo(1)-C(10)	2.362(2)
Mo(1)-C(5)	2.362(2)
Mo(1)-C(4)	2.365(2)
Mo(1)-C(11)	2.389(2)
Mo(1)-S(2)	2.4731(6)
Mo(1)-S(1)	2.4766(6)
S(1)-C(1)	1.815(2)
S(2)-C(2)	1.814(2)
C(1)-H(1A)	0.97(3)
C(1)-H(1B)	0.94(2)
C(1)-H(1C)	0.96(2)
C(2)-H(2A)	0.94(3)
C(2)-H(2B)	0.98(3)
C(2)-H(2C)	0.92(3)
C(3)-C(7)	1.406(3)
C(3)-C(4)	1.418(3)
C(3)-H(3)	0.87(3)
C(4)-C(5)	1.393(3)
C(4)-H(4)	0.87(2)
C(5)-C(6)	1.409(3)
C(5)-H(5)	0.91(2)
C(6)-C(7)	1.420(3)
C(6)-H(6)	0.90(2)
C(7)-H(7)	0.91(2)
C(8)-C(12)	1.413(3)
C(8)-C(9)	1.414(3)
C(8)-H(8)	0.89(3)
C(9)-C(10)	1.413(3)

C(9)-H(9)	0.92(2)
C(10)-C(11)	1.387(3)
C(10)-H(10)	0.93(3)
C(11)-C(12)	1.405(3)
C(11)-H(11)	0.93(2)
C(12)-H(12)	0.93(2)

C(8)-Mo(1)-C(6)	134.56(8)
C(8)-Mo(1)-C(7)	106.98(8)
C(6)-Mo(1)-C(7)	36.08(8)
C(8)-Mo(1)-C(9)	36.00(8)
C(6)-Mo(1)-C(9)	148.06(8)
C(7)-Mo(1)-C(9)	139.82(9)
C(8)-Mo(1)-C(12)	35.84(8)
C(6)-Mo(1)-C(12)	136.21(8)
C(7)-Mo(1)-C(12)	100.16(8)
C(9)-Mo(1)-C(12)	59.79(8)
C(8)-Mo(1)-C(3)	76.38(8)
C(6)-Mo(1)-C(3)	58.84(8)
C(7)-Mo(1)-C(3)	35.40(8)
C(9)-Mo(1)-C(3)	104.99(9)
C(12)-Mo(1)-C(3)	85.75(8)
C(8)-Mo(1)-C(10)	58.42(8)
C(6)-Mo(1)-C(10)	165.05(8)
C(7)-Mo(1)-C(10)	157.95(8)
C(9)-Mo(1)-C(10)	35.29(8)
C(12)-Mo(1)-C(10)	58.09(8)
C(3)-Mo(1)-C(10)	134.80(8)
C(8)-Mo(1)-C(5)	114.09(8)
C(6)-Mo(1)-C(5)	35.22(7)
C(7)-Mo(1)-C(5)	59.02(8)
C(9)-Mo(1)-C(5)	113.18(8)
C(12)-Mo(1)-C(5)	141.13(8)
C(3)-Mo(1)-C(5)	57.94(8)
C(10)-Mo(1)-C(5)	139.92(8)
C(8)-Mo(1)-C(4)	81.11(8)

C(6)-Mo(1)-C(4)	58.33(8)
C(7)-Mo(1)-C(4)	58.95(8)
C(9)-Mo(1)-C(4)	92.15(8)
C(12)-Mo(1)-C(4)	107.48(8)
C(3)-Mo(1)-C(4)	35.16(8)
C(10)-Mo(1)-C(4)	127.26(8)
C(5)-Mo(1)-C(4)	34.26(8)
C(8)-Mo(1)-C(11)	58.00(8)
C(6)-Mo(1)-C(11)	153.07(8)
C(7)-Mo(1)-C(11)	125.45(8)
C(9)-Mo(1)-C(11)	58.14(8)
C(12)-Mo(1)-C(11)	34.72(8)
C(3)-Mo(1)-C(11)	120.21(8)
C(10)-Mo(1)-C(11)	33.94(8)
C(5)-Mo(1)-C(11)	171.08(8)
C(4)-Mo(1)-C(11)	138.85(8)
C(8)-Mo(1)-S(2)	131.11(6)
C(6)-Mo(1)-S(2)	81.93(6)
C(7)-Mo(1)-S(2)	85.45(6)
C(9)-Mo(1)-S(2)	128.14(6)
C(12)-Mo(1)-S(2)	96.16(6)
C(3)-Mo(1)-S(2)	119.18(6)
C(10)-Mo(1)-S(2)	92.91(6)
C(5)-Mo(1)-S(2)	112.71(6)
C(4)-Mo(1)-S(2)	139.68(6)
C(11)-Mo(1)-S(2)	76.03(6)
C(8)-Mo(1)-S(1)	127.20(6)
C(6)-Mo(1)-S(1)	85.83(6)
C(7)-Mo(1)-S(1)	121.28(6)
C(9)-Mo(1)-S(1)	91.27(6)
C(12)-Mo(1)-S(1)	136.45(6)
C(3)-Mo(1)-S(1)	135.83(6)
C(10)-Mo(1)-S(1)	79.29(6)
C(5)-Mo(1)-S(1)	77.89(6)
C(4)-Mo(1)-S(1)	105.22(6)
C(11)-Mo(1)-S(1)	103.36(6)

S(2)-Mo(1)-S(1)	75.990(19)
C(1)-S(1)-Mo(1)	106.79(8)
C(2)-S(2)-Mo(1)	107.82(8)
S(1)-C(1)-H(1A)	112.8(15)
S(1)-C(1)-H(1B)	112.1(14)
H(1A)-C(1)-H(1B)	110(2)
S(1)-C(1)-H(1C)	109.4(13)
H(1A)-C(1)-H(1C)	105.8(19)
H(1B)-C(1)-H(1C)	106.0(19)
S(2)-C(2)-H(2A)	108.4(17)
S(2)-C(2)-H(2B)	112.3(14)
H(2A)-C(2)-H(2B)	109(2)
S(2)-C(2)-H(2C)	112.6(15)
H(2A)-C(2)-H(2C)	107(2)
H(2B)-C(2)-H(2C)	107(2)
C(7)-C(3)-C(4)	108.7(2)
C(7)-C(3)-Mo(1)	71.11(12)
C(4)-C(3)-Mo(1)	73.90(12)
C(7)-C(3)-H(3)	127.3(17)
C(4)-C(3)-H(3)	123.9(17)
Mo(1)-C(3)-H(3)	123.3(16)
C(5)-C(4)-C(3)	107.9(2)
C(5)-C(4)-Mo(1)	72.76(12)
C(3)-C(4)-Mo(1)	70.94(12)
C(5)-C(4)-H(4)	126.7(16)
C(3)-C(4)-H(4)	125.4(16)
Mo(1)-C(4)-H(4)	120.7(15)
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C(6)-C(5)-Mo(1)	69.58(11)
C(4)-C(5)-H(5)	125.3(14)
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C(7)-C(6)-Mo(1)	72.20(12)

C(5)-C(6)-H(6)	126.3(15)
C(7)-C(6)-H(6)	125.3(15)
Mo(1)-C(6)-H(6)	117.9(15)
C(3)-C(7)-C(6)	106.8(2)
C(3)-C(7)-Mo(1)	73.49(12)
C(6)-C(7)-Mo(1)	71.73(12)
C(3)-C(7)-H(7)	125.1(16)
C(6)-C(7)-H(7)	127.8(16)
Mo(1)-C(7)-H(7)	125.5(15)
C(12)-C(8)-C(9)	108.8(2)
C(12)-C(8)-Mo(1)	73.48(12)
C(9)-C(8)-Mo(1)	72.72(12)
C(12)-C(8)-H(8)	125.1(17)
C(9)-C(8)-H(8)	126.2(17)
Mo(1)-C(8)-H(8)	121.0(17)
C(8)-C(9)-C(10)	106.5(2)
C(8)-C(9)-Mo(1)	71.29(12)
C(10)-C(9)-Mo(1)	74.89(13)
C(8)-C(9)-H(9)	132.2(16)
C(10)-C(9)-H(9)	121.3(16)
Mo(1)-C(9)-H(9)	119.8(15)
C(11)-C(10)-C(9)	108.9(2)
C(11)-C(10)-Mo(1)	74.08(13)
C(9)-C(10)-Mo(1)	69.83(12)
C(11)-C(10)-H(10)	126.7(16)
C(9)-C(10)-H(10)	124.5(16)
Mo(1)-C(10)-H(10)	120.8(15)
C(10)-C(11)-C(12)	108.8(2)
C(10)-C(11)-Mo(1)	71.98(13)
C(12)-C(11)-Mo(1)	69.74(12)
C(10)-C(11)-H(11)	127.6(15)
C(12)-C(11)-H(11)	123.6(15)
Mo(1)-C(11)-H(11)	123.4(15)
C(11)-C(12)-C(8)	106.9(2)
C(11)-C(12)-Mo(1)	75.54(13)
C(8)-C(12)-Mo(1)	70.69(12)

C(11)-C(12)-H(12)	126.1(15)
C(8)-C(12)-H(12)	126.8(15)
Mo(1)-C(12)-H(12)	122.3(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for lkuo3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	13(1)	15(1)	17(1)	1(1)	1(1)	1(1)
S(1)	16(1)	26(1)	23(1)	-2(1)	3(1)	1(1)
S(2)	16(1)	24(1)	26(1)	-5(1)	-2(1)	1(1)
C(1)	26(1)	28(1)	23(1)	-2(1)	3(1)	3(1)
C(2)	27(1)	31(1)	39(1)	-14(1)	-2(1)	3(1)
C(3)	20(1)	23(1)	36(1)	8(1)	12(1)	0(1)
C(4)	25(1)	22(1)	32(1)	5(1)	-4(1)	-10(1)
C(5)	29(1)	14(1)	26(1)	3(1)	7(1)	-1(1)
C(6)	24(1)	19(1)	23(1)	6(1)	-1(1)	1(1)
C(7)	33(1)	23(1)	18(1)	2(1)	6(1)	-1(1)
C(8)	16(1)	24(1)	38(1)	9(1)	-4(1)	4(1)
C(9)	35(1)	30(1)	24(1)	2(1)	-9(1)	8(1)
C(10)	28(1)	30(1)	30(1)	15(1)	6(1)	7(1)
C(11)	30(1)	17(1)	41(1)	9(1)	-7(1)	-1(1)
C(12)	31(1)	20(1)	28(1)	3(1)	2(1)	11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for lkuo3.

	x	y	z	U(eq)
H(1A)	3730(40)	5526(19)	-1277(19)	39(7)
H(1B)	3630(30)	6525(18)	-1922(18)	33(7)
H(1C)	5430(30)	5893(17)	-1906(17)	26(6)
H(2A)	5620(40)	9530(20)	2650(20)	48(8)
H(2B)	3880(40)	8847(19)	2925(19)	35(7)
H(2C)	3770(40)	9651(19)	2082(18)	36(7)
H(3)	-910(40)	7200(18)	1573(19)	32(7)
H(4)	-320(30)	6032(17)	189(18)	30(7)
H(5)	2860(30)	5323(18)	419(17)	27(6)
H(6)	4360(30)	6182(18)	1933(17)	29(6)
H(7)	1920(30)	7296(17)	2720(20)	30(7)
H(8)	-1160(40)	8017(19)	-93(19)	39(7)
H(9)	1110(40)	7612(17)	-1550(20)	32(7)
H(10)	3860(40)	8689(19)	-1294(19)	36(7)
H(11)	3410(30)	9760(19)	278(18)	34(7)
H(12)	350(30)	9303(18)	1045(19)	34(7)

Table 6. Torsion angles [°] for lkuo3.

C(8)-Mo(1)-S(1)-C(1)	-43.56(11)
C(6)-Mo(1)-S(1)-C(1)	102.32(10)
C(7)-Mo(1)-S(1)-C(1)	109.35(11)
C(9)-Mo(1)-S(1)-C(1)	-45.83(10)
C(12)-Mo(1)-S(1)-C(1)	-90.82(12)
C(3)-Mo(1)-S(1)-C(1)	67.37(12)
C(10)-Mo(1)-S(1)-C(1)	-79.20(10)
C(5)-Mo(1)-S(1)-C(1)	67.62(10)
C(4)-Mo(1)-S(1)-C(1)	46.75(10)
C(11)-Mo(1)-S(1)-C(1)	-103.33(10)
S(2)-Mo(1)-S(1)-C(1)	-174.96(9)
C(8)-Mo(1)-S(2)-C(2)	46.94(13)
C(6)-Mo(1)-S(2)-C(2)	-97.83(11)
C(7)-Mo(1)-S(2)-C(2)	-61.69(11)
C(9)-Mo(1)-S(2)-C(2)	94.09(13)
C(12)-Mo(1)-S(2)-C(2)	38.07(12)
C(3)-Mo(1)-S(2)-C(2)	-50.49(12)
C(10)-Mo(1)-S(2)-C(2)	96.28(12)
C(5)-Mo(1)-S(2)-C(2)	-115.32(11)
C(4)-Mo(1)-S(2)-C(2)	-88.38(13)
C(11)-Mo(1)-S(2)-C(2)	66.57(12)
S(1)-Mo(1)-S(2)-C(2)	174.48(10)
C(8)-Mo(1)-C(3)-C(7)	-149.28(15)
C(6)-Mo(1)-C(3)-C(7)	38.78(13)
C(9)-Mo(1)-C(3)-C(7)	-171.37(13)
C(12)-Mo(1)-C(3)-C(7)	-114.21(14)
C(10)-Mo(1)-C(3)-C(7)	-149.05(14)
C(5)-Mo(1)-C(3)-C(7)	80.38(14)
C(4)-Mo(1)-C(3)-C(7)	116.84(19)
C(11)-Mo(1)-C(3)-C(7)	-109.82(14)
S(2)-Mo(1)-C(3)-C(7)	-19.53(15)
S(1)-Mo(1)-C(3)-C(7)	80.66(15)
C(8)-Mo(1)-C(3)-C(4)	93.88(14)
C(6)-Mo(1)-C(3)-C(4)	-78.06(14)

C(7)-Mo(1)-C(3)-C(4)	-116.84(19)
C(9)-Mo(1)-C(3)-C(4)	71.79(14)
C(12)-Mo(1)-C(3)-C(4)	128.95(14)
C(10)-Mo(1)-C(3)-C(4)	94.12(16)
C(5)-Mo(1)-C(3)-C(4)	-36.46(13)
C(11)-Mo(1)-C(3)-C(4)	133.34(13)
S(2)-Mo(1)-C(3)-C(4)	-136.37(12)
S(1)-Mo(1)-C(3)-C(4)	-36.18(17)
C(7)-C(3)-C(4)-C(5)	0.8(2)
Mo(1)-C(3)-C(4)-C(5)	63.85(15)
C(7)-C(3)-C(4)-Mo(1)	-63.04(15)
C(8)-Mo(1)-C(4)-C(5)	164.50(15)
C(6)-Mo(1)-C(4)-C(5)	-36.93(13)
C(7)-Mo(1)-C(4)-C(5)	-79.44(14)
C(9)-Mo(1)-C(4)-C(5)	130.12(14)
C(12)-Mo(1)-C(4)-C(5)	-170.95(13)
C(3)-Mo(1)-C(4)-C(5)	-116.6(2)
C(10)-Mo(1)-C(4)-C(5)	126.22(14)
C(11)-Mo(1)-C(4)-C(5)	170.70(13)
S(2)-Mo(1)-C(4)-C(5)	-47.93(17)
S(1)-Mo(1)-C(4)-C(5)	38.22(14)
C(8)-Mo(1)-C(4)-C(3)	-78.95(14)
C(6)-Mo(1)-C(4)-C(3)	79.62(14)
C(7)-Mo(1)-C(4)-C(3)	37.11(13)
C(9)-Mo(1)-C(4)-C(3)	-113.33(14)
C(12)-Mo(1)-C(4)-C(3)	-54.40(15)
C(10)-Mo(1)-C(4)-C(3)	-117.23(14)
C(5)-Mo(1)-C(4)-C(3)	116.6(2)
C(11)-Mo(1)-C(4)-C(3)	-72.75(18)
S(2)-Mo(1)-C(4)-C(3)	68.62(16)
S(1)-Mo(1)-C(4)-C(3)	154.77(12)
C(3)-C(4)-C(5)-C(6)	-1.7(2)
Mo(1)-C(4)-C(5)-C(6)	61.01(14)
C(3)-C(4)-C(5)-Mo(1)	-62.66(15)
C(8)-Mo(1)-C(5)-C(4)	-16.82(16)
C(6)-Mo(1)-C(5)-C(4)	117.55(19)

C(7)-Mo(1)-C(5)-C(4)	79.20(15)
C(9)-Mo(1)-C(5)-C(4)	-56.23(15)
C(12)-Mo(1)-C(5)-C(4)	13.8(2)
C(3)-Mo(1)-C(5)-C(4)	37.43(13)
C(10)-Mo(1)-C(5)-C(4)	-85.74(17)
C(11)-Mo(1)-C(5)-C(4)	-43.3(5)
S(2)-Mo(1)-C(5)-C(4)	148.62(12)
S(1)-Mo(1)-C(5)-C(4)	-142.37(14)
C(8)-Mo(1)-C(5)-C(6)	-134.36(13)
C(7)-Mo(1)-C(5)-C(6)	-38.35(13)
C(9)-Mo(1)-C(5)-C(6)	-173.77(13)
C(12)-Mo(1)-C(5)-C(6)	-103.72(16)
C(3)-Mo(1)-C(5)-C(6)	-80.12(14)
C(10)-Mo(1)-C(5)-C(6)	156.71(14)
C(4)-Mo(1)-C(5)-C(6)	-117.55(19)
C(11)-Mo(1)-C(5)-C(6)	-160.9(5)
S(2)-Mo(1)-C(5)-C(6)	31.07(14)
S(1)-Mo(1)-C(5)-C(6)	100.08(13)
C(4)-C(5)-C(6)-C(7)	1.9(2)
Mo(1)-C(5)-C(6)-C(7)	65.07(14)
C(4)-C(5)-C(6)-Mo(1)	-63.18(15)
C(8)-Mo(1)-C(6)-C(5)	66.33(17)
C(7)-Mo(1)-C(6)-C(5)	115.39(19)
C(9)-Mo(1)-C(6)-C(5)	10.9(2)
C(12)-Mo(1)-C(6)-C(5)	118.24(14)
C(3)-Mo(1)-C(6)-C(5)	77.36(14)
C(10)-Mo(1)-C(6)-C(5)	-80.7(3)
C(4)-Mo(1)-C(6)-C(5)	35.91(13)
C(11)-Mo(1)-C(6)-C(5)	173.56(16)
S(2)-Mo(1)-C(6)-C(5)	-151.26(13)
S(1)-Mo(1)-C(6)-C(5)	-74.84(12)
C(8)-Mo(1)-C(6)-C(7)	-49.05(17)
C(9)-Mo(1)-C(6)-C(7)	-104.52(18)
C(12)-Mo(1)-C(6)-C(7)	2.86(19)
C(3)-Mo(1)-C(6)-C(7)	-38.03(13)
C(10)-Mo(1)-C(6)-C(7)	164.0(3)

C(5)-Mo(1)-C(6)-C(7)	-115.39(19)
C(4)-Mo(1)-C(6)-C(7)	-79.48(14)
C(11)-Mo(1)-C(6)-C(7)	58.2(2)
S(2)-Mo(1)-C(6)-C(7)	93.35(12)
S(1)-Mo(1)-C(6)-C(7)	169.77(13)
C(4)-C(3)-C(7)-C(6)	0.3(2)
Mo(1)-C(3)-C(7)-C(6)	-64.49(14)
C(4)-C(3)-C(7)-Mo(1)	64.84(15)
C(5)-C(6)-C(7)-C(3)	-1.4(2)
Mo(1)-C(6)-C(7)-C(3)	65.67(14)
C(5)-C(6)-C(7)-Mo(1)	-67.04(14)
C(8)-Mo(1)-C(7)-C(3)	31.27(15)
C(6)-Mo(1)-C(7)-C(3)	-114.49(19)
C(9)-Mo(1)-C(7)-C(3)	13.0(2)
C(12)-Mo(1)-C(7)-C(3)	67.52(14)
C(10)-Mo(1)-C(7)-C(3)	76.5(3)
C(5)-Mo(1)-C(7)-C(3)	-77.06(14)
C(4)-Mo(1)-C(7)-C(3)	-36.86(13)
C(11)-Mo(1)-C(7)-C(3)	93.71(15)
S(2)-Mo(1)-C(7)-C(3)	162.98(13)
S(1)-Mo(1)-C(7)-C(3)	-126.44(12)
C(8)-Mo(1)-C(7)-C(6)	145.75(13)
C(9)-Mo(1)-C(7)-C(6)	127.47(15)
C(12)-Mo(1)-C(7)-C(6)	-177.99(13)
C(3)-Mo(1)-C(7)-C(6)	114.49(19)
C(10)-Mo(1)-C(7)-C(6)	-169.0(2)
C(5)-Mo(1)-C(7)-C(6)	37.42(13)
C(4)-Mo(1)-C(7)-C(6)	77.63(14)
C(11)-Mo(1)-C(7)-C(6)	-151.81(13)
S(2)-Mo(1)-C(7)-C(6)	-82.54(12)
S(1)-Mo(1)-C(7)-C(6)	-11.96(15)
C(6)-Mo(1)-C(8)-C(12)	111.53(15)
C(7)-Mo(1)-C(8)-C(12)	83.82(14)
C(9)-Mo(1)-C(8)-C(12)	-116.3(2)
C(3)-Mo(1)-C(8)-C(12)	101.84(15)
C(10)-Mo(1)-C(8)-C(12)	-77.97(15)

C(5)-Mo(1)-C(8)-C(12)	146.88(13)
C(4)-Mo(1)-C(8)-C(12)	137.40(15)
C(11)-Mo(1)-C(8)-C(12)	-37.80(13)
S(2)-Mo(1)-C(8)-C(12)	-15.19(17)
S(1)-Mo(1)-C(8)-C(12)	-120.20(12)
C(6)-Mo(1)-C(8)-C(9)	-132.14(14)
C(7)-Mo(1)-C(8)-C(9)	-159.85(14)
C(12)-Mo(1)-C(8)-C(9)	116.3(2)
C(3)-Mo(1)-C(8)-C(9)	-141.83(15)
C(10)-Mo(1)-C(8)-C(9)	38.37(14)
C(5)-Mo(1)-C(8)-C(9)	-96.78(14)
C(4)-Mo(1)-C(8)-C(9)	-106.27(15)
C(11)-Mo(1)-C(8)-C(9)	78.54(15)
S(2)-Mo(1)-C(8)-C(9)	101.15(14)
S(1)-Mo(1)-C(8)-C(9)	-3.86(16)
C(12)-C(8)-C(9)-C(10)	-2.0(2)
Mo(1)-C(8)-C(9)-C(10)	-67.19(15)
C(12)-C(8)-C(9)-Mo(1)	65.15(15)
C(6)-Mo(1)-C(9)-C(8)	92.77(19)
C(7)-Mo(1)-C(9)-C(8)	30.7(2)
C(12)-Mo(1)-C(9)-C(8)	-37.39(13)
C(3)-Mo(1)-C(9)-C(8)	38.45(15)
C(10)-Mo(1)-C(9)-C(8)	-113.7(2)
C(5)-Mo(1)-C(9)-C(8)	99.56(14)
C(4)-Mo(1)-C(9)-C(8)	71.64(14)
C(11)-Mo(1)-C(9)-C(8)	-78.10(15)
S(2)-Mo(1)-C(9)-C(8)	-109.96(13)
S(1)-Mo(1)-C(9)-C(8)	176.92(13)
C(8)-Mo(1)-C(9)-C(10)	113.7(2)
C(6)-Mo(1)-C(9)-C(10)	-153.48(15)
C(7)-Mo(1)-C(9)-C(10)	144.45(14)
C(12)-Mo(1)-C(9)-C(10)	76.36(15)
C(3)-Mo(1)-C(9)-C(10)	152.19(14)
C(5)-Mo(1)-C(9)-C(10)	-146.69(13)
C(4)-Mo(1)-C(9)-C(10)	-174.62(14)
C(11)-Mo(1)-C(9)-C(10)	35.64(13)

S(2)-Mo(1)-C(9)-C(10)	3.78(17)
S(1)-Mo(1)-C(9)-C(10)	-69.33(13)
C(8)-C(9)-C(10)-C(11)	0.5(2)
Mo(1)-C(9)-C(10)-C(11)	-64.25(16)
C(8)-C(9)-C(10)-Mo(1)	64.73(15)
C(8)-Mo(1)-C(10)-C(11)	78.42(15)
C(6)-Mo(1)-C(10)-C(11)	-128.7(3)
C(7)-Mo(1)-C(10)-C(11)	25.6(3)
C(9)-Mo(1)-C(10)-C(11)	117.6(2)
C(12)-Mo(1)-C(10)-C(11)	36.00(13)
C(3)-Mo(1)-C(10)-C(11)	78.15(18)
C(5)-Mo(1)-C(10)-C(11)	169.21(13)
C(4)-Mo(1)-C(10)-C(11)	124.34(15)
S(2)-Mo(1)-C(10)-C(11)	-59.44(13)
S(1)-Mo(1)-C(10)-C(11)	-134.59(14)
C(8)-Mo(1)-C(10)-C(9)	-39.16(14)
C(6)-Mo(1)-C(10)-C(9)	113.7(3)
C(7)-Mo(1)-C(10)-C(9)	-92.0(3)
C(12)-Mo(1)-C(10)-C(9)	-81.58(15)
C(3)-Mo(1)-C(10)-C(9)	-39.43(19)
C(5)-Mo(1)-C(10)-C(9)	51.63(19)
C(4)-Mo(1)-C(10)-C(9)	6.76(18)
C(11)-Mo(1)-C(10)-C(9)	-117.6(2)
S(2)-Mo(1)-C(10)-C(9)	-177.02(13)
S(1)-Mo(1)-C(10)-C(9)	107.83(14)
C(9)-C(10)-C(11)-C(12)	1.3(2)
Mo(1)-C(10)-C(11)-C(12)	-60.28(15)
C(9)-C(10)-C(11)-Mo(1)	61.55(15)
C(8)-Mo(1)-C(11)-C(10)	-79.77(15)
C(6)-Mo(1)-C(11)-C(10)	153.60(17)
C(7)-Mo(1)-C(11)-C(10)	-168.51(13)
C(9)-Mo(1)-C(11)-C(10)	-37.07(14)
C(12)-Mo(1)-C(11)-C(10)	-118.8(2)
C(3)-Mo(1)-C(11)-C(10)	-126.53(14)
C(5)-Mo(1)-C(11)-C(10)	-51.1(6)
C(4)-Mo(1)-C(11)-C(10)	-87.00(18)

S(2)-Mo(1)-C(11)-C(10)	117.60(14)
S(1)-Mo(1)-C(11)-C(10)	45.99(14)
C(8)-Mo(1)-C(11)-C(12)	39.05(14)
C(6)-Mo(1)-C(11)-C(12)	-87.6(2)
C(7)-Mo(1)-C(11)-C(12)	-49.69(17)
C(9)-Mo(1)-C(11)-C(12)	81.75(15)
C(3)-Mo(1)-C(11)-C(12)	-7.70(17)
C(10)-Mo(1)-C(11)-C(12)	118.8(2)
C(5)-Mo(1)-C(11)-C(12)	67.8(5)
C(4)-Mo(1)-C(11)-C(12)	31.8(2)
S(2)-Mo(1)-C(11)-C(12)	-123.58(14)
S(1)-Mo(1)-C(11)-C(12)	164.81(13)
C(10)-C(11)-C(12)-C(8)	-2.5(2)
Mo(1)-C(11)-C(12)-C(8)	-64.18(14)
C(10)-C(11)-C(12)-Mo(1)	61.68(15)
C(9)-C(8)-C(12)-C(11)	2.8(2)
Mo(1)-C(8)-C(12)-C(11)	67.46(15)
C(9)-C(8)-C(12)-Mo(1)	-64.66(15)
C(8)-Mo(1)-C(12)-C(11)	-114.1(2)
C(6)-Mo(1)-C(12)-C(11)	139.16(14)
C(7)-Mo(1)-C(12)-C(11)	140.87(14)
C(9)-Mo(1)-C(12)-C(11)	-76.59(15)
C(3)-Mo(1)-C(12)-C(11)	173.33(15)
C(10)-Mo(1)-C(12)-C(11)	-35.19(14)
C(5)-Mo(1)-C(12)-C(11)	-166.78(13)
C(4)-Mo(1)-C(12)-C(11)	-158.67(14)
S(2)-Mo(1)-C(12)-C(11)	54.40(14)
S(1)-Mo(1)-C(12)-C(11)	-21.71(18)
C(6)-Mo(1)-C(12)-C(8)	-106.70(15)
C(7)-Mo(1)-C(12)-C(8)	-104.99(14)
C(9)-Mo(1)-C(12)-C(8)	37.56(13)
C(3)-Mo(1)-C(12)-C(8)	-72.53(14)
C(10)-Mo(1)-C(12)-C(8)	78.96(15)
C(5)-Mo(1)-C(12)-C(8)	-52.63(19)
C(4)-Mo(1)-C(12)-C(8)	-44.52(15)
C(11)-Mo(1)-C(12)-C(8)	114.1(2)

S(2)-Mo(1)-C(12)-C(8)	168.55(13)
S(1)-Mo(1)-C(12)-C(8)	92.43(14)

Symmetry transformations used to generate equivalent atoms: