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Chiral undecagold clusters: synthesis, characterization and investigation in catalysis

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X-Ray crystal structure analysis:

General: Data were collected at 150.0-(1) K on a Nonius Kappa CCD diffractometer using a Mo Kα (λ = 0.71070 Å) X-ray source and a graphite monochromator. All data were measured using phi and omega scans. Experimental details are described in Tables S1-1 – S3-1. The crystal structures were solved using SIR 97[1] and Shelxl-97.[2] ORTEP drawings were made using ORTEP III for Windows.[3] CCDC 775545 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at **www.ccdc.cam.ac.uk/conts/** retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk

Crystallographic data for 2*S*:

Figure S1: Molecular structure of 2*S*

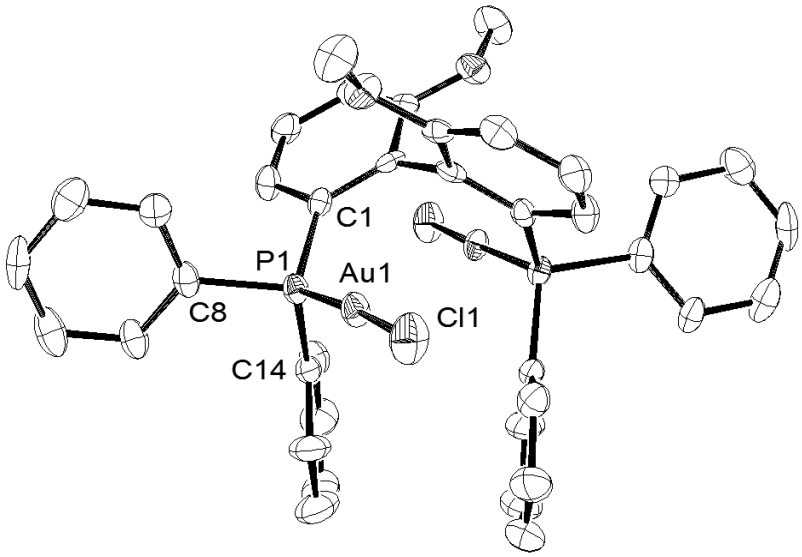

Table S1-1. Crystal data for 2*S*

Compound	**2*S***
Molecular formula	$C_{38}H_{32}Au_2Cl_2O_2P_2$
Molecular weight	1047.41
Crystal habit	Pale Yellow Block
Crystal dimensions(mm)	0.20x0.14x0.10
Crystal system	trigonal
Space group	P3121
a(Å)	10.462(1)
b(Å)	10.462(1)
c(Å)	27.906(1)
α(°)	90.00
β(°)	90.00
γ(°)	120.00
V(Å^3)	2645.2(4)
Z	3
d(g-cm^{-3})	1.973
F(000)	1494
μ(cm^{-1})	8.585
Absorption corrections	multi-scan ; 0.2786 min, 0.4806 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-13 8 ; -7 14 ; -39 39
Reflections measured	9420
Unique data	4524
Rint	0.0447
Reflections used	3722
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	209
Reflections / parameter	17
wR2	0.0583
R1	0.0352
Flack's parameter	-0.015(8)
Weights a, b	0.0169 ; 0.0000
GoF	0.968
difference peak / hole (e Å^{-3})	1.311(0.173) / -1.701(0.173)

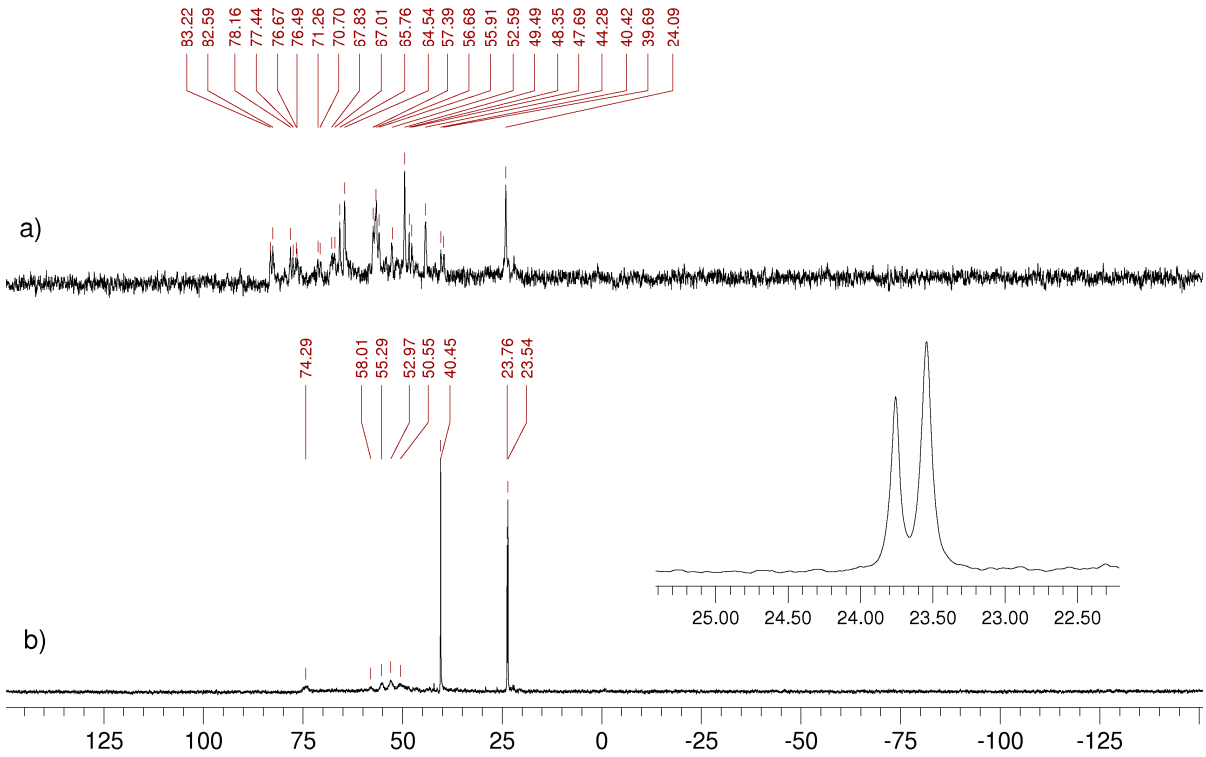

Figure S2. a) ^{31}P NMR spectrum of the reaction mixture between cluster **3***S* and AgOTf in dichloromethane, showing the decomposition of the initial cluster; b) ^{31}P NMR spectrum of the reaction mixture between cluster **3***S* and AgOTf in the presence of free ligand **1***S*.

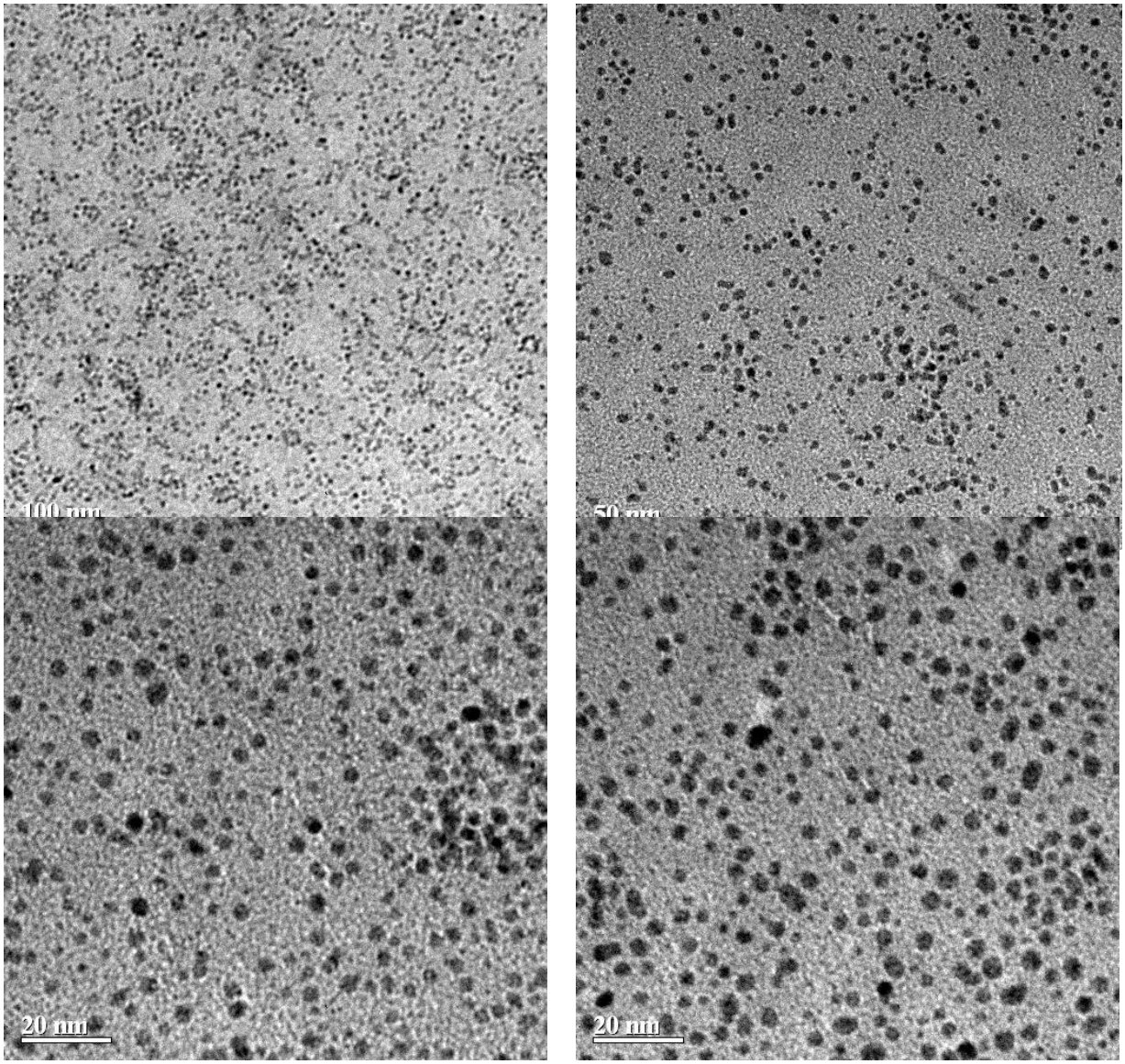

Figure S3. Additional TEM images (at different magnifications) of the cluster species **3***S* after the catalytic reaction (Table 1, entry 4).

1 A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *SIR97, an integrated package of computer programs for the solution and refinement of crystal structures using single crystal data.*

2 G. M. Sheldrick, in: *SHELXL-97* Universität Göttingen, Göttingen, Germany, 1997.

3 L. J. Farrugia, *ORTEP-3;* Department of Chemistry, University of Glasgow