Supporting Information

Synthesis, Structure, and Reactions of a (η^3-α-silabenzyl)molybdenum Complex: A Synthetic Equivalent of a Coordinatively Unsaturated Silyl Complex

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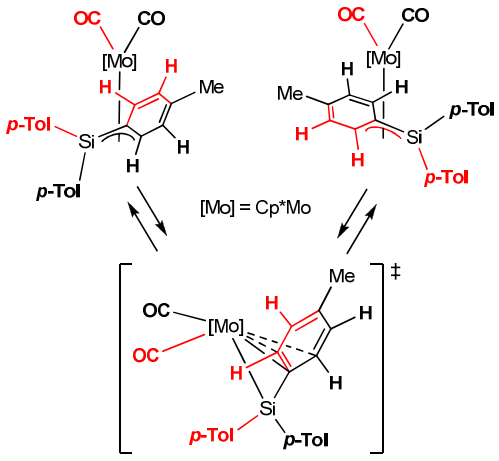
Scheme S1. A Possible Mechanism of the Dynamic Behavior of η^3-α-Silabenzyl Complex Cp*Mo(CO)$_2$\{η^3(*Si*,*C*,*C*)-Si(*p*-Tol)$_3$\} (1)



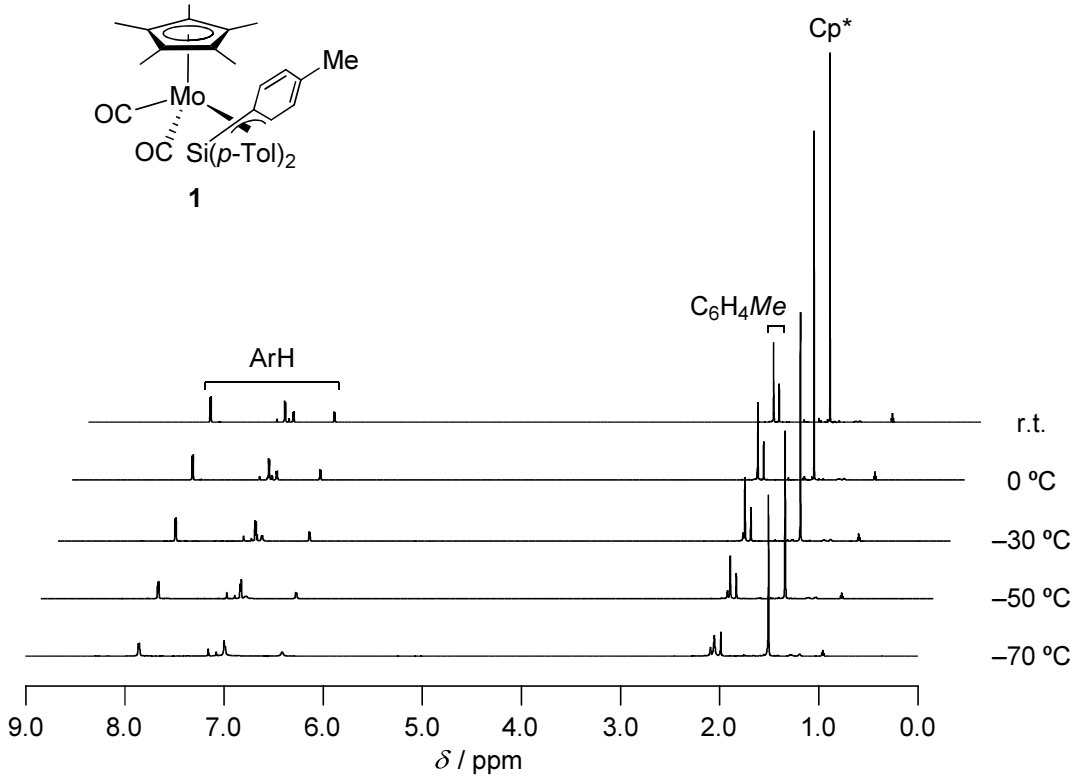


Figure S1. Variable temperature ^{1}H NMR spectra of Cp*Mo(CO)$_2${η^3(*Si,C,C*)-Si(*p*-Tol)$_3$} (**1**) in toluene-d_8.

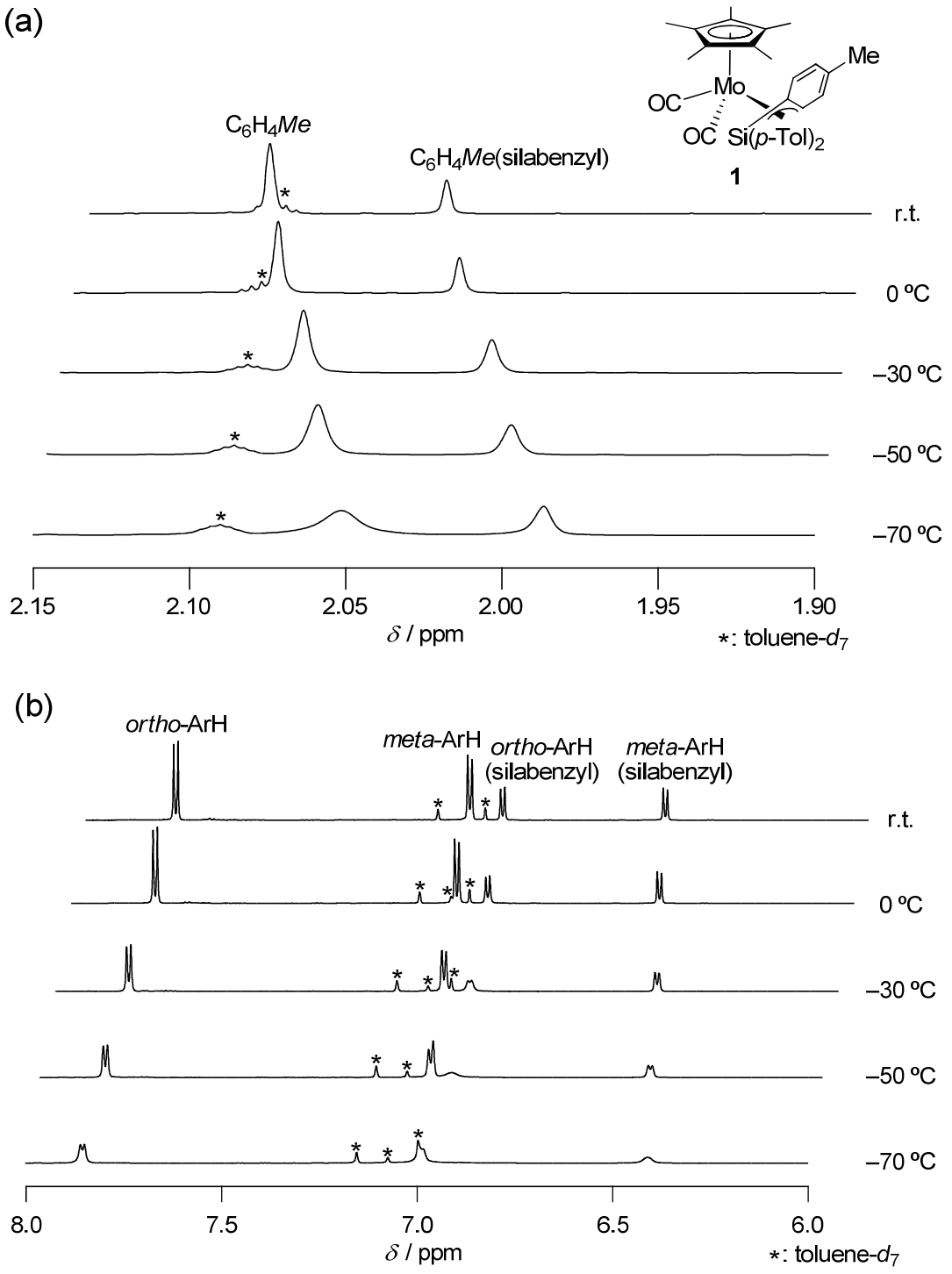


Figure S2. Expanded views of the signals for (a) methyl protons of *p*-tolyl groups and (b) aromatic protons in variable temperature ^{1}H NMR spectra of **1** in toluene-d_8.

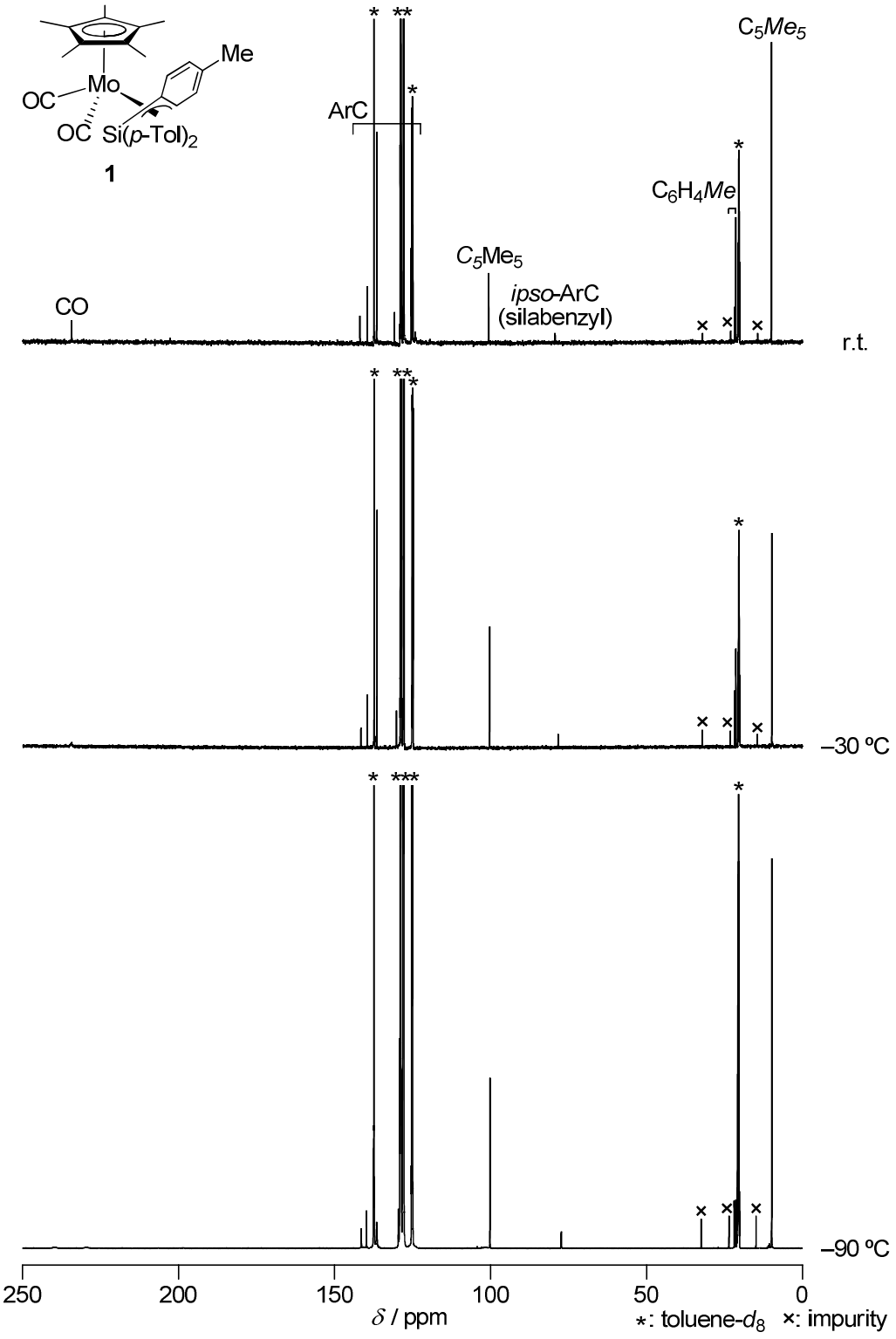


Figure S3. Variable temperature $^{13}C\{^1H\}$ NMR spectra of Cp*Mo(CO)$_2${η^3(*Si,C,C*)-Si(*p*-Tol)$_3$} (**1**) in toluene-d_8.

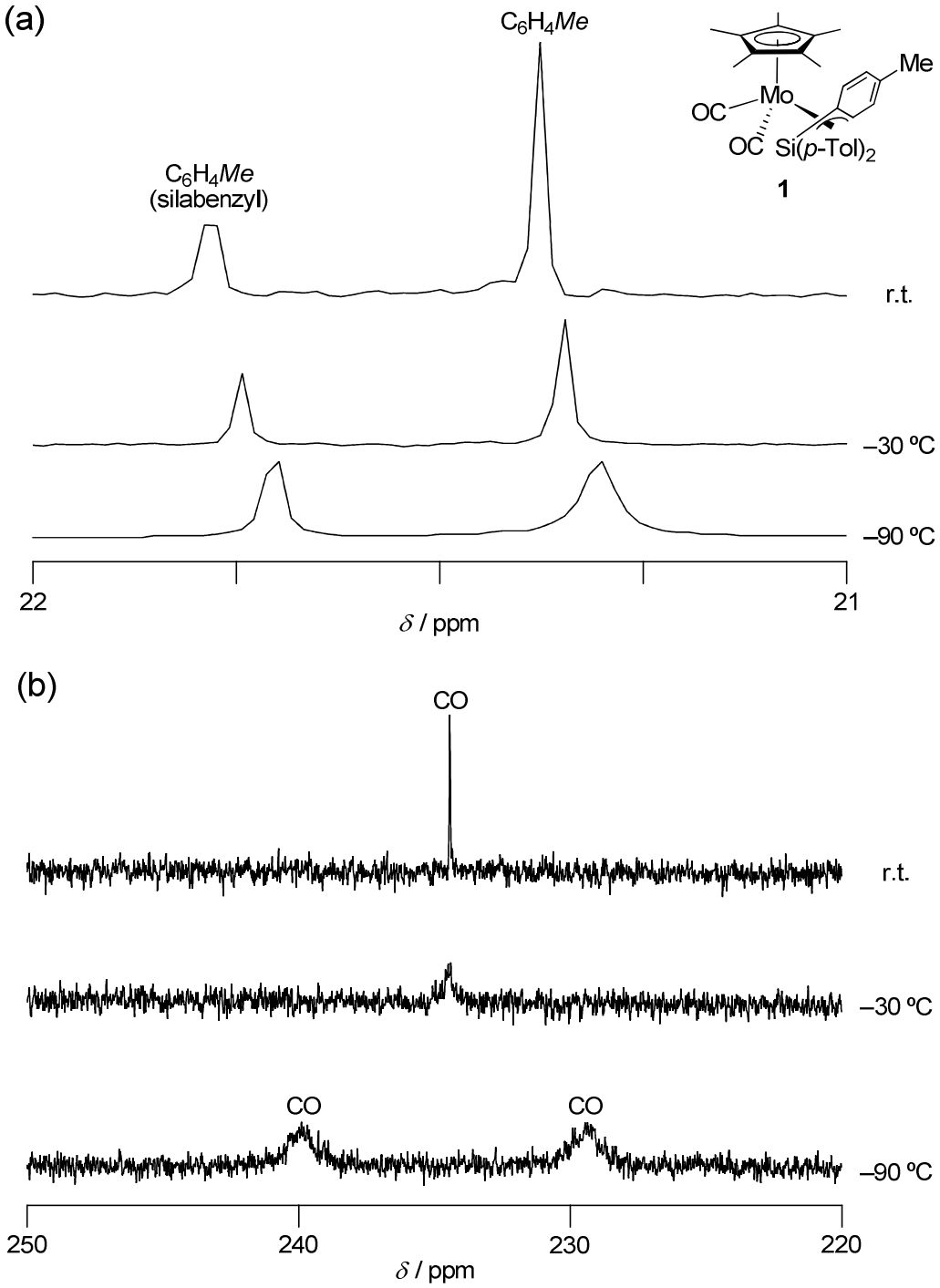


Figure S4. Expanded views of the signals for (a) methyl carbons of *p*-tolyl groups and (b) carbonyl ligands in variable temperature $^{13}C\{^{1}H\}$ NMR spectra of **1** in toluene-d_8.

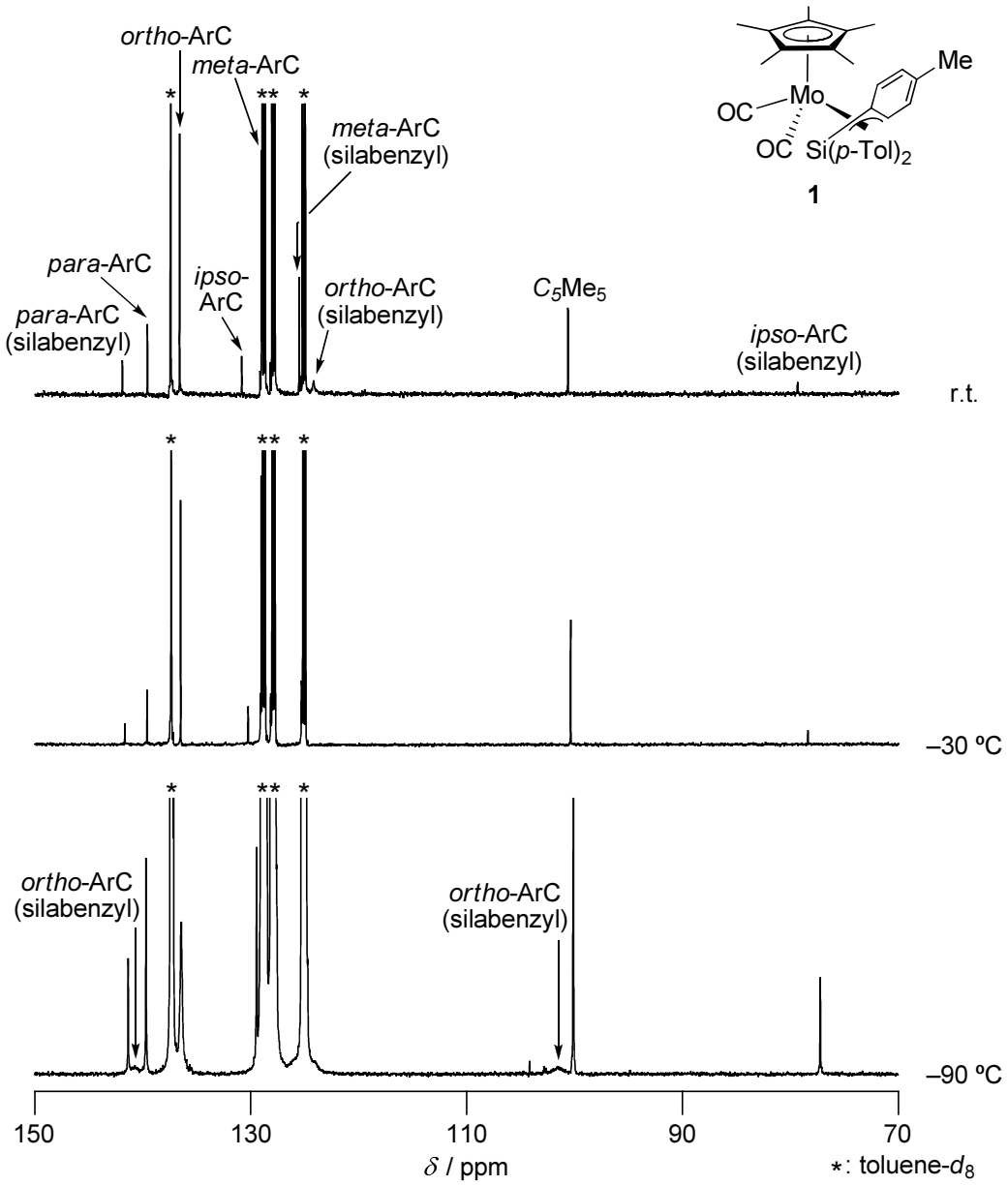


Figure S5. Expanded views of the signals for aromatic carbons in variable temperature $^{13}C\{^{1}H\}$ NMR spectra of **1** in toluene-d_8.

Table S1 Crystallographic Data for Cp*Mo(CO)$_2${η^3(*Si,C,C*)-Si(*p*-Tol)$_3$} (1), Cp*Mo(CO)$_2$(DMAP){Si(*p*-Tol)$_3$} (2), and Cp*Mo(CO)$_2${η^2(*C,N*)-C(Me)=NSi(*p*-Tol)$_3$} (4)

compound	**1**	**2**•1.5THF	**4**•0.5hexane
formula	$C_{33}H_{36}O_2SiMo$	$C_{46}H_{58}N_2O_{3.5}SiMo$	$C_{38}H_{46}NO_2SiMo$
formula weight	588.65	818.97	672.79
crystal system	monoclinic	monoclinic	monoclinic
crystal size/mm^3	0.27 × 0.19 × 0.10	0.37 × 0.20 × 0.12	0.35 × 0.35 × 0.33
space group	$P2_1/c$ (No. 14)	$C2/c$ (No. 15)	$P2_1/c$ (No. 14)
a/Å	8.4574(2)	20.6607(10)	21.7540(6)
b/Å	32.8279(7)	20.3913(7)	8.6383(3)
c/Å	10.3808(3)	20.7670(9)	20.4816(5)
β/°	92.5371(11)	101.6454(15)	113.4531(10)
V/Å^3	2879.29(12)	8569.0(6)	3530.88(18)
Z	4	8	4
D_{calcd}/g·cm^{-3}	1.358	1.270	1.266
F(000)	1224	3456	1412
μ(Mo-Kα)/mm^{-1}	0.525	0.376	0.437
reflections collected	21553	34029	52632
unique reflections (R_{int})	6349 (0.0378)	9369 (0.0428)	8038 (0.0279)
refined parameters	346	461	398
$R1$, $wR2$ (all data)	0.0508, 0.1073	0.0751, 0.1724	0.0300, 0.0910
$R1$, $wR2$ [$I > 2\ \sigma(I)$]	0.0429, 0.0988	0.0556, 0.1556	0.0257, 0.0791
GOF	1.295	1.167	1.266
Largest residual peak, hole/e·Å^{-3}	0.445, –0.621	1.142, –0.718	0.442, –0.634