One-Pot Synthesis of Substituted Benzene via Intermolecular [2+2+2] Cycloaddition Catalyzed by Air Stable Ru(II)-Complex

Chung-Yeh Wu, Ying-Chih Lin,* Pi-Tai Chou,Yu Wang, Yi-Hung Liu

Department of Chemistry, National Taiwan University
Taipei, 106 (Taiwan)
Fax: (+886) 223636359
E-mail: yclin@ntu.edu.tw

Table s1. Crystal Data and Collection and Refinement Parameters.

	4ga	**4gs**	**6p**	**7**
formula	$C_{34}H_{26}O_8$	$C_{34}H_{26}O_8$	$C_{69}H_{61}Cl_4O_{24.5}$	$C_{22}H_{16}O_8S_2$
formula weight	562.55	562.55	1423.98	472.47
crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$P2_1/c$
a(Å)	8.79121(1)	11.9034(6)	12.0972(3)	9.0718(3)
b(Å)	13.56521(1)	11.1168(5)	14.9120(4)	19.0514(9)
c(Å)	24.5222(2)	21.4260(9)	20.7722(6)	11.6545(4)
α(deg)	90°	90°	72.261(2)°	90°
β(deg)	98.6201(1)°	97.873(4)°	77.370(2)°	91.567(4)°
γ(deg)	90°	90°	89.011(2)°	90°
V(Å^3)	2891.35(5)	2808.5(2)	3477.73(16)	2013.50(14)
Z	4	4	2	4
reflns collected	23056	12030	28484	11482
Indep reflns (Rint)	5278(0.0174)	5030(0.0578)	12637(0.0331)	3633(0.0524)
Goodness-of-fit on F^2	1.454	1.779	1.555	1.434
R_1/wR_2 [$I>2\sigma(I)$]	0.0405/0.1572	0.1341/0.3213	0.0739/0.2115	0.0668/0.1909
R_1/wR_2 (all data)	0.0441/0.1623	0.2295/0.3622	0.0939/0.2212	0.0882/0.2088

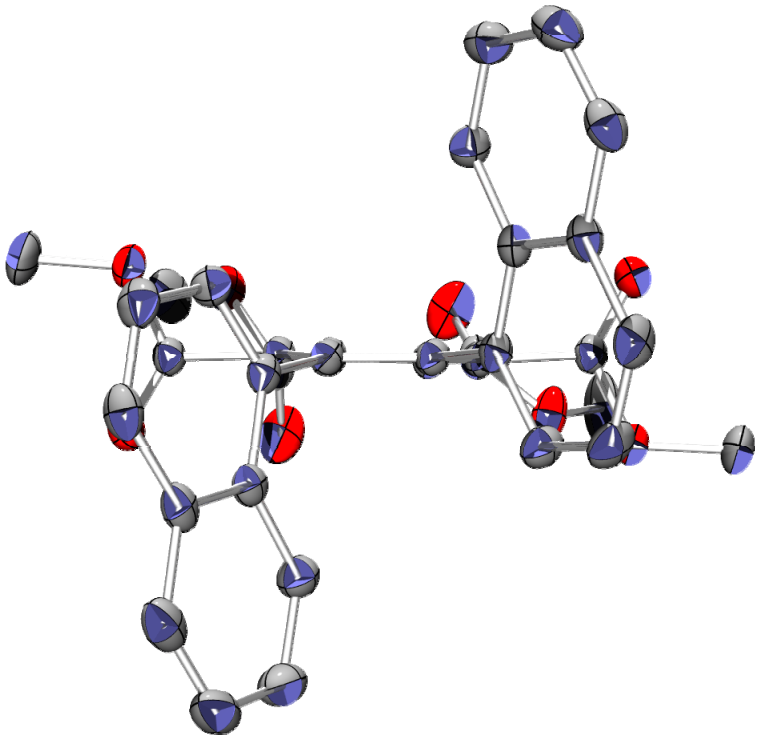

Figure S1. X-ray crystal structure of **4ga** with hydrogen atoms are omitted for clarity. (thermal ellipsoids are set at 30% probability level)

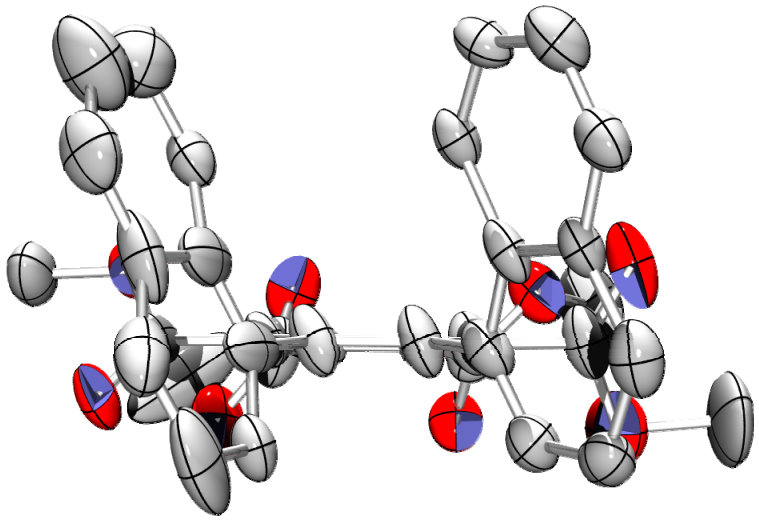

Figure S2. X-ray crystal structure of **4gs** with hydrogen atoms are omitted for clarity. (thermal ellipsoids are set at 30% probability level)

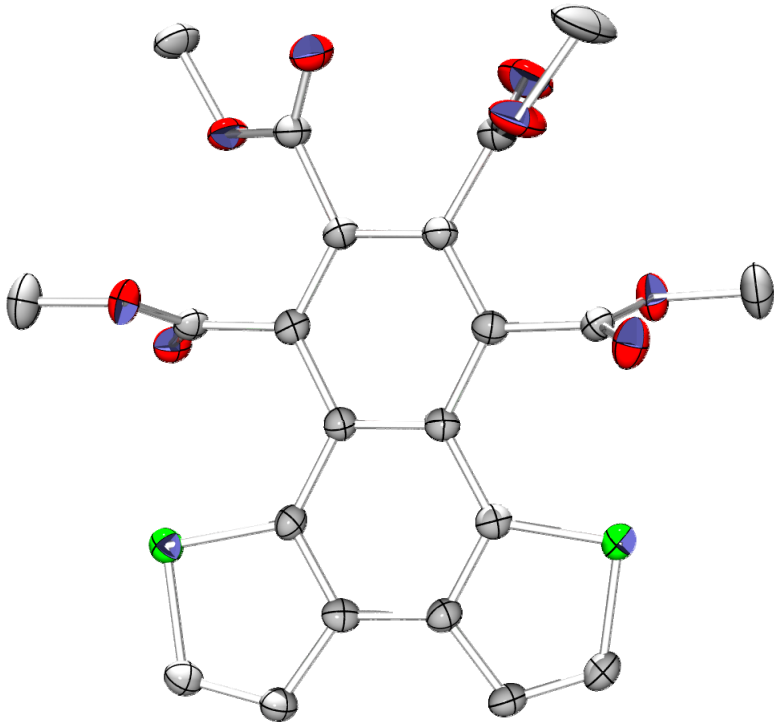

Figure S3. X-ray crystal structure of **7** with hydrogen atoms are omitted for clarity. (thermal ellipsoids are set at 30% probability level)