Supplementary Information

Atomically Precise Structure of $Pt_2(S\text{-}Adam)_4(PPh_3)_2$ Complexes and Catalytic Application in Propane Dehydrogenation

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1. Figures

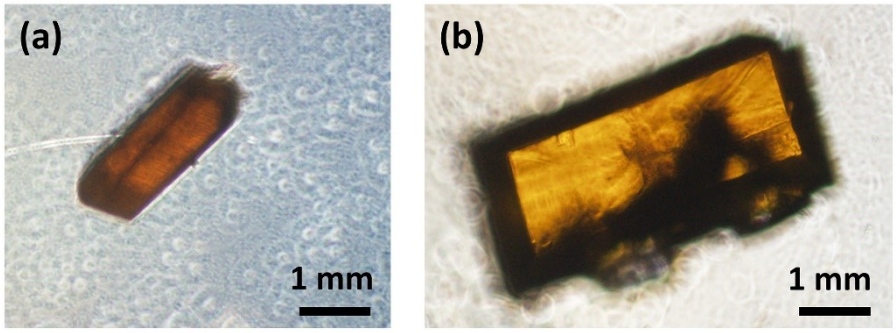

Figure S1. The photos of Pt_2-A crystals (a) and Pt_2-B crystals (b) taken by optical electron microscopy.

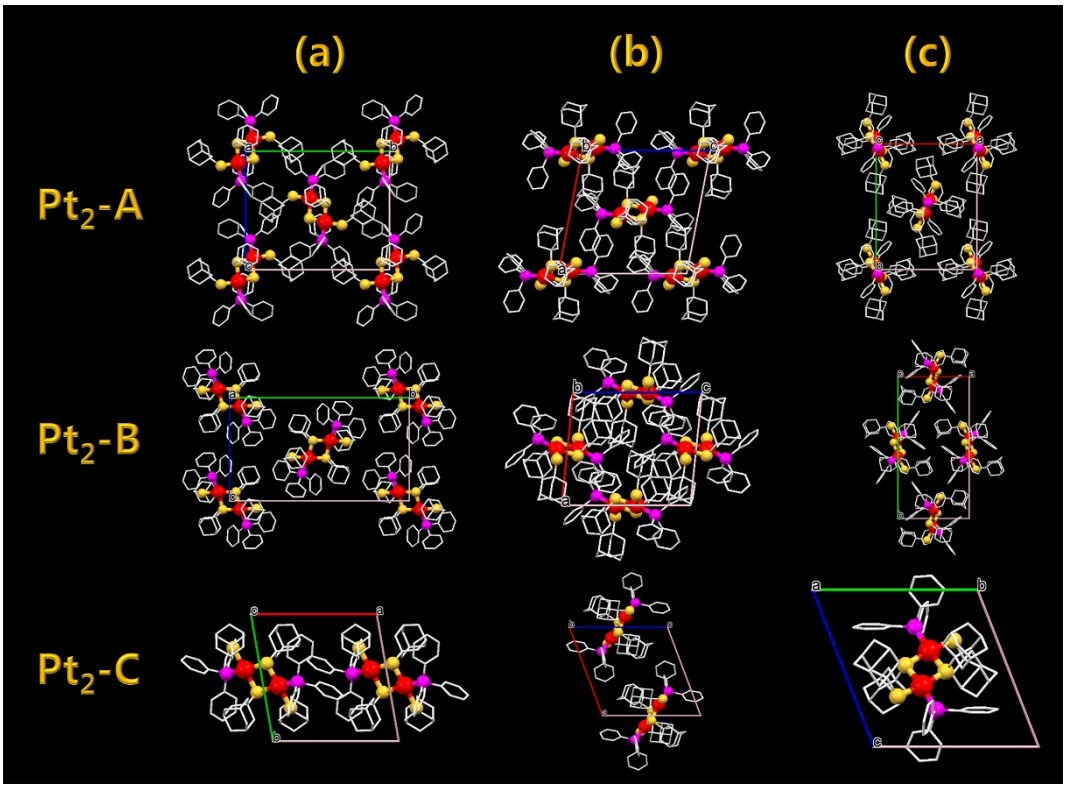

Figure S2. (a-c) Packing of Pt_2 complexes isomers from a, b, c directions in a unit cell, respectively. Color legend: Pt, red; S, yellow; P, purple; C, light grey. Hydrogen atoms are omitted for clarity.

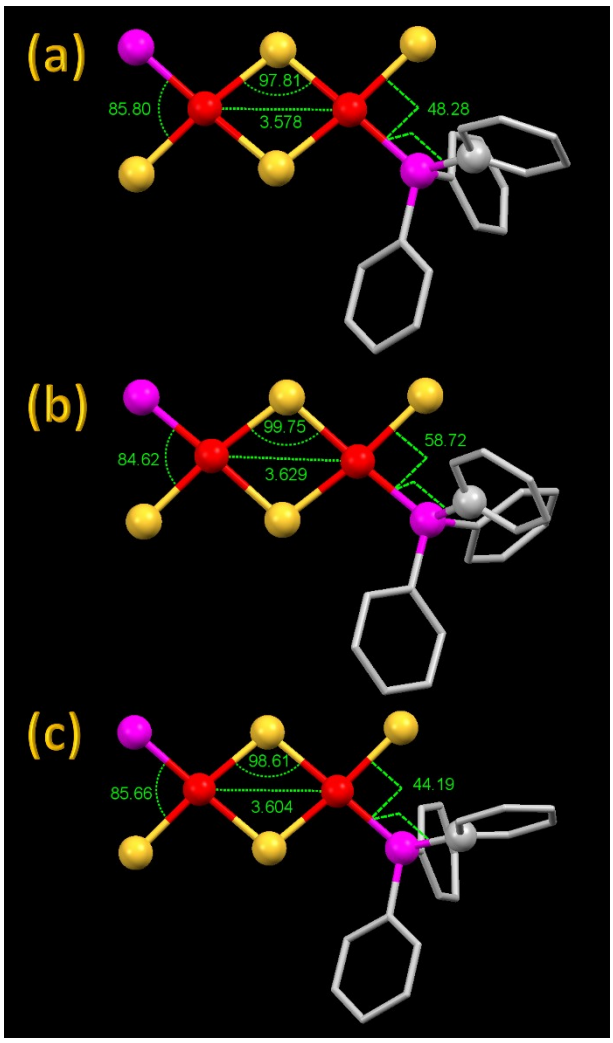

Figure S3. (a-c) Comparative analysis of structural angels and lengths for Pt_2 complexes isomers. The unit of distances is Å and the unit of angles is °. Color legend: Pt, red; S, yellow; P, purple; C, light grey.

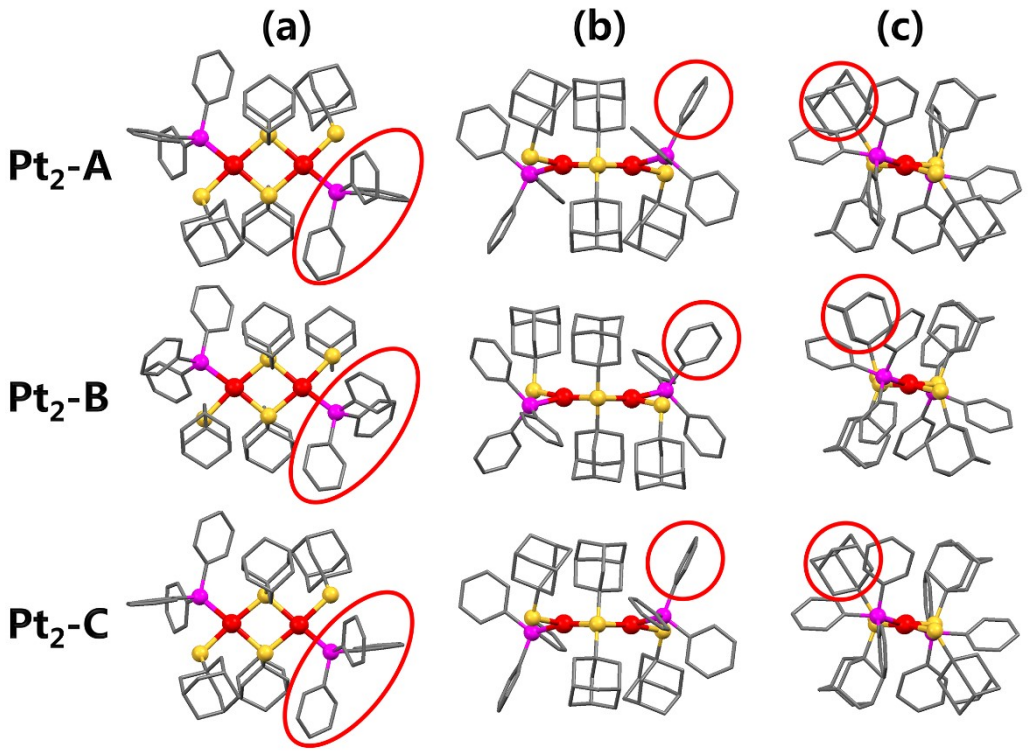

Figure S4. Total structures of Pt_2 complexes from (a) top view, (b) front view, and (c) side view, respectively. Color legend: Pt, red; S, yellow; P, purple; C, grey. Hydrogen atoms are omitted for clarity.

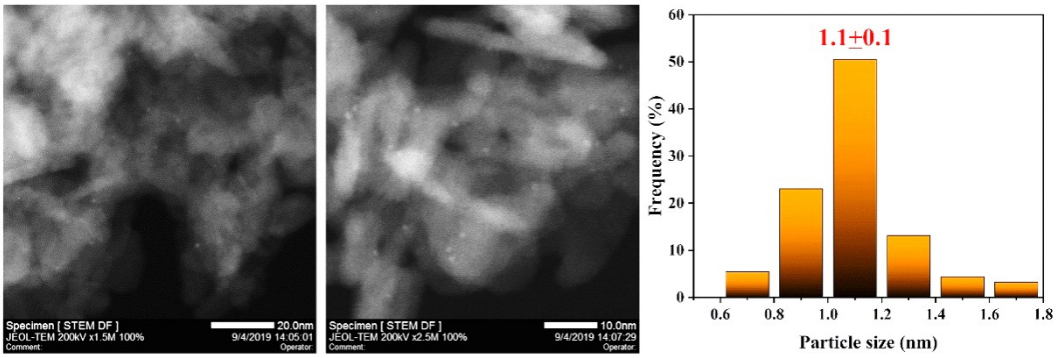

Figure S5. STEM images of $Pt_2/\gamma\text{-}Al_2O_3\text{-}600\text{-}N_2$.

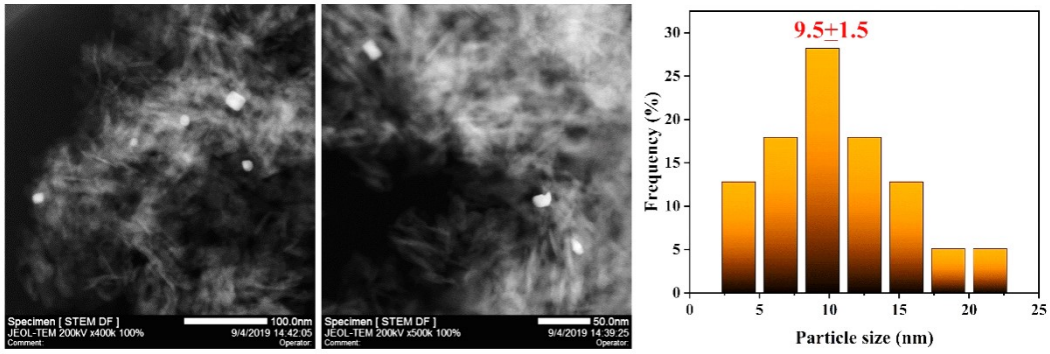

Figure S6. STEM images of $Pt_2/\gamma\text{-}Al_2O_3\text{-}600\text{-}O_2$.

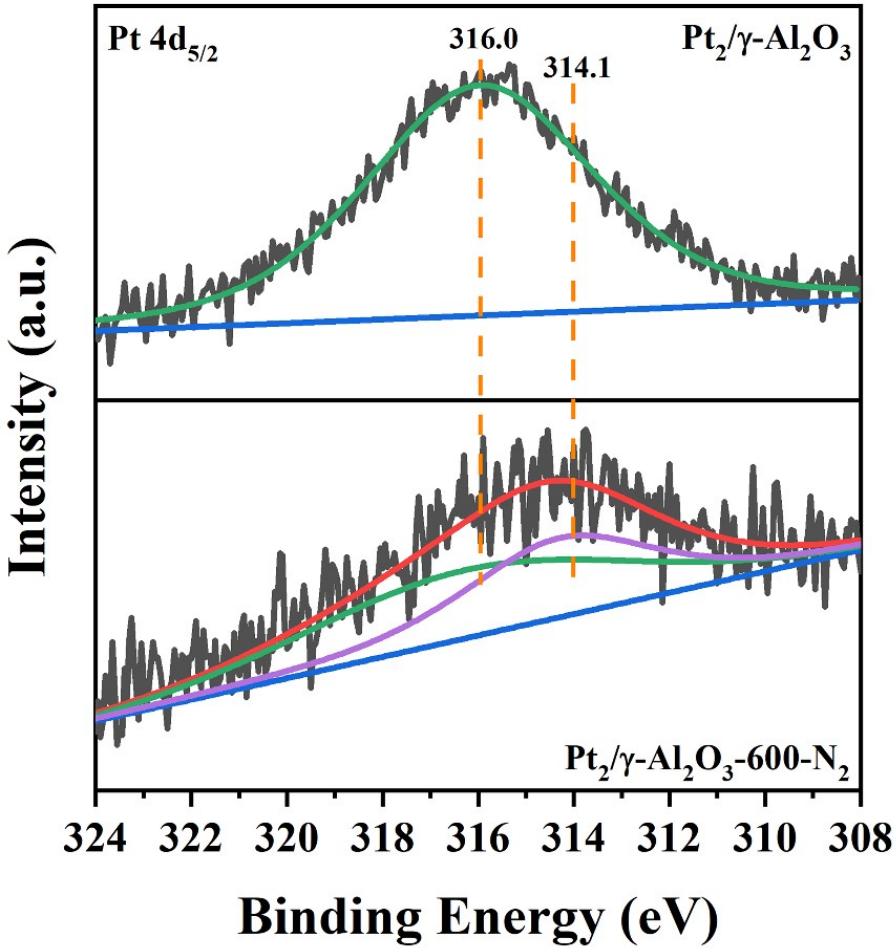

Figure S7. Pt $4d_{5/2}$ XPS spectra of $Pt_2/\gamma\text{-}Al_2O_3$ and $Pt_2/\gamma\text{-}Al_2O_3\text{-}600\text{-}N_2$.

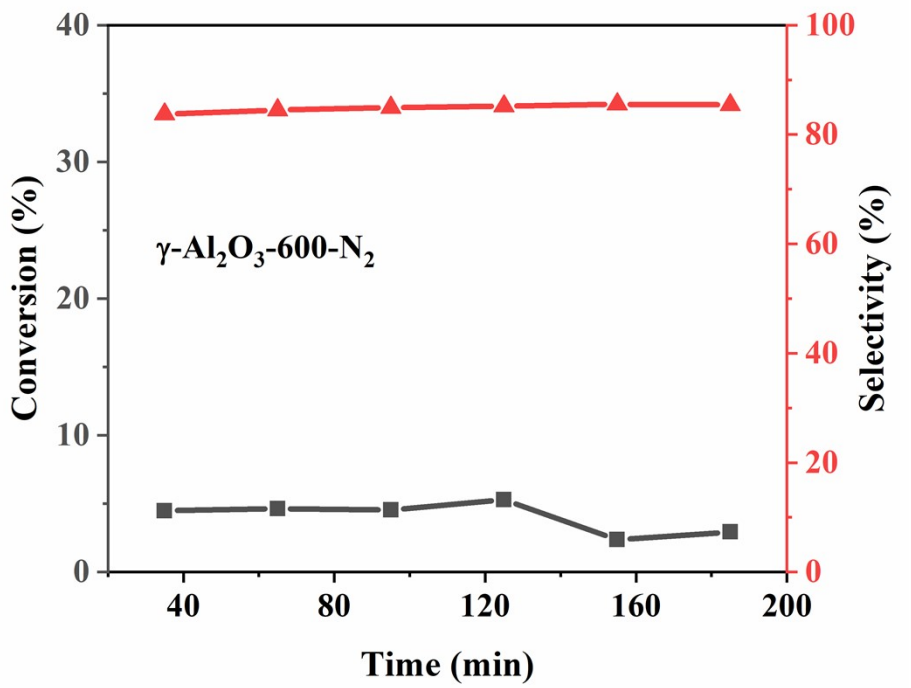

Figure S8. The catalytic performance of γ-Al_2O_3-600-N_2 in propane dehydrogenation.

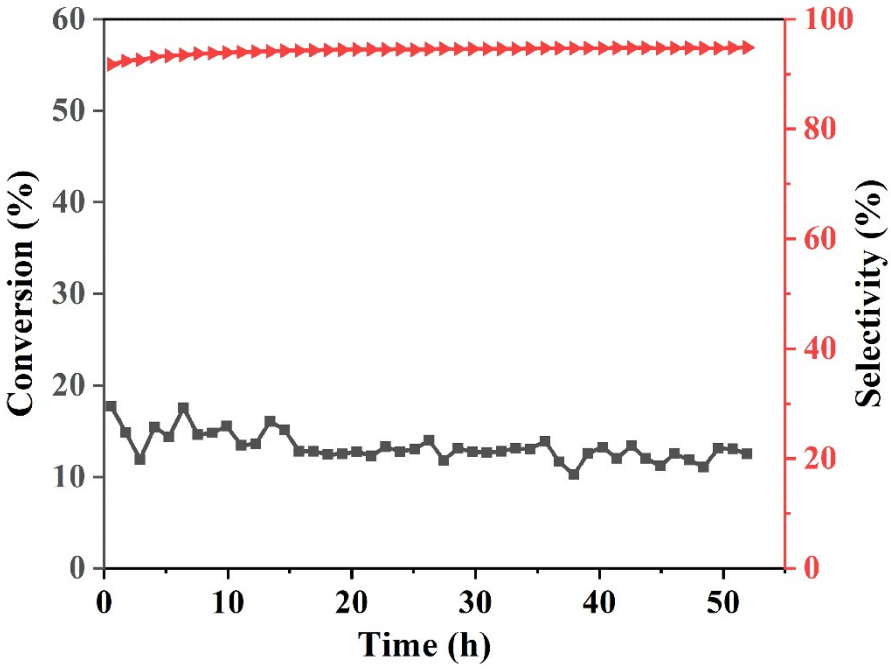

Figure S9. The catalytic stability of $Pt_2/\gamma\text{-}Al_2O_3\text{-}600\text{-}N_2$ in propane dehydrogenation.

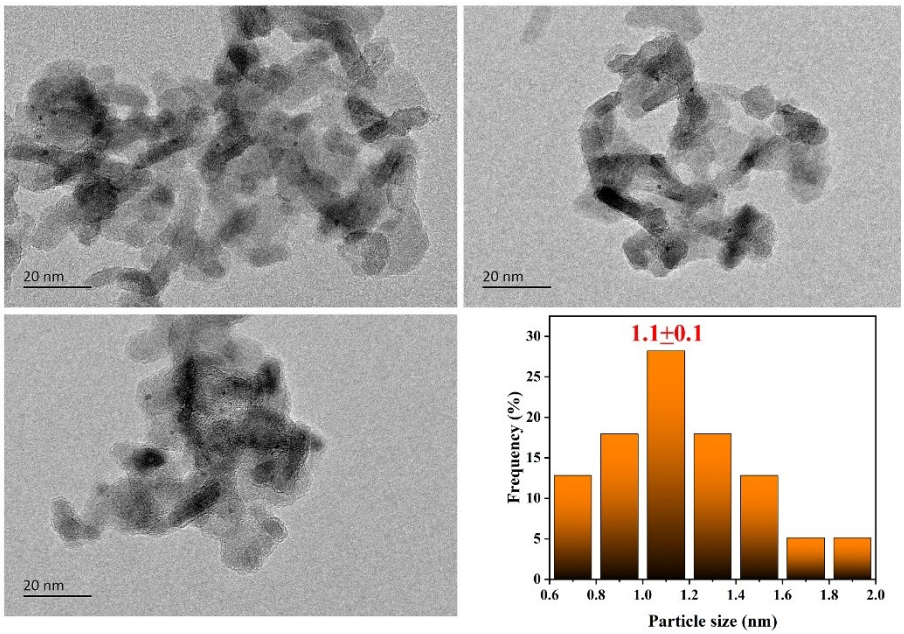

Figure S10. The HRTEM images of the spent Pt_2/γ-Al_2O_3-600-N_2 catalyst after catalytic propane dehydrogenation for 50 h.

2. Tables

Table S1. Crystal data and structure refinement for three Pt_2 complexes (A, B and C).

	A	B	C
Compound	$Pt_2(PPh_3)_2(SC_{10}H_{15})_4$	$Pt_2(PPh_3)_2(SC_{10}H_{15})_4$	$Pt_2(PPh_3)_2(SC_{10}H_{15})_4$
Empirical formula	C76 H90 P2 Pt2 S4'	C76 H90 P2 Pt2 S4'	C76 H90 P2 Pt2 S4'
Formula weight	1583.83	1583.83	1583.83
Crystal system	monoclinic	monoclinic	triclinic
Temperature (K)	100	293	293
Radiation type, wavelength (Å)	synchrotron radiation, 0.6229	0.71073	0.71073
Space group	P 21/n	P 21/n	P -1
a, b, c (Å)	14.310(3), 17.506(4), 14.665(3	11.7531(5), 23.1655(12), 13.3165(7)	13.016(2), 13.366(3), 14.337(2)
α, β, γ (°)	90, 100.92(3), 90	90, 95.940(5), 90	62.656(18), 63.186(19), 69.974(17)
V ($Å^3$)	3607.2(13)	3606.2(3)	1948.3(7)
Z	2	2	1
Density (mg /m^3)	1.458	1.231	1.350
Crystal size (mm^3)	2.2*0.8*0.6	3.1*1.5*0.2	1.2*0.7*0.3
Absorption coefficient	4.074	4.227	3.771
F(000)	1592	1760	796
Theta range for data collection	2.05 to 27.56	2.818 to 29.815	3.377 to 22.389
Index ranges	-19<=h<=0, -23<=k<=23, -18<=l<=19	-14<=h<=15, -25<=k<=32, -17<=l<=18	-15<=h<=15, -15<=k<=14, -17<=l<=15

Reflections collected	9340	8797	6837
Independent reflections	8800	7056	3874
Goodness-of-fit on F2	1.025	1.091	0.938
Final R indices [I>2sigma(I)]	R1=0.0288, wR2= 0.0761	R1=0.0312, wR2= 0.0624	R1=0.0911, wR2= 0.2075
R indices (all data)	R1= 0.0303, wR2= 0.0776	R1=0.0486, wR2= 0.0707	R1= 0.1450, wR2= 0.2333

Table S2. Crystal data comparison of three Pt_2 complexes isomers (A, B and C)

	A	**B**	**C**
Formula	C76 H90 P2 Pt2 S4	C76 H90 P2 Pt2 S4	C76 H90 P2 Pt2 S4
Crystal system	monoclinic	monoclinic	triclinic
Space group	P 21/n	P 21/n	P -1
a, b, c (Å)	14.310(3), 17.506(4), 14.665(3)	11.7531(5), 23.1655(12), 13.3165(7)	13.016(2), 13.366(3), 14.337(2)
α, β, γ (°)	90, 100.92(3), 90	90, 95.940(5), 90	62.656(18), 63.186(19), 69.974(17)
V ($Å^3$)	3607.2(13)	3606.2(3)	1948.3(7)

Table S3. Structural analysis of three Pt_2 complexes isomers (A, B and C)

	A	**B**	**C**
Pt--Pt distance (Å)	3.578	3.629	3.604
Pt-S lengths (Å)	2.3639 (2.3442-2.3789)	2.365(2.349-2.378)	2.369(2.351-2.391)
Pt-P lengths	2.2707	2.2868	2.273
Pt-S-Pt angles (°)	97.81	99.75	98.60