

Supporting Information

Synthesis and Characterization of Conjugated Diallenes and their Binuclear Ruthenium η^3 -Allyl Complexes

Jian-Long Xia, Xianghua Wu, Yinghui Lu, Gang Chen, Shan Jin, Guang-ao Yu, Sheng Hua Liu*

Key Laboratory of Pesticide and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

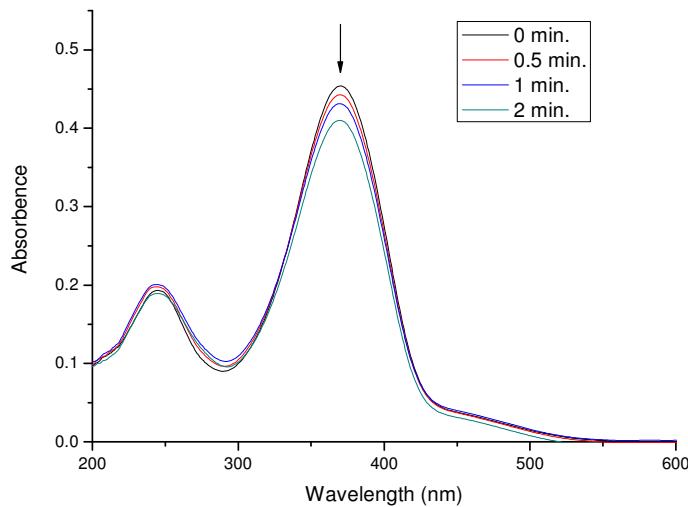


Figure S1 UV/Vis absorption spectral change of compound **4** (1×10^{-5} mol/L) in CH_2Cl_2 upon the UV light irradiation at 0, 0.5, 1, 2 min..

Table S1. Bond lengths (\AA) and angles ($^\circ$) for compound **4**.

| | |
|----------------|------------|
| C(1)-C(2) | 1.374(2) |
| C(1)-C(6) | 1.387(2) |
| C(1)-N(1) | 1.423(2) |
| C(2)-C(3) | 1.370(3) |
| C(2)-H(2) | 0.9300 |
| C(3)-C(4) | 1.394(2) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.385(2) |
| C(4)-C(7) | 1.467(3) |
| C(5)-C(6) | 1.373(2) |
| C(5)-H(5) | 0.9300 |
| C(6)-H(6) | 0.9300 |
| C(7)-C(8) | 1.302(2) |
| C(7)-H(7) | 1.0507 |
| C(8)-C(9) | 1.283(3) |
| C(9)-H(9A) | 0.9603 |
| C(9)-H(9B) | 1.0691 |
| N(1)-N(1)#1 | 1.251(3) |
| | |
| C(2)-C(1)-C(6) | 118.98(18) |
| C(2)-C(1)-N(1) | 116.44(16) |
| C(6)-C(1)-N(1) | 124.57(16) |
| C(3)-C(2)-C(1) | 121.01(17) |
| C(3)-C(2)-H(2) | 119.5 |
| C(1)-C(2)-H(2) | 119.5 |
| C(2)-C(3)-C(4) | 120.88(17) |
| C(2)-C(3)-H(3) | 119.6 |
| C(4)-C(3)-H(3) | 119.6 |
| C(5)-C(4)-C(3) | 117.41(18) |
| C(5)-C(4)-C(7) | 120.35(18) |
| C(3)-C(4)-C(7) | 122.21(16) |
| C(6)-C(5)-C(4) | 121.85(17) |
| C(6)-C(5)-H(5) | 119.1 |
| C(4)-C(5)-H(5) | 119.1 |
| C(5)-C(6)-C(1) | 119.86(16) |

| | |
|------------------|------------|
| C(5)-C(6)-H(6) | 120.1 |
| C(1)-C(6)-H(6) | 120.1 |
| C(8)-C(7)-C(4) | 125.91(18) |
| C(8)-C(7)-H(7) | 120.1 |
| C(4)-C(7)-H(7) | 113.8 |
| C(9)-C(8)-C(7) | 179.4(2) |
| C(8)-C(9)-H(9A) | 133.6 |
| C(8)-C(9)-H(9B) | 121.0 |
| H(9A)-C(9)-H(9B) | 102.7 |
| N(1)#1-N(1)-C(1) | 114.56(18) |
