Supplementary Materials: Impact of the Subunit Arrangement on the Nonlinear Absorption Properties of Organometallic Complexes with Ruthenium(II) σ-Acetylide and Benzothiadiazole as Building Units

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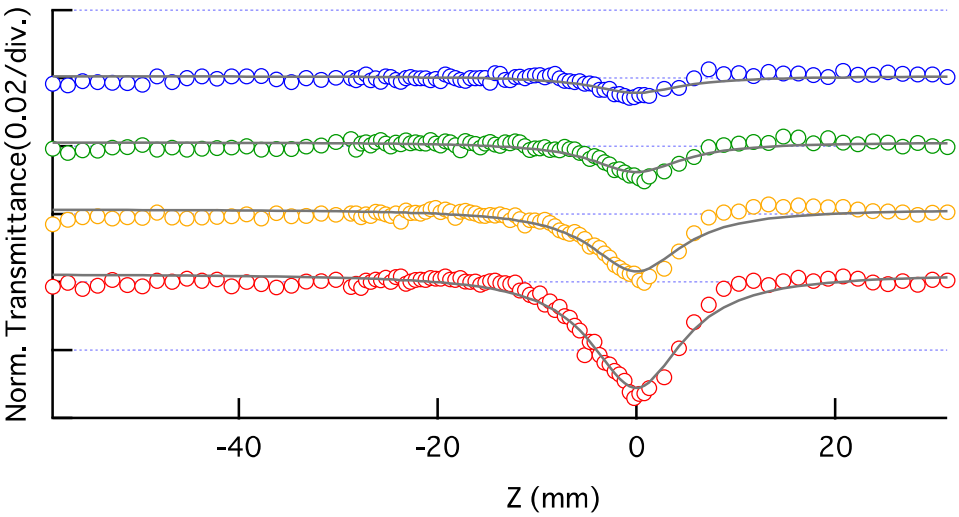

Figure S1. Open-aperture Z-scan traces at different incident powers (0.19, 0.23, 0.32, 0.42 mW from top to bottom) of **Ru-1** in dichloromethane excited at 800 nm. Solid curves are theoretical fits.

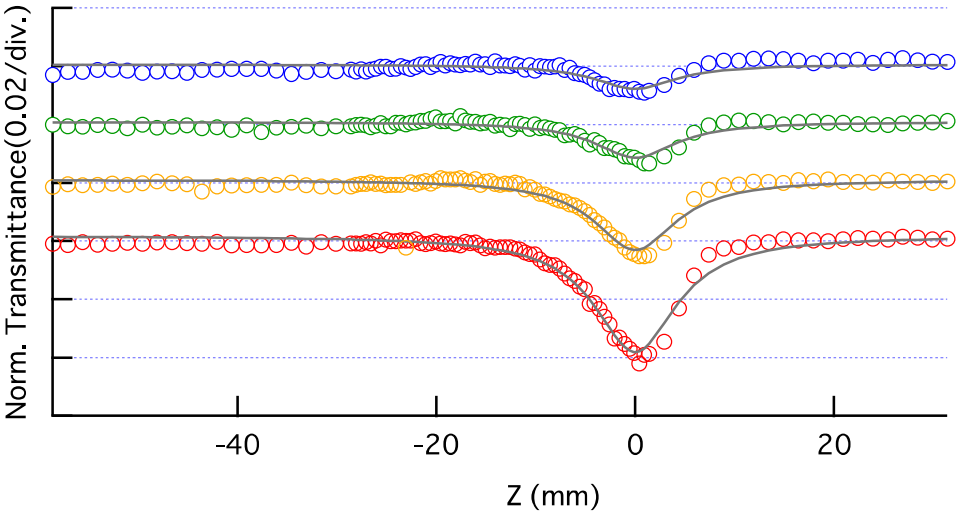

Figure S2. Open-aperture Z-scan traces at different incident powers (0.18, 0.22, 0.29, 0.39 mW from top to bottom) of **Ru-1** in dichloromethane excited at 840 nm. Solid curves are theoretical fits.

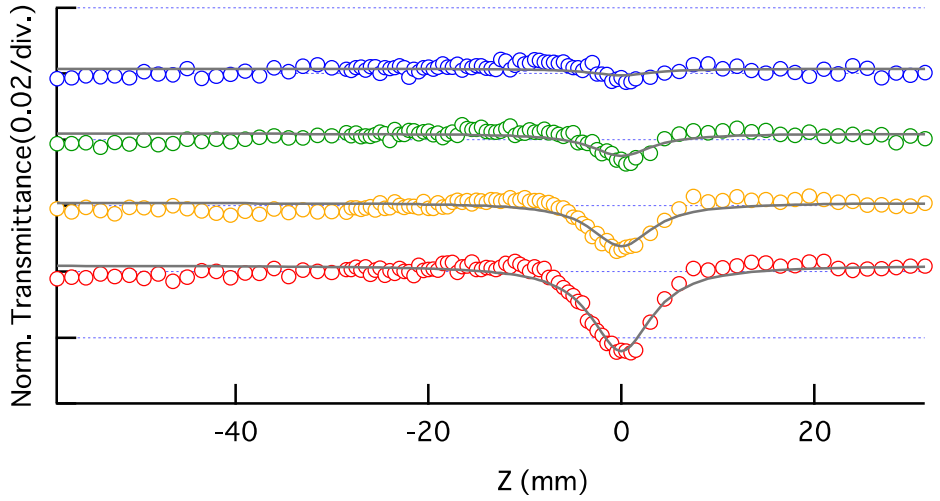

Figure S3. Open-aperture Z-scan traces at different incident powers (0.22, 0.25, 0.34, 0.44 mW from top to bottom) of **Ru-1** in dichloromethane excited at 960 nm. Solid curves are theoretical fits.

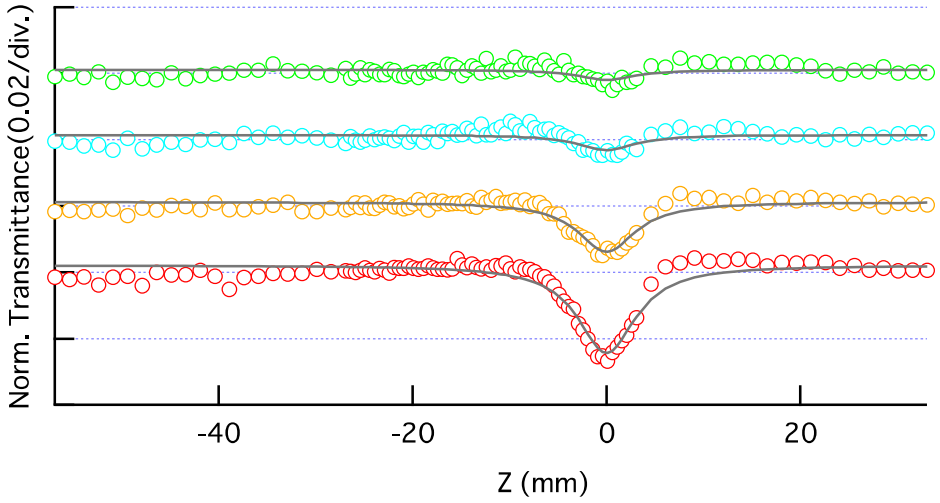

Figure S4. Open-aperture Z-scan traces at different incident powers (0.25, 0.29, 0.39, 0.50 mW from top to bottom) of **Ru-1** in dichloromethane excited at 970 nm. Solid curves are theoretical fits.

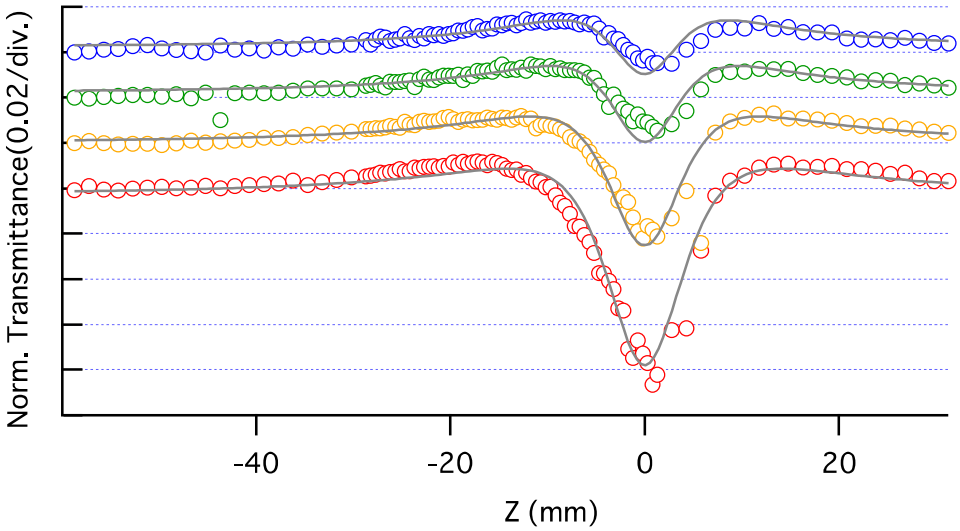

Figure S5. Open-aperture Z-scan traces at different incident powers (0.19, 0.22, 0.31, 0.42 mW from top to bottom) of **Ru-2** in dichloromethane excited at 800 nm. Solid curves are theoretical fits assuming the saturable absorption.

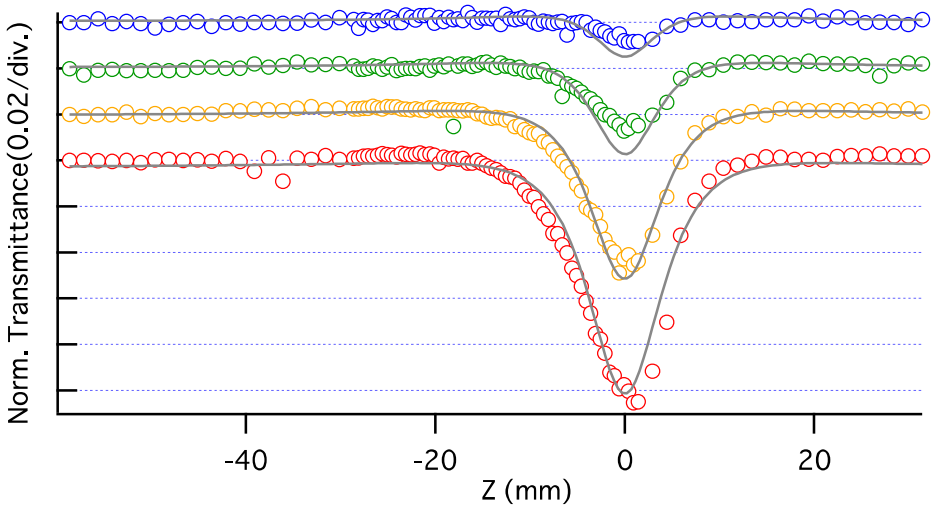

Figure S6. Open-aperture Z-scan traces at different incident powers (0.11, 0.28, 0.29, 0.39 mW from top to bottom) of **Ru-2** in dichloromethane excited at 840 nm. Solid curves are theoretical fits assuming the saturable absorption.

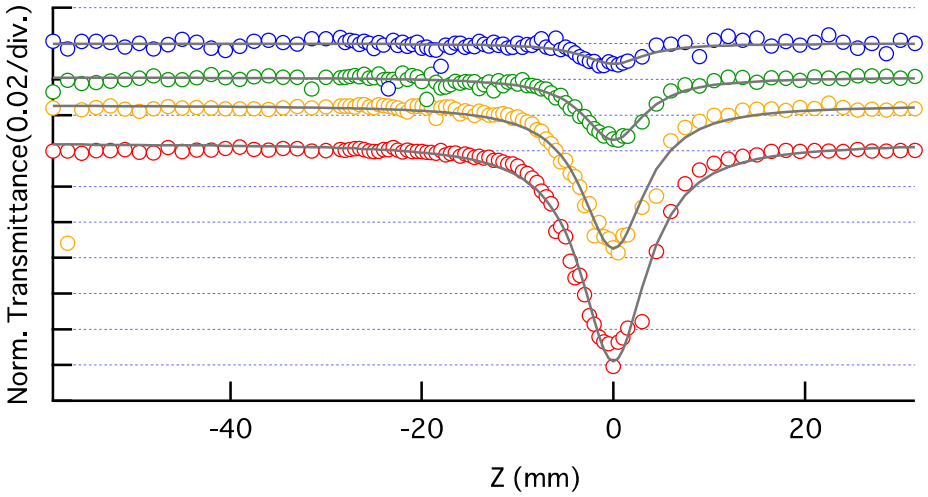

Figure S7. Open-aperture Z-scan traces at different incident powers (0.12, 0.22, 0.38, 0.44 mW from top to bottom) of **Ru-2** in dichloromethane excited at 960 nm. Solid curves are theoretical fits.

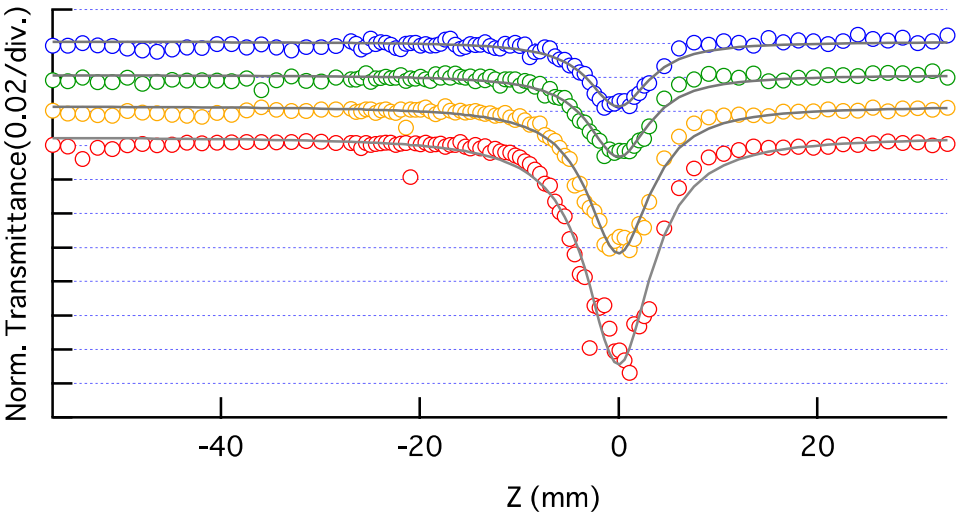

Figure S8. Open-aperture Z-scan traces at different incident powers (0.25, 0.29, 0.39, 0.50 mW from top to bottom) of **Ru-2** in dichloromethane excited at 970 nm. Solid curves are theoretical fits.

Table S1. Summary of the TD-DFT calculations of transition energy, wavelength, oscillator strength, electronic configuration and the contribution of the 12 lowest excited states of Ru-1 and Ru-2 calculated at the B3LYP/6-31G(d) (lanl2DZ for Ru) level.

Ru-1 (HOMO: orbital 383; LUMO: orbital 384)			
Excited State 1	1.7217 eV	720.11 nm	*f*=0.8670
	382 → 385	-0.11458	
	383 → 384	0.68509	
	383 → 385	0.11653	
Excited State 2	1.7979 eV	689.60 nm	*f* =0.0465
	383 → 384	-0.11921	
	383 → 385	0.69191	
Excited State 3	2.0192 eV	614.03 nm	*f*=0.0776
	382 → 384	0.67523	
	382 → 385	-0.16890	
Excited State 4	2.0321 eV	610.14 nm	*f*=0.1895
	382 → 384	0.17403	
	382 → 385	0.66917	
Excited State 5	2.4556 eV	504.91 nm	*f*=0.0118
	381 → 384	0.69470	
Excited State 6	2.4867 eV	498.59 nm	*f*=0.0133
	381 → 385	0.69298	
Excited State 7	2.6025 eV	476.40 nm	*f*=0.0004
	380 → 386	0.16191	
	383 → 386	0.66606	
Excited State 8	2.7333 eV	453.61 nm	*f*=0.0092
	379 → 385	0.14558	
	380 → 384	0.67217	
Excited State 9	2.7618 eV	448.93 nm	*f*=0.0201
	379 → 384	0.15514	
	380 → 385	0.67070	
Excited State 10	2.9157 eV	425.23 nm	f=0.0010
	381 → 386	0.36859	
	382 → 386	0.57089	
Excited State 11	3.0374 eV	408.19 nm	*f*=1.2070
	382 → 388	-0.15883	
	383 → 387	0.66262	
Excited State 12	3.1037 eV	399.47 nm	*f*=0.0227
	378 → 384	0.10993	
	378 → 385	-0.15095	
	379 → 384	0.63485	
	380 → 385	-0.12978	
	383 → 388	-0.11123	

Table S1. (***continued***)

Ru-2 (HOMO: orbital 577; LUMO: orbital 578)			
Excited State 1	1.6468 eV	752.86 nm	*f*=0.8802
	577 → 578	0.70356	
Excited State 2	2.1033 eV	589.46 nm	*f*=0.0318
	575 → 578	-0.11271	
	576 → 578	0.69293	
Excited State 3	2.1631 eV	573.19 nm	*f*=0.0151
	575 → 578	0.69108	
	576 → 578	0.11265	
Excited State 4	2.3624 eV	524.83 nm	*f*=0.0004
	574 → 578	0.69978	
Excited State 5	2.5364 eV	488.83 nm	*f*=0.0003
	573 → 578	0.23534	
	575 → 580	0.12445	
	576 → 580	0.30107	
	577 → 580	0.55134	
Excited State 6	2.5435 eV	487.46 nm	*f*=0.0044
	573 → 578	0.65459	
	576 → 580	-0.10929	
	577 → 580	-0.19261	
Excited State 7	2.5987 eV	477.09 nm	*f*=0.0002
	573 → 579	0.13038	
	576 → 579	-0.38141	
	577 → 579	0.54917	
Excited State 8	2.7338 eV	453.52 nm	*f*=0.0003
	573 → 579	-0.10552	
	575 → 579	0.61281	
	575 → 617	-0.11202	
	576 → 579	-0.17899	
	577 → 579	-0.18236	
Excited State 9	2.8537 eV	434.47 nm	*f*=0.0942
	572 → 578	0.66408	
	577 → 581	-0.20256	
Excited State 10	2.9065 eV	426.58 nm	*f*=1.3085
	572 → 578	0.20280	
	577 → 581	0.65108	
Excited State 11	2.9266 eV	423.65 nm	*f*=0.0087
	574 → 580	0.66474	
	574 → 618	0.13483	
Excited State 12	3.0571 eV	405.57 nm	*f*=0.0171
	571 → 578	0.68731	