

## Supporting information

# **The molecular picture for Amplified Spontaneous Emission of star-shaped functionalized-truxene derivates**

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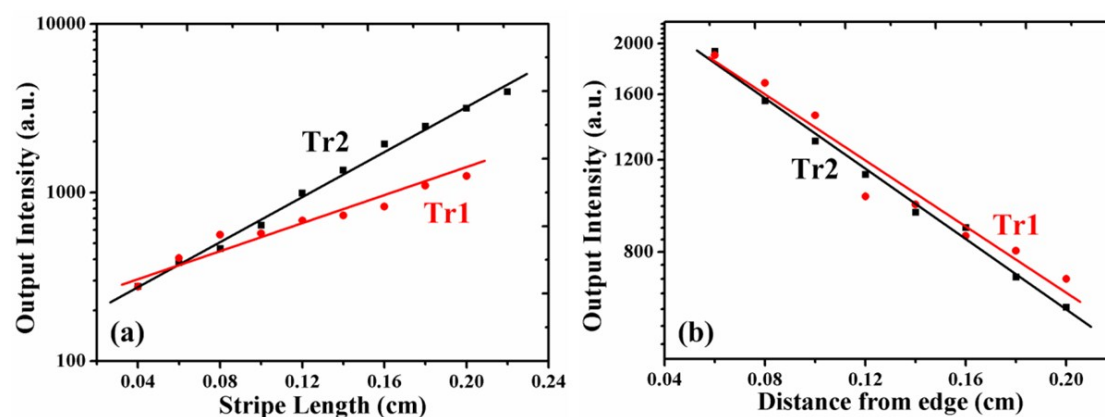
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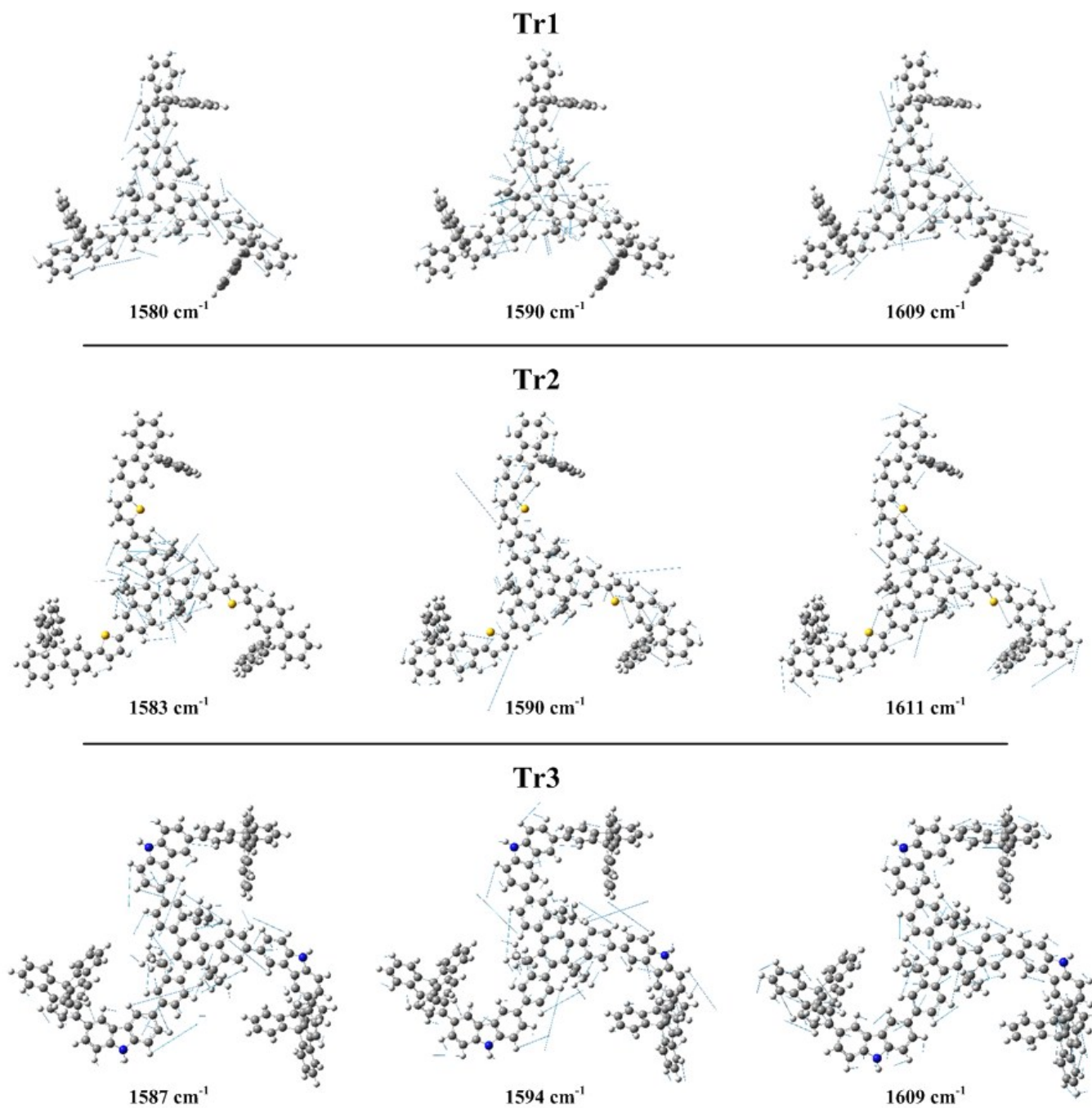
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## Optical gain and waveguide losses

Figure S1 shows the ASE output intensity as a function of pump stripe length at the pump intensity  $0.78 \text{ mJ/cm}^2$ . The net gain coefficients were found to be as high as  $19 \text{ cm}^{-1}$  for Tr1 and  $32 \text{ cm}^{-1}$  for Tr2. If instead of changing the length of the stripe we vary the distance between the stripe and the edge of the film, the output intensity  $I_{out}$  is given by  $I_{out} = I_0 \exp(-\alpha x)$ , where  $\alpha$  is the optical loss coefficient and  $x$  is the distance from the end of the stripe to the edge of the film. The results of optical loss measurements are shown in Figure S1(b). In the semi-log graph, the slope of the lines corresponds to loss coefficients of  $3.4 \text{ cm}^{-1}$  for Tr1 and  $3.2 \text{ cm}^{-1}$  for Tr2, relatively low value compared to other star-shaped organic emitters.<sup>[1]</sup>



**Figure S1** ASE measurements on the Tr1 and Tr2 showing (a) optical gain measurements and (b) waveguide losses. The pump intensity is  $0.78 \text{ mJ/cm}^2$  which is above the ASE thresholds of the compounds.



**Figure S2** Calculated vibrational eigenvectors of some high-frequency modes. The contribution of each mode to the total deformation of samples is enlarged by the same factor.

**Table SI** Selected normal modes and relevant parameters of Tr1, Tr2 and Tr3.

Selected vibrational frequencies ( $\hbar\omega_j$ ), Huang-Rhys factors ( $S_j$ ) and reorganization energies ( $\lambda_j$ ) of the ground state of compound Tr1.

	$\hbar\omega_j$ ( $\text{cm}^{-1}$ )	$S_j$	$\lambda_j$ ( $\text{cm}^{-1}$ )
Low-frequency Modes	27	0.488072	13.3
	136	0.4811805	65.3

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137	0.4598405	62.9	
138	0.2132045	29.4	
155	0.346112	53.9	
167	0.4232	70.6	
172	0.293378	50.5	
207	0.2865245	59.4	
208	1.131008	235.7	
222	0.553352	122.8	
225	0.3570125	80.4	
232	0.2003445	46.5	
275	1.2121245	332.8	
276	1.3861125	381.5	
278	0.9261605	257.6	
284	1.0731125	304.6	
349	0.2972205	103.8	
350	0.3096845	108.4	
365	0.294912	107.9	
437	0.3898445	170	
439	0.492032	215.7	
439	0.245	107.5	
490	0.4608	225.6	
507	0.4636845	234.7	
508	0.32805	166.6	
644	0.213858	137.1	
715	0.209952	150.2	
722	0.8911125	643.7	
724	0.5408	391.8	
741	0.4522005	334.8	
742	0.390728	289.8	
782	0.272322	212.6	
785	0.2987645	234.9	
835	0.3112605	259.8	
838	0.2028845	169.9	
841	0.6061005	509.6	
871	0.2686445	233.8	
874	0.2211125	193	
879	0.21125	185.9	
889	0.249218	221.5	
1167	0.376712	439.3	
1299	0.118098	153.2	
High-frequency Modes	1580	0.1305605	206.2
	1590	0.07605	120.8
	1609	0.019217	30..9

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Selected vibrational frequencies ( $\hbar\omega_j$ ), Huang-Rhys factors ( $S_j$ ) and reorganization energies ( $\lambda_j$ ) of the ground state of compound Tr2.

	$\hbar\omega_j$ (cm <sup>-1</sup> )	$S_j$	$\lambda_j$ (cm <sup>-1</sup> )
	4	0.88445	3.5
	6	0.69974	3.9
	8	2.31289	18.5
	11	1.3300805	14.6
	13	0.581042	7.6
	14	0.2443005	3.3
	21	0.2686445	5.6
	26	0.3638045	9.7
	45	1.0039445	44.8
	48	2.455328	118.4
	49	1.6562	80.5
	50	0.753992	37.9
	58	0.5951405	34.4
	59	0.647522	38
Low-frequency Modes	127	0.2820005	35.7
	129	0.4772645	61.4
	131	0.8515125	111.1
	132	1.1873405	156.6
	134	0.919368	123.1
	137	1.6909605	231.1
	140	0.5995125	84.2
	155	0.5171445	80.2
	157	1.8605205	292.2
	165	0.3192005	52.7
	169	0.445568	75.1
	179	0.31205	55.9
	201	0.2820005	56.7
	385	0.2527605	97.5
	387	0.240818	93.1
	1168	0.1990125	231.8
	1302	0.1417605	184.5
High-frequency Modes	1583	0.359552	564.9
	1590	0.082205	127.2
	1611	0.01283	20.8

Selected vibrational frequencies ( $\hbar\omega_j$ ), Huang-Rhys factors ( $S_j$ ) and reorganization energies ( $\lambda_j$ ) of the ground state of compound Tr3.

	$\hbar\omega_j$ (cm <sup>-1</sup> )	$S_j$	$\omega_j$ (cm <sup>-1</sup> )
	7	0.96605	6.7
	8	0.8129845	6.6
	9	0.21424	1.8
	49	0.591872	29.1
	51	0.334562	17.2
	54	0.739328	39.7
	54	0.741762	40.3
	56	0.22445	12.6
	59	0.2642645	15.6
	67	0.202248	13.5
	112	0.326432	36.7
	120	0.3049805	36.5
	124	0.32805	40.5
	132	0.406802	53.5
	136	0.8857805	120.9
	157	0.8725205	137.4
	195	0.445568	347.7
	197	1.7653205	52.7
	214	0.246402	57.9
	270	0.2145125	227.9
Low-frequency Modes	281	0.8102645	88.4
	296	0.2987645	409.7
	300	1.367858	119.7
	315	0.380192	115.4
	322	0.357858	185.5
	385	0.482162	99.3
	472	0.209952	101.5
	477	0.212552	202.3
	492	0.4113245	151.7
	494	0.3065445	139.9
	516	0.2715845	147.7
	519	0.284258	118.4
	525	0.225792	134.2
	561	0.239432	550.5
	580	0.9480645	259.2
	619	0.4186125	139.9
	654	1.9110125	1248.4
	657	0.2926125	223.9
	704	0.3176045	248
	712	0.3486125	548.6
	727	0.7552205	276
	742	0.371522	119.3

	907	0.239432	217
	1166	0.313632	365.4
	1299	0.152488	198
High-frequency Modes	1587	0.1529045	240.8
	1594	0.024537	39.1
	1609	0.0321805	51.5

### Theoretical model: Elongation of vibrational modes

Under the adiabatic approximation, the electronic ground and excited state wave functions can be expressed as products of an electronic and nuclear part. Assuming a single vibronic coordinate for simplicity, the vibronic part of the total wave function contributes only a Frank-Condon overlap factors. The probability to emit through a transition from the lowest vibronic level  $|0_e\rangle$  of the first excited-state vibronic to the electronic ground state vibronic level  $|n_g\rangle$  with an electric field  $E$  at energy  $E_L$  is given by Fermi's golden rule: [2]

$$P(|0_e\rangle \rightarrow |n_g\rangle) = \frac{2\pi}{\hbar} |E \cdot \mu|^2 |\langle 0_e | n_g \rangle|^2 \times \delta(E_L + E_{HOMO} - E_{LUMO} - n_g \hbar \omega) \quad (1)$$

where  $\mu$  is the electronic transition dipole and the Franck-Condon factor can be defined as Poisson distribution:

$$|\langle 0_e | n_g \rangle|^2 = \frac{S^n}{n!} e^{-S} \quad (2)$$

In the Poisson distribution over the vibronic levels,  $S$  is Huang-Rhys factor which represents the vibronic coupling strength:

$$S_j = \frac{\omega(\Delta Q_j)^2}{2\hbar} \quad (3)$$

where  $\Delta Q_j$  represents the displacement along the normal mode  $(NM)_j$  between the equilibrium positions of the two electronic states.

## References:

- [1] Y. Wang, G. Tsiminis, Y. Yang, A. Ruseckas, A. L. Kanibolotsky, I. F. Perepichka, P. J. Skabara, G. A. Turnbull, I. D. W. Samuel, *Synth. Met.* **2010**, *160*, 1397.
- [2] I. Vragovic, R. Scholz, M. Schreiber, *Euro. Phys. Lett.* **2002**, *57*, 288-294.