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以主族元素为桥的梯形化合物的光电性质

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Optoelectronic Properties for Main Group Element-Bridged Ladder Compounds

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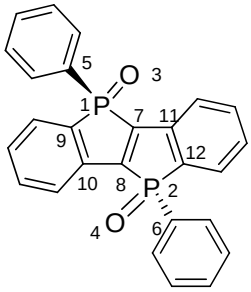
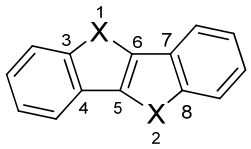
Table S1 Selected bond length (Å) and bond angles (º) of the *trans*-**4a** in the ground state together with the experimental values



trans-**4a**

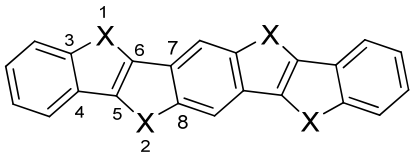
	B3LYP			
	6-31g(d)	6-31+g(d)	6-311+g(d)	exp[1]
P1-O3	1.501	1.504	1.499	1.483(2)
P1-C9	1.835	1.836	1.835	1.812(3)
P1-C7	1.835	1.836	1.837	1.812(3)
C9-C10	1.415	1.415	1.412	1.411(3)
C8-C10	1.468	1.469	1.468	1.468(3)
C7-C8	1.358	1.359	1.354	1.348(3)
P1-C5	1.826	1.828	1.827	1.794(3)
C9-P1-C7	90.71	90.74	90.71	91.38(14)
P1-C9-C10	110.25	110.23	110.20	110.02(13)
P1-C7-C8	110.32	110.24	110.13	110.4(2)
C9-C10-C8	112.40	112.38	112.41	112.15(13)
C10-C8-C7	116.31	116.40	116.54	116.0(2)

Table S2 Selected bond length (Å) and bond angles (º) of the compounds **1a**, **2a**, **3a**, and *cis*-**4a** in the ground-state



	1	**2**	*cis*-**3**	*trans*-**3**	*cis*-**4**
X1-C3	1.536	1.888	1.843	1.843	1.835
X1-C6	1.517	1.891	1.833	1.831	1.835
C3-C4	1.420	1.424	1.420	1.420	1.415
C4-C5	1.457	1.475	1.458	1.457	1.468
C5-C6	1.358	1.373	1.370	1.371	1.358
C3-X1-C6	100.06	91.16	88.86	88.90	90.74
C5-X1-C8	100.06	91.16	88.86	88.90	90.74
X1-C3-C4	110.64	107.94	111.30	111.34	110.20
X1-C6-C5	112.25	108.97	112.01	112.02	110.29
C3-C4-C5	107.02	115.20	112.12	112.12	112.44
C4-C5-C6	110.03	117.73	115.05	115.02	116.29

Table S3 Selected bond length (Å) and bond angles (°) of the compounds **1b-4b** in the ground-state



Ground state

DFT	**1b**	**2b**	*cis*-**3b**	*trans*-**3b**	*cis*-**4b**	*trans*-**4b**
X1-C3	1.536	1.888	1.843	1.842	1.834	1.835
X1-C6	1.517	1.891	1.834	1.832	1.837	1.837
C3-C4	1.420	1.424	1.420	1.421	1.415	1.415
C4-C5	1.456	1.474	1.457	1.456	1.467	1.467
C5-C6	1.359	1.374	1.371	1.372	1.360	1.360
C3-X1-C6	100.11	91.22	88.85	88.90	90.67	90.63
C5-X2-C8	100.18	91.27	88.91	88.96	90.69	90.65
X1-C3-C4	110.60	107.91	111.37	111.37	110.32	110.33
X1-C6-C5	112.15	108.88	111.98	111.96	110.24	110.30
C3-C4-C5	107.06	115.23	112.13	112.14	112.41	112.40
C4-C5-C6	110.08	116.76	115.07	115.05	116.33	116.33

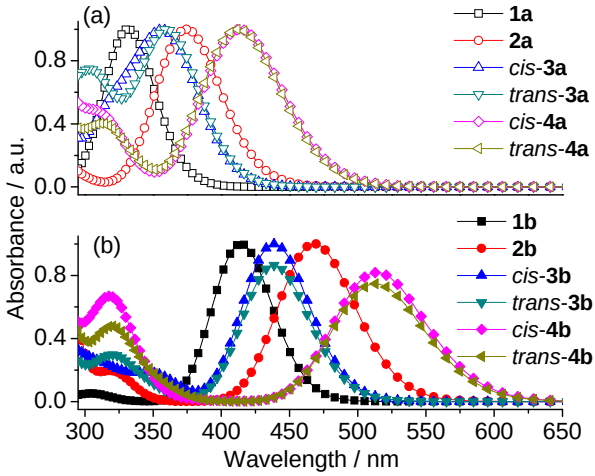


Fig.S1 The simulated absorption spectra of **1-4** in CH_2Cl_2 solution

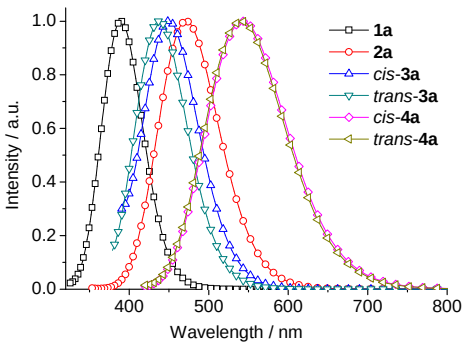


Fig.S2 The simulated emission spectra of **1a-4a** in CH_2Cl_2 solutions