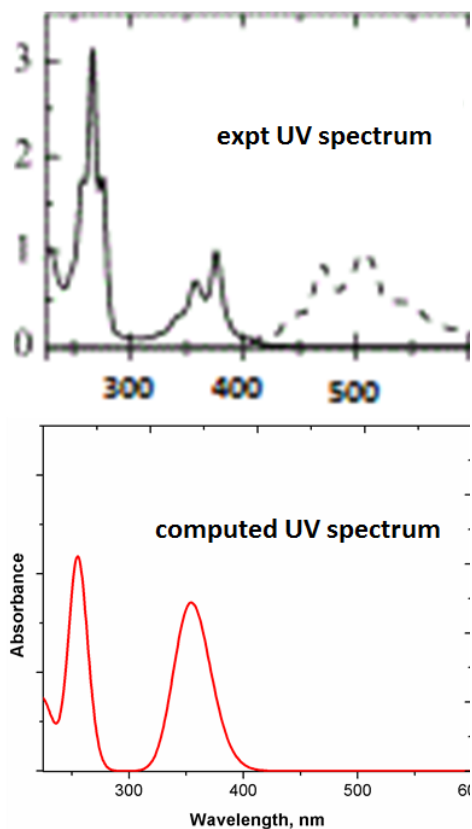


## Electronic Supporting Information

# Design of novel tetra-hetero[8]circulenes: A theoretical study of electronic structure and charge transport characteristics

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**Supporting Information Available:** Table S1 contains the Cartesian coordinates for optimized geometries, Table S2 contains the intermolecular interaction energies of dimmers 1a-4a obtained at M06.



**Figure S1.** The experimental (up) and theoretical (down) UV spectra of compound **1a**. The experimental spectrum was obtained from ref. 18.

**Table S1.** Optimized geometries of the molecules at the B3LYP/6-31+G(d,p) level. Cartesian coordinates in angstroms

<b>Comp</b>	<b>XYZ-coordinate</b>				<b>Comp</b>	<b>XYZ-coordinate</b>			
<b>1a</b>	6	0.698105000	1.710155000	0.000000000	<b>1b</b>	6	0.698480000	1.712737000	0.000000000
	6	-0.698105000	1.710155000	0.000000000		6	-0.698480000	1.712737000	0.000000000
	6	0.698105000	-1.710155000	0.000000000		6	0.698480000	-1.712737000	0.000000000
	6	-1.710155000	0.698105000	0.000000000		6	-1.712737000	0.698480000	0.000000000
	6	-0.698105000	-1.710155000	0.000000000		6	-0.698480000	-1.712737000	0.000000000
	6	-1.710155000	-0.698105000	0.000000000		6	-1.712737000	-0.698480000	0.000000000
	6	1.710155000	0.698105000	0.000000000		6	1.712737000	0.698480000	0.000000000
	6	1.710155000	-0.698105000	0.000000000		6	1.712737000	-0.698480000	0.000000000
	6	2.937181000	-1.372047000	0.000000000		6	2.933027000	-1.382612000	0.000000000
	6	2.937181000	1.372047000	0.000000000		6	2.933027000	1.382612000	0.000000000
	6	1.372047000	2.937181000	0.000000000		6	1.382612000	2.933027000	0.000000000
	6	-1.372047000	2.937181000	0.000000000		6	-1.382612000	2.933027000	0.000000000
	6	-2.937181000	1.372047000	0.000000000		6	-2.933027000	1.382612000	0.000000000
	6	-2.937181000	-1.372047000	0.000000000		6	-2.933027000	-1.382612000	0.000000000
	6	-1.372047000	-2.937181000	0.000000000		6	-1.382612000	-2.933027000	0.000000000
	6	1.372047000	-2.937181000	0.000000000		6	1.382612000	-2.933027000	0.000000000
	6	-4.166548000	0.701163000	0.000000000		6	-4.156771000	0.700401000	0.000000000
	6	-4.166548000	-0.701163000	0.000000000		6	-4.156771000	-0.700401000	0.000000000
	6	-0.701163000	4.166548000	0.000000000		6	-0.700401000	4.156771000	0.000000000
	6	0.701163000	4.166548000	0.000000000		6	0.700401000	4.156771000	0.000000000
	6	4.166548000	0.701163000	0.000000000		6	4.156771000	0.700401000	0.000000000
	6	4.166548000	-0.701163000	0.000000000		6	4.156771000	-0.700401000	0.000000000
	6	0.701163000	-4.166548000	0.000000000		6	0.700401000	-4.156771000	0.000000000
	6	-0.701163000	-4.166548000	0.000000000		6	-0.700401000	-4.156771000	0.000000000
	1	1.252591000	-5.099793000	0.000000000		8	2.749425000	-2.749425000	0.000000000
	1	-1.252591000	-5.099793000	0.000000000		8	2.749425000	2.749425000	0.000000000
	1	-5.099793000	1.252591000	0.000000000		8	-2.749425000	2.749425000	0.000000000
	1	-5.099793000	-1.252591000	0.000000000		8	-2.749425000	-2.749425000	0.000000000
1	-1.252591000	5.099793000	0.000000000	9	1.356660000	-5.321319000	0.000000000		
1	1.252591000	5.099793000	0.000000000	9	-1.356660000	-5.321319000	0.000000000		
1	5.099793000	1.252591000	0.000000000	9	5.321319000	-1.356660000	0.000000000		
1	5.099793000	-1.252591000	0.000000000	9	5.321319000	1.356660000	0.000000000		
8	2.743704000	-2.743704000	0.000000000	9	1.356660000	5.321319000	0.000000000		

	8	2.743704000	2.743704000	0.000000000		9	-1.356660000	5.321319000	0.000000000
	8	-2.743704000	2.743704000	0.000000000		9	-5.321319000	1.356660000	0.000000000
	8	-2.743704000	-2.743704000	0.000000000		9	-5.321319000	-1.356660000	0.000000000
<b>2a</b>	6	0.723758000	1.772717000	0.001335000	<b>2b</b>	6	1.609436000	-1.027439000	0.000010000
	6	-0.723758000	1.772717000	-0.001338000		6	1.868876000	0.391290000	-0.000005000
	6	0.723758000	-1.772717000	-0.001338000		6	-1.868876000	-0.391290000	-0.000005000
	6	-1.772717000	0.723758000	-0.001335000		6	1.027439000	1.609436000	-0.000010000
	6	-0.723758000	-1.772717000	0.001335000		6	-1.609436000	1.027439000	0.000010000
	6	-1.772717000	-0.723758000	0.001338000		6	-0.391290000	1.868876000	0.000005000
	6	1.772717000	0.723758000	0.001338000		6	0.391290000	-1.868876000	0.000005000
	6	1.772717000	-0.723758000	-0.001335000		6	-1.027439000	-1.609436000	-0.000010000
	6	3.064997000	-1.332359000	-0.003467000		6	-1.868876000	-2.759922000	-0.000024000
	6	3.064997000	1.332359000	0.003472000		6	0.770870000	-3.242783000	0.000014000
	6	1.332359000	3.064997000	0.003467000		6	2.759922000	-1.868876000	0.000024000
	6	-1.332359000	3.064997000	-0.003472000		6	3.242783000	0.770870000	-0.000014000
	6	-3.064997000	1.332359000	-0.003467000		6	1.868876000	2.759922000	-0.000024000
	6	-3.064997000	-1.332359000	0.003472000		6	-0.770870000	3.242783000	0.000014000
	6	-1.332359000	-3.064997000	0.003467000		6	-2.759922000	1.868876000	0.000024000
	6	1.332359000	-3.064997000	-0.003472000		6	-3.242783000	-0.770870000	-0.000014000
	6	-4.302756000	0.683192000	-0.002080000		6	1.441057000	4.085174000	-0.000022000
	6	-4.302756000	-0.683192000	0.002090000		6	0.098397000	4.330743000	0.000002000
	6	-0.683192000	4.302756000	-0.002090000		6	4.330743000	-0.098397000	-0.000002000
	6	0.683192000	4.302756000	0.002080000		6	4.085174000	-1.441057000	0.000022000
	6	4.302756000	0.683192000	0.002090000		6	-0.098397000	-4.330743000	0.000002000
	6	4.302756000	-0.683192000	-0.002080000		6	-1.441057000	-4.085174000	-0.000022000
	6	0.683192000	-4.302756000	-0.002090000		6	-4.330743000	0.098397000	-0.000002000
	6	-0.683192000	-4.302756000	0.002080000		6	-4.085174000	1.441057000	0.000022000
	1	1.257696000	-5.223064000	-0.003816000		16	3.579350000	2.472362000	-0.000036000
	1	-1.257696000	-5.223064000	0.003804000		16	2.472362000	-3.579350000	0.000036000
	1	-5.223064000	1.257696000	-0.003804000		16	-3.579350000	-2.472362000	-0.000036000
	1	-5.223064000	-1.257696000	0.003816000		16	-2.472362000	3.579350000	0.000036000
	1	-1.257696000	5.223064000	-0.003816000		9	-5.577814000	-0.394882000	-0.000010000
	1	1.257696000	5.223064000	0.003804000		9	-5.076995000	2.343689000	0.000036000
	1	5.223064000	1.257696000	0.003816000		9	-0.394882000	5.577814000	0.000010000
	1	5.223064000	-1.257696000	-0.003804000		9	2.343689000	5.076995000	-0.000036000
	16	-3.064647000	3.064647000	-0.006835000		9	5.076995000	-2.343689000	0.000036000
	16	3.064647000	3.064647000	0.006835000		9	5.577814000	0.394882000	-0.000010000

	16	3.064647000	-3.064647000	-0.006835000		9	0.394882000	-5.577814000	0.000010000
	16	-3.064647000	-3.064647000	0.006835000		9	-2.343689000	-5.076995000	-0.000036000
<b>3a</b>	6	-0.824315000	1.695803000	0.182027000	<b>3b</b>	6	-0.298873000	-1.882605000	0.123824000
	6	-1.765340000	0.659991000	-0.187750000		6	1.092471000	-1.562507000	-0.120070000
	6	1.765337000	-0.659973000	-0.187759000		6	-1.092472000	1.562504000	-0.120102000
	6	-1.695800000	-0.824307000	-0.182012000		6	1.882607000	-0.298876000	-0.123801000
	6	0.824312000	-1.695786000	0.181998000		6	0.298875000	1.882609000	0.123769000
	6	-0.659982000	-1.765329000	0.187738000		6	1.562506000	1.092473000	0.120064000
	6	0.659982000	1.765345000	0.187763000		6	-1.562505000	-1.092470000	0.120108000
	6	1.695792000	0.824318000	-0.182022000		6	-1.882607000	0.298873000	-0.123792000
	6	2.965708000	1.404722000	-0.470211000		6	-3.266683000	0.581673000	-0.317343000
	6	1.117206000	3.082756000	0.484335000		6	-2.684076000	-1.952620000	0.308304000
	6	-1.404732000	2.965719000	0.470213000		6	-0.581676000	-3.266678000	0.317398000
	6	-3.082762000	1.117192000	-0.484316000		6	1.952622000	-2.684082000	-0.308237000
	6	-2.965709000	-1.404723000	-0.470214000		6	3.266681000	-0.581681000	-0.317358000
	6	-1.117180000	-3.082753000	0.484327000		6	2.684079000	1.952628000	0.308225000
	6	1.404713000	-2.965698000	0.470207000		6	0.581678000	3.266686000	0.317303000
	6	3.082751000	-1.117195000	-0.484349000		6	-1.952625000	2.684074000	-0.308292000
	6	-3.333969000	-2.735335000	-0.267677000		6	4.312600000	0.323004000	-0.199406000
	6	-2.409637000	-3.573846000	0.295736000		6	4.019809000	1.597588000	0.181391000
	6	-3.573866000	2.409636000	-0.295700000		6	1.597585000	-4.019810000	-0.181384000
	6	-2.735341000	3.333985000	0.267678000		6	0.323009000	-4.312598000	0.199439000
	6	2.409687000	3.573821000	0.295824000		6	-4.019807000	-1.597583000	0.181473000
	6	3.334025000	2.735299000	-0.267578000		6	-4.312602000	-0.323010000	-0.199356000
	6	3.573805000	-2.409688000	-0.295856000		6	-1.597587000	4.019805000	-0.181480000
	6	2.735291000	-3.334009000	0.267578000		6	-0.323007000	4.312604000	0.199323000
	1	4.605203000	-2.646233000	-0.534524000		34	3.754241000	-2.349810000	-0.640209000
	1	3.068163000	-4.340399000	0.497970000		34	-2.349799000	-3.754235000	0.640286000
	1	-4.340327000	-3.068245000	-0.498164000		34	2.349805000	3.754252000	0.640161000
	1	-2.646132000	-4.605283000	0.534283000		34	-3.754247000	2.349793000	-0.640238000
	1	-4.605319000	2.646105000	-0.534187000		9	5.575853000	-0.088351000	-0.399829000
	1	-3.068248000	4.340348000	0.498145000		9	4.976495000	2.520731000	0.375840000
	1	2.646204000	4.605236000	0.534438000		9	0.088348000	5.575861000	0.399727000
	1	4.340422000	3.068169000	-0.497945000		9	-2.520727000	4.976488000	-0.375955000
	34	-4.289276000	-0.205549000	-1.007190000		9	-5.575857000	0.088340000	-0.399780000
	34	-0.205514000	4.289318000	1.007124000		9	-4.976492000	-2.520720000	0.375956000
	34	0.205515000	-4.289230000	1.007244000		9	-0.088344000	-5.575850000	0.399882000

	34	4.289279000	0.205480000	-1.007174000		9	2.520724000	-4.976499000	-0.375841000
<b>4a</b>	6	0.705947000	1.723322000	0.000000000	<b>4b</b>	6	0.705902000	1.723486000	0.000000000
	6	-0.705947000	1.723322000	0.000000000		6	-0.705902000	1.723486000	0.000000000
	6	0.705947000	-1.723322000	0.000000000		6	0.705902000	-1.723486000	0.000000000
	6	-1.723322000	0.705947000	0.000000000		6	-1.723486000	0.705902000	0.000000000
	6	-0.705947000	-1.723322000	0.000000000		6	-0.705902000	-1.723486000	0.000000000
	6	-1.723322000	-0.705947000	0.000000000		6	-1.723486000	-0.705902000	0.000000000
	6	1.723322000	0.705947000	0.000000000		6	1.723486000	0.705902000	0.000000000
	6	1.723322000	-0.705947000	0.000000000		6	1.723486000	-0.705902000	0.000000000
	6	2.974301000	-1.373960000	0.000000000		6	2.966638000	-1.381980000	0.000000000
	6	2.974301000	1.373960000	0.000000000		6	2.966638000	1.381980000	0.000000000
	6	1.373960000	2.974301000	0.000000000		6	1.381980000	2.966638000	0.000000000
	6	-1.373960000	2.974301000	0.000000000		6	-1.381980000	2.966638000	0.000000000
	6	-2.974301000	1.373960000	0.000000000		6	-2.966638000	1.381980000	0.000000000
	6	-2.974301000	-1.373960000	0.000000000		6	-2.966638000	-1.381980000	0.000000000
	6	-1.373960000	-2.974301000	0.000000000		6	-1.381980000	-2.966638000	0.000000000
	6	1.373960000	-2.974301000	0.000000000		6	1.381980000	-2.966638000	0.000000000
	6	-4.205052000	0.694587000	0.000000000		6	-4.188344000	0.691968000	0.000000000
	6	-4.205052000	-0.694587000	0.000000000		6	-4.188344000	-0.691968000	0.000000000
	6	-0.694587000	4.205052000	0.000000000		6	-0.691968000	4.188344000	0.000000000
	6	0.694587000	4.205052000	0.000000000		6	0.691968000	4.188344000	0.000000000
	6	4.205052000	0.694587000	0.000000000		6	4.188344000	0.691968000	0.000000000
	6	4.205052000	-0.694587000	0.000000000		6	4.188344000	-0.691968000	0.000000000
	6	0.694587000	-4.205052000	0.000000000		6	0.691968000	-4.188344000	0.000000000
	6	-0.694587000	-4.205052000	0.000000000		6	-0.691968000	-4.188344000	0.000000000
	1	1.243223000	-5.142221000	0.000000000		7	-2.747165000	2.747165000	0.000000000
	1	-1.243223000	-5.142221000	0.000000000		7	2.747165000	2.747165000	0.000000000
	1	-5.142221000	1.243223000	0.000000000		7	2.747165000	-2.747165000	0.000000000
	1	-5.142221000	-1.243223000	0.000000000		7	-2.747165000	-2.747165000	0.000000000
	1	-1.243223000	5.142221000	0.000000000		9	-1.379296000	-5.349039000	0.000000000
	1	1.243223000	5.142221000	0.000000000		9	1.379296000	-5.349039000	0.000000000
	1	5.142221000	1.243223000	0.000000000		9	5.349039000	-1.379296000	0.000000000
	1	5.142221000	-1.243223000	0.000000000		9	5.349039000	1.379296000	0.000000000
	1	-3.451823000	3.451823000	0.000000000		9	1.379296000	5.349039000	0.000000000
	1	-3.451823000	-3.451823000	0.000000000		9	-1.379296000	5.349039000	0.000000000
1	3.451823000	-3.451823000	0.000000000	9	-5.349039000	1.379296000	0.000000000		
1	3.451823000	3.451823000	0.000000000	9	-5.349039000	-1.379296000	0.000000000		

7	-2.740524000	2.740524000	0.000000000	1	3.458641000	-3.458641000	0.000000000
7	2.740524000	2.740524000	0.000000000	1	3.458641000	3.458641000	0.000000000
7	2.740524000	-2.740524000	0.000000000	1	-3.458641000	3.458641000	0.000000000
7	-2.740524000	-2.740524000	0.000000000	1	-3.458641000	-3.458641000	0.000000000

**Table S2** The intermolecular interaction energies of dimers **1a-4a** obtained by using functional M06 in conjugation with three different basis sets

	6-31G(d,p)	6-311G(d,p)	6-311+G(d,p)
<b>1a</b>	1.12	1.30	1.33
<b>2a</b>	1.4	1.66	1.75
<b>3a</b>	1.34	1.57	1.64
<b>4a</b>	1.12	1.32	1.35