

Design of A-D-A-Type Organic Third-Order Nonlinear Optical Materials Based on Benzodithiophene: A DFT Study

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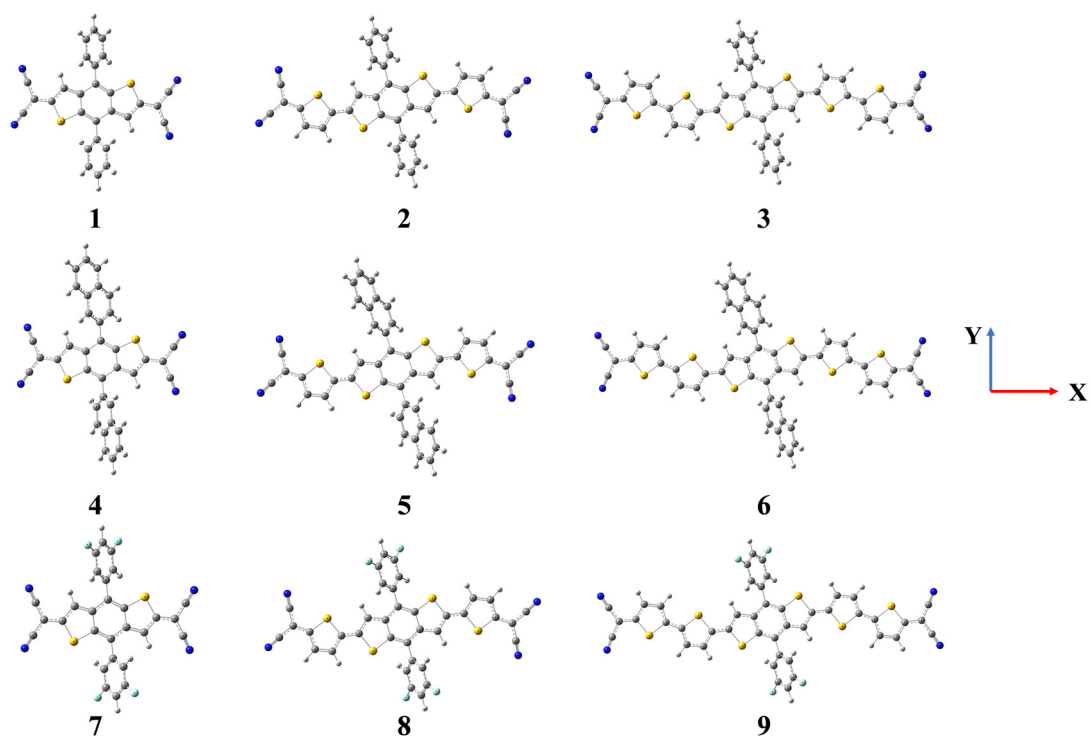


Figure S1. The front view of the optimized molecules.

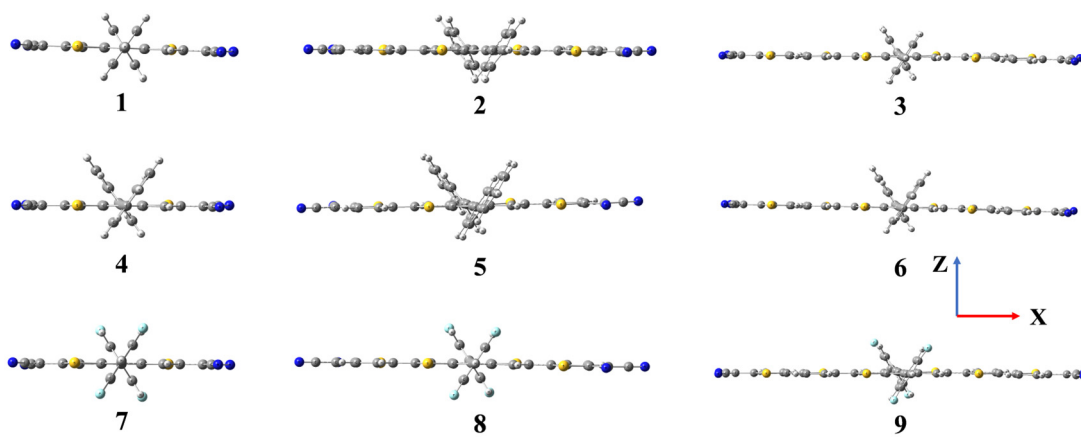


Figure S2. The side view of the optimized molecules.

Table S1. Static third-order NLO coefficients (γ) of the nine molecules.

molecules	γ_{total}	γ_x	γ_y	γ_z
1	1049.01004	917.64652	454.71147	227.12199
2	3075.94347	3001.97982	604.22474	290.61633
3	7944.82987	7909.6953	656.73289	354.60379
4	1513.12745	990.54997	1101.50398	308.30895
5	3527.2009	3321.45702	1127.27715	371.90817
6	8296.9846	8209.45886	1119.63029	437.22615
7	1319.91511	762.73198	1052.00201	231.749
8	3190.42442	3100.18606	693.86384	293.6109
9	8081.39683	8039.38096	741.86364	356.32401

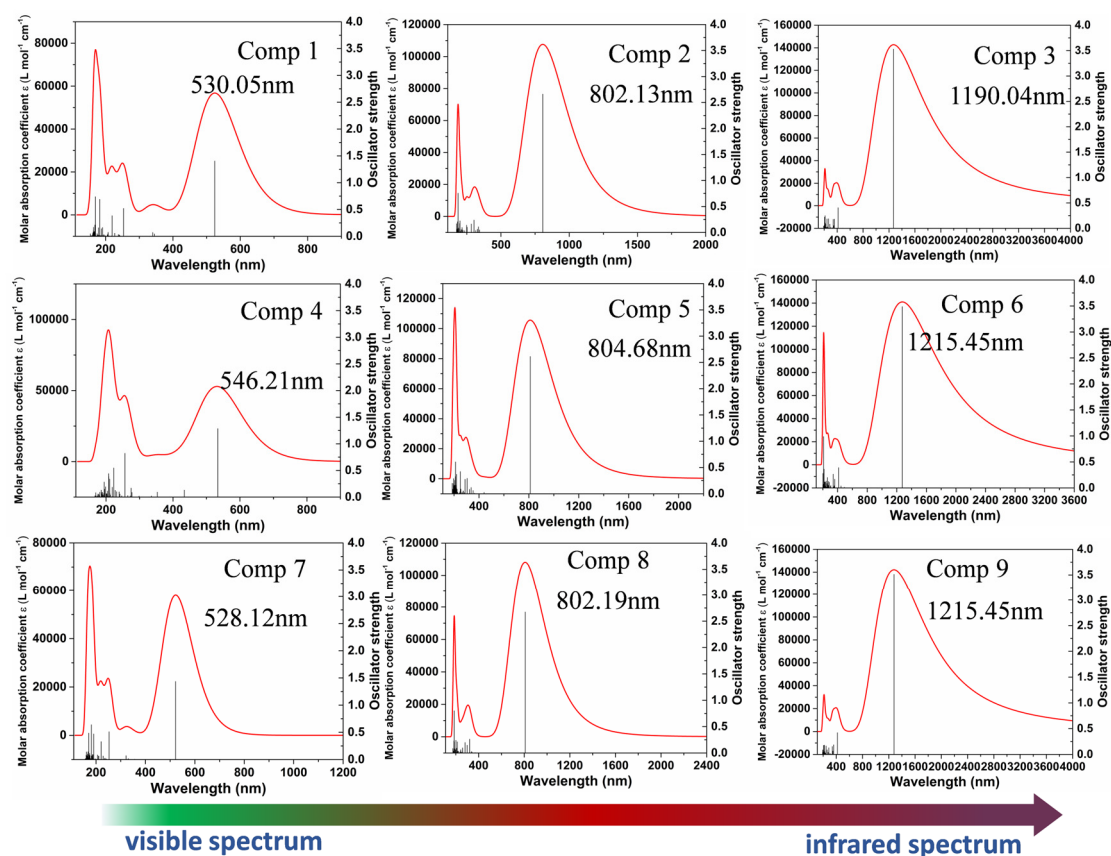


Figure S3. The UV-vis spectra of the nine compounds calculated under the wB97XD/def2-SVP level.