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Molecular electrostatic potential for exploring π-conjugation: A density-functional investigation

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Optimized geometries and energies of the building blocks of the π-conjugated molecular systems and their dimers studied in the present work at B3LYP/6-311++G(2d,2p) level of DFT. All co-ordinates are in Å.

ethylene: (Energy = -78.62066 a.u.)

C	0.000000	0.000000	0.662786
C	0.000000	0.000000	-0.662786
H	0.000000	0.920643	1.231528
H	0.000000	-0.920643	1.231528
H	0.000000	0.920643	-1.231528
H	0.000000	-0.920643	-1.231528

acetylene: (Energy = -77.36064 a.u.)

C	0.000000	0.000000	0.597943
C	0.000000	0.000000	-0.597943
H	0.000000	0.000000	1.659441
H	0.000000	0.000000	-1.659441

benezene: (Energy = -232.32418 a.u.)

C	-0.000026	1.391935	0.000000
C	0.000026	-1.391935	0.000000
C	-1.205482	0.695921	0.000000
C	1.205482	-0.695921	0.000000
C	-1.205482	-0.696028	0.000000
C	1.205482	0.696028	0.000000
H	-0.000064	2.473576	0.000000

H	0.000064	-2.473576	0.000000
H	-2.142217	1.236733	0.000000
H	2.142217	-1.236733	0.000000
H	-2.142194	-1.236872	0.000000
H	2.142194	1.236872	0.000000

furan: (Energy = -230.09932 a.u.)

O	0.000000	0.000000	1.158519
C	0.000000	1.093670	0.345588
C	0.000000	-1.093670	0.345588
C	0.000000	0.716458	-0.956209
C	0.000000	-0.716458	-0.956209
H	0.000000	-2.047269	0.839882
H	0.000000	2.047269	0.839882
H	0.000000	-1.370355	-1.810233
H	0.000000	1.370355	-1.810233

pyrrole: (Energy = -210.24102 a.u.)

C	0.000000	1.122970	0.330481
C	0.000000	0.711078	-0.980317
C	0.000000	-0.711078	-0.980317
C	0.000000	-1.122970	0.330481
N	0.000000	0.000000	1.119248
H	0.000000	2.107587	0.761928
H	0.000000	1.356184	-1.841380
H	0.000000	-1.356184	-1.841380
H	0.000000	-2.107587	0.761928
H	0.000000	0.000000	2.122202

thiophene: (Energy = -553.08647 a.u.)

S	0.000000	0.000000	1.194615
C	0.000000	1.239319	-0.010891
C	0.000000	0.712147	-1.268077
C	0.000000	-0.712147	-1.268077
C	0.000000	-1.239319	-0.010891
H	0.000000	-2.275251	0.280336
H	0.000000	-1.314875	-2.163451
H	0.000000	1.314875	-2.163451
H	0.000000	2.275251	0.280336

phenylvinylene: (Energy = -309.74806 a.u.)

C	-1.357627	1.324617	0.000068
C	0.008445	1.088348	0.000091
C	0.513040	-0.219830	0.000004
C	-0.405291	-1.276855	-0.000105
C	-1.775323	-1.042346	-0.000129
C	-2.257858	0.260617	-0.000042

C	1.950251	-0.527496	0.000022
C	2.967507	0.334543	0.000081
H	-1.724797	2.342089	0.000138
H	0.688893	1.928232	0.000181
H	-0.035936	-2.294479	-0.000173
H	-2.463690	-1.876597	-0.000214
H	-3.322741	0.448423	-0.000059
H	2.182936	-1.587335	-0.000022
H	2.827246	1.406829	0.000122
H	3.989224	-0.016749	0.000087

***trans* 1,3-butadiene:** (Energy = -156.05031 a.u.)

C	0.600608	1.744528	0.000000
C	0.600608	0.409567	0.000000
C	-0.600608	-0.409567	0.000000
C	-0.600608	-1.744528	0.000000
H	1.520398	2.311570	0.000000
H	-0.323506	2.308751	0.000000
H	1.546541	-0.122554	0.000000
H	-1.546541	0.122554	0.000000
H	0.323506	-2.308751	0.000000
H	-1.520398	-2.311570	0.000000

biacetylene: (Energy = -153.53811 a.u.)

C	0.000000	0.000000	1.886966
C	0.000000	0.000000	0.682921
C	0.000000	0.000000	-0.682921
C	0.000000	0.000000	-1.886966
H	0.000000	0.000000	2.947865
H	0.000000	0.000000	-2.947865

biphenyl: (Energy = -463.44758 a.u.)

C	-0.411063	1.127911	1.462143
C	-0.411498	1.128349	2.851534
C	0.000000	0.000000	3.553141
C	0.411498	-1.128349	2.851534
C	0.411063	-1.127911	1.462143
C	0.000000	0.000000	0.741773
C	0.000000	0.000000	-0.741773
C	-0.411063	-1.127911	-1.462143
C	-0.411498	-1.128349	-2.851534
C	0.000000	0.000000	-3.553141
C	0.411498	1.128349	-2.851534
C	0.411063	1.127911	-1.462143
H	0.741930	2.008536	-3.386455
H	0.000000	0.000000	-4.634482
H	-0.741930	-2.008536	-3.386455

H	0.741930	-2.008536	3.386455
H	0.000000	0.000000	4.634482
H	-0.741930	2.008536	3.386455
H	0.755318	-2.003548	0.929042
H	-0.755318	-2.003548	-0.929042
H	-0.755318	2.003548	0.929042
H	0.755318	2.003548	-0.929042

2,2'-bifuran: (Energy = -459.00759 a.u.)

O	-1.061122	1.462983	0.000000
O	1.061122	-1.462983	0.000000
C	-0.676224	2.771471	0.000000
C	0.676224	2.867254	0.000000
C	1.175284	1.529714	0.000000
C	0.081424	0.712681	0.000000
C	-0.081424	-0.712681	0.000000
C	0.676224	-2.771471	0.000000
C	-0.676224	-2.867254	0.000000
C	-1.175284	-1.529714	0.000000
H	2.201514	1.210014	0.000000
H	1.250158	3.776960	0.000000
H	-1.471142	3.493636	0.000000
H	-2.201514	-1.210014	0.000000
H	1.471142	-3.493636	0.000000
H	-1.250158	-3.776960	0.000000

2,2'-bipyrrole: (Energy = -419.28816 a.u.)

N	-1.033289	1.526677	-0.227482
N	1.033289	-1.526677	-0.227482
C	0.669248	2.898297	0.142745
C	-0.669248	-2.898297	0.142745
C	-0.669248	2.848308	-0.161945
C	0.669248	-2.848308	-0.161945
C	1.128124	1.560506	0.263308
C	-1.128124	-1.560506	0.263308
C	0.053367	0.721157	0.025080
C	-0.053367	-0.721157	0.025080
H	-1.383773	3.632289	-0.336439
H	1.383773	-3.632289	-0.336439
H	1.250577	3.793617	0.277292
H	-1.250577	-3.793617	0.277292
H	2.120349	1.247262	0.539899
H	-2.120349	-1.247262	0.539899
H	1.936090	-1.185584	-0.503504
H	-1.936090	1.185584	-0.503504

2,2'-bithiophene: (Energy = -1104.97505 a.u.)

S	-1.164608	1.847212	-0.258106
S	1.164608	-1.847212	-0.258106
C	-0.106687	3.198408	-0.058469
C	1.164608	2.799731	0.231217
C	1.296153	1.389078	0.309159
C	0.123092	0.713579	0.076840
C	-0.123092	-0.713579	0.076840
C	0.106687	-3.198408	-0.058469
C	-1.164608	-2.799731	0.231217
C	-1.296153	-1.389078	0.309159
H	2.220528	0.886406	0.551056
H	1.979479	3.488643	0.393271
H	-0.486301	4.199506	-0.167117
H	-2.220528	-0.886406	0.551056
H	0.486301	-4.199506	-0.167117
H	-1.979479	-3.488643	0.393271