Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supporting Information

The π-Conjugated P-flowers $C_{16}(PH)_8$ and $C_{16}(PF)_8$ Are Potential Materials for Organic n-Type Semiconductors

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Supporting Information Available: Table containing the Cartesian coordinates of the optimized geometries.

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

Structure	Geometry (Cartesian Coordinates)			
$C_{16}(PH)_8$-D_{4d}	6	1.359582000	1.359582000	0.000000000
	6	0.000000000	1.922697000	0.000000000
	6	0.000000000	-1.922697000	0.000000000
	6	-1.359582000	1.359582000	0.000000000
	6	-1.359582000	-1.359582000	0.000000000
	6	-1.922697000	0.000000000	0.000000000
	6	1.922697000	0.000000000	0.000000000
	6	1.359582000	-1.359582000	0.000000000
	6	2.336897000	-2.336897000	0.000000000
	6	3.304905000	0.000000000	0.000000000
	6	2.336897000	2.336897000	0.000000000
	6	0.000000000	3.304905000	0.000000000
	6	-2.336897000	2.336897000	0.000000000
	6	-3.304905000	0.000000000	0.000000000
	6	-2.336897000	-2.336897000	0.000000000
	6	0.000000000	-3.304905000	0.000000000
	15	4.010831000	1.661340000	0.141231000
	15	1.661340000	4.010831000	-0.141231000
	15	-1.661340000	4.010831000	0.141231000
	15	-4.010831000	1.661340000	-0.141231000
	15	-4.010831000	-1.661340000	0.141231000
	15	-1.661340000	-4.010831000	-0.141231000

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	15	1.661340000	-4.010831000	0.141231000
	15	4.010831000	-1.661340000	-0.141231000
	1	-1.854293000	4.476538000	-1.190262000
	1	1.854293000	4.476538000	1.190262000
	1	4.476538000	1.854293000	-1.190262000
	1	4.476538000	-1.854293000	1.190262000
	1	1.854293000	-4.476538000	-1.190262000
	1	-1.854293000	-4.476538000	1.190262000
	1	-4.476538000	-1.854293000	-1.190262000
	1	-4.476538000	1.854293000	1.190262000
$C_{16}(PH)_8$-C_{8v}	6	0.000000000	1.922993000	0.023010000
	6	-1.359761000	1.359761000	0.023010000
	6	1.359761000	-1.359761000	0.023010000
	6	-1.922993000	0.000000000	0.023010000
	6	0.000000000	-1.922993000	0.023010000
	6	-1.359761000	-1.359761000	0.023010000
	6	1.359761000	1.359761000	0.023010000
	6	1.922993000	0.000000000	0.023010000
	6	3.307584000	0.000000000	0.074701000
	6	2.338815000	2.338815000	0.074701000
	6	0.000000000	3.307584000	0.074701000
	6	-2.338815000	2.338815000	0.074701000
	6	-3.307584000	0.000000000	0.074701000
	6	-2.338815000	-2.338815000	0.074701000
	6	0.000000000	-3.307584000	0.074701000
	6	2.338815000	-2.338815000	0.074701000
	15	1.657911000	4.002550000	-0.117965000
	15	-1.657911000	4.002550000	-0.117965000
	15	-4.002550000	1.657911000	-0.117965000
	15	-4.002550000	-1.657911000	-0.117965000
	15	-1.657911000	-4.002550000	-0.117965000
	15	1.657911000	-4.002550000	-0.117965000
	15	4.002550000	-1.657911000	-0.117965000
	15	4.002550000	1.657911000	-0.117965000
	1	-4.540067000	1.880557000	1.183212000
	1	-1.880557000	4.540067000	1.183212000
	1	1.880557000	4.540067000	1.183212000
	1	4.540067000	1.880557000	1.183212000
	1	4.540067000	-1.880557000	1.183212000
	1	1.880557000	-4.540067000	1.183212000
	1	-1.880557000	-4.540067000	1.183212000
	1	-4.540067000	-1.880557000	1.183212000
$C_{16}(PH)_8^{+}$-D_{4d}	6	1.793051000	0.652071000	0.005712000
	6	1.732712000	-0.798713000	0.007086000
	6	-1.732699000	0.798706000	0.007085000
	6	0.660498000	-1.791601000	-0.006905000

	6	-1.793041000	-0.652072000	0.005761000
	6	-0.808370000	-1.729782000	-0.008003000
	6	0.808372000	1.729778000	-0.008069000
	6	-0.660490000	1.791591000	-0.006954000
	6	-1.139331000	3.093523000	-0.020502000
	6	1.394988000	2.987973000	-0.023734000
	6	3.109764000	1.132088000	0.017525000
	6	3.003796000	-1.386218000	0.021656000
	6	1.139330000	-3.093528000	-0.020417000
	6	-1.394992000	-2.987973000	-0.023627000
	6	-3.109762000	-1.132085000	0.017615000
	6	-3.003791000	1.386217000	0.021655000
	15	3.199007000	2.923160000	-0.178770000
	15	4.350897000	-0.180817000	0.203399000
	15	2.941246000	-3.176459000	-0.174032000
	15	-0.181022000	-4.298488000	0.150964000
	15	-3.199016000	-2.923161000	-0.178632000
	15	-4.350892000	0.180826000	0.203478000
	15	-2.941248000	3.176451000	-0.174113000
	15	0.181019000	4.298494000	0.150838000
	1	3.345177000	-3.601354000	1.119216000
	1	4.896508000	-0.203567000	-1.109004000
	1	3.631472000	3.306651000	1.118507000
	1	0.209255000	4.946551000	-1.110017000
	1	-3.345178000	3.601405000	1.119116000
	1	-4.896541000	0.203542000	-1.108910000
	1	-3.631472000	-3.306595000	1.118665000
	1	-0.209294000	-4.946579000	-1.109872000
$C_{16}(PH)_8^+$-C_{8v}	6	1.353881000	1.345126000	0.008848000
	6	0.000000000	1.908870000	0.041580000
	6	0.000000000	-1.908870000	0.041580000
	6	-1.353881000	1.345126000	0.008848000
	6	-1.353881000	-1.345126000	0.008848000
	6	-1.907315000	0.000000000	-0.017077000
	6	1.907315000	0.000000000	-0.017077000
	6	1.353881000	-1.345126000	0.008848000
	6	2.344586000	-2.328482000	0.079486000
	6	3.312998000	0.000000000	0.021206000
	6	2.344586000	2.328482000	0.079486000
	6	0.000000000	3.293855000	0.153612000
	6	-2.344586000	2.328482000	0.079486000
	6	-3.312998000	0.000000000	0.021206000
	6	-2.344586000	-2.328482000	0.079486000
	6	0.000000000	-3.293855000	0.153612000
	15	4.015130000	1.658659000	-0.150270000
	15	1.650875000	3.974897000	-0.079026000

	15	-1.650875000	3.974897000	-0.079026000
	15	-4.015130000	1.658659000	-0.150270000
	15	-4.015130000	-1.658659000	-0.150270000
	15	-1.650875000	-3.974897000	-0.079026000
	15	1.650875000	-3.974897000	-0.079026000
	15	4.015130000	-1.658659000	-0.150270000
	1	-1.968192000	4.574300000	1.167983000
	1	1.968192000	4.574300000	1.167983000
	1	4.579923000	1.832304000	1.143480000
	1	4.579923000	-1.832304000	1.143480000
	1	1.968192000	-4.574300000	1.167983000
	1	-1.968192000	-4.574300000	1.167983000
	1	-4.579923000	-1.832304000	1.143480000
	1	-4.579923000	1.832304000	1.143480000
$C_{16}(PH)_8$-D_{4d}	6	1.352059000	1.352059000	0.000000000
	6	0.000000000	1.912060000	0.000000000
	6	0.000000000	-1.912060000	0.000000000
	6	-1.352059000	1.352059000	0.000000000
	6	-1.352059000	-1.352059000	0.000000000
	6	-1.912060000	0.000000000	0.000000000
	6	1.912060000	0.000000000	0.000000000
	6	1.352059000	-1.352059000	0.000000000
	6	2.335486000	-2.335486000	0.000000000
	6	3.302913000	0.000000000	0.000000000
	6	2.335486000	2.335486000	0.000000000
	6	0.000000000	3.302913000	0.000000000
	6	-2.335486000	2.335486000	0.000000000
	6	-3.302913000	0.000000000	0.000000000
	6	-2.335486000	-2.335486000	0.000000000
	6	0.000000000	-3.302913000	0.000000000
	15	4.012144000	1.661884000	0.103783000
	15	1.661884000	4.012144000	-0.103783000
	15	-1.661884000	4.012144000	0.103783000
	15	-4.012144000	1.661884000	-0.103783000
	15	-4.012144000	-1.661884000	0.103783000
	15	-1.661884000	-4.012144000	-0.103783000
	15	1.661884000	-4.012144000	0.103783000
	15	4.012144000	-1.661884000	-0.103783000
	1	-1.848664000	4.463191000	-1.247004000
	1	1.848664000	4.463191000	1.247004000
	1	4.463191000	1.848664000	-1.247004000
	1	4.463191000	-1.848664000	1.247004000
	1	1.848664000	-4.463191000	-1.247004000
	1	-1.848664000	-4.463191000	1.247004000
	1	-4.463191000	-1.848664000	-1.247004000
	1	-4.463191000	1.848664000	1.247004000

$C_{16}(PH)_8^-$-C_{8v}	6	0.000000000	1.913120000	0.047956000
	6	-1.352769000	1.352769000	0.048234000
	6	1.352769000	-1.352769000	0.048234000
	6	-1.913120000	0.000000000	0.047956000
	6	0.000000000	-1.913120000	0.047956000
	6	-1.352769000	-1.352769000	0.048234000
	6	1.352769000	1.352769000	0.048234000
	6	1.913120000	0.000000000	0.047956000
	6	3.306017000	0.000000000	0.060744000
	6	2.337775000	2.337775000	0.061580000
	6	0.000000000	3.306017000	0.060744000
	6	-2.337775000	2.337775000	0.061580000
	6	-3.306017000	0.000000000	0.060744000
	6	-2.337775000	-2.337775000	0.061580000
	6	0.000000000	-3.306017000	0.060744000
	6	2.337775000	-2.337775000	0.061580000
	15	1.658179000	4.003069000	-0.123300000
	15	-1.658179000	4.003069000	-0.123300000
	15	-4.003069000	1.658179000	-0.123300000
	15	-4.003069000	-1.658179000	-0.123300000
	15	-1.658179000	-4.003069000	-0.123300000
	15	1.658179000	-4.003069000	-0.123300000
	15	4.003069000	-1.658179000	-0.123300000
	15	4.003069000	1.658179000	-0.123300000
	1	-4.534743000	1.877563000	1.193963000
	1	-1.877563000	4.534743000	1.193963000
	1	1.877563000	4.534743000	1.193963000
	1	4.534743000	1.877563000	1.193963000
	1	4.534743000	-1.877563000	1.193963000
	1	1.877563000	-4.534743000	1.193963000
	1	-1.877563000	-4.534743000	1.193963000
	1	-4.534743000	-1.877563000	1.193963000
$C_{16}(PF)_8$-D_{4d}	6	0.739920000	1.786324000	0.000000000
	6	-0.739920000	1.786324000	0.000000000
	6	0.739920000	-1.786324000	0.000000000
	6	-1.786324000	0.739920000	0.000000000
	6	-0.739920000	-1.786324000	0.000000000
	6	-1.786324000	-0.739920000	0.000000000
	6	1.786324000	0.739920000	0.000000000
	6	1.786324000	-0.739920000	0.000000000
	6	3.057501000	-1.266459000	0.000000000
	6	3.057501000	1.266459000	0.000000000
	6	1.266459000	3.057501000	0.000000000
	6	-1.266459000	3.057501000	0.000000000
	6	-3.057501000	1.266459000	0.000000000
	6	-3.057501000	-1.266459000	0.000000000

	6	-1.266459000	-3.057501000	0.000000000
	6	1.266459000	-3.057501000	0.000000000
	15	3.060636000	3.060636000	0.263067000
	15	0.000000000	4.328393000	-0.263067000
	15	-3.060636000	3.060636000	0.263067000
	15	-4.328393000	0.000000000	-0.263067000
	15	-3.060636000	-3.060636000	0.263067000
	15	0.000000000	-4.328393000	-0.263067000
	15	3.060636000	-3.060636000	0.263067000
	15	4.328393000	0.000000000	-0.263067000
	9	5.224690000	0.000000000	1.089986000
	9	0.000000000	5.224690000	1.089986000
	9	0.000000000	-5.224690000	1.089986000
	9	-5.224690000	0.000000000	1.089986000
	9	-3.694413000	-3.694413000	-1.089986000
	9	3.694413000	-3.694413000	-1.089986000
	9	-3.694413000	3.694413000	-1.089986000
	9	3.694413000	3.694413000	-1.089986000
$C_{16}(PF)_8$-C_{8v}	6	-1.929683000	0.000000000	-0.149905000
	6	-1.364492000	-1.364492000	-0.149905000
	6	1.364492000	1.364492000	-0.149905000
	6	0.000000000	-1.929683000	-0.149905000
	6	1.929683000	0.000000000	-0.149905000
	6	1.364492000	-1.364492000	-0.149905000
	6	-1.364492000	1.364492000	-0.149905000
	6	0.000000000	1.929683000	-0.149905000
	6	0.000000000	3.313046000	-0.083848000
	6	-2.342677000	2.342677000	-0.083848000
	6	-3.313046000	0.000000000	-0.083848000
	6	-2.342677000	-2.342677000	-0.083848000
	6	0.000000000	-3.313046000	-0.083848000
	6	2.342677000	-2.342677000	-0.083848000
	6	3.313046000	0.000000000	-0.083848000
	6	2.342677000	2.342677000	-0.083848000
	15	-3.976476000	1.647110000	-0.418178000
	15	-3.976476000	-1.647110000	-0.418178000
	15	-1.647110000	-3.976476000	-0.418178000
	15	1.647110000	-3.976476000	-0.418178000
	15	3.976476000	-1.647110000	-0.418178000
	15	3.976476000	1.647110000	-0.418178000
	15	1.647110000	3.976476000	-0.418178000
	15	-1.647110000	3.976476000	-0.418178000
	9	-4.902870000	2.030835000	0.852799000
	9	-2.030835000	4.902870000	0.852799000
	9	2.030835000	4.902870000	0.852799000
	9	4.902870000	2.030835000	0.852799000

	9	4.902870000	-2.030835000	0.852799000
	9	2.030835000	-4.902870000	0.852799000
	9	-2.030835000	-4.902870000	0.852799000
	9	-4.902870000	-2.030835000	0.852799000
$C_{16}(PF)_8^+$-D_{4d}	6	0.732657000	1.768790000	0.000000000
	6	-0.732657000	1.768790000	0.000000000
	6	0.732657000	-1.768790000	0.000000000
	6	-1.768790000	0.732657000	0.000000000
	6	-0.732657000	-1.768790000	0.000000000
	6	-1.768790000	-0.732657000	0.000000000
	6	1.768790000	0.732657000	0.000000000
	6	1.768790000	-0.732657000	0.000000000
	6	3.049072000	-1.262967000	0.000000000
	6	3.049072000	1.262967000	0.000000000
	6	1.262967000	3.049072000	0.000000000
	6	-1.262967000	3.049072000	0.000000000
	6	-3.049072000	1.262967000	0.000000000
	6	-3.049072000	-1.262967000	0.000000000
	6	-1.262967000	-3.049072000	0.000000000
	6	1.262967000	-3.049072000	0.000000000
	15	3.050864000	3.050864000	0.356205000
	15	0.000000000	4.314573000	-0.356205000
	15	-3.050864000	3.050864000	0.356205000
	15	-4.314573000	0.000000000	-0.356205000
	15	-3.050864000	-3.050864000	0.356205000
	15	0.000000000	-4.314573000	-0.356205000
	15	3.050864000	-3.050864000	0.356205000
	15	4.314573000	0.000000000	-0.356205000
	9	5.291518000	0.000000000	0.922707000
	9	0.000000000	-5.291518000	0.922707000
	9	0.000000000	5.291518000	0.922707000
	9	-5.291518000	0.000000000	0.922707000
	9	-3.741668000	3.741668000	-0.922707000
	9	-3.741668000	-3.741668000	-0.922707000
	9	3.741668000	-3.741668000	-0.922707000
	9	3.741668000	3.741668000	-0.922707000
$C_{16}(PF)_8^+$-C_{8v}	6	1.358547000	1.353226000	-0.181363000
	6	0.000000000	1.918983000	-0.128937000
	6	0.000000000	-1.918983000	-0.128937000
	6	-1.358547000	1.353226000	-0.181363000
	6	-1.358547000	-1.353226000	-0.181363000
	6	-1.913495000	0.000000000	-0.226709000
	6	1.913495000	0.000000000	-0.226709000
	6	1.358547000	-1.353226000	-0.181363000
	6	2.352253000	-2.328339000	-0.078409000
	6	3.312247000	0.000000000	-0.183559000

	6	2.352253000	2.328339000	-0.078409000
	6	0.000000000	3.300412000	0.041429000
	6	-2.352253000	2.328339000	-0.078409000
	6	-3.312247000	0.000000000	-0.183559000
	6	-2.352253000	-2.328339000	-0.078409000
	6	0.000000000	-3.300412000	0.041429000
	15	3.993732000	1.655794000	-0.462644000
	15	1.635419000	3.951410000	-0.333591000
	15	-1.635419000	3.951410000	-0.333591000
	15	-3.993732000	1.655794000	-0.462644000
	15	-3.993732000	-1.655794000	-0.462644000
	15	-1.635419000	-3.951410000	-0.333591000
	15	1.635419000	-3.951410000	-0.333591000
	15	3.993732000	-1.655794000	-0.462644000
	9	2.109163000	4.915611000	0.851419000
	9	-2.109163000	4.915611000	0.851419000
	9	-4.918288000	1.962900000	0.814746000
	9	-4.918288000	-1.962900000	0.814746000
	9	-2.109163000	-4.915611000	0.851419000
	9	2.109163000	-4.915611000	0.851419000
	9	4.918288000	-1.962900000	0.814746000
	9	4.918288000	1.962900000	0.814746000
$C_{16}(PF)_8^-$-D_{4d}	6	0.734997000	1.774439000	0.000000000
	6	-0.734997000	1.774439000	0.000000000
	6	0.734997000	-1.774439000	0.000000000
	6	-1.774439000	0.734997000	0.000000000
	6	-0.734997000	-1.774439000	0.000000000
	6	-1.774439000	-0.734997000	0.000000000
	6	1.774439000	0.734997000	0.000000000
	6	1.774439000	-0.734997000	0.000000000
	6	3.052243000	-1.264281000	0.000000000
	6	3.052243000	1.264281000	0.000000000
	6	1.264281000	3.052243000	0.000000000
	6	-1.264281000	3.052243000	0.000000000
	6	-3.052243000	1.264281000	0.000000000
	6	-3.052243000	-1.264281000	0.000000000
	6	-1.264281000	-3.052243000	0.000000000
	6	1.264281000	-3.052243000	0.000000000
	15	3.068253000	3.068253000	0.173735000
	15	0.000000000	4.339164000	-0.173735000
	15	-3.068253000	3.068253000	0.173735000
	15	-4.339164000	0.000000000	-0.173735000
	15	-3.068253000	-3.068253000	0.173735000
	15	0.000000000	-4.339164000	-0.173735000
	15	3.068253000	-3.068253000	0.173735000
	15	4.339164000	0.000000000	-0.173735000

	9	0.000000000	-5.112418000	1.276920000
	9	-5.112418000	0.000000000	1.276920000
	9	0.000000000	5.112418000	1.276920000
	9	5.112418000	0.000000000	1.276920000
	9	3.615025000	3.615025000	-1.276920000
	9	3.615025000	-3.615025000	-1.276920000
	9	-3.615025000	-3.615025000	-1.276920000
	9	-3.615025000	3.615025000	-1.276920000
$C_{16}(PF)_8^-$-C_{8v}	6	-1.917641000	0.000000000	-0.143403000
	6	-1.355977000	-1.355977000	-0.143403000
	6	1.355977000	1.355977000	-0.143403000
	6	0.000000000	-1.917641000	-0.143403000
	6	1.917641000	0.000000000	-0.143403000
	6	1.355977000	-1.355977000	-0.143403000
	6	-1.355977000	1.355977000	-0.143403000
	6	0.000000000	1.917641000	-0.143403000
	6	0.000000000	3.308354000	-0.123838000
	6	-2.339360000	2.339360000	-0.123838000
	6	-3.308354000	0.000000000	-0.123838000
	6	-2.339360000	-2.339360000	-0.123838000
	6	0.000000000	-3.308354000	-0.123838000
	6	2.339360000	-2.339360000	-0.123838000
	6	3.308354000	0.000000000	-0.123838000
	6	2.339360000	2.339360000	-0.123838000
	15	-3.978694000	1.648029000	-0.431421000
	15	-3.978694000	-1.648029000	-0.431421000
	15	-1.648029000	-3.978694000	-0.431421000
	15	1.648029000	-3.978694000	-0.431421000
	15	3.978694000	-1.648029000	-0.431421000
	15	3.978694000	1.648029000	-0.431421000
	15	1.648029000	3.978694000	-0.431421000
	15	-1.648029000	3.978694000	-0.431421000
	9	-4.863530000	2.014540000	0.897197000
	9	-2.014540000	4.863530000	0.897197000
	9	2.014540000	4.863530000	0.897197000
	9	4.863530000	2.014540000	0.897197000
	9	4.863530000	-2.014540000	0.897197000
	9	2.014540000	-4.863530000	0.897197000
	9	-2.014540000	-4.863530000	0.897197000
	9	-4.863530000	-2.014540000	0.897197000