Supporting Information

Theoretical Investigation of Charge Transfer in Metal Organic Frameworks (MOFs) For Electrochemical Device Applications

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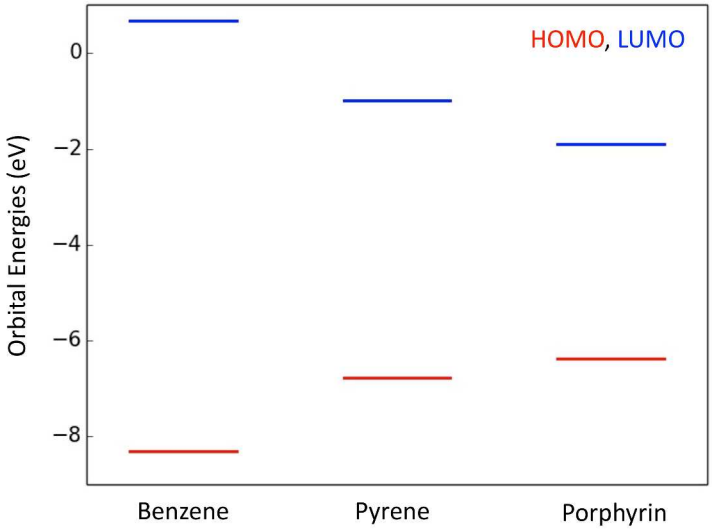


Figure S1. Energy levels associated with the HOMO and LUMO orbitals of benzene, pyrene and porphyrin molecules in gas phase (M06-2X xc-functional, TZP basis set).

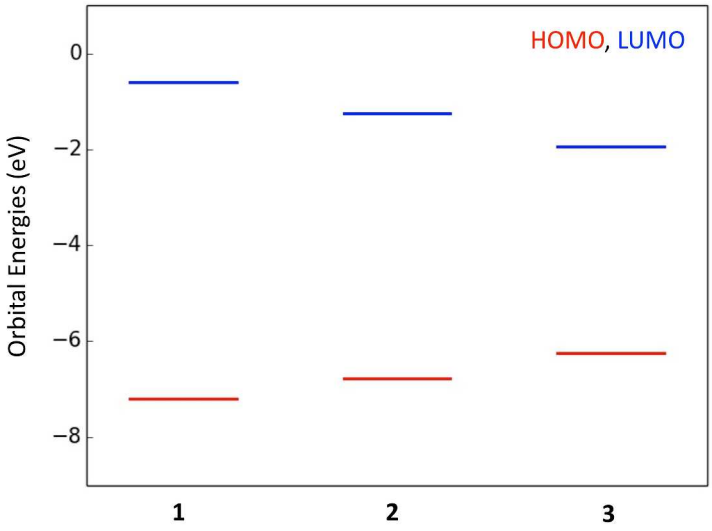


Figure S2. Energy levels associated with the HOMO and LUMO orbitals of **1**, **2** and **3**.

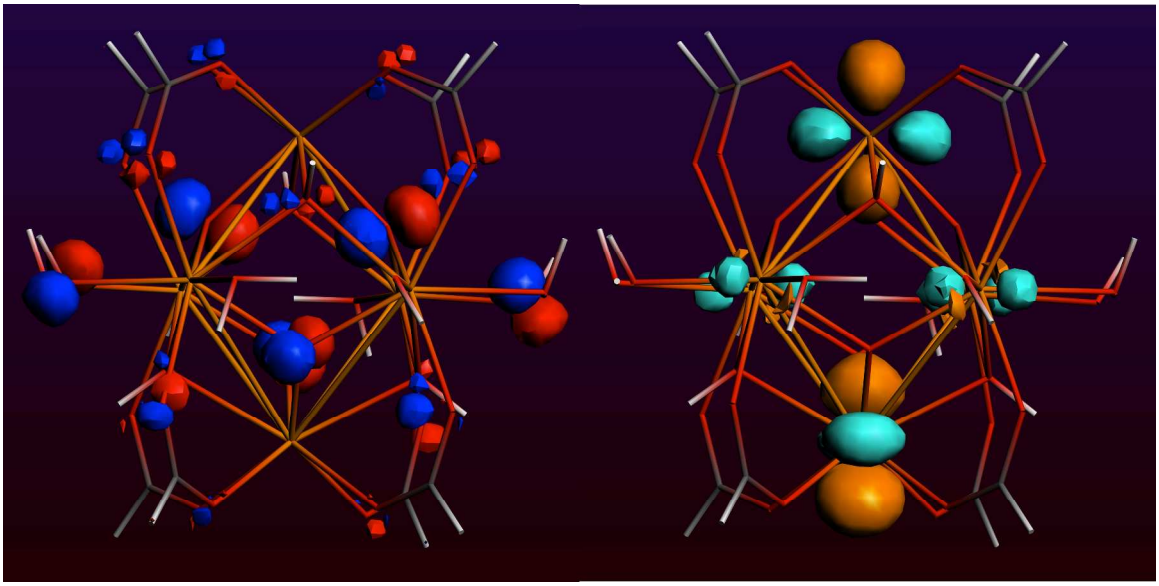


Figure S3. The frontier orbitals isosurfaces of the $Zr^{(IV)}$-node at 0.05 a.u. (left: HOMO, right: LUMO). The frontier orbitals largely consist of hydroxyl groups and oxygen atoms forming μ-oxo bonds, with some contribution from pendent carboxylate groups of the linkers.

Table S1: Internal reorganization energy λ_h as a function of rotation angle θ for linker **2**. 0° corresponds to the 54.9° equilibrium geometry in the gas phase (see Figure 3). During geometry optimizations, all four phenyl rotations were fixed at θ.

θ in degrees	λ(θ) in eV
-30	0.24176
-20	0.24079
-10	0.24428
0	0.24950
10	0.25008
20	0.25331
30	0.25439

Structural coordinates that were used to calculate charge transfer integrals in different directions in NU-1000.

Direction *a*-*b*

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C	6.30740451	-4.35917736	1.51850100
C	-10.84428649	9.87325464	6.15611500
C	3.56016151	-5.19382836	5.72741500
H	3.51316351	-5.83687936	6.59724100
H	7.55234451	-4.53833636	4.72829100
C	3.56016151	-5.19382836	-5.72741500
O	-3.20163349	-1.65864836	-5.87720000
C	2.41291251	-4.41320936	5.38334700
C	7.55254951	-4.50527736	3.64688700
C	1.13205651	-4.45480036	6.15611500
H	5.60612451	-5.79706636	-5.32843700
C	5.14229951	-4.50812136	-0.74237400
C	-6.30392749	2.11505464	-3.78710000
H	4.19556151	-4.73740136	-1.20566600
H	3.51316351	-5.83687936	-6.59724100
H	-3.46515149	0.08956864	-3.89658400
C	2.41291251	-4.41320936	-5.38334700
C	2.61424551	-3.60024236	4.22872900
H	1.81014451	-2.95612536	3.89658400
C	-9.36312349	9.01692064	4.22872900
O	-3.20163349	-1.65864836	5.87720000
C	-6.95779849	3.21275564	2.98276300
C	-6.92886049	3.28278364	1.51850100
C	-6.27806849	0.48627664	5.72741500
H	-6.81146749	0.12404964	6.59724100
C	-8.75276149	7.95476664	3.46032700
C	10.30451251	-5.16254736	-4.98353000
C	1.13205651	-4.45480036	-6.15611500
C	3.83927851	-3.60273136	3.46032700
H	11.20815151	-2.92555436	-2.61820900
C	4.80017651	-5.16254736	-4.98353000
H	3.89653751	-2.92555436	2.61820900
C	4.98365451	-4.40183436	3.78710000
H	-9.55727349	7.07888064	-1.20566600
C	4.80017651	-5.16254736	4.98353000
C	-8.87261749	6.56415564	3.78710000
H	-4.48187349	1.91172364	-2.61820900
H	5.60612451	-5.79706636	5.32843700
C	5.14229951	-4.50812136	0.74237400

H	-7.70648649	4.27135364	-4.72829100
H	4.19556151	-4.73740136	1.20566600
O	-10.58959249	11.13767264	5.87720000
C	-9.62315249	6.34269564	4.98353000
H	13.29454451	-2.95612536	-3.89658400
C	7.55213951	-4.31047836	0.78905600
O	14.94030451	-3.60202036	-5.87720000
O	0.99886051	-5.35450236	-7.09982600
C	6.26122651	-4.41925236	-2.98276300
O	-11.69004949	9.53875464	-7.09982600
C	8.84346251	-4.41925236	-2.98276300
C	3.83927851	-3.60273136	-3.46032700
O	0.99886051	-5.35450236	7.09982600
C	-7.50905249	4.38510564	-0.78905600
C	-7.67795949	4.28806164	-3.64688700
H	-10.85064849	7.12011564	6.59724100
H	-7.82346949	1.95651364	5.32843700
H	7.55234451	-4.53833636	-4.72829100
C	7.55213951	-4.50527736	-3.64688700
C	7.55254951	-4.31047836	-0.78905600
O	0.16438451	-3.60202036	5.87720000
C	6.26122651	-4.41925236	2.98276300
C	-6.47529649	2.19930164	0.74237400
C	10.12103451	-4.40183436	-3.78710000
H	-7.70648649	4.27135364	4.72829100
C	12.49044351	-3.60024236	-4.22872900
C	13.97263251	-4.45480036	-6.15611500
C	8.79728451	-4.35917736	-1.51850100
C	-7.67775449	4.28770564	3.64688700
O	14.10582851	-5.35450236	-7.09982600
C	-5.03969549	1.52354664	3.46032700
H	-4.48187349	1.91172364	2.61820900
C	-10.16784049	8.78479664	5.38334700
C	-8.17380149	5.43908364	1.51850100
C	-6.87098549	1.57580164	-4.98353000
C	-5.03969549	1.52354664	-3.46032700
H	3.89653751	-2.92555436	-2.61820900
C	-8.24891649	5.44903664	2.98276300
C	12.69177651	-4.41320936	-5.38334700
C	4.98365451	-4.40183436	-3.78710000
C	-8.88534249	6.37362164	0.74237400
H	10.90912751	-4.73740136	1.20566600
O	14.10582851	-5.35450236	7.09982600
H	-6.81146749	0.12404964	-6.59724100
C	-6.87098549	1.57580164	4.98353000
C	-5.02840749	-0.11696136	-5.38334700

C	-4.42399849	-1.24701036	-6.15611500
O	-5.13656549	-1.81221236	7.09982600
O	-5.13656549	-1.81221236	-7.09982600
H	-7.82346949	1.95651364	-5.32843700
C	-6.47529649	2.19930164	-0.74237400
H	-6.20049049	1.26476264	-1.20566600
O	14.94030451	-3.60202036	5.87720000
C	8.84346251	-4.41925236	2.98276300
C	8.79728451	-4.35917736	1.51850100
C	11.54452751	-5.19382836	5.72741500
C	11.26541051	-3.60273136	-3.46032700
C	-6.30392749	2.11505464	3.78710000
H	11.59152551	-5.83687936	6.59724100
C	-10.27025149	7.40093964	5.72741500
C	-7.50925849	4.38546064	0.78905600
C	12.69177651	-4.41320936	5.38334700
H	-6.20049049	1.26476264	1.20566600
H	-9.55727349	7.07888064	1.20566600
C	13.97263251	-4.45480036	6.15611500
H	1.81014451	-2.95612536	-3.89658400
O	-11.69004949	9.53875464	7.09982600
H	-9.20735149	10.03535064	3.89658400
H	-8.13768049	8.24376664	2.61820900
C	-5.02840749	-0.11696136	5.38334700
C	12.49044351	-3.60024236	4.22872900
H	13.29454451	-2.95612536	3.89658400
C	11.26541051	-3.60273136	3.46032700
O	-10.58959249	11.13767264	-5.87720000
C	-8.24891649	5.44903664	-2.98276300
C	-4.42399849	-1.24701036	6.15611500
C	-8.17380149	5.43908364	-1.51850100
C	-4.42502449	0.46388164	4.22872900
C	-10.27025149	7.40093964	-5.72741500
O	0.16438451	-3.60202036	-5.87720000
H	-10.85064849	7.12011564	-6.59724100
C	-10.16784049	8.78479664	-5.38334700
C	-10.84428649	9.87325464	-6.15611500
H	9.49856451	-5.79706636	-5.32843700
C	9.96238951	-4.50812136	-0.74237400
C	-9.36312349	9.01692064	-4.22872900
C	-6.95779849	3.21275564	-2.98276300
H	-9.20735149	10.03535064	-3.89658400
C	-8.75276149	7.95476664	-3.46032700
H	10.90912751	-4.73740136	-1.20566600
H	-8.13768049	8.24376664	-2.61820900
C	-8.87261749	6.56415564	-3.78710000

C	-6.92886049	3.28278364	-1.51850100
C	-9.62315249	6.34269564	-4.98353000
C	2.61424551	-3.60024236	-4.22872900
H	-9.76968849	5.32746464	-5.32843700
C	-8.88534249	6.37362164	-0.74237400
C	6.30740451	-4.35917736	-1.51850100
H	-9.76968849	5.32746464	5.32843700
C	-4.42502449	0.46388164	-4.22872900
H	11.20815151	-2.92555436	2.61820900
C	11.54452751	-5.19382836	-5.72741500
H	11.59152551	-5.83687936	-6.59724100
C	10.12103451	-4.40183436	3.78710000
C	10.30451251	-5.16254736	4.98353000
H	9.49856451	-5.79706636	5.32843700
H	-3.46515149	0.08956864	3.89658400
C	9.96238951	-4.50812136	0.74237400
C	-6.27806849	0.48627664	-5.72741500
H	14.66177154	-3.02445097	5.16275408
H	14.66176992	-3.02444818	-5.16275696
H	0.44291910	-3.02444818	5.16275697
H	0.44291748	-3.02445096	-5.16275408
H	-2.84071045	-1.12864692	5.16275404
H	-2.84070885	-1.12864413	-5.16275692
H	-9.95013620	11.18524020	-5.16275407
H	-9.95013298	11.18524019	5.16275695

Direction *a*+*b*

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H	16.75969600	3.04569400	29.08458400
C	16.30510600	5.12627800	28.64832700
H	15.69002500	4.83727800	27.80620900
C	16.42496200	6.51688900	28.97510000
C	17.17549700	6.73834800	30.17153000
H	17.32203300	7.75358000	30.51643700
C	17.95456000	18.06443300	21.40090000
C	16.43768700	6.70742200	25.93037400
H	17.10961800	6.00216400	26.39366600
O	12.68891000	14.89325700	18.08817400
O	10.75397800	14.73969300	19.31080000
C	14.51014300	9.86828900	22.20523700
C	14.48120500	9.79826100	23.66949900
C	13.83041300	12.59476800	19.46058500
H	14.36381200	12.95699500	18.59075900
C	12.58075200	13.19800600	19.80465300

C	11.97634300	14.32805500	19.03188500
C	11.97736900	12.61716300	20.95927100
H	11.01749600	12.99147600	21.29141600
C	12.59204000	11.55749700	21.72767300
C	17.77108200	17.30372000	20.20447000
O	19.24239400	3.54229000	18.08817400
O	18.14193700	1.94337200	19.31080000
C	15.80126100	7.63200800	22.20523700
C	15.72614600	7.64196100	23.66949900
C	17.82259600	5.68010500	19.46058500
C	23.27541800	17.30372000	20.20447000
H	12.03421800	11.16932100	22.56979100
C	13.85627200	10.96599000	21.40090000
C	14.42333000	11.50524300	20.20447000
H	15.37581400	11.12453100	19.85956300
C	14.02764100	10.88174300	24.44562600
H	13.75283500	11.81628200	23.98233400
C	19.23213200	18.04701500	28.17076300
C	19.27831000	18.10709000	23.66949900
C	23.09194000	18.06443300	21.40090000
O	13.13529000	18.86424700	19.31080000
H	24.17905700	19.54071300	27.80620900
C	23.09194000	18.06443300	28.97510000
C	23.27541800	17.30372000	30.17153000
H	22.46947000	16.66920100	30.51643700
H	20.52325000	17.92793100	20.45970900
C	20.52304500	17.96099000	21.54111300
C	20.52345500	18.15578900	24.39894400
C	25.66268200	18.05305800	19.80465300
C	22.93329500	17.95814600	25.93037400
C	19.27831000	18.10709000	26.70650100
C	16.81018400	18.86353600	21.72767300
H	20.52325000	17.92793100	29.91629100
C	16.53106700	17.27243900	19.46058500
C	25.46134900	18.86602500	20.95927100
C	20.52345500	17.96099000	28.83488700
H	16.48406900	16.62938800	18.59075900
O	27.07673400	17.11176500	18.08817400
C	15.38381800	18.05305800	19.80465300
C	16.53106700	17.27243900	30.91541500
H	16.48406900	16.62938800	31.78524100
O	27.07673400	17.11176500	32.28782600
C	14.10296200	18.01146700	19.03188500
O	27.91121000	18.86424700	19.31080000
O	13.96976600	17.11176500	18.08817400
O	27.91121000	18.86424700	31.06520000

C	21.81436800	18.04701500	28.17076300
C	21.76819000	18.10709000	26.70650100
C	24.51543300	17.27243900	30.91541500
H	24.56243100	16.62938800	31.78524100
H	26.26545000	19.51014200	21.29141600
C	15.38381800	18.05305800	30.57134700
C	25.66268200	18.05305800	30.57134700
C	20.52304500	18.15578900	25.97705600
C	26.94353800	18.01146700	31.34411500
C	14.10296200	18.01146700	31.34411500
C	15.58515100	18.86602500	29.41672900
C	25.46134900	18.86602500	29.41672900
H	26.26545000	19.51014200	29.08458400
C	24.23631600	18.86353600	28.64832700
H	14.78105000	19.51014200	29.08458400
C	15.58515100	18.86602500	20.95927100
C	16.81018400	18.86353600	28.64832700
H	24.17905700	19.54071300	22.56979100
C	26.94353800	18.01146700	19.03188500
H	16.86744300	19.54071300	27.80620900
H	18.40299300	5.96092900	18.59075900
C	17.72018500	4.29624800	19.80465300
C	18.39663100	3.20778900	19.03188500
C	16.91546800	4.06412400	20.95927100
H	16.75969600	3.04569400	21.29141600
C	17.95456000	18.06443300	28.97510000
C	16.30510600	5.12627800	21.72767300
H	15.69002500	4.83727800	22.56979100
C	16.42496200	6.51688900	21.40090000
C	17.17549700	6.73834800	20.20447000
H	17.32203300	7.75358000	19.85956300
C	16.43768700	6.70742200	24.44562600
H	17.10961800	6.00216400	23.98233400
C	24.23631600	18.86353600	21.72767300
H	15.25883100	8.80969000	20.45970900
C	15.23030400	8.79298300	21.54111300
C	15.06139700	8.69593900	24.39894400
H	18.57703000	16.66920100	19.85956300
C	21.81436800	18.04701500	22.20523700
C	18.11320500	17.95814600	24.44562600
H	23.88003300	17.72886600	26.39366600
C	17.77108200	17.30372000	30.17153000
H	16.86744300	19.54071300	22.56979100
H	17.16646700	17.72886600	23.98233400
O	13.96976600	17.11176500	32.28782600
O	13.13529000	18.86424700	31.06520000

C	19.23213200	18.04701500	22.20523700
H	18.57703000	16.66920100	30.51643700
C	18.11320500	17.95814600	25.93037400
C	21.76819000	18.10709000	23.66949900
H	17.16646700	17.72886600	26.39366600
O	12.68891000	14.89325700	32.28782600
O	10.75397800	14.73969300	31.06520000
C	14.51014300	9.86828900	28.17076300
C	14.48120500	9.79826100	26.70650100
C	13.83041300	12.59476800	30.91541500
H	14.36381200	12.95699500	31.78524100
C	12.58075200	13.19800600	30.57134700
C	11.97634300	14.32805500	31.34411500
C	11.97736900	12.61716300	29.41672900
H	22.46947000	16.66920100	19.85956300
C	22.93329500	17.95814600	24.44562600
H	11.01749600	12.99147600	29.08458400
C	12.59204000	11.55749700	28.64832700
H	12.03421800	11.16932100	27.80620900
H	14.78105000	19.51014200	21.29141600
H	23.88003300	17.72886600	23.98233400
C	13.85627200	10.96599000	28.97510000
C	14.42333000	11.50524300	30.17153000
H	15.37581400	11.12453100	30.51643700
C	14.02764100	10.88174300	25.93037400
H	15.25883100	8.80969000	29.91629100
C	15.23009900	8.79333900	28.83488700
C	15.06160300	8.69558300	25.97705600
H	13.75283500	11.81628200	26.39366600
O	19.24239400	3.54229000	32.28782600
O	18.14193700	1.94337200	31.06520000
C	15.80126100	7.63200800	28.17076300
C	24.51543300	17.27243900	19.46058500
H	24.56243100	16.62938800	18.59075900
C	15.72614600	7.64196100	26.70650100
C	17.82259600	5.68010500	30.91541500
H	18.40299300	5.96092900	31.78524100
C	17.72018500	4.29624800	30.57134700
C	18.39663100	3.20778900	31.34411500
C	16.91546800	4.06412400	29.41672900
H	13.41382459	19.44181918	30.35075697
H	13.41382297	19.44181640	20.02524592
H	10.39305336	14.20968877	20.02524308
H	10.39305496	14.20969156	30.35075404
H	17.50247749	1.89580466	30.35075694
H	17.50248071	1.89580464	20.02524594

H	27.63267541	19.44181918	20.02524304
H	27.63267703	19.44181639	30.35075408

Direction *c*

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O	19.24239400	3.54229000	1.29617400
O	18.14193700	1.94337200	2.51880000
C	15.80126100	7.63200800	5.41323700
C	15.72614600	7.64196100	6.87749900
C	17.82259600	5.68010500	2.66858500
H	18.40299300	5.96092900	1.79875900
C	17.72018500	4.29624800	3.01265300
C	18.39663100	3.20778900	2.23988500
C	16.91546800	4.06412400	4.16727100
H	16.75969600	3.04569400	4.49941600
C	16.30510600	5.12627800	4.93567300
H	15.69002500	4.83727800	5.77779100
C	16.42496200	6.51688900	4.60890000
C	17.17549700	6.73834800	3.41247000
H	17.32203300	7.75358000	3.06756300
C	16.43768700	6.70742200	7.65362600
H	17.10961800	6.00216400	7.19033400
H	15.25883100	8.80969000	3.66770900
C	15.23030400	8.79298300	4.74911300
C	15.06139700	8.69593900	7.60694400
H	16.75969600	3.04569400	29.08458400
O	19.24239400	3.54229000	18.08817400
O	18.14193700	1.94337200	19.31080000
C	15.80126100	7.63200800	22.20523700
C	15.72614600	7.64196100	23.66949900
C	17.82259600	5.68010500	19.46058500
C	16.30510600	5.12627800	28.64832700
H	15.69002500	4.83727800	27.80620900
O	12.68891000	14.89325700	15.49582600
O	10.75397800	14.73969300	14.27320000
C	14.51014300	9.86828900	11.37876300
C	14.48120500	9.79826100	9.91450100
C	13.83041300	12.59476800	14.12341500
H	14.36381200	12.95699500	14.99324100
C	12.58075200	13.19800600	13.77934700
C	11.97634300	14.32805500	14.55211500
C	11.97736900	12.61716300	12.62472900
H	11.01749600	12.99147600	12.29258400
C	12.59204000	11.55749700	11.85632700

H	12.03421800	11.16932100	11.01420900
C	13.85627200	10.96599000	12.18310000
C	14.42333000	11.50524300	13.37953000
H	15.37581400	11.12453100	13.72443700
C	14.02764100	10.88174300	9.13837400
H	15.25883100	8.80969000	13.12429100
C	15.23009900	8.79333900	12.04288700
C	15.06160300	8.69558300	9.18505600
H	13.75283500	11.81628200	9.60166600
O	19.24239400	3.54229000	15.49582600
O	18.14193700	1.94337200	14.27320000
C	15.80126100	7.63200800	11.37876300
C	15.72614600	7.64196100	9.91450100
C	17.82259600	5.68010500	14.12341500
H	18.40299300	5.96092900	14.99324100
C	17.72018500	4.29624800	13.77934700
C	18.39663100	3.20778900	14.55211500
C	16.91546800	4.06412400	12.62472900
H	16.75969600	3.04569400	12.29258400
C	16.30510600	5.12627800	11.85632700
H	15.69002500	4.83727800	11.01420900
C	16.42496200	6.51688900	12.18310000
C	17.17549700	6.73834800	13.37953000
H	17.32203300	7.75358000	13.72443700
C	16.43768700	6.70742200	9.13837400
H	17.10961800	6.00216400	9.60166600
O	12.68891000	14.89325700	1.29617400
O	10.75397800	14.73969300	2.51880000
C	14.51014300	9.86828900	5.41323700
C	14.48120500	9.79826100	6.87749900
C	13.83041300	12.59476800	2.66858500
H	14.36381200	12.95699500	1.79875900
C	12.58075200	13.19800600	3.01265300
C	11.97634300	14.32805500	2.23988500
C	11.97736900	12.61716300	4.16727100
H	11.01749600	12.99147600	4.49941600
C	12.59204000	11.55749700	4.93567300
H	12.03421800	11.16932100	5.77779100
C	13.85627200	10.96599000	4.60890000
C	14.42333000	11.50524300	3.41247000
H	15.37581400	11.12453100	3.06756300
C	14.02764100	10.88174300	7.65362600
H	13.75283500	11.81628200	7.19033400
H	18.40299300	5.96092900	18.59075900
C	17.72018500	4.29624800	19.80465300
C	18.39663100	3.20778900	19.03188500

C	16.91546800	4.06412400	20.95927100
H	16.75969600	3.04569400	21.29141600
C	16.42496200	6.51688900	28.97510000
C	16.30510600	5.12627800	21.72767300
H	15.69002500	4.83727800	22.56979100
C	16.42496200	6.51688900	21.40090000
C	17.17549700	6.73834800	20.20447000
H	17.32203300	7.75358000	19.85956300
C	16.43768700	6.70742200	24.44562600
H	17.10961800	6.00216400	23.98233400
C	17.17549700	6.73834800	30.17153000
H	15.25883100	8.80969000	20.45970900
C	15.23030400	8.79298300	21.54111300
C	15.06139700	8.69593900	24.39894400
H	17.32203300	7.75358000	30.51643700
H	13.75283500	11.81628200	23.98233400
C	16.43768700	6.70742200	25.93037400
H	17.10961800	6.00216400	26.39366600
O	12.68891000	14.89325700	18.08817400
O	10.75397800	14.73969300	19.31080000
C	14.51014300	9.86828900	22.20523700
C	14.48120500	9.79826100	23.66949900
C	13.83041300	12.59476800	19.46058500
H	14.36381200	12.95699500	18.59075900
C	12.58075200	13.19800600	19.80465300
C	11.97634300	14.32805500	19.03188500
C	11.97736900	12.61716300	20.95927100
H	11.01749600	12.99147600	21.29141600
O	12.68891000	14.89325700	32.28782600
O	10.75397800	14.73969300	31.06520000
C	14.51014300	9.86828900	28.17076300
C	14.48120500	9.79826100	26.70650100
C	13.83041300	12.59476800	30.91541500
H	14.36381200	12.95699500	31.78524100
C	12.58075200	13.19800600	30.57134700
C	11.97634300	14.32805500	31.34411500
C	11.97736900	12.61716300	29.41672900
C	12.59204000	11.55749700	21.72767300
H	12.03421800	11.16932100	22.56979100
H	11.01749600	12.99147600	29.08458400
C	12.59204000	11.55749700	28.64832700
H	12.03421800	11.16932100	27.80620900
C	13.85627200	10.96599000	21.40090000
C	14.42333000	11.50524300	20.20447000
C	13.85627200	10.96599000	28.97510000
C	14.42333000	11.50524300	30.17153000

H	15.37581400	11.12453100	30.51643700
C	14.02764100	10.88174300	25.93037400
H	15.25883100	8.80969000	29.91629100
C	15.23009900	8.79333900	28.83488700
C	15.06160300	8.69558300	25.97705600
H	13.75283500	11.81628200	26.39366600
O	19.24239400	3.54229000	32.28782600
O	18.14193700	1.94337200	31.06520000
C	15.80126100	7.63200800	28.17076300
H	15.37581400	11.12453100	19.85956300
C	14.02764100	10.88174300	24.44562600
C	15.72614600	7.64196100	26.70650100
C	17.82259600	5.68010500	30.91541500
H	18.40299300	5.96092900	31.78524100
C	17.72018500	4.29624800	30.57134700
C	18.39663100	3.20778900	31.34411500
C	16.91546800	4.06412400	29.41672900
H	10.39305496	14.20969156	30.35075404
H	10.39305336	14.20968877	20.02524308
H	10.39305496	14.20969156	13.55875404
H	10.39305336	14.20968877	3.23324308
H	17.50248071	1.89580464	3.23324594
H	17.50247749	1.89580466	13.55875694
H	17.50248071	1.89580464	20.02524594
H	17.50247749	1.89580466	30.35075694

Structural coordinates that were used to calculate binding energy (for the calculation of ΔG) of PF6- ions with Py(+).

H 0.092429 -0.014412 4.486487
C -0.09664200000000001 2.432306 0.5826030000000001
H -0.081882 3.375668 1.108156
H 0.008651000000000001 -3.389222 1.090057
H -0.126617 3.381051 -1.313
C -0.09439599999999998 1.216448 -2.959158
C -0.093643 1.23099 -1.527175
C -0.10097 2.435487 -0.791839
C 0.141146 -1.223818 2.729888
C 0.031032 -1.238679 1.30229
C -0.017829 -2.443558 0.569356
C -0.089627 1.203095 2.744258
C -0.089784 1.224398 1.312351
C -0.294734 -1.213211 -2.956168
C -0.184055 -1.233408 -1.528636
C -0.111431 -0.002569 -0.821075
C -0.220494 0.002964 -3.62495
H -0.26233 0.005048 -4.707151
C -0.119271 -2.440993000000001 -0.801357
H -0.13296 -3.384445 -1.326537
C -0.05685 -0.005553 0.600486
C 0.051393 -0.011858 3.404346
H 1.760331 3.198753 -2.737856
H -1.255004 -1.993749 4.894328
H -1.969402 3.162647 2.531156
H -2.129621 -3.192995 -2.596768
C -0.473522 -2.445815 -3.753562
C 0.332968 -2.667288 -4.875895
C 0.161566 -3.806883 -5.650442
C -0.831369 -4.727504 -5.327331
C -1.65341 -4.504008 -4.226356
C -1.474568 -3.373248 -3.440122
H 1.110225 -1.955101 -5.124655
H 0.803401 -3.976086 -6.505459
H -0.967276 -5.613887 -5.933769
H -2.436977 -5.209158999999999 -3.980929
C 0.019582 2.452359 -3.763498
C -0.87308 2.676327 -4.818152000000001
C -0.764568 3.81858 -5.600104
C 0.249407 4.739725 -5.352948
C 1.15546 4.514258 -4.32044
C 1.040702 3.380634 -3.526429
H -1.666283 1.963502 -5.007832999999999

H -1.471555 3.98921 -6.401776
H 0.3361140000000001 5.628192 -5.965304
H 1.954933 5.219889 -4.135009
C -0.220072 2.433452 3.554588
C 0.668365 2.663195 4.611564
C 0.544247 3.799735 5.399506
C -0.481199 4.70908 5.156037000000001
C -1.383097 4.477507 4.121238
C -1.252873 3.349707 3.321337
H 1.47036 1.959545 4.7985
H 1.247963 3.975066 6.203037999999999
H -0.580113 5.592997 5.773107
H -2.191455 5.173707 3.938702
C 0.335157 -2.457919 3.521412
C 1.347601 -3.371365 3.20359
C 1.540246 -4.503714 3.984267
C 0.720709 -4.742892 5.083815
C -0.283736 -3.836333 5.411094
C -0.468968 -2.695049 4.64224
H 2.000459 -3.178906 2.361222
H 2.332562 -5.197868 3.735592
H 0.867371 -5.630589 5.685806
H -0.923804 -4.017848 6.264908
P 3.743835 0.087899 0.444586
F 2.774981 1.233808 -0.16475
F 2.853339 0.054126 1.796972
F 4.712689 -1.058009 1.053921
F 4.687982999999999 1.231939 1.094842
F 4.634331 0.121675 -0.9078009999999999
F 2.799688 -1.05614 -0.205671

Structural coordinates that were used to calculate binding energy (for the calculation of ΔG) of PF6- ions with Py(0).

H -0.058991 0.05512 4.572691
C -0.179154 2.516588 0.662031
H -0.225024 3.455513 1.196086
H 0.096859 -3.335597 1.185797
H -0.148658 3.461803 -1.219175
C -0.029157 1.28633 -2.851399
C -0.065567 1.297683 -1.442739
C -0.127844 2.520418 -0.687901
C 0.06560199999999999 -1.157064 2.818014
C 0.026243 -1.171069 1.409468
C 0.048475 -2.39519 0.654641
C -0.189072 1.272294 2.821899

C -0.154286 1.290297 1.413284
C -0.111704 -1.154923 -2.854728
C -0.071884 -1.170284 -1.446221
C -0.067704 0.062677 -0.734758
C -0.071231 0.06664100000000002 -3.5213
H -0.07239 0.06816899999999999 -4.605801
C -0.007521 -2.395145 -0.695069
H 0.011276 -3.33493 -1.229183
C -0.06518699999999999 0.060622 0.701682
C -0.060545 0.056679 3.488184
H 1.843373 3.25246 -2.715008
H -1.552793 -2.076353 4.775962
H -2.196372 3.100976 2.69208
H -1.983678 -3.121697 -2.721146
C -0.19102 -2.401584 -3.665038
C 0.753548 -2.652641 -4.663948
C 0.6657999999999999 -3.796169 -5.451158999999999
C -0.373974 -4.700109000000001 -5.256296
C -1.32618 -4.453924 -4.270679
C -1.234465 -3.314521 -3.480049
H 1.56735 -1.953009 -4.814988
H 1.410973 -3.980712 -6.214803
H -0.444153 -5.589612 -5.869651
H -2.14432 -5.1471 -4.120215
C 0.049245 2.535192 -3.658421
C -0.896133 2.788878 -4.655886
C -0.808737 3.93423 -5.440482
C 0.23129 4.837553 -5.244251
C 1.184218 4.588882 -4.260014
C 1.093005 3.447527 -3.472209
H -1.710255 2.089809 -4.807851
H -1.554528 4.120796 -6.203022
H 0.301072 5.728606 -5.855392
H 2.00254 5.281601 -4.108398
C -0.355274 2.510127 3.632591
C 0.57039 2.827409 4.630342
C 0.402516 3.961449 5.418269
C -0.6990619999999999 4.789312 5.225081
C -1.632605 4.47647 4.240566
C -1.46121 3.346684 3.449456
H 1.432183 2.187469 4.779915
H 1.13371 4.198278 6.180989
H -0.831421 5.671476 5.838761
H -2.498085 5.109845 4.091304
C 0.232441 -2.397409 3.624748
C 1.337229 -3.23453 3.437186

C 1.508483 -4.367070999999999 4.224439
C 0.576044 -4.682099 5.209363
C -0.5243409999999999 -3.853648 5.406882999999999
C -0.692009 -2.716824 4.622953
H 2.070972 -2.987548 2.678869
H 2.372994 -5.000964 4.071875
H 0.7083789999999999 -5.566322 5.820087999999999
H -1.254637 -4.092062 6.169976
P 3.788065 0.214494 0.85738
F 2.809596 1.300392 0.159886
F 2.843106 0.207881 2.172707
F 4.766535 -0.871404 1.554874
F 4.667113 1.4161 1.494948
F 4.733024 0.221107 -0.457946
F 2.909017 -0.987112 0.219812