

Electronic Supplementary Information

Tetraquinolines; Four Linked Quinoline Units or Porphyrinoids

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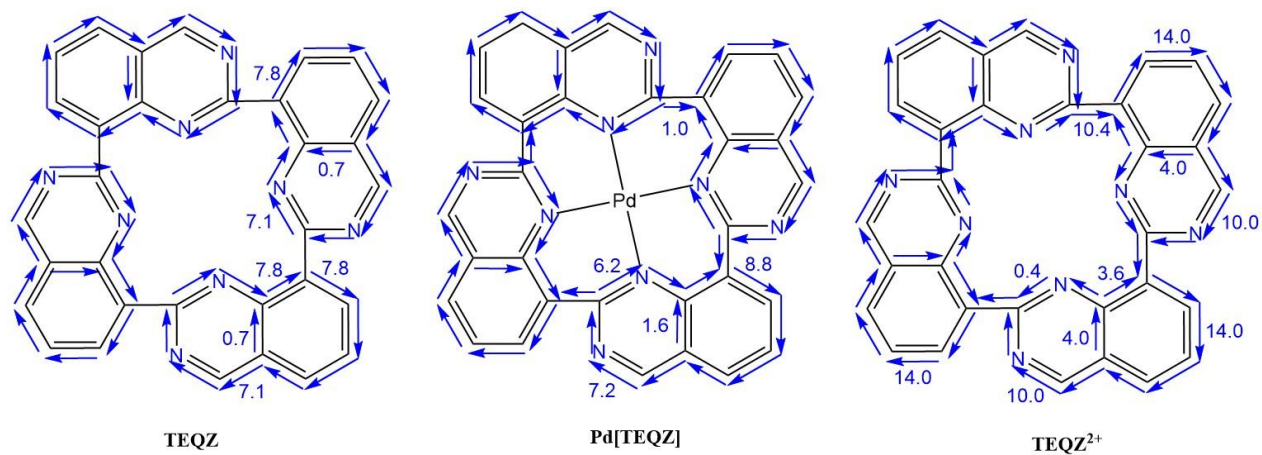


Fig. S1. Current density in nA/T for TEQZ derivatives.

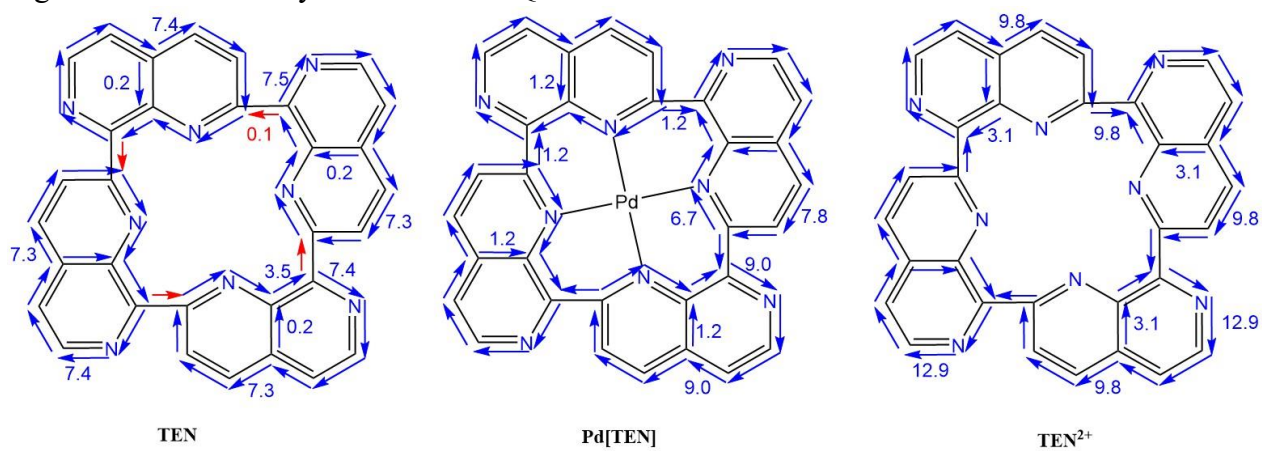


Fig. S2. Current density in nA/T for TEN derivatives.

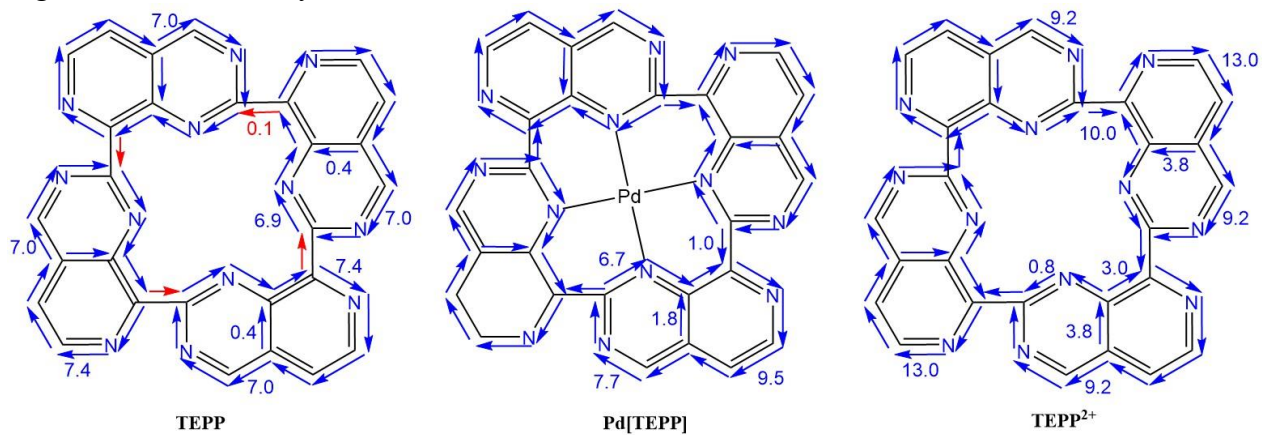


Fig. S3. Current density in nA/T for TEPP derivatives.

Table S1. AV1245 values for the selected systems.

Molecule	Pathway	AV1245	Molecule	Pathway	AV1245
Zn[Por]	Outer rim	2.547	TEQ ²⁺	Outer rim	2.270
	Inner rim	1.778		Inner rim	-0.124
Ni[Nor]	Outer rim	3.301	Pd[TEQ]	Qn	3.599
	Inner rim	1.105		Outer rim	2.330
TEQ	Outer rim	2.198		Inner rim	-0.128
	Inner rim	-0.607		Qn	4.394
	Qn	5.657			

Cartesian Coordinates of Optimized Systems

TEQ

E(RB3LYP) = -1603.66695412

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6   -3.122506000   2.571877000   1.913419000
6   -2.218785000   2.154842000   0.966165000
6   -0.869492000   2.600675000   1.041934000
6   -0.479034000   3.441349000   2.124324000
6   -1.435289000   3.828775000   3.089661000
6   -2.733596000   3.407507000   2.980661000
1   -4.148458000   2.233655000   1.850246000
6    0.869492000   3.857848000   2.163473000
1   -1.126136000   4.464785000   3.909493000
1   -3.467748000   3.705912000   3.716618000
6    1.728078000   3.457677000   1.178866000
6    1.240505000   2.635825000   0.131635000
1    2.768075000   3.751137000   1.184545000
6    2.154842000   2.218785000  -0.966165000
6    2.600675000   0.869492000  -1.041934000
6    2.571877000   3.122506000  -1.913419000
6    3.441349000   0.479034000  -2.124324000
6    3.407507000   2.733596000  -2.980661000
1    2.233655000   4.148458000  -1.850246000
6    2.635825000  -1.240505000  -0.131635000
6    3.857848000  -0.869492000  -2.163473000
6    3.828775000   1.435289000  -3.089661000
1    3.705912000   3.467748000  -3.716618000
6    3.457677000  -1.728078000  -1.178866000
1    4.490262000  -1.207178000  -2.975039000
1    4.464785000   1.126136000  -3.909493000
1    3.751137000  -2.768075000  -1.184545000
6    2.218785000  -2.154842000   0.966165000
6    0.869492000  -2.600675000   1.041934000
6    3.122506000  -2.571877000   1.913419000

```

6	0.479034000	-3.441349000	2.124324000
6	2.733596000	-3.407507000	2.980661000
1	4.148458000	-2.233655000	1.850246000
6	-1.240505000	-2.635825000	0.131635000
6	1.435289000	-3.828775000	3.089661000
1	3.467748000	-3.705912000	3.716618000
1	1.126136000	-4.464785000	3.909493000
6	-2.154842000	-2.218785000	-0.966165000
6	-2.600675000	-0.869492000	-1.041934000
6	-2.571877000	-3.122506000	-1.913419000
6	-3.441349000	-0.479034000	-2.124324000
6	-3.407507000	-2.733596000	-2.980661000
1	-2.233655000	-4.148458000	-1.850246000
6	-2.635825000	1.240505000	-0.131635000
6	-3.857848000	0.869492000	-2.163473000
6	-3.828775000	-1.435289000	-3.089661000
1	-3.705912000	-3.467748000	-3.716618000
6	-3.457677000	1.728078000	-1.178866000
1	-4.490262000	1.207178000	-2.975039000
1	-4.464785000	-1.126136000	-3.909493000
1	-3.751137000	2.768075000	-1.184545000
7	-0.005541000	2.230672000	0.065302000
7	2.230672000	0.005541000	-0.065302000
7	0.005541000	-2.230672000	0.065302000
7	-2.230672000	-0.005541000	-0.065302000
6	-0.869492000	-3.857848000	2.163473000
6	-1.728078000	-3.457677000	1.178866000
1	-2.768075000	-3.751137000	1.184545000
1	-1.207178000	-4.490262000	2.975039000
1	1.207178000	4.490262000	2.975039000

Pd[TEQ]

E(RB3LYP) = -1731.25701472

6	-2.982899000	-2.593252000	2.182990000
6	-2.340562000	-1.852750000	1.205915000
6	-2.705759000	-0.496079000	1.025969000
6	-3.844492000	0.000000000	1.716802000
6	-4.454379000	-0.781969000	2.720810000
6	-3.997816000	-2.047324000	2.981464000
1	-2.705004000	-3.628241000	2.325413000
6	-4.357361000	1.251810000	1.322278000
1	-5.297557000	-0.373197000	3.260349000
1	-4.451294000	-2.648388000	3.755860000

6	-3.760508000	1.939610000	0.306097000
6	-2.549370000	1.465745000	-0.247074000
1	-4.149756000	2.889338000	-0.023228000
6	-1.852750000	2.340562000	-1.205915000
6	-0.496079000	2.705759000	-1.025969000
6	-2.593252000	2.982899000	-2.182990000
6	0.000000000	3.844492000	-1.716802000
6	-2.047324000	3.997816000	-2.981464000
1	-3.628241000	2.705004000	-2.325413000
6	1.465745000	2.549370000	0.247074000
6	1.251810000	4.357361000	-1.322278000
6	-0.781969000	4.454379000	-2.720810000
1	-2.648388000	4.451294000	-3.755860000
6	1.939610000	3.760508000	-0.306097000
1	1.649797000	5.231931000	-1.819056000
1	-0.373197000	5.297557000	-3.260349000
1	2.889338000	4.149756000	0.023228000
6	2.340562000	1.852750000	1.205915000
6	2.705759000	0.496079000	1.025969000
6	2.982899000	2.593252000	2.182990000
6	3.844492000	0.000000000	1.716802000
6	3.997816000	2.047324000	2.981464000
1	2.705004000	3.628241000	2.325413000
6	2.549370000	-1.465745000	-0.247074000
6	4.454379000	0.781969000	2.720810000
1	4.451294000	2.648388000	3.755860000
1	5.297557000	0.373197000	3.260349000
6	1.852750000	-2.340562000	-1.205915000
6	0.496079000	-2.705759000	-1.025969000
6	2.593252000	-2.982899000	-2.182990000
6	0.000000000	-3.844492000	-1.716802000
6	2.047324000	-3.997816000	-2.981464000
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6	-1.465745000	-2.549370000	0.247074000
6	-1.251810000	-4.357361000	-1.322278000
6	0.781969000	-4.454379000	-2.720810000
1	2.648388000	-4.451294000	-3.755860000
6	-1.939610000	-3.760508000	-0.306097000
1	-1.649797000	-5.231931000	-1.819056000
1	0.373197000	-5.297557000	-3.260349000
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7	-2.022699000	0.308661000	0.146084000
7	0.308661000	2.022699000	-0.146084000

7	2.022699000	-0.308661000	0.146084000
7	-0.308661000	-2.022699000	-0.146084000
6	4.357361000	-1.251810000	1.322278000
6	3.760508000	-1.939610000	0.306097000
1	4.149756000	-2.889338000	-0.023228000
1	5.231931000	-1.649797000	1.819056000
1	-5.231931000	1.649797000	1.819056000
46	0.000000000	0.000000000	0.000000000

TEQ²⁺

E(RB3LYP) = -1603.04066291

6	-3.286323000	2.780424000	1.594639000
6	-2.291638000	2.196148000	0.821463000
6	-0.923267000	2.590765000	1.018278000
6	-0.626457000	3.552716000	2.035511000
6	-1.653818000	4.044975000	2.848180000
6	-2.970164000	3.658550000	2.630101000
1	-4.318373000	2.507276000	1.426165000
6	0.693842000	4.054488000	2.093729000
1	-1.421481000	4.767507000	3.619078000
1	-3.757281000	4.049172000	3.259195000
6	1.601047000	3.658550000	1.152864000
6	1.225809000	2.675385000	0.205466000
1	2.608235000	4.046863000	1.152554000
6	2.196148000	2.291638000	-0.821463000
6	2.590765000	0.923267000	-1.018278000
6	2.780424000	3.286323000	-1.594639000
6	3.552716000	0.626457000	-2.035511000
6	3.658550000	2.970164000	-2.630101000
1	2.507276000	4.318373000	-1.426165000
6	2.675385000	-1.225809000	-0.205466000
6	4.054488000	-0.693842000	-2.093729000
6	4.044975000	1.653818000	-2.848180000
1	4.049172000	3.757281000	-3.259195000
6	3.658550000	-1.601047000	-1.152864000
1	4.766943000	-0.963344000	-2.861927000
1	4.767507000	1.421481000	-3.619078000
1	4.046863000	-2.608235000	-1.152554000
6	2.291638000	-2.196148000	0.821463000
6	0.923267000	-2.590765000	1.018278000
6	3.286323000	-2.780424000	1.594639000
6	0.626457000	-3.552716000	2.035511000

6	2.970164000	-3.658550000	2.630101000
1	4.318373000	-2.507276000	1.426165000
6	-1.225809000	-2.675385000	0.205466000
6	1.653818000	-4.044975000	2.848180000
1	3.757281000	-4.049172000	3.259195000
1	1.421481000	-4.767507000	3.619078000
6	-2.196148000	-2.291638000	-0.821463000
6	-2.590765000	-0.923267000	-1.018278000
6	-2.780424000	-3.286323000	-1.594639000
6	-3.552716000	-0.626457000	-2.035511000
6	-3.658550000	-2.970164000	-2.630101000
1	-2.507276000	-4.318373000	-1.426165000
6	-2.675385000	1.225809000	-0.205466000
6	-4.054488000	0.693842000	-2.093729000
6	-4.044975000	-1.653818000	-2.848180000
1	-4.049172000	-3.757281000	-3.259195000
6	-3.658550000	1.601047000	-1.152864000
1	-4.766943000	0.963344000	-2.861927000
1	-4.767507000	-1.421481000	-3.619078000
1	-4.046863000	2.608235000	-1.152554000
7	-0.002171000	2.147268000	0.155539000
7	2.147268000	0.002171000	-0.155539000
7	0.002171000	-2.147268000	0.155539000
7	-2.147268000	-0.002171000	-0.155539000
6	-0.693842000	-4.054488000	2.093729000
6	-1.601047000	-3.658550000	1.152864000
1	-2.608235000	-4.046863000	1.152554000
1	-0.963344000	-4.766943000	2.861927000
1	0.963344000	4.766943000	2.861927000

TEQZ

E(RB3LYP) = -1667.83900688

6	-3.159315000	2.732395000	1.784142000
6	-2.248902000	2.209299000	0.896862000
6	-0.898080000	2.642552000	0.961596000
6	-0.525261000	3.582263000	1.959741000
6	-1.477871000	4.065846000	2.880416000
6	-2.778681000	3.648045000	2.786488000
1	-4.193819000	2.425464000	1.712290000
6	0.818012000	4.012961000	1.926191000
1	-1.170619000	4.774001000	3.639383000
1	-3.524235000	4.019075000	3.476039000

6	1.222823000	2.686383000	0.125597000
6	2.209299000	2.248902000	-0.896862000
6	2.642552000	0.898080000	-0.961596000
6	2.732395000	3.159315000	-1.784142000
6	3.582263000	0.525261000	-1.959741000
6	3.648045000	2.778681000	-2.786488000
1	2.425464000	4.193819000	-1.712290000
6	2.686383000	-1.222823000	-0.125597000
6	4.012961000	-0.818012000	-1.926191000
6	4.065846000	1.477871000	-2.880416000
1	4.019075000	3.524235000	-3.476039000
1	4.736982000	-1.169048000	-2.656672000
1	4.774001000	1.170619000	-3.639383000
6	2.248902000	-2.209299000	0.896862000
6	0.898080000	-2.642552000	0.961596000
6	3.159315000	-2.732395000	1.784142000
6	0.525261000	-3.582263000	1.959741000
6	2.778681000	-3.648045000	2.786488000
1	4.193819000	-2.425464000	1.712290000
6	-1.222823000	-2.686383000	0.125597000
6	1.477871000	-4.065846000	2.880416000
1	3.524235000	-4.019075000	3.476039000
1	1.170619000	-4.774001000	3.639383000
6	-2.209299000	-2.248902000	-0.896862000
6	-2.642552000	-0.898080000	-0.961596000
6	-2.732395000	-3.159315000	-1.784142000
6	-3.582263000	-0.525261000	-1.959741000
6	-3.648045000	-2.778681000	-2.786488000
1	-2.425464000	-4.193819000	-1.712290000
6	-2.686383000	1.222823000	-0.125597000
6	-4.012961000	0.818012000	-1.926191000
6	-4.065846000	-1.477871000	-2.880416000
1	-4.019075000	-3.524235000	-3.476039000
1	-4.736982000	1.169048000	-2.656672000
1	-4.774001000	-1.170619000	-3.639383000
7	0.005983000	2.209299000	0.049258000
7	2.209299000	-0.005983000	-0.049258000
7	-0.005983000	-2.209299000	0.049258000
7	-2.209299000	0.005983000	-0.049258000
6	-0.818012000	-4.012961000	1.926191000
1	-1.169048000	-4.736982000	2.656672000
1	1.169048000	4.736982000	2.656672000
7	1.680149000	3.593363000	1.035006000

7	3.593363000	-1.680149000	-1.035006000
7	-1.680149000	-3.593363000	1.035006000
7	-3.593363000	1.680149000	-1.035006000

Pd[TEQZ]

E(RB3LYP) = -1795.40862433

6	2.734363000	3.049508000	2.064342000
6	2.097096000	2.204897000	1.164968000
6	2.657747000	0.934959000	0.915971000
6	3.941891000	0.651290000	1.448419000
6	4.541614000	1.515563000	2.384244000
6	3.912067000	2.685290000	2.727431000
1	2.320518000	4.034017000	2.221964000
6	4.609319000	-0.462985000	0.903132000
1	5.507629000	1.256835000	2.796061000
1	4.352930000	3.360739000	3.445590000
6	2.772694000	-1.028952000	-0.327976000
6	2.204897000	-2.097096000	-1.164968000
6	0.934959000	-2.657747000	-0.915971000
6	3.049508000	-2.734363000	-2.064342000
6	0.651290000	-3.941891000	-1.448419000
6	2.685290000	-3.912067000	-2.727431000
1	4.034017000	-2.320518000	-2.221964000
6	-1.028952000	-2.772694000	0.327976000
6	-0.462985000	-4.609319000	-0.903132000
6	1.515563000	-4.541614000	-2.384244000
1	3.360739000	-4.352930000	-3.445590000
1	-0.692291000	-5.625593000	-1.206004000
1	1.256835000	-5.507629000	-2.796061000
6	-2.097096000	-2.204897000	1.164968000
6	-2.657747000	-0.934959000	0.915971000
6	-2.734363000	-3.049508000	2.064342000
6	-3.941891000	-0.651290000	1.448419000
6	-3.912067000	-2.685290000	2.727431000
1	-2.320518000	-4.034017000	2.221964000
6	-2.772694000	1.028952000	-0.327976000
6	-4.541614000	-1.515563000	2.384244000
1	-4.352930000	-3.360739000	3.445590000
1	-5.507629000	-1.256835000	2.796061000
6	-2.204897000	2.097096000	-1.164968000
6	-0.934959000	2.657747000	-0.915971000
6	-3.049508000	2.734363000	-2.064342000
6	-0.651290000	3.941891000	-1.448419000

6	-2.685290000	3.912067000	-2.727431000
1	-4.034017000	2.320518000	-2.221964000
6	1.028952000	2.772694000	0.327976000
6	0.462985000	4.609319000	-0.903132000
6	-1.515563000	4.541614000	-2.384244000
1	-3.360739000	4.352930000	-3.445590000
1	0.692291000	5.625593000	-1.206004000
1	-1.256835000	5.507629000	-2.796061000
7	2.049802000	0.000000000	0.107632000
7	0.000000000	-2.049802000	-0.107632000
7	-2.049802000	0.000000000	0.107632000
7	0.000000000	2.049802000	-0.107632000
6	-4.609319000	0.462985000	0.903132000
1	-5.625593000	0.692291000	1.206004000
1	5.625593000	-0.692291000	1.206004000
7	4.066616000	-1.233773000	-0.002453000
7	-1.233773000	-4.066616000	0.002453000
7	-4.066616000	1.233773000	-0.002453000
7	1.233773000	4.066616000	0.002453000
46	0.000000000	0.000000000	0.000000000

TEQZ²⁺

E(RB3LYP) = -1667.19141101

6	-3.468918000	3.002231000	1.023605000
6	-2.403539000	2.272328000	0.498595000
6	-1.060666000	2.657084000	0.852514000
6	-0.888295000	3.708636000	1.805783000
6	-1.990185000	4.329978000	2.393619000
6	-3.276159000	3.983933000	1.989822000
1	-4.469162000	2.760976000	0.696472000
6	0.439386000	4.153692000	2.014472000
1	-1.837817000	5.109270000	3.128822000
1	-4.131256000	4.481544000	2.424548000
6	1.169918000	2.729113000	0.401885000
6	2.272328000	2.403539000	-0.498595000
6	2.657084000	1.060666000	-0.852514000
6	3.002231000	3.468918000	-1.023605000
6	3.708636000	0.888295000	-1.805783000
6	3.983933000	3.276159000	-1.989822000
1	2.760976000	4.469162000	-0.696472000
6	2.729113000	-1.169918000	-0.401885000
6	4.153692000	-0.439386000	-2.014472000
6	4.329978000	1.990185000	-2.393619000

1	4.481544000	4.131256000	-2.424548000
1	4.921413000	-0.649649000	-2.752151000
1	5.109270000	1.837817000	-3.128822000
6	2.403539000	-2.272328000	0.498595000
6	1.060666000	-2.657084000	0.852514000
6	3.468918000	-3.002231000	1.023605000
6	0.888295000	-3.708636000	1.805783000
6	3.276159000	-3.983933000	1.989822000
1	4.469162000	-2.760976000	0.696472000
6	-1.169918000	-2.729113000	0.401885000
6	1.990185000	-4.329978000	2.393619000
1	4.131256000	-4.481544000	2.424548000
1	1.837817000	-5.109270000	3.128822000
6	-2.272328000	-2.403539000	-0.498595000
6	-2.657084000	-1.060666000	-0.852514000
6	-3.002231000	-3.468918000	-1.023605000
6	-3.708636000	-0.888295000	-1.805783000
6	-3.983933000	-3.276159000	-1.989822000
1	-2.760976000	-4.469162000	-0.696472000
6	-2.729113000	1.169918000	-0.401885000
6	-4.153692000	0.439386000	-2.014472000
6	-4.329978000	-1.990185000	-2.393619000
1	-4.481544000	-4.131256000	-2.424548000
1	-4.921413000	0.649649000	-2.752151000
1	-5.109270000	-1.837817000	-3.128822000
7	-0.015857000	2.149492000	0.190081000
7	2.149492000	0.015857000	-0.190081000
7	0.015857000	-2.149492000	0.190081000
7	-2.149492000	-0.015857000	-0.190081000
6	-0.439386000	-4.153692000	2.014472000
1	-0.649649000	-4.921413000	2.752151000
1	0.649649000	4.921413000	2.752151000
7	1.438603000	3.708636000	1.300315000
7	3.708636000	-1.438603000	-1.300315000
7	-1.438603000	-3.708636000	1.300315000
7	-3.708636000	1.438603000	-1.300315000

TEN

$E(\text{RB3LYP}) = -1667.82422559$

6	-2.265709000	2.198644000	0.883021000
6	-0.912046000	2.633159000	0.988100000
6	-0.598103000	3.553774000	2.022008000
6	-1.636236000	3.975637000	2.878149000

6	-2.905769000	3.516814000	2.654326000
6	0.734151000	4.020122000	2.095822000
1	-1.431505000	4.670430000	3.682150000
1	-3.732097000	3.840251000	3.274718000
6	1.636236000	3.594388000	1.165484000
6	1.220121000	2.678823000	0.164112000
1	2.657809000	3.945042000	1.166496000
6	2.198644000	2.265709000	-0.883021000
6	2.633159000	0.912046000	-0.988100000
6	3.553774000	0.598103000	-2.022008000
6	3.516814000	2.905769000	-2.654326000
6	2.678823000	-1.220121000	-0.164112000
6	4.020122000	-0.734151000	-2.095822000
6	3.975637000	1.636236000	-2.878149000
1	3.840251000	3.732097000	-3.274718000
6	3.594388000	-1.636236000	-1.165484000
1	4.719557000	-1.015373000	-2.872472000
1	4.670430000	1.431505000	-3.682150000
1	3.945042000	-2.657809000	-1.166496000
6	2.265709000	-2.198644000	0.883021000
6	0.912046000	-2.633159000	0.988100000
6	0.598103000	-3.553774000	2.022008000
6	2.905769000	-3.516814000	2.654326000
6	-1.220121000	-2.678823000	0.164112000
6	1.636236000	-3.975637000	2.878149000
1	3.732097000	-3.840251000	3.274718000
1	1.431505000	-4.670430000	3.682150000
6	-2.198644000	-2.265709000	-0.883021000
6	-2.633159000	-0.912046000	-0.988100000
6	-3.553774000	-0.598103000	-2.022008000
6	-3.516814000	-2.905769000	-2.654326000
6	-2.678823000	1.220121000	-0.164112000
6	-4.020122000	0.734151000	-2.095822000
6	-3.975637000	-1.636236000	-2.878149000
1	-3.840251000	-3.732097000	-3.274718000
6	-3.594388000	1.636236000	-1.165484000
1	-4.719557000	1.015373000	-2.872472000
1	-4.670430000	-1.431505000	-3.682150000
1	-3.945042000	2.657809000	-1.166496000
7	-0.000670000	2.210026000	0.079865000
7	2.210026000	0.000670000	-0.079865000
7	0.000670000	-2.210026000	0.079865000
7	-2.210026000	-0.000670000	-0.079865000

6	-0.734151000	-4.020122000	2.095822000
6	-1.636236000	-3.594388000	1.165484000
1	-2.657809000	-3.945042000	1.166496000
1	-1.015373000	-4.719557000	2.872472000
1	1.015373000	4.719557000	2.872472000
7	-3.222072000	2.649813000	1.663312000
7	-2.649813000	-3.222072000	-1.663312000
7	3.222072000	-2.649813000	1.663312000
7	2.649813000	3.222072000	-1.663312000

Pd[TEN]

E(RB3LYP) = -1795.39237637

6	-2.690522000	1.345832000	1.202564000
6	-1.635630000	2.261181000	0.958752000
6	-1.763362000	3.549119000	1.538314000
6	-2.766946000	3.759155000	2.500186000
6	-3.641606000	2.737054000	2.779989000
6	-0.907297000	4.572874000	1.069414000
1	-2.863331000	4.722180000	2.981523000
1	-4.413439000	2.839793000	3.530239000
6	0.000000000	4.287102000	0.096750000
6	0.185430000	2.945833000	-0.320660000
1	0.636988000	5.043113000	-0.332183000
6	1.345832000	2.690522000	-1.202564000
6	2.261181000	1.635630000	-0.958752000
6	3.549119000	1.763362000	-1.538314000
6	2.737054000	3.641606000	-2.779989000
6	2.945833000	-0.185430000	0.320660000
6	4.572874000	0.907297000	-1.069414000
6	3.759155000	2.766946000	-2.500186000
1	2.839793000	4.413439000	-3.530239000
6	4.287102000	0.000000000	-0.096750000
1	5.573226000	0.998332000	-1.470201000
1	4.722180000	2.863331000	-2.981523000
1	5.043113000	-0.636988000	0.332183000
6	2.690522000	-1.345832000	1.202564000
6	1.635630000	-2.261181000	0.958752000
6	1.763362000	-3.549119000	1.538314000
6	3.641606000	-2.737054000	2.779989000
6	-0.185430000	-2.945833000	-0.320660000
6	2.766946000	-3.759155000	2.500186000
1	4.413439000	-2.839793000	3.530239000
1	2.863331000	-4.722180000	2.981523000

6	-1.345832000	-2.690522000	-1.202564000
6	-2.261181000	-1.635630000	-0.958752000
6	-3.549119000	-1.763362000	-1.538314000
6	-2.737054000	-3.641606000	-2.779989000
6	-2.945833000	0.185430000	0.320660000
6	-4.572874000	-0.907297000	-1.069414000
6	-3.759155000	-2.766946000	-2.500186000
1	-2.839793000	-4.413439000	-3.530239000
6	-4.287102000	0.000000000	-0.096750000
1	-5.573226000	-0.998332000	-1.470201000
1	-4.722180000	-2.863331000	-2.981523000
1	-5.043113000	0.636988000	0.332183000
7	-0.586038000	1.963638000	0.124698000
7	1.963638000	0.586038000	-0.124698000
7	0.586038000	-1.963638000	0.124698000
7	-1.963638000	-0.586038000	-0.124698000
6	0.907297000	-4.572874000	1.069414000
6	0.000000000	-4.287102000	0.096750000
1	-0.636988000	-5.043113000	-0.332183000
1	0.998332000	-5.573226000	1.470201000
1	-0.998332000	5.573226000	1.470201000
7	-3.643572000	1.592806000	2.076881000
7	-1.592806000	-3.643572000	-2.076881000
7	3.643572000	-1.592806000	2.076881000
7	1.592806000	3.643572000	-2.076881000
46	0.000000000	0.000000000	0.000000000

TEN²⁺

E(RB3LYP) = -1667.17128608

6	-2.345983000	2.264006000	0.664678000
6	-0.984674000	2.652553000	0.927094000
6	-0.778948000	3.669222000	1.913867000
6	-1.889631000	4.182751000	2.581011000
6	-3.162827000	3.772057000	2.192304000
6	0.530668000	4.193669000	2.053810000
1	-1.774833000	4.958636000	3.325765000
1	-4.044339000	4.209808000	2.642411000
6	1.498606000	3.772057000	1.195216000
6	1.205341000	2.726189000	0.278370000
1	2.491758000	4.192182000	1.210947000
6	2.264006000	2.345983000	-0.664678000
6	2.652553000	0.984674000	-0.927094000
6	3.669222000	0.778948000	-1.913867000

6	3.772057000	3.162827000	-2.192304000
6	2.726189000	-1.205341000	-0.278370000
6	4.193669000	-0.530668000	-2.053810000
6	4.182751000	1.889631000	-2.581011000
1	4.209808000	4.044339000	-2.642411000
6	3.772057000	-1.498606000	-1.195216000
1	4.949282000	-0.732208000	-2.800896000
1	4.958636000	1.774833000	-3.325765000
1	4.192182000	-2.491758000	-1.210947000
6	2.345983000	-2.264006000	0.664678000
6	0.984674000	-2.652553000	0.927094000
6	0.778948000	-3.669222000	1.913867000
6	3.162827000	-3.772057000	2.192304000
6	-1.205341000	-2.726189000	0.278370000
6	1.889631000	-4.182751000	2.581011000
1	4.044339000	-4.209808000	2.642411000
1	1.774833000	-4.958636000	3.325765000
6	-2.264006000	-2.345983000	-0.664678000
6	-2.652553000	-0.984674000	-0.927094000
6	-3.669222000	-0.778948000	-1.913867000
6	-3.772057000	-3.162827000	-2.192304000
6	-2.726189000	1.205341000	-0.278370000
6	-4.193669000	0.530668000	-2.053810000
6	-4.182751000	-1.889631000	-2.581011000
1	-4.209808000	-4.044339000	-2.642411000
6	-3.772057000	1.498606000	-1.195216000
1	-4.949282000	0.732208000	-2.800896000
1	-4.958636000	-1.774833000	-3.325765000
1	-4.192182000	2.491758000	-1.210947000
7	-0.002290000	2.168516000	0.163947000
7	2.168516000	0.002290000	-0.163947000
7	0.002290000	-2.168516000	0.163947000
7	-2.168516000	-0.002290000	-0.163947000
6	-0.530668000	-4.193669000	2.053810000
6	-1.498606000	-3.772057000	1.195216000
1	-2.491758000	-4.192182000	1.210947000
1	-0.732208000	-4.949282000	2.800896000
1	0.732208000	4.949282000	2.800896000
7	-3.376013000	2.869606000	1.230205000
7	-2.869606000	-3.376013000	-1.230205000
7	3.376013000	-2.869606000	1.230205000
7	2.869606000	3.376013000	-1.230205000

TEPP

E(RB3LYP) = -1731.97752009

6	-2.254293000	2.208283000	0.899139000
6	-0.898715000	2.644055000	0.945763000
6	-0.537858000	3.554928000	1.963188000
6	-1.524950000	3.988110000	2.868854000
6	-2.801217000	3.516905000	2.710363000
6	0.816075000	3.968728000	1.965898000
1	-1.279795000	4.683269000	3.660909000
1	-3.597059000	3.830144000	3.373781000
6	1.217695000	2.689566000	0.130541000
6	2.208283000	2.254293000	-0.899139000
6	2.644055000	0.898715000	-0.945763000
6	3.554928000	0.537858000	-1.963188000
6	3.516905000	2.801217000	-2.710363000
6	2.689566000	-1.217695000	-0.130541000
6	3.968728000	-0.816075000	-1.965898000
6	3.988110000	1.524950000	-2.868854000
1	3.830144000	3.597059000	-3.373781000
1	4.659406000	-1.171656000	-2.725088000
1	4.683269000	1.279795000	-3.660909000
6	2.254293000	-2.208283000	0.899139000
6	0.898715000	-2.644055000	0.945763000
6	0.537858000	-3.554928000	1.963188000
6	2.801217000	-3.516905000	2.710363000
6	-1.217695000	-2.689566000	0.130541000
6	1.524950000	-3.988110000	2.868854000
1	3.597059000	-3.830144000	3.373781000
1	1.279795000	-4.683269000	3.660909000
6	-2.208283000	-2.254293000	-0.899139000
6	-2.644055000	-0.898715000	-0.945763000
6	-3.554928000	-0.537858000	-1.963188000
6	-3.516905000	-2.801217000	-2.710363000
6	-2.689566000	1.217695000	-0.130541000
6	-3.968728000	0.816075000	-1.965898000
6	-3.988110000	-1.524950000	-2.868854000
1	-3.830144000	-3.597059000	-3.373781000
1	-4.659406000	1.171656000	-2.725088000
1	-4.683269000	-1.279795000	-3.660909000
7	0.000532000	2.221789000	0.026507000
7	2.221789000	-0.000532000	-0.026507000
7	-0.000532000	-2.221789000	0.026507000
7	-2.221789000	0.000532000	-0.026507000

6	-0.816075000	-3.968728000	1.965898000
1	-1.171656000	-4.659406000	2.725088000
1	1.171656000	4.659406000	2.725088000
7	1.678326000	3.553770000	1.075905000
7	3.553770000	-1.678326000	-1.075905000
7	-1.678326000	-3.553770000	1.075905000
7	-3.553770000	1.678326000	-1.075905000
7	-3.161546000	2.644055000	1.738549000
7	-2.644055000	-3.161546000	-1.738549000
7	3.161546000	-2.644055000	1.738549000
7	2.644055000	3.161546000	-1.738549000

Pd[TEPP]

E(RB3LYP) = -1859.50490340

6	-2.243535000	2.102835000	1.117778000
6	-0.959279000	2.654404000	0.911822000
6	-0.714823000	3.926645000	1.478608000
6	-1.645181000	4.469323000	2.376435000
6	-2.793525000	3.752539000	2.635917000
6	0.463280000	4.585649000	1.045788000
1	-1.468786000	5.433027000	2.833663000
1	-3.525803000	4.094291000	3.354491000
6	1.040309000	2.790773000	-0.241058000
6	2.102835000	2.243535000	-1.117778000
6	2.654404000	0.959279000	-0.911822000
6	3.926645000	0.714823000	-1.478608000
6	3.752539000	2.793525000	-2.635917000
6	2.790773000	-1.040309000	0.241058000
6	4.585649000	-0.463280000	-1.045788000
6	4.469323000	1.645181000	-2.376435000
1	4.094291000	3.525803000	-3.354491000
1	5.570689000	-0.714212000	-1.425441000
1	5.433027000	1.468786000	-2.833663000
6	2.243535000	-2.102835000	1.117778000
6	0.959279000	-2.654404000	0.911822000
6	0.714823000	-3.926645000	1.478608000
6	2.793525000	-3.752539000	2.635917000
6	-1.040309000	-2.790773000	-0.241058000
6	1.645181000	-4.469323000	2.376435000
1	3.525803000	-4.094291000	3.354491000
1	1.468786000	-5.433027000	2.833663000
6	-2.102835000	-2.243535000	-1.117778000
6	-2.654404000	-0.959279000	-0.911822000

6	-3.926645000	-0.714823000	-1.478608000
6	-3.752539000	-2.793525000	-2.635917000
6	-2.790773000	1.040309000	0.241058000
6	-4.585649000	0.463280000	-1.045788000
6	-4.469323000	-1.645181000	-2.376435000
1	-4.094291000	-3.525803000	-3.354491000
1	-5.570689000	0.714212000	-1.425441000
1	-5.433027000	-1.468786000	-2.833663000
7	0.000000000	2.056399000	0.130710000
7	2.056399000	0.000000000	-0.130710000
7	0.000000000	-2.056399000	0.130710000
7	-2.056399000	0.000000000	-0.130710000
6	-0.463280000	-4.585649000	1.045788000
1	-0.714212000	-5.570689000	1.425441000
1	0.714212000	5.570689000	1.425441000
7	1.272030000	4.054415000	0.171948000
7	4.054415000	-1.272030000	-0.171948000
7	-1.272030000	-4.054415000	0.171948000
7	-4.054415000	1.272030000	-0.171948000
7	-3.103873000	2.639454000	1.955429000
7	-2.639454000	-3.103873000	-1.955429000
7	3.103873000	-2.639454000	1.955429000
7	2.639454000	3.103873000	-1.955429000
46	0.000000000	0.000000000	0.000000000

TEPP²⁺

E(RB3LYP) = -1731.29011309

6	-2.367268000	2.349848000	0.414597000
6	-1.022640000	2.703219000	0.792285000
6	-0.875597000	3.747223000	1.752695000
6	-2.008588000	4.367818000	2.263175000
6	-3.257606000	3.991295000	1.756983000
6	0.461874000	4.126536000	2.063350000
1	-1.929425000	5.166644000	2.988583000
1	-4.158575000	4.495042000	2.083145000
6	1.219134000	2.703219000	0.461750000
6	2.349848000	2.367268000	-0.414597000
6	2.703219000	1.022640000	-0.792285000
6	3.747223000	0.875597000	-1.752695000
6	3.991295000	3.257606000	-1.756983000
6	2.703219000	-1.219134000	-0.461750000
6	4.126536000	-0.461874000	-2.063350000
6	4.367818000	2.008588000	-2.263175000

1	4.495042000	4.158575000	-2.083145000
1	4.847980000	-0.662508000	-2.848899000
1	5.166644000	1.929425000	-2.988583000
6	2.367268000	-2.349848000	0.414597000
6	1.022640000	-2.703219000	0.792285000
6	0.875597000	-3.747223000	1.752695000
6	3.257606000	-3.991295000	1.756983000
6	-1.219134000	-2.703219000	0.461750000
6	2.008588000	-4.367818000	2.263175000
1	4.158575000	-4.495042000	2.083145000
1	1.929425000	-5.166644000	2.988583000
6	-2.349848000	-2.367268000	-0.414597000
6	-2.703219000	-1.022640000	-0.792285000
6	-3.747223000	-0.875597000	-1.752695000
6	-3.991295000	-3.257606000	-1.756983000
6	-2.703219000	1.219134000	-0.461750000
6	-4.126536000	0.461874000	-2.063350000
6	-4.367818000	-2.008588000	-2.263175000
1	-4.495042000	-4.158575000	-2.083145000
1	-4.847980000	0.662508000	-2.848899000
1	-5.166644000	-1.929425000	-2.988583000
7	0.032874000	2.160946000	0.177352000
7	2.160946000	-0.032874000	-0.177352000
7	-0.032874000	-2.160946000	0.177352000
7	-2.160946000	0.032874000	-0.177352000
6	-0.461874000	-4.126536000	2.063350000
1	-0.662508000	-4.847980000	2.848899000
1	0.662508000	4.847980000	2.848899000
7	1.475991000	3.645215000	1.403727000
7	3.645215000	-1.475991000	-1.403727000
7	-1.475991000	-3.645215000	1.403727000
7	-3.645215000	1.475991000	-1.403727000
7	-3.415511000	3.029989000	0.846903000
7	-3.029989000	-3.415511000	-0.846903000
7	3.415511000	-3.029989000	0.846903000
7	3.029989000	3.415511000	-0.846903000