

## Supramolecular D $\cdots$ A - layered structures based on germanium complexes with 2,3-dihydroxynaphthalene and N,N'-bidentate ligands

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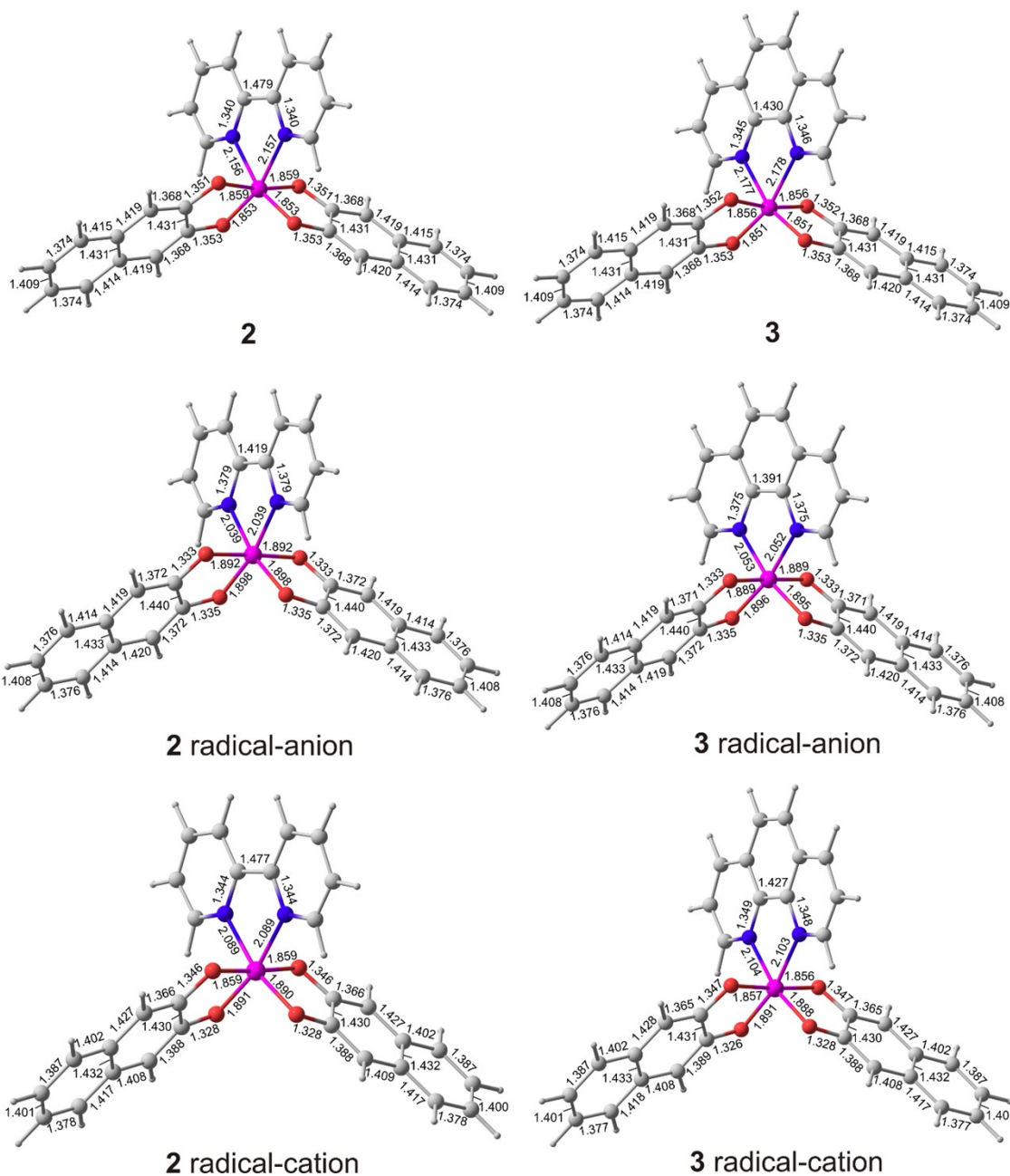
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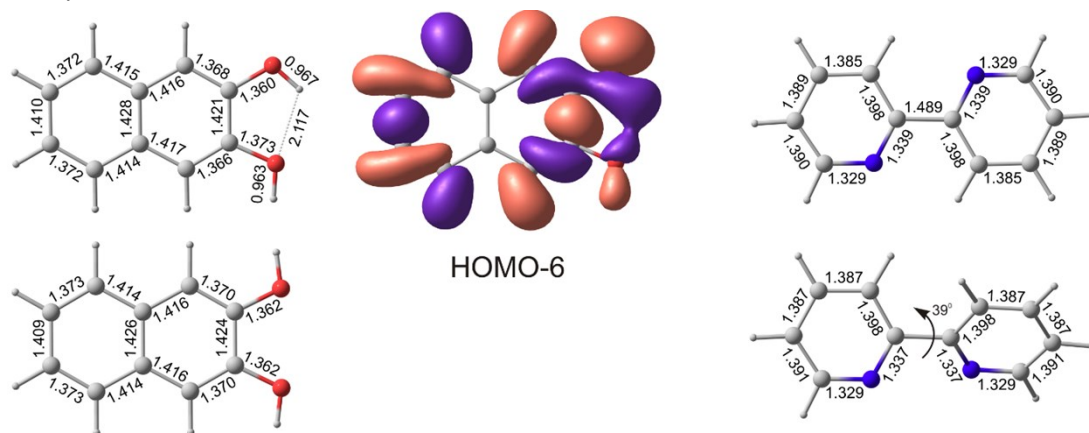
### Supporting Information

**Table S1.** Total energies without ( $E_{\text{total}}$ , a.u.) and with taking into account for the energies of zero-point harmonic vibrations ( $E_{\text{total}}^{\text{ZPE}}$ , a.u.), relative energies without ( $E$ , kcal mol<sup>-1</sup>) and with taking into account for the energies of zero-point harmonic vibrations ( $E^{\text{ZPE}}$ , kcal mol<sup>-1</sup>) calculated by DFT B3LYP/Def2TZVP method.

Structure	$E_{\text{total}}$	$E$	$E_{\text{total}}^{\text{ZPE}}$	$E^{\text{ZPE}}$
<b>1</b>	-3147.806967		-3147.537973	
<b>2</b>	-3643.407174	0.0	-3642.977600	0.0
<b>2</b> radical-anion	-3643.490719	-219.5	-3643.065475	-230.9
<b>2</b> radical-cation	-3643.178121	601.8	-3642.749546	599.2
<b>3</b>	-3719.662628	0.0	-3719.220326	0.0
<b>3</b> radical-anion	-3719.743689	-213.0	-3719.306163	-225.5
<b>3</b> radical-cation	-3719.434095	600.4	-3718.992614	598.3
2,3-dihydroxynaphthalene <i>H-bond</i>	-536.545378	0.0	-536.390113	0.0
2,3-dihydroxynaphthalene	-536.539653	3.6	-536.384476	3.5
2,2'-bipyridine <i>flat</i>	-495.567323	0.0	-495.409680	0.0
2,2'-bipyridine <i>twisted</i>	-495.557411	6.2	-495.400135	6.0
1,10-phenanthroline	-571.813563		-571.643488	



**Figure S1.** Bond lengths in **2**, **3** and their radical-anion and radical-cation forms calculated by DFT B3LYP/Def2TZVP method.



**Figure S2.** Geometry characteristics of 2,3-dihydroxynaphthalene and 2,2'-bipyridine molecules calculated by DFT B3LYP/Def2TZVP method.

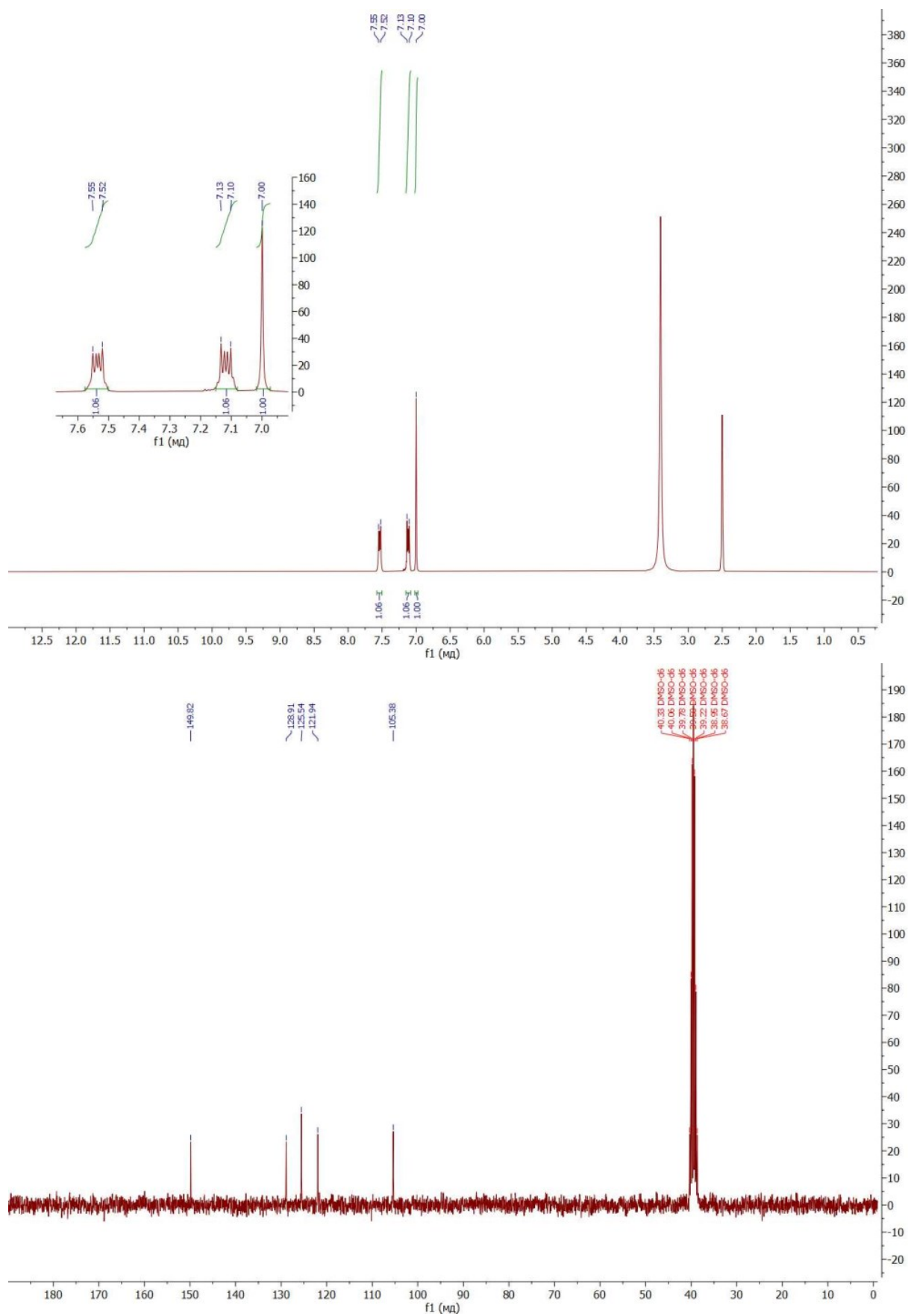
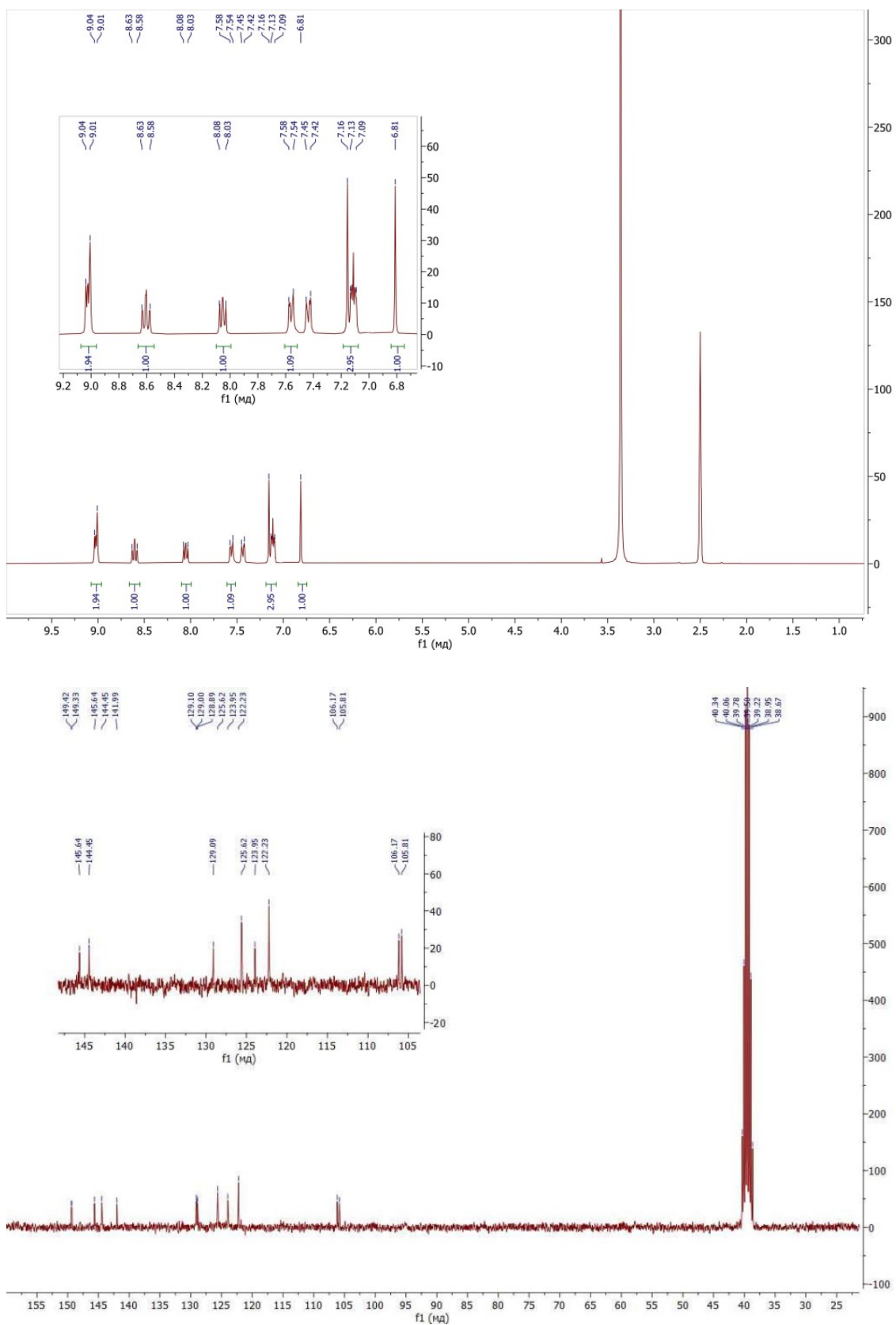
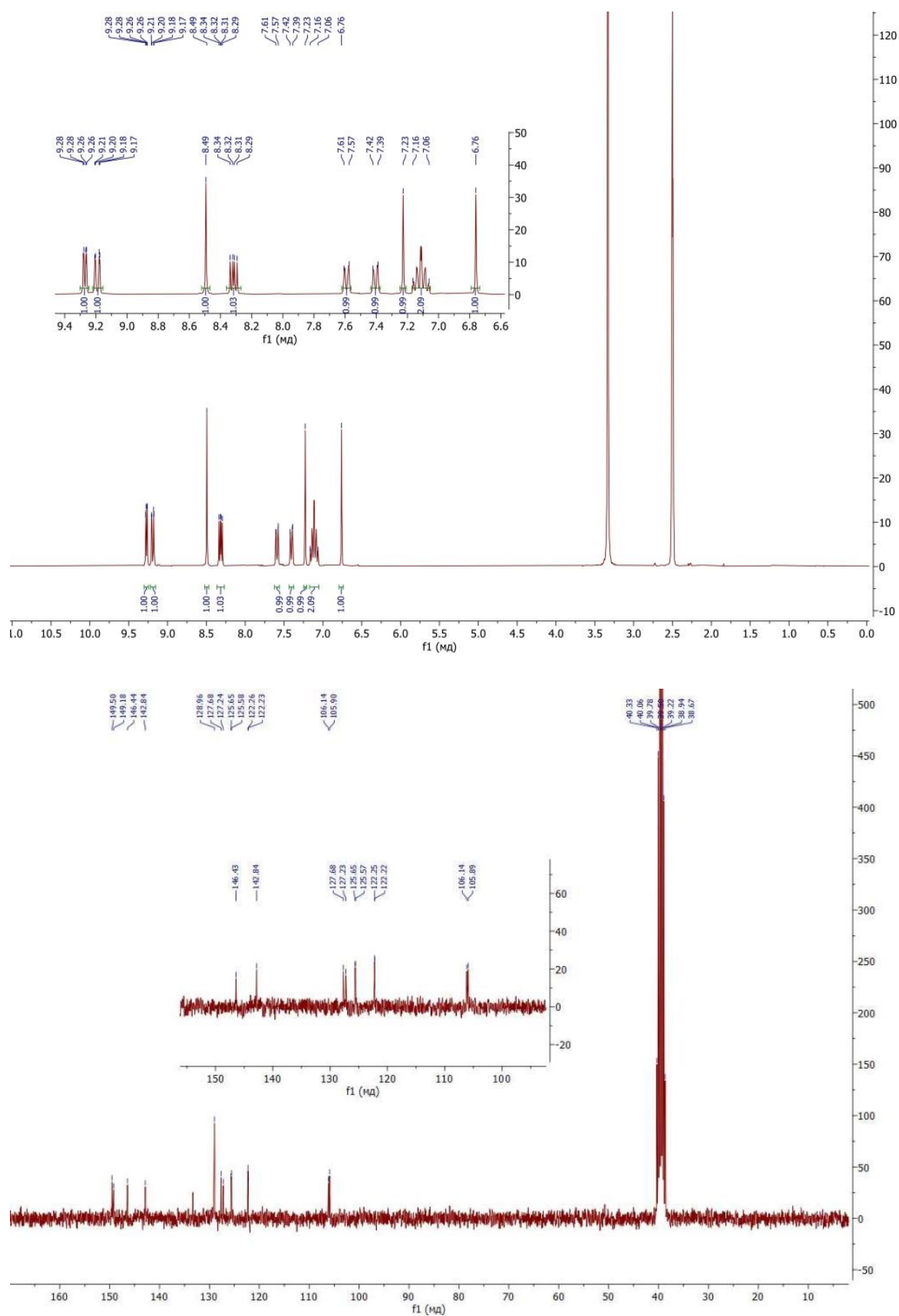


Figure S3. <sup>1</sup>H (top) and <sup>13</sup>C (bottom) NMR spectra of 1 in DMSO-d<sub>6</sub>.



**Figure S4.** <sup>1</sup>H (top) and <sup>13</sup>C (bottom) NMR spectra of **2** in DMSO-d<sub>6</sub>. DEPT135 is shown in the inset.



**Figure S5.** <sup>1</sup>H (*top*) and <sup>13</sup>C (*bottom*) NMR spectra of **3** in DMSO-d<sub>6</sub>. DEPT135 is shown in the inset (CH only).

Cartesian coordinates of the structures calculated by the DFT B3LYP/Def2TZVP

1  
32 0.000528000 0.002333000 0.004735000  
8 -1.114965000 -0.793301000 1.143851000  
8 -1.299808000 0.820786000 -0.897936000  
8 1.118764000 -1.034508000 -0.917494000  
8 1.297483000 1.016298000 0.686036000  
6 2.498057000 0.537801000 0.197477000  
6 3.707082000 1.080170000 0.514768000  
1 3.762390000 1.930601000 1.181773000  
6 4.887727000 0.518824000 -0.037507000  
6 6.168939000 1.042141000 0.257891000  
1 6.242599000 1.893673000 0.923954000  
6 7.300558000 0.487959000 -0.284226000  
1 8.272918000 0.900956000 -0.047504000  
6 7.203824000 -0.619915000 -1.150625000  
1 8.102527000 -1.050537000 -1.573696000  
6 5.977408000 -1.151887000 -1.457951000  
1 5.902425000 -2.003389000 -2.123900000  
6 4.789523000 -0.605342000 -0.916688000  
6 3.513088000 -1.143772000 -1.224380000  
1 3.420554000 -1.994020000 -1.887515000  
6 2.400058000 -0.579832000 -0.676424000  
6 -2.398461000 -0.416499000 0.799139000  
6 -3.509836000 -0.843135000 1.462191000  
1 -3.414518000 -1.512664000 2.307081000  
6 -4.788338000 -0.401131000 1.033194000  
6 -5.975057000 -0.812951000 1.684958000  
1 -5.897619000 -1.483208000 2.532853000  
6 -7.203399000 -0.376555000 1.258014000  
1 -8.101202000 -0.701462000 1.768380000  
6 -7.303268000 0.495462000 0.154834000  
1 -8.277121000 0.834613000 -0.174832000  
6 -6.172859000 0.913934000 -0.499843000  
1 -6.248981000 1.584276000 -1.347790000  
6 -4.889677000 0.483654000 -0.086310000  
6 -3.710337000 0.907288000 -0.752369000  
1 -3.768373000 1.576463000 -1.600922000  
6 -2.499081000 0.463092000 -0.313653000

2

32	-0.000265000	0.169409000	-0.001244000
8	-1.021513000	-0.961416000	-1.055550000
8	-1.447880000	0.307048000	1.156875000
8	1.447821000	0.306709000	-1.158987000
8	1.018915000	-0.964998000	1.051153000
7	0.705938000	1.882445000	1.101858000
7	-0.704134000	1.885529000	-1.101894000
6	1.401558000	1.749601000	2.230024000
1	1.593895000	0.732856000	2.543587000
6	1.840861000	2.853584000	2.945912000
1	2.406848000	2.713914000	3.855880000
6	1.537796000	4.119052000	2.466518000
1	1.865503000	5.002558000	2.998624000
6	0.804922000	4.245748000	1.294913000
6	-0.802225000	4.249409000	-1.288710000
6	-1.536229000	4.125994000	-2.460026000
1	-1.863800000	5.011036000	-2.989632000
6	-1.840319000	2.861993000	-2.942346000
1	-2.407198000	2.724839000	-3.852135000
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6	-0.393903000	3.098664000	-0.623402000
6	0.396465000	3.096806000	0.626431000
6	2.229955000	-1.177776000	0.486704000
6	3.190884000	-1.994301000	1.016853000
1	2.990116000	-2.535635000	1.933354000
6	4.440061000	-2.143590000	0.359618000
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6	6.663623000	-3.112944000	0.220549000
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1	7.851483000	-2.519886000	-1.486013000
6	5.931700000	-1.590069000	-1.499576000
1	6.113553000	-1.051541000	-2.422894000
6	4.681616000	-1.430272000	-0.857174000
6	3.666435000	-0.589661000	-1.383895000
1	3.833248000	-0.049228000	-2.307660000
6	2.469674000	-0.467892000	-0.732568000
6	-2.231773000	-1.175429000	-0.489854000
6	-3.193325000	-1.991036000	-1.020113000
1	-2.994337000	-2.530149000	-1.938295000

6	-4.441616000	-2.141760000	-0.361225000
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6	-6.664119000	-3.113086000	-0.220014000
1	-7.431488000	-3.760546000	-0.625970000
6	-6.900930000	-2.412130000	0.978913000
1	-7.849620000	-2.523527000	1.489380000
6	-5.930582000	-1.592209000	1.501256000
1	-6.111237000	-1.055203000	2.425711000
6	-4.681550000	-1.430504000	0.856963000
6	-3.665959000	-0.590269000	1.383537000
1	-3.831980000	-0.050551000	2.307816000
6	-2.470119000	-0.467314000	0.730809000
1	-0.552124000	5.227204000	-0.905389000
1	0.555885000	5.224567000	0.913526000

## 2 radical-anion

32	0.000324000	0.458020000	0.000101000
8	-0.946273000	-0.797829000	-1.061957000
8	-1.510391000	0.425659000	1.138370000
8	1.510909000	0.426120000	-1.138369000
8	0.948442000	-0.795611000	1.063362000
7	0.670443000	2.032170000	1.109337000
7	-0.671638000	2.030348000	-1.110466000
6	1.333221000	1.911137000	2.269345000
1	1.514877000	0.894603000	2.589339000
6	1.751368000	2.997443000	3.000328000
1	2.286762000	2.851767000	3.927188000
6	1.462773000	4.291114000	2.502444000
1	1.779285000	5.170667000	3.049488000
6	0.776858000	4.425562000	1.325345000
6	-0.783147000	4.423391000	-1.327418000
6	-1.469267000	4.286945000	-2.504168000
1	-1.787999000	5.165581000	-3.051381000
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1	-2.290680000	2.845363000	-3.928103000
6	-1.334658000	1.907387000	-2.270143000
1	-1.514152000	0.890318000	-2.589633000
6	-0.365907000	3.278183000	-0.609594000
6	0.362352000	3.279123000	0.607876000
6	2.114987000	-1.129324000	0.506667000
6	2.991626000	-2.045346000	1.029909000
1	2.737469000	-2.560527000	1.948962000



6	4.219278000	-2.325579000	0.374682000
6	5.148423000	-3.263354000	0.880594000
1	4.905991000	-3.785779000	1.800115000
6	6.335926000	-3.521678000	0.234518000
1	7.030748000	-4.246151000	0.643391000
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1	7.582906000	-3.047581000	-1.468576000
6	5.764475000	-1.925972000	-1.479355000
1	6.003255000	-1.404463000	-2.400401000
6	4.535935000	-1.637359000	-0.841813000
6	3.613503000	-0.695155000	-1.366085000
1	3.839206000	-0.169553000	-2.286522000
6	2.430730000	-0.442457000	-0.719137000
6	-2.112984000	-1.131459000	-0.505588000
6	-2.988923000	-2.048432000	-1.028355000
1	-2.734154000	-2.564329000	-1.946833000
6	-4.216833000	-2.328528000	-0.373523000
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1	-4.902011000	-3.790608000	-1.797756000
6	-6.333088000	-3.525308000	-0.233406000
1	-7.027324000	-4.250596000	-0.641826000
6	-6.646097000	-2.846690000	0.959604000
1	-7.581442000	-3.049740000	1.468295000
6	-5.763421000	-1.927438000	1.479047000
1	-6.003034000	-1.404871000	2.399275000
6	-4.534553000	-1.639114000	0.842000000
6	-3.612768000	-0.696063000	1.365892000
1	-3.839220000	-0.169564000	2.285620000
6	-2.429676000	-0.443627000	0.719426000
1	-0.553430000	5.406554000	-0.940881000
1	0.545259000	5.408027000	0.938163000

## 2 radical-cation

32	-0.000269000	0.455065000	-0.000083000
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8	1.519298000	0.501948000	-1.070259000
8	0.929825000	-0.789217000	1.077570000
7	0.618170000	2.085178000	1.151056000
7	-0.618351000	2.085082000	-1.150625000
6	1.209861000	1.949306000	2.339683000
1	1.379916000	0.934888000	2.671341000
6	1.573726000	3.051741000	3.096074000

1	2.052757000	2.911346000	4.054381000
6	1.306316000	4.318295000	2.596817000
1	1.577123000	5.200431000	3.161655000
6	0.680235000	4.447992000	1.364628000
6	-0.679282000	4.447856000	-1.365048000
6	-1.304993000	4.318045000	-2.597346000
1	-1.575262000	5.200056000	-3.162641000
6	-1.573102000	3.051377000	-3.096162000
1	-2.052042000	2.910971000	-4.054512000
6	-1.210140000	1.949052000	-2.339344000
1	-1.380791000	0.934543000	-2.670389000
6	-0.340031000	3.302903000	-0.655506000
6	0.340442000	3.303024000	0.655481000
6	2.088814000	-1.120127000	0.520683000
6	2.936396000	-2.092655000	1.033698000
1	2.646942000	-2.629200000	1.928386000
6	4.155899000	-2.374150000	0.387942000
6	5.048760000	-3.359040000	0.879353000
1	4.780509000	-3.904540000	1.775948000
6	6.236277000	-3.625804000	0.233876000
1	6.907569000	-4.381122000	0.619844000
6	6.572360000	-2.916213000	-0.925919000
1	7.504778000	-3.125643000	-1.433818000
6	5.718380000	-1.946673000	-1.431332000
1	5.989566000	-1.407148000	-2.330613000
6	4.502609000	-1.651609000	-0.798912000
6	3.609125000	-0.662537000	-1.309712000
1	3.864199000	-0.121068000	-2.211742000
6	2.430888000	-0.404044000	-0.669141000
6	-2.088892000	-1.119868000	-0.520415000
6	-2.936617000	-2.091566000	-1.033962000
1	-2.647368000	-2.627761000	-1.928930000
6	-4.156479000	-2.373220000	-0.388215000
6	-5.049636000	-3.357198000	-0.880294000
1	-4.781762000	-3.902109000	-1.777373000
6	-6.237352000	-3.624114000	-0.234762000
1	-6.908978000	-4.378766000	-0.621447000
6	-6.572975000	-2.915588000	0.925546000
1	-7.505371000	-3.125087000	1.433417000
6	-5.718443000	-1.946846000	1.431634000
1	-5.989035000	-1.408148000	2.331592000
6	-4.502683000	-1.651655000	0.799076000
6	-3.608833000	-0.663284000	1.310379000

1	-3.863494000	-0.122328000	2.212838000
6	-2.430504000	-0.404614000	0.669632000
1	-0.456448000	5.427578000	-0.970363000
1	0.457686000	5.427729000	0.969818000

### 3

32	-0.001654000	-0.124179000	0.000471000
8	-1.037343000	-1.241328000	-1.050697000
8	-1.436960000	0.028156000	1.167546000
8	1.434227000	0.027158000	-1.166337000
8	1.031247000	-1.246534000	1.049081000
7	0.737281000	1.599276000	1.107199000
7	-0.735100000	1.603865000	-1.104270000
6	1.460428000	1.534391000	2.210326000
1	1.687708000	0.540857000	2.573015000
6	1.900932000	2.693515000	2.866153000
1	2.494023000	2.598664000	3.764801000
6	1.573189000	3.928065000	2.355574000
1	1.905090000	4.834843000	2.846252000
6	0.797148000	4.013232000	1.183134000
6	0.390583000	5.239904000	0.565964000
1	0.696773000	6.173688000	1.020575000
6	-0.362533000	5.242255000	-0.564822000
1	-0.661952000	6.177947000	-1.020045000
6	-0.777902000	4.018138000	-1.181244000
6	-1.555192000	3.937978000	-2.353306000
1	-1.880452000	4.846965000	-2.844320000
6	-1.892090000	2.705619000	-2.863005000
1	-2.486616000	2.614316000	-3.761069000
6	-1.459129000	1.543650000	-2.206894000
1	-1.693197000	0.551633000	-2.569493000
6	-0.391804000	2.800405000	-0.593524000
6	0.402423000	2.797841000	0.595984000
6	2.244905000	-1.438787000	0.483514000
6	3.221231000	-2.236792000	1.013956000
1	3.031429000	-2.779738000	1.931832000
6	4.471798000	-2.365528000	0.355019000
6	5.507362000	-3.183027000	0.865023000
1	5.332667000	-3.728035000	1.785898000
6	6.711607000	-3.296441000	0.214197000
1	7.490605000	-3.929474000	0.620778000
6	6.935676000	-2.592277000	-0.985232000
1	7.886093000	-2.686963000	-1.495849000

6	5.950510000	-1.790483000	-1.508101000
1	6.121261000	-1.251006000	-2.432980000
6	4.698976000	-1.651022000	-0.863863000
6	3.668361000	-0.829447000	-1.390760000
1	3.823975000	-0.288351000	-2.316075000
6	2.470715000	-0.727649000	-0.737913000
6	-2.251198000	-1.432605000	-0.485150000
6	-3.229399000	-2.227065000	-1.017263000
1	-3.041719000	-2.767380000	-1.937108000
6	-4.479999000	-2.354932000	-0.357936000
6	-5.517253000	-3.169378000	-0.869377000
1	-5.344073000	-3.712194000	-1.791787000
6	-6.721246000	-3.282395000	-0.218066000
1	-7.501552000	-3.913285000	-0.625456000
6	-6.943316000	-2.580800000	0.983308000
1	-7.893614000	-2.675126000	1.494222000
6	-5.956450000	-1.782111000	1.507607000
1	-6.125618000	-1.244546000	2.433897000
6	-4.704978000	-1.643214000	0.862852000
6	-3.672556000	-0.824866000	1.391275000
1	-3.827019000	-0.285054000	2.317490000
6	-2.475051000	-0.723781000	0.738087000

### 3 radical-anion

32	-0.000930000	0.176327000	0.002288000
8	-0.958438000	-1.065338000	-1.062382000
8	-1.504062000	0.153189000	1.146583000
8	1.502717000	0.152288000	-1.141509000
8	0.955940000	-1.065921000	1.067267000
7	0.690521000	1.754872000	1.118664000
7	-0.689498000	1.755503000	-1.112787000
6	1.373901000	1.701228000	2.268187000
1	1.586331000	0.707674000	2.638255000
6	1.781085000	2.839860000	2.939257000
1	2.334555000	2.739102000	3.862047000
6	1.472815000	4.108891000	2.411046000
1	1.787320000	5.010954000	2.922166000
6	0.756827000	4.196573000	1.224521000
6	0.367887000	5.418821000	0.575792000
1	0.653054000	6.357124000	1.038244000
6	-0.337385000	5.419077000	-0.585055000
1	-0.614994000	6.357619000	-1.051630000
6	-0.736174000	4.197243000	-1.228856000

6	-1.451578000	4.110729000	-2.415796000
1	-1.757878000	5.013146000	-2.931182000
6	-1.769172000	2.841660000	-2.939319000
1	-2.322457000	2.741600000	-3.862313000
6	-1.371568000	1.702765000	-2.263771000
1	-1.590648000	0.709445000	-2.630493000
6	-0.359325000	2.984637000	-0.592012000
6	0.369299000	2.984338000	0.593160000
6	2.123801000	-1.392232000	0.508587000
6	3.009214000	-2.299489000	1.032420000
1	2.761760000	-2.813332000	1.954028000
6	4.236783000	-2.572864000	0.374246000
6	5.174477000	-3.501971000	0.880489000
1	4.938987000	-4.022811000	1.802688000
6	6.361556000	-3.754003000	0.231269000
1	7.063021000	-4.471889000	0.640347000
6	6.664509000	-3.078885000	-0.966328000
1	7.599278000	-3.277291000	-1.477855000
6	5.772786000	-2.168902000	-1.486573000
1	6.004514000	-1.649223000	-2.410424000
6	4.544367000	-1.886988000	-0.845837000
6	3.613168000	-0.953713000	-1.370625000
1	3.831675000	-0.430017000	-2.293857000
6	2.430771000	-0.707781000	-0.720737000
6	-2.128513000	-1.387521000	-0.505826000
6	-3.016584000	-2.290828000	-1.031897000
1	-2.769873000	-2.804546000	-1.953776000
6	-4.246198000	-2.560193000	-0.375781000
6	-5.186522000	-3.485412000	-0.884221000
1	-4.951624000	-4.006202000	-1.806588000
6	-6.375394000	-3.733789000	-0.236856000
1	-7.078877000	-4.448775000	-0.647535000
6	-6.677540000	-3.058692000	0.960957000
1	-7.613703000	-3.254214000	1.471046000
6	-5.783206000	-2.152513000	1.483360000
1	-6.014318000	-1.632886000	2.407402000
6	-4.552885000	-1.874421000	0.844564000
6	-3.619046000	-0.945000000	1.371498000
1	-3.837109000	-0.421112000	2.294722000
6	-2.434771000	-0.702831000	0.723583000

**3 radical-cation**

32	-0.002331000	0.174153000	-0.001032000
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8	-0.942137000	-1.059546000	-1.077489000
8	-1.512645000	0.232546000	1.076733000
8	1.511228000	0.228526000	-1.075752000
8	0.934904000	-1.068026000	1.073688000
7	0.645064000	1.804885000	1.160915000
7	-0.638724000	1.810393000	-1.159244000
6	1.259773000	1.736783000	2.331126000
1	1.456098000	0.745571000	2.716038000
6	1.628479000	2.894261000	3.028617000
1	2.130537000	2.798094000	3.980722000
6	1.347566000	4.130883000	2.492785000
1	1.628515000	5.035245000	3.017902000
6	0.685383000	4.220068000	1.252361000
6	0.337043000	5.447398000	0.601077000
1	0.597363000	6.380780000	1.083262000
6	-0.304690000	5.450092000	-0.596726000
1	-0.558487000	6.385636000	-1.078178000
6	-0.661642000	4.225806000	-1.248999000
6	-1.323717000	4.142134000	-2.489851000
1	-1.598014000	5.048746000	-3.014633000
6	-1.613182000	2.907918000	-3.026692000
1	-2.115258000	2.816122000	-3.979216000
6	-1.253466000	1.747352000	-2.329776000
1	-1.457173000	0.757720000	-2.714962000
6	-0.335176000	3.010491000	-0.624491000
6	0.349922000	3.007648000	0.627145000
6	2.095263000	-1.388214000	0.516762000
6	2.951403000	-2.354787000	1.028949000
1	2.666058000	-2.893883000	1.923386000
6	4.171898000	-2.626214000	0.382425000
6	5.072318000	-3.606073000	0.872000000
1	4.808487000	-4.154015000	1.768368000
6	6.259997000	-3.864240000	0.224893000
1	6.936770000	-4.615860000	0.608476000
6	6.589874000	-3.150616000	-0.934944000
1	7.522945000	-3.353585000	-1.444293000
6	5.729454000	-2.186122000	-1.438257000
1	5.996240000	-1.643883000	-2.337197000
6	4.512410000	-1.899784000	-0.804433000
6	3.611282000	-0.916832000	-1.314130000
1	3.862000000	-0.373088000	-2.215972000
6	2.431550000	-0.668450000	-0.673747000
6	-2.103726000	-1.379201000	-0.518620000

6	-2.962483000	-2.341636000	-1.031504000
1	-2.679956000	-2.880186000	-1.927193000
6	-4.183747000	-2.611119000	-0.383900000
6	-5.087972000	-3.585924000	-0.875161000
1	-4.827057000	-4.132562000	-1.773228000
6	-6.276508000	-3.841486000	-0.227704000
1	-6.956477000	-4.589197000	-0.613313000
6	-6.602827000	-3.130336000	0.934208000
1	-7.536170000	-3.331265000	1.443831000
6	-5.738113000	-2.170664000	1.439331000
1	-6.001800000	-1.629859000	2.340062000
6	-4.520527000	-1.887091000	0.804867000
6	-3.615391000	-0.908608000	1.315696000
1	-3.862440000	-0.366390000	2.219477000
6	-2.435910000	-0.662100000	0.673450000

2,3-dihydroxynaphthalene *H-bond*

8	-2.964567000	1.253858000	0.000065000
8	-2.895517000	-1.406514000	0.000421000
6	-1.713322000	-0.734109000	0.000225000
6	-0.524969000	-1.411539000	0.000055000
1	-0.539852000	-2.494107000	0.000144000
6	0.708755000	-0.716474000	-0.000122000
6	1.953094000	-1.390935000	-0.000266000
1	1.957858000	-2.474576000	-0.000277000
6	3.134796000	-0.693579000	-0.000395000
1	4.077769000	-1.225660000	-0.000505000
6	3.128440000	0.716200000	-0.000385000
1	4.065960000	1.257737000	-0.000488000
6	1.939071000	1.400802000	-0.000244000
1	1.933122000	2.484763000	-0.000241000
6	0.704276000	0.711469000	-0.000108000
6	-0.541045000	1.388510000	-0.000048000
1	-0.556574000	2.473670000	-0.000230000
6	-1.713553000	0.687307000	0.000156000
1	-2.895875000	2.214570000	0.003279000
1	-3.614993000	-0.761062000	0.001224000

2,3-dihydroxynaphthalene

8	2.951581000	-1.315273000	-0.000675000
8	2.951604000	1.315275000	-0.000160000
6	1.730139000	0.712140000	0.000169000
6	0.541145000	1.391958000	0.000163000

1	0.548103000	2.477428000	0.000720000
6	-0.701987000	0.713017000	0.000171000
6	-1.940478000	1.395827000	0.000170000
1	-1.940220000	2.479718000	0.000346000
6	-3.126479000	0.704737000	0.000039000
1	-4.066763000	1.241491000	0.000052000
6	-3.126494000	-0.704696000	-0.000143000
1	-4.066791000	-1.241428000	-0.000259000
6	-1.940508000	-1.395813000	-0.000215000
1	-1.940269000	-2.479703000	-0.000298000
6	-0.702003000	-0.713031000	0.000008000
6	0.541121000	-1.391990000	-0.000218000
1	0.548090000	-2.477456000	-0.000953000
6	1.730109000	-0.712165000	0.000269000
1	2.832445000	-2.271965000	0.006472000
1	2.832540000	2.272003000	-0.001884000

*2,2'-bipyridine flat*

7	1.158064000	1.383252000	0.000510000
7	-1.158064000	-1.383252000	0.000510000
6	1.158064000	2.712539000	0.000553000
1	2.132483000	3.190859000	0.001017000
6	-0.001504000	3.479060000	0.000078000
1	0.055860000	4.559548000	0.000232000
6	-1.222337000	2.816414000	-0.000492000
1	-2.151890000	3.372191000	-0.000866000
6	-1.236037000	1.431060000	-0.000560000
6	1.236037000	-1.431060000	-0.000560000
6	1.222337000	-2.816414000	-0.000492000
1	2.151890000	-3.372191000	-0.000866000
6	0.001504000	-3.479060000	0.000078000
1	-0.055860000	-4.559548000	0.000232000
6	-1.158064000	-2.712539000	0.000553000
1	-2.132483000	-3.190859000	0.001017000
6	0.018632000	-0.744056000	-0.000086000
6	-0.018632000	0.744056000	-0.000086000
1	2.158020000	-0.868925000	-0.000908000
1	-2.158020000	0.868925000	-0.000908000

*2,2'-bipyridine twisted*

7	-0.390089000	1.356305000	-1.120439000
7	0.390089000	-1.356305000	-1.120439000
6	-0.397109000	2.685083000	-1.145669000



1	-0.727053000	3.141807000	-2.073730000
6	-0.014035000	3.479858000	-0.070204000
1	-0.036759000	4.558766000	-0.149166000
6	0.397112000	2.847262000	1.094152000
1	0.715513000	3.422020000	1.954977000
6	0.404305000	1.460857000	1.134368000
6	-0.404305000	-1.460857000	1.134368000
6	-0.397112000	-2.847262000	1.094152000
1	-0.715513000	-3.422020000	1.954977000
6	0.014035000	-3.479858000	-0.070204000
1	0.036759000	-4.558766000	-0.149166000
6	0.397109000	-2.685083000	-1.145669000
1	0.727053000	-3.141807000	-2.073730000
6	-0.002299000	-0.745548000	0.002454000
6	0.002299000	0.745548000	0.002454000
1	-0.740729000	-0.939310000	2.020409000
1	0.740729000	0.939310000	2.020409000

1,10-phenanthroline

7	1.382042000	-1.555718000	0.000399000
7	-1.382054000	-1.555734000	-0.000525000
6	2.698807000	-1.543323000	0.000601000
1	3.186775000	-2.513613000	0.001172000
6	3.470845000	-0.369931000	0.000091000
1	4.551689000	-0.427392000	0.000031000
6	2.818869000	0.838232000	-0.000458000
1	3.371282000	1.770733000	-0.001190000
6	1.412612000	0.866207000	-0.000324000
6	0.677057000	2.092805000	-0.000243000
1	1.226391000	3.027184000	-0.000562000
6	-0.677063000	2.092796000	0.000134000
1	-1.226410000	3.027166000	0.000394000
6	-1.412598000	0.866182000	0.000290000
6	-2.818884000	0.838226000	0.000587000
1	-3.371247000	1.770757000	0.001366000
6	-3.470853000	-0.369911000	0.000091000
1	-4.551693000	-0.427425000	0.000370000
6	-2.698783000	-1.543327000	-0.000592000
1	-3.186805000	-2.513596000	-0.001239000
6	-0.727980000	-0.378440000	-0.000020000
6	0.727989000	-0.378459000	-0.000067000