Supporting Information

Clamshell-type Bis-phthalocyanines as Color-Changing Optical Limiters: TDDFT Modeling of Electrically Induced Absorption for Real-Time Color Indication of Optical Limiter Efficiency in Nonlinear Laser Protection

Alexander Yu. Tolbin [a*]

[a] FSBIS Institute of Physiologically Active Compounds of the Russian Academy of Sciences, Russian Academy of Sciences, 142432, Chernogolovka, Severny proezd, 1, Moscow Region, Russian Federation

[*]Corresponding author. Tel.: +7 496 5242566, e-mail address: tolbin@ipac.ac.ru (Prof. A.Yu. Tolbin), ORCID 0000-0002-5541-5401.

TABLE OF CONTENTS

1. DFT-optimized geometries of bis-phthalocyanines 1a-c

Quantum chemical calculations were performed using density functional theory (DFT) implemented with exchange-correlation functional M06-2X [1] and aug-cc-pVDZ basis set.[2] Optimized geometries are presented in GAMESS-US format.

1.1. Phthalocyanine 1a

```
Molecule specification
Cl
N  7.000000 -0.882000 1.227000 8.871000
N  7.000000 1.850000 1.622000 8.382000
N  7.000000 -0.046000 3.161000 7.051000
P  15.000000 0.660000 0.860000 9.153000
P  15.000000 1.487000 2.928000 7.492000
P  15.000000 -1.234000 2.476000 7.901000
Cl  17.000000 -2.231000 3.895000 8.990000
Cl  17.000000 0.996000 0.952000 11.180000
C  6.000000 2.474000 7.817000 -1.038000
C  6.000000 2.469000 7.756000 -2.447000
C  6.000000 2.381000 6.537000 -3.117000
C  6.000000 2.297000 5.374000 -2.348000
C  6.000000 2.302000 5.435000 -0.933000
C  6.000000 2.392000 6.659000 -0.266000
C  6.000000 2.192000 3.974000 -2.728000
N  7.000000 2.143000 3.261000 -1.548000
C  6.000000 2.203000 4.072000 -0.433000
C  6.000000 2.257000 2.210000 5.042000
C  6.000000 2.228000 2.890000 3.824000
C  6.000000 2.126000 2.113000 2.676000
C  6.000000 2.039000 0.711000 2.742000
C  6.000000 2.062000 0.047000 3.966000
C  6.000000 2.182000 0.811000 5.130000
C  6.000000 2.104000 2.447000 1.245000
N  7.000000 2.010000 1.314000 0.485000
C  6.000000 1.966000 0.253000 1.350000
C  6.000000 1.745000 -2.913000 -0.558000
C  6.000000 1.735000 -2.972000 -1.973000
C  6.000000 1.647000 -4.196000 -2.641000
C  6.000000 1.572000 -5.353000 -1.868000
C  6.000000 1.582000 -5.295000 -0.460000
C  6.000000 1.668000 -4.076000 0.211000
C  6.000000 1.836000 -1.511000 -0.178000
N  7.000000 1.872000 -0.796000 -1.358000
C  6.000000 1.818000 -1.608000 -2.473000
C  6.000000 2.012000 2.417000 -6.873000
C  6.000000 1.930000 1.642000 -8.035000
C  6.000000 1.830000 0.241000 -7.969000
C  6.000000 1.811000 -0.425000 -6.738000
C  6.000000 1.895000 0.349000 -5.583000
C  6.000000 1.992000 1.751000 -5.649000
C  6.000000 1.904000 0.018000 -4.152000
N  7.000000 1.997000 1.150000 -3.390000
C  6.000000 2.053000 2.210000 -4.255000
N  7.000000 2.151000 3.510000 -3.961000
N  7.000000 1.832000 -1.252000 -3.741000
N  7.000000 2.186000 3.716000 0.835000
N  7.000000 1.880000 -1.048000 1.055000
O  8.000000 2.451000 3.003000 6.188000
H  1.000000 2.547000 8.790000 -0.547000
H  1.000000 2.537000 8.684000 -3.021000
H  1.000000 2.379000 6.478000 -4.208000
H  1.000000 2.398000 6.694000 0.825000
H  1.000000 2.297000 3.979000 3.787000
H  1.000000 2.001000 -1.042000 4.013000
H  1.000000 2.232000 0.335000 6.111000
H  1.000000 1.631000 -4.229000 -3.732000
H  1.000000 1.498000 -6.326000 -2.360000
H  1.000000 1.515000 -6.223000 0.113000
H  1.000000 1.673000 -4.018000 1.302000
H  1.000000 2.091000 3.506000 -6.914000
H  1.000000 1.944000 2.131000 -9.013000
H  1.000000 1.769000 -0.334000 -8.896000
H  1.000000 1.731000 -1.512000 -6.674000
H  1.000000 2.062000 2.239000 -1.509000
H  1.000000 1.940000 0.227000 -1.399000
```

```
Cl  17.000000 2.233000 4.587000 8.441000
Cl  17.000000 0.904000 -1.154000 8.814000
C  6.000000 -2.581000 -7.640000 2.594000
C  6.000000 -2.566000 -8.063000 1.249000
C  6.000000 -2.471000 -7.145000 0.205000
C  6.000000 -2.389000 -5.789000 0.532000
C  6.000000 -2.403000 -5.364000 1.883000
C  6.000000 -2.501000 -6.289000 2.926000
C  6.000000 -2.282000 -4.603000 -0.302000
N  7.000000 -2.235000 -3.530000 0.564000
C  6.000000 -2.307000 -3.912000 1.889000
C  6.000000 -2.443000 -0.289000 6.415000
C  6.000000 -2.404000 -1.333000 5.488000
C  6.000000 -2.261000 -1.008000 4.141000
C  6.000000 -2.149000 0.330000 3.723000
C  6.000000 -2.172000 1.382000 4.634000
C  6.000000 -2.328000 1.039000 5.977000
C  6.000000 -2.221000 -1.812000 2.914000
N  7.000000 -2.099000 -1.010000 1.811000
C  6.000000 -2.047000 0.281000 2.258000
C  6.000000 -1.733000 2.600000 -0.611000
C  6.000000 -1.705000 2.172000 -1.961000
C  6.000000 -1.584000 3.093000 -3.004000
C  6.000000 -1.490000 4.443000 -2.672000
C  6.000000 -1.516000 4.869000 -1.329000
C  6.000000 -1.639000 3.955000 -0.283000
C  6.000000 -1.862000 1.415000 0.224000
N  7.000000 -1.902000 0.340000 -0.642000
C  6.000000 -1.815000 0.721000 -1.966000
C  6.000000 -2.107000 -4.558000 -4.729000
C  6.000000 -2.013000 -4.230000 -6.085000
C  6.000000 -1.880000 -2.893000 -6.501000
C  6.000000 -1.840000 -1.847000 -5.573000
C  6.000000 -1.938000 -2.178000 -4.224000
C  6.000000 -2.067000 -3.515000 -3.807000
C  6.000000 -1.933000 -1.378000 -2.992000
N  7.000000 -2.046000 -2.178000 -1.888000
C  6.000000 -2.127000 -3.468000 -2.340000
N  7.000000 -2.239000 -4.588000 -1.619000
N  7.000000 -1.827000 -0.046000 -3.037000
N  7.000000 -2.306000 -3.145000 2.960000
N  7.000000 -1.931000 1.402000 1.539000
H  1.000000 -2.563000 -0.481000 7.483000
H  1.000000 -2.659000 -8.388000 3.387000
H  1.000000 -2.634000 -9.131000 1.025000
H  1.000000 -2.462000 -7.460000 -0.841000
H  1.000000 -2.514000 -5.950000 3.965000
H  1.000000 -2.497000 -2.374000 5.806000
H  1.000000 -2.086000 2.424000 4.323000
O  8.000000 -2.466000 2.084000 6.915000
H  1.000000 -1.559000 2.751000 -4.042000
H  1.000000 -1.388000 5.188000 -3.465000
H  1.000000 -1.433000 5.935000 -1.106000
H  1.000000 -1.656000 4.273000 0.761000
H  1.000000 -2.210000 -5.593000 -4.394000
H  1.000000 -2.043000 -5.023000 -6.837000
H  1.000000 -1.806000 -2.670000 -7.569000
H  1.000000 -1.730000 -0.807000 -5.886000
H  1.000000 -2.152000 -2.555000 0.255000
H  1.000000 -1.990000 -0.634000 -0.333000
 $END
```

1.2. Phthalocyanine 1b

```
Molecule specification
C1
N  7.000000 -0.847000 1.197000 8.881000
N  7.000000 1.868000 1.623000 8.329000
N  7.000000 -0.074000 3.152000 7.056000
P  15.000000 0.705000 0.841000 9.122000
P  15.000000 1.471000 2.935000 7.465000
P  15.000000 -1.235000 2.447000 7.927000
Cl  17.000000 -2.230000 3.848000 9.038000
Cl  17.000000 1.089000 0.914000 11.140000
C  6.000000 2.578000 7.973000 -1.045000
C  6.000000 2.588000 7.931000 -2.452000
C  6.000000 2.496000 6.718000 -3.139000
C  6.000000 2.393000 5.548000 -2.385000
C  6.000000 2.383000 5.591000 -0.972000
C  6.000000 2.476000 6.804000 -0.288000
C  6.000000 2.278000 4.139000 -2.764000
N  7.000000 2.207000 3.388000 -1.615000
C  6.000000 2.262000 4.207000 -0.511000
C  6.000000 2.202000 2.270000 4.984000
C  6.000000 2.207000 2.969000 3.779000
C  6.000000 2.093000 2.217000 2.612000
C  6.000000 1.963000 0.810000 2.655000
```

```
C  6.000000 1.954000 0.130000 3.873000
C  6.000000 2.085000 0.870000 5.048000
C  6.000000 2.101000 2.598000 1.199000
N  7.000000 1.980000 1.453000 0.447000
C  6.000000 1.893000 0.354000 1.267000
C  6.000000 1.660000 -2.764000 -0.729000
C  6.000000 1.687000 -2.807000 -2.142000
C  6.000000 1.606000 -4.020000 -2.826000
C  6.000000 1.498000 -5.189000 -2.070000
C  6.000000 1.471000 -5.147000 -0.663000
C  6.000000 1.552000 -3.934000 0.025000
C  6.000000 1.761000 -1.354000 -0.350000
N  7.000000 1.838000 -0.601000 -1.499000
C  6.000000 1.799000 -1.422000 -2.602000
C  6.000000 2.147000 2.654000 -6.988000
C  6.000000 2.077000 1.899000 -8.161000
C  6.000000 1.956000 0.497000 -8.119000
C  6.000000 1.902000 -0.187000 -6.902000
C  6.000000 1.973000 0.565000 -5.728000
C  6.000000 2.093000 1.973000 -5.770000
C  6.000000 1.945000 0.187000 -4.314000
N  7.000000 2.042000 1.333000 -3.560000
C  6.000000 2.136000 2.433000 -4.381000
N  7.000000 2.246000 3.710000 -4.024000
N  7.000000 1.844000 -1.068000 -3.884000
N  7.000000 2.219000 3.852000 0.771000
N  7.000000 1.778000 -0.924000 0.910000
O  8.000000 2.407000 3.040000 6.143000
H  1.000000 2.653000 8.940000 -0.540000
H  1.000000 2.671000 8.865000 -3.014000
H  1.000000 2.505000 6.674000 -4.230000
H  1.000000 2.469000 6.826000 0.804000
H  1.000000 2.309000 4.055000 3.760000
H  1.000000 1.862000 -0.958000 3.902000
H  1.000000 2.114000 0.376000 6.021000
H  1.000000 1.620000 -4.041000 -3.918000
H  1.000000 1.426000 -6.155000 -2.576000
H  1.000000 1.379000 -6.081000 -0.102000
H  1.000000 1.531000 -3.892000 1.116000
H  1.000000 2.243000 3.742000 -7.009000
H  1.000000 2.117000 2.403000 -9.130000
H  1.000000 1.904000 -0.062000 -9.056000
H  1.000000 1.808000 -1.274000 -6.856000
Zn  30.000000 1.975000 1.399000 -1.559000
Cl  17.000000 2.214000 4.592000 8.418000
Cl  17.000000 0.959000 -1.165000 8.753000
C  6.000000 -2.814000 -7.757000 2.756000
C  6.000000 -2.800000 -8.198000 1.419000
C  6.000000 -2.661000 -7.295000 0.363000
C  6.000000 -2.536000 -5.940000 0.675000
C  6.000000 -2.550000 -5.498000 2.018000
C  6.000000 -2.691000 -6.402000 3.071000
C  6.000000 -2.378000 -4.748000 -0.159000
N  7.000000 -2.298000 -3.652000 0.666000
C  6.000000 -2.402000 -4.042000 1.982000
C  6.000000 -2.504000 -0.338000 6.496000
C  6.000000 -2.476000 -1.396000 5.589000
C  6.000000 -2.300000 -1.102000 4.236000
C  6.000000 -2.145000 0.234000 3.797000
C  6.000000 -2.161000 1.299000 4.696000
C  6.000000 -2.350000 0.982000 6.038000
C  6.000000 -2.262000 -1.944000 3.042000
N  7.000000 -2.091000 -1.131000 1.947000
C  6.000000 -2.014000 0.184000 2.340000
C  6.000000 -1.615000 2.422000 -0.590000
C  6.000000 -1.584000 1.975000 -1.932000
C  6.000000 -1.448000 2.878000 -2.988000
C  6.000000 -1.339000 4.235000 -2.675000
C  6.000000 -1.366000 4.679000 -1.340000
C  6.000000 -1.506000 3.779000 -0.281000
C  6.000000 -1.779000 1.232000 0.245000
N  7.000000 -1.838000 0.130000 -0.578000
C  6.000000 -1.732000 0.519000 -1.893000
C  6.000000 -2.166000 -4.799000 -4.631000
C  6.000000 -2.047000 -4.495000 -5.989000
C  6.000000 -1.866000 -3.169000 -6.425000
C  6.000000 -1.802000 -2.111000 -5.514000
C  6.000000 -1.924000 -2.413000 -4.158000
C  6.000000 -2.102000 -3.744000 -3.719000
C  6.000000 -1.900000 -1.575000 -2.957000
N  7.000000 -2.052000 -2.389000 -1.859000
C  6.000000 -2.174000 -3.700000 -2.258000
N  7.000000 -2.325000 -4.776000 -1.489000
N  7.000000 -1.754000 -0.253000 -2.978000
N  7.000000 -2.389000 -3.270000 3.065000
N  7.000000 -1.862000 1.261000 1.573000
H  1.000000 -2.647000 -0.509000 7.564000
H  1.000000 -2.926000 -8.491000 3.558000
H  1.000000 -2.901000 -9.266000 1.208000
H  1.000000 -2.652000 -7.625000 -0.679000
```

```
H  1.000000 -2.703000 -6.050000 4.105000
H  1.000000 -2.600000 -2.429000 5.921000
H  1.000000 -2.045000 2.334000 4.369000
O  8.000000 -2.480000 2.040000 6.962000
H  1.000000 -1.430000 2.524000 -4.022000
H  1.000000 -1.226000 4.967000 -3.479000
H  1.000000 -1.272000 5.748000 -1.132000
H  1.000000 -1.530000 4.115000 0.758000
H  1.000000 -2.305000 -5.824000 -4.281000
H  1.000000 -2.095000 -5.298000 -6.729000
H  1.000000 -1.775000 -2.966000 -7.495000
H  1.000000 -1.656000 -1.079000 -5.842000
Zn  30.000000 -2.031000 -1.766000 0.045000
 $END
```

1.3. Phthalocyanine 1c

```
Molecule specification
Cl
N  7.000000 -0.828000 1.191000 8.946000
N  7.000000 1.853000 1.634000 8.257000
N  7.000000 -0.164000 3.125000 7.056000
P  15.000000 0.738000 0.862000 9.126000
P  15.000000 1.400000 2.922000 7.385000
P  15.000000 -1.278000 2.412000 7.981000
Cl  17.000000 -2.270000 3.805000 9.101000
Cl  17.000000 1.214000 0.997000 11.121000
C  6.000000 2.488000 7.691000 -1.223000
C  6.000000 2.504000 7.614000 -2.628000
C  6.000000 2.394000 6.385000 -3.285000
C  6.000000 2.266000 5.241000 -2.497000
C  6.000000 2.247000 5.319000 -1.096000
C  6.000000 2.360000 6.542000 -0.437000
C  6.000000 2.125000 3.830000 -2.834000
N  7.000000 2.024000 3.074000 -1.677000
C  6.000000 2.101000 3.953000 -0.609000
C  6.000000 2.029000 2.201000 4.883000
C  6.000000 2.060000 2.867000 3.656000
C  6.000000 1.920000 2.084000 2.515000
C  6.000000 1.736000 0.695000 2.594000
C  6.000000 1.700000 0.043000 3.827000
C  6.000000 1.859000 0.810000 4.983000
C  6.000000 1.938000 2.422000 1.097000
N  7.000000 1.783000 1.278000 0.338000
C  6.000000 1.658000 0.212000 1.224000
C  6.000000 1.485000 -2.915000 -0.651000
C  6.000000 1.572000 -2.992000 -2.050000
C  6.000000 1.580000 -4.220000 -2.711000
C  6.000000 1.507000 -5.376000 -1.928000
C  6.000000 1.429000 -5.300000 -0.526000
C  6.000000 1.417000 -4.065000 0.133000
C  6.000000 1.526000 -1.495000 -0.314000
N  7.000000 1.648000 -0.737000 -1.470000
C  6.000000 1.665000 -1.624000 -2.534000
C  6.000000 2.093000 2.285000 -6.968000
C  6.000000 2.105000 1.494000 -8.122000
C  6.000000 2.038000 0.091000 -8.045000
C  6.000000 1.957000 -0.561000 -6.811000
C  6.000000 1.945000 0.231000 -5.663000
C  6.000000 2.009000 1.631000 -5.740000
C  6.000000 1.866000 -0.100000 -4.246000
N  7.000000 1.891000 1.064000 -3.485000
C  6.000000 1.987000 2.122000 -4.366000
N  7.000000 2.092000 3.409000 -4.082000
N  7.000000 1.772000 -1.342000 -3.822000
N  7.000000 2.074000 3.666000 0.677000
N  7.000000 1.522000 -1.066000 0.937000
O  8.000000 2.265000 3.001000 6.012000
H  1.000000 2.578000 8.668000 -0.741000
H  1.000000 2.607000 8.532000 -3.212000
H  1.000000 2.409000 6.311000 -4.375000
H  1.000000 2.347000 6.589000 0.654000
H  1.000000 2.203000 3.947000 3.606000
H  1.000000 1.566000 -1.039000 3.884000
H  1.000000 1.872000 0.338000 5.967000
H  1.000000 1.642000 -4.264000 -3.801000
H  1.000000 1.508000 -6.357000 -2.410000
H  1.000000 1.370000 -6.222000 0.058000
H  1.000000 1.353000 -3.997000 1.221000
H  1.000000 2.148000 3.375000 -7.016000
H  1.000000 2.168000 1.972000 -9.103000
H  1.000000 2.052000 -0.496000 -8.966000
H  1.000000 1.903000 -1.649000 -6.734000
Co  27.000000 1.812000 1.169000 -1.575000
Cl  17.000000 2.183000 4.606000 8.255000
Cl  17.000000 1.003000 -1.151000 8.800000
C  6.000000 -2.377000 -7.601000 2.519000
```

```
C  6.000000 -2.376000 -7.985000 1.166000
C  6.000000 -2.294000 -7.034000 0.145000
C  6.000000 -2.210000 -5.693000 0.518000
C  6.000000 -2.215000 -5.309000 1.868000
C  6.000000 -2.298000 -6.255000 2.889000
C  6.000000 -2.115000 -4.464000 -0.260000
N  7.000000 -2.054000 -3.369000 0.587000
C  6.000000 -2.126000 -3.854000 1.883000
C  6.000000 -2.406000 -0.400000 6.508000
C  6.000000 -2.308000 -1.421000 5.561000
C  6.000000 -2.178000 -1.059000 4.221000
C  6.000000 -2.146000 0.289000 3.832000
C  6.000000 -2.233000 1.322000 4.763000
C  6.000000 -2.366000 0.943000 6.098000
C  6.000000 -2.084000 -1.843000 2.997000
N  7.000000 -1.987000 -1.004000 1.903000
C  6.000000 -2.016000 0.298000 2.381000
C  6.000000 -1.684000 2.634000 -0.398000
C  6.000000 -1.568000 2.247000 -1.741000
C  6.000000 -1.496000 3.191000 -2.765000
C  6.000000 -1.521000 4.540000 -2.399000
C  6.000000 -1.621000 4.929000 -1.051000
C  6.000000 -1.709000 3.978000 -0.030000
C  6.000000 -1.787000 1.406000 0.379000
N  7.000000 -1.740000 0.305000 -0.457000
C  6.000000 -1.600000 0.786000 -1.753000
C  6.000000 -2.094000 -4.345000 -4.675000
C  6.000000 -2.006000 -3.982000 -6.022000
C  6.000000 -1.802000 -2.643000 -6.403000
C  6.000000 -1.682000 -1.630000 -5.446000
C  6.000000 -1.772000 -1.997000 -4.105000
C  6.000000 -1.976000 -3.332000 -3.725000
C  6.000000 -1.707000 -1.223000 -2.871000
N  7.000000 -1.852000 -2.061000 -1.776000
C  6.000000 -2.005000 -3.347000 -2.267000
N  7.000000 -2.119000 -4.467000 -1.579000
N  7.000000 -1.573000 0.090000 -2.875000
N  7.000000 -2.130000 -3.163000 3.007000
N  7.000000 -1.923000 1.418000 1.693000
H  1.000000 -2.512000 -0.620000 7.572000
H  1.000000 -2.444000 -8.370000 3.293000
H  1.000000 -2.443000 -9.046000 0.912000
H  1.000000 -2.295000 -7.318000 -0.910000
H  1.000000 -2.304000 -5.944000 3.936000
H  1.000000 -2.340000 -2.472000 5.856000
H  1.000000 -2.204000 2.373000 4.471000
O  8.000000 -2.543000 1.956000 7.064000
H  1.000000 -1.417000 2.879000 -3.809000
H  1.000000 -1.457000 5.310000 -3.173000
H  1.000000 -1.632000 5.992000 -0.802000
H  1.000000 -1.798000 4.267000 1.020000
H  1.000000 -2.252000 -5.381000 -4.366000
H  1.000000 -2.098000 -4.749000 -6.796000
H  1.000000 -1.735000 -2.393000 -7.465000
H  1.000000 -1.518000 -0.588000 -5.730000
Co  27.000000 -1.880000 -1.533000 0.064000
 $END
```

2. Calculation of the color of a substance

The method of calculating colours based on electronic spectra obtained by the quantum-chemical TDDFT method is described in Section 4 of the main text. The essence of the method is as follows: the absorption spectrum is divided into conventional sections by the colours of the rainbow. The ranges are presented in Table 1 (see main text). Next, the zones are integrated, and the integral shares are calculated, which are then multiplied by the hexadecimal codes of the corresponding colours. After that, the numbers are added to obtain the absorbed colour. To calculate the colour that we observe in reflected light, the absorbed colour is subtracted from the colour of the light source, i.e., white, with the code #FFFFFF.

Here is the full version of the program in PHP, which calculates the colour of a substance based on its electronic absorption spectrum according to the algorithm described in the article.

```
<?php
/*
How to work. It's simple :)
Export the absorption spectrum to an ASCII text file which contains two columns: X – wavelengths, Y – intensities.
Columns must be separated by tabs. Name the file uvvis.txt and run the program.
Have a nice work!

Written by Prof. A. Yu. Tolbin (tolbin@ipac.ac.ru), 2024.

Please cite this article if you use this program :)
*/

$color = color :: uvvis($uvvis_file = "uvvis.txt",   /* X;Y columns, TAB delimiter */
          $illuminator = "#FFFFFF");

echo "The calculated color of the substance is $color \n";

exit;

/*
The program text follows. No changes are needed, except for the color codes
in static $color_data. You can play with them and see the result.
*/

class color {
   static $color_data = array(
      array("#800080", "Violet",    array(380, 440)),
      array("#0000FF", "Indigo",    array(440, 485)),
      array("#00FFFF", "Blue",      array(485, 500)),
      array("#00FF00", "Green",     array(500, 565)),
      array("#FFFF00", "Yellow",    array(565, 590)),
      array("#FF8000", "Orange",    array(590, 625)),
      array("#FF0000", "Red",       array(625, 780))
      );

   static function uvvis($uvvis_file = "uvvis.txt", $illuminator = "#FFFFFF")
   {
      if (!file_exists($uvvis_file)) return -1;
         // reading uvvis spectrum
      $data = file($uvvis_file);
      $spec = array();
      for($i = 0;$i < count($data);$i++) {
         $line = $data[$i];
         $elem = explode("\t", $line);
         $x = intval($elem[0]);
```

```
        $y = floatval($elem[1]);

        $spec[$x] = $y;
    }
    ksort($spec, SORT_NUMERIC);

        // calculating integrals
    self::calc_integrals ($spec);

        // calculating color
    $color = self::calc_color ($illuminator);

    return $color;
}

static function calc_integrals($spec)       // calculating integrals
{
    $index = 0;
    foreach(self::$color_data as $color_data_element) {
        $range_left = $color_data_element[2][0];
        $range_right = $color_data_element[2][1];

        $wavelengths = array_keys($spec);
        $integralValue = 0.0;
        for($i = 1; $i < count($wavelengths); $i++)
        if ($wavelengths[$i] >= $range_left && $wavelengths[$i] <= $range_right) {
            $x = $wavelengths[$i];
            $x_1 = $wavelengths[$i-1];
            $y = $spec[$x];
            $y_1 = $spec[$x_1];
            $integralValue += ($x - $x_1) * ($y + $y_1);
        }
        $integralValue /= 2.0;

        self::$color_data[$index][] = $integralValue;
        $index++;
    }

    return 1;
}

static function calc_color ($illuminator = "#FFFFFF") // calculating color
{
    $sum = 0.0;
    foreach(self::$color_data as $color_data_element)
            $sum += $color_data_element[3];

    $colors = array();
    $portions = array();
```

```
    for($i = 0; $i < count(self::$color_data); $i++) {
        $colors[] = self::$color_data[$i][0];
        $integral = self::$color_data[$i][3];
        $portions[] = $integral / $sum;
    }

    return self::subtract($illuminator, self::color_mix($colors, $portions));
}

static function color_mix($colors, $portions)        // mixing colors
{
    $colors_rgb = array();
    for($i = 0;$i < count($portions);$i++) {
        $portion = $portions[$i];
        $color = self::hex2rgb($colors[$i]);
        for($j = 0;$j < count($color);$j++) $color[$j] *= $portion;
        $colors_rgb[] = $color;
    }

    $R = 0;
    $G = 0;
    $B = 0;
    foreach($colors_rgb as $color_rgb) {
        $R += $color_rgb[0];
        $G += $color_rgb[1];
        $B += $color_rgb[2];
    }

    $color_rgb = array(round($R), round($G), round($B));
    for($i = 0; $i < count($color_rgb); $i++)
            $color_rgb[$i] = ($color_rgb[$i] > 255) ? 255 : $color_rgb[$i];
    $color_mix = self::rgb2hex($color_rgb);

    return $color_mix;
}

static function subtract($color1, $color2)  // subtract absorbed color from illuminator
{
    $color1 = self::hex2rgb($color1);
    $color2 = self::hex2rgb($color2);

    $result_color = array();
    for($i = 0;$i < count($color1);$i++) {
        $delta = $color1[$i] - $color2[$i];
        $result_color[$i] = ($delta < 0) ? 0 : $delta;
    }
    return self::rgb2hex($result_color);
}
```

```
    // technic functions for conversion hex <-> dec

    static function hex2rgb($hex = '#000000')
    {
        if (!function_exists('_hex2rgb_f')) {
            function _hex2rgb_f($x)
            {
                return hexdec($x);
            }
        }
        return array_map('_hex2rgb_f', str_split(str_replace("#", "", $hex), 2));
    }

    static function rgb2hex($rgb = array(0, 0, 0))
    {
        if (!function_exists('_rgb2hex_f')) {
            function _rgb2hex_f($x)
            {
                return str_pad(dechex($x), 2, "0", STR_PAD_LEFT);
            }
        }

        return "#" . implode("", array_map('_rgb2hex_f', $rgb));
    }
}

?>
```

3. References

1. Y. Zhao and D. G. Truhlar, *Theoretical Chemistry Accounts*, 2008, **120**, 215-241.
2. T. H. Dunning, *The Journal of Chemical Physics*, 1989, **90**, 1007-1023.