

Supporting Information

Halogen-free GeO₂ conversion: electrochemical reduction vs. complexation in (DTBC)₂Ge[Py(CN)_n] (n = 0..2) complexes

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Table S1. Total energies without (E_{total} , given in a.u.), with ($E_{\text{total}}^{\text{ZPE}}$, given in a.u.) taking into account for zero-point harmonic vibrations and total enthalpies (H_{total}^{298} , given in a.u.), stabilization energies without (E_{stab} , given in kcal/mol), with ($E_{\text{stab}}^{\text{ZPE}}$, given in kcal/mol) taking into account the energies of zero-point harmonic vibrations and relative enthalpies (ΔH^{298} , given in kcal/mol) calculated by DFT B3LYP/def2tzvp method.

| Structure | E_{total} | E_{stab} | $E_{\text{total}}^{\text{ZPE}}$ | $E_{\text{stab}}^{\text{ZPE}}$ | H_{total}^{298} | ΔH^{298} |
|-------------------------------------------------------|--------------------|-------------------|---------------------------------|--------------------------------|--------------------------|------------------|
| 4-Cyanopyridine | -340.6525191 | | -340.565324 | | -340.558403 | |
| 3-Cyanopyridine | -340.6538251 | | -340.566602 | | -340.559675 | |
| Pyridine | -248.3789962 | | -248.290394 | | -248.285181 | |
| 2-Cyanopyridine | -340.6519659 | | -340.564919 | | -340.558000 | |
| 2,6-Dicyanopyridine | -432.9206996 | | -432.835399 | | -432.826696 | |
| 3,5-di-tert-butylcatecholate germanium complex | -3469.652377 | | -3469.029081 | | -3468.992438 | |
| Complex 1 | -4150.993055 | -22.4 | -4150.191583 | -20.0 | -4150.139849 | -19.2 |
| Complex 2 | -4150.993910 | -21.3 | -4150.192272 | -18.8 | -4150.140586 | -18.1 |
| Complex 3 | -3966.453661 | -27.2 | -3965.648752 | -24.4 | -3965.600834 | -23.9 |
| Complex 4 | -4150.972501 | -10.2 | -4150.171541 | -7.9 | -4150.119754 | -7.1 |
| Complex 5 | -4335.476352 | 10.9 | -4334.680056 | 12.4 | -4334.624041 | 13.7 |

Table S2. Total energies without ($E_{\text{total}}^{\text{S}}$, given in a.u.), with ($E_{\text{total}}^{\text{S,ZPE}}$, given in a.u.) taking into account for zero-point harmonic vibrations and total enthalpies ($H_{\text{total}}^{\text{S},298}$, given in a.u.), stabilization energies without ($E_{\text{stab}}^{\text{S}}$, given in kcal/mol), with ($E_{\text{stab}}^{\text{S,ZPE}}$, given in kcal/mol) taking into account the energies of zero-point harmonic vibrations and relative enthalpies ($\Delta H^{\text{S},298}$, given in kcal/mol) taking into account the nonspecific solvation (SMD, solvent – toluene) calculated by DFT B3LYP/def2tzvp method.

| Structure | $E_{\text{Total}}^{\text{S}}$ | $E_{\text{stab}}^{\text{S}}$ | $E_{\text{total}}^{\text{S,ZPE}}$ | $E_{\text{stab}}^{\text{S,ZPE}}$ | $H_{\text{total}}^{\text{S},298}$ | $\Delta H^{\text{S},298}$ |
|-------------------------------------------------------|-------------------------------|------------------------------|-----------------------------------|----------------------------------|-----------------------------------|---------------------------|
| 4-Cyanopyridine | -340.661238 | | -340.573910 | | -340.567002 | |
| 3-Cyanopyridine | -340.662875 | | -340.575532 | | -340.568614 | |
| Pyridine | -248.386621 | | -248.297919 | | -248.292711 | |
| 2-Cyanopyridine | -340.661209 | | -340.574029 | | -340.567119 | |
| 2,6-Dicyanopyridine | -432.931225 | | -432.845795 | | -432.837110 | |
| 3,5-di-tert-butylcatecholate germanium complex | -3469.672597 | | -3469.049484 | | -3469.012902 | |
| Complex 1 | -4151.030848 | -22.4 | -4150.229522 | -20.2 | -4150.177806 | -19.4 |
| Complex 2 | -4151.032516 | -21.4 | -4150.230777 | -19.0 | -4150.179171 | -18.2 |
| Complex 3 | -3966.489043 | -27.1 | -3965.684423 | -24.5 | -3965.636451 | -23.9 |
| Complex 4 | -4151.010545 | -9.7 | -4150.209710 | -7.6 | -4150.158006 | -6.8 |
| Complex 5 | -4335.516877 | 11.4 | -4334.720634 | 12.8 | -4334.665541 | 13.5 |

Optimized geometries calculated by DFT B3LYP/def2tzvp

4-Cyanopyridine

| | | | |
|---|--------------|--------------|--------------|
| 7 | 0.000000000 | 0.000000000 | -2.189552000 |
| 6 | 0.000440000 | 1.140691000 | -1.500062000 |
| 1 | 0.000066000 | 2.055423000 | -2.082792000 |
| 6 | 0.000000000 | 1.200662000 | -0.113107000 |
| 1 | -0.000201000 | 2.150579000 | 0.402865000 |
| 6 | 0.000000000 | 0.000000000 | 0.598588000 |
| 6 | 0.000000000 | -1.200662000 | -0.113107000 |
| 1 | 0.000201000 | -2.150579000 | 0.402865000 |
| 6 | -0.000440000 | -1.140691000 | -1.500062000 |
| 1 | -0.000066000 | -2.055423000 | -2.082792000 |
| 6 | 0.000000000 | 0.000000000 | 2.030054000 |
| 7 | 0.000000000 | 0.000000000 | 3.181843000 |

3-Cyanopyridine

| | | | |
|---|--------------|--------------|--------------|
| 7 | -1.444134000 | -1.246590000 | -0.000025000 |
| 6 | -0.118362000 | -1.186499000 | 0.000178000 |
| 1 | 0.418131000 | -2.128828000 | 0.000090000 |
| 6 | 0.592333000 | 0.020636000 | 0.000021000 |
| 6 | -0.128500000 | 1.217394000 | 0.000068000 |
| 1 | 0.391407000 | 2.166001000 | 0.000100000 |
| 6 | -1.511249000 | 1.152755000 | 0.000024000 |
| 1 | -2.109749000 | 2.053626000 | 0.000124000 |
| 6 | -2.121308000 | -0.097510000 | -0.000161000 |
| 1 | -3.202963000 | -0.179706000 | -0.000143000 |
| 6 | 2.020639000 | 0.017565000 | -0.000033000 |
| 7 | 3.172971000 | 0.009855000 | -0.000083000 |

Pyridine

| | | | |
|---|--------------|--------------|--------------|
| 7 | 0.000004000 | 1.412081000 | 0.000000000 |
| 6 | 1.139485000 | 0.719764000 | -0.000443000 |
| 1 | 2.054442000 | 1.303688000 | 0.000209000 |
| 6 | 1.193796000 | -0.669726000 | 0.000185000 |
| 1 | 2.149004000 | -1.178456000 | 0.000595000 |
| 6 | -0.000004000 | -1.378943000 | 0.000000000 |
| 1 | -0.000007000 | -2.461921000 | 0.000000000 |
| 6 | -1.193799000 | -0.669720000 | -0.000185000 |
| 1 | -2.149010000 | -1.178446000 | -0.000594000 |
| 6 | -1.139482000 | 0.719770000 | 0.000443000 |
| 1 | -2.054435000 | 1.303700000 | -0.000209000 |

2-Cyanopyridine

| | | | |
|---|-------------|--------------|--------------|
| 7 | 0.044590000 | -1.206201000 | -0.000081000 |
| 6 | 1.373735000 | -1.204892000 | 0.000100000 |

| | | | |
|---|--------------|--------------|--------------|
| 6 | 2.140873000 | -0.042991000 | -0.000007000 |
| 1 | 3.220951000 | -0.104406000 | -0.000020000 |
| 6 | 1.490355000 | 1.182679000 | 0.000013000 |
| 1 | 2.050878000 | 2.108498000 | 0.000068000 |
| 6 | 0.103566000 | 1.202943000 | -0.000021000 |
| 1 | -0.451746000 | 2.130567000 | 0.000002000 |
| 6 | -0.570878000 | -0.019208000 | -0.000052000 |
| 6 | -2.011728000 | -0.033112000 | -0.000028000 |
| 7 | -3.162549000 | -0.003504000 | 0.000065000 |
| 1 | 1.850091000 | -2.179238000 | 0.000026000 |

2,6-Dicyanopyridine

| | | | |
|---|--------------|--------------|--------------|
| 7 | 0.000001000 | 0.751080000 | -0.000006000 |
| 6 | 1.138496000 | 0.057697000 | -0.000083000 |
| 6 | 1.194517000 | -1.338874000 | -0.000017000 |
| 1 | 2.150455000 | -1.843438000 | 0.000041000 |
| 6 | -0.000001000 | -2.041945000 | 0.000003000 |
| 1 | -0.000003000 | -3.123746000 | 0.000004000 |
| 6 | -1.194518000 | -1.338871000 | 0.000018000 |
| 1 | -2.150458000 | -1.843433000 | -0.000034000 |
| 6 | -1.138496000 | 0.057698000 | 0.000072000 |
| 6 | 2.362473000 | 0.816917000 | 0.000030000 |
| 7 | 3.363788000 | 1.383986000 | 0.000011000 |
| 6 | -2.362472000 | 0.816917000 | -0.000033000 |
| 7 | -3.363786000 | 1.383987000 | 0.000001000 |

3,5-di-tert-butylcatecholate germanium complex

| | | | |
|----|--------------|--------------|--------------|
| 32 | -0.000020000 | 0.000013000 | -0.272938000 |
| 8 | -1.222862000 | -0.907792000 | 0.651315000 |
| 8 | -1.209281000 | 0.932041000 | -1.187263000 |
| 6 | -2.476371000 | -0.473503000 | 0.232562000 |
| 6 | -2.458559000 | 0.515931000 | -0.756099000 |
| 6 | -3.620260000 | 1.046196000 | -1.271697000 |
| 1 | -3.547113000 | 1.808793000 | -2.034593000 |
| 6 | -4.850495000 | 0.583491000 | -0.794619000 |
| 6 | -4.843562000 | -0.404055000 | 0.191508000 |
| 1 | -5.788602000 | -0.762953000 | 0.561229000 |
| 6 | -3.678023000 | -0.964927000 | 0.737553000 |
| 6 | -6.149030000 | 1.173872000 | -1.368590000 |
| 6 | -6.181663000 | 2.694559000 | -1.108980000 |
| 1 | -7.097732000 | 3.129518000 | -1.516012000 |
| 1 | -5.336903000 | 3.203750000 | -1.574404000 |
| 1 | -6.151120000 | 2.907640000 | -0.038579000 |
| 6 | -6.203000000 | 0.917004000 | -2.889138000 |
| 1 | -6.187861000 | -0.153344000 | -3.104098000 |
| 1 | -5.358869000 | 1.373036000 | -3.407776000 |

| | | | |
|---|--------------|--------------|--------------|
| 1 | -7.119257000 | 1.335665000 | -3.312510000 |
| 6 | -7.406012000 | 0.557086000 | -0.737601000 |
| 1 | -8.295112000 | 1.010546000 | -1.179867000 |
| 1 | -7.449275000 | 0.731788000 | 0.339104000 |
| 1 | -7.464216000 | -0.518782000 | -0.913078000 |
| 6 | -3.718173000 | -2.052504000 | 1.823515000 |
| 6 | -3.003916000 | -1.546997000 | 3.095586000 |
| 1 | -3.495844000 | -0.653140000 | 3.485196000 |
| 1 | -1.959860000 | -1.306595000 | 2.904825000 |
| 1 | -3.038332000 | -2.315029000 | 3.872074000 |
| 6 | -3.024435000 | -3.331704000 | 1.307569000 |
| 1 | -1.981234000 | -3.152529000 | 1.054887000 |
| 1 | -3.531363000 | -3.714177000 | 0.419041000 |
| 1 | -3.058618000 | -4.109019000 | 2.074774000 |
| 6 | -5.156444000 | -2.427168000 | 2.214100000 |
| 1 | -5.127132000 | -3.199648000 | 2.984652000 |
| 1 | -5.720095000 | -2.827486000 | 1.369332000 |
| 1 | -5.705591000 | -1.576775000 | 2.622607000 |
| 8 | 1.222855000 | 0.908061000 | 0.651039000 |
| 8 | 1.209212000 | -0.932257000 | -1.187051000 |
| 6 | 2.476351000 | 0.473629000 | 0.232397000 |
| 6 | 2.458504000 | -0.516067000 | -0.756001000 |
| 6 | 3.620185000 | -1.046508000 | -1.271464000 |
| 1 | 3.547011000 | -1.809307000 | -2.034154000 |
| 6 | 4.850438000 | -0.583729000 | -0.794510000 |
| 6 | 4.843544000 | 0.404081000 | 0.191353000 |
| 1 | 5.788598000 | 0.763046000 | 0.560982000 |
| 6 | 3.678033000 | 0.965149000 | 0.737244000 |
| 6 | 6.148949000 | -1.174342000 | -1.368299000 |
| 6 | 6.202946000 | -0.917962000 | -2.888928000 |
| 1 | 7.119186000 | -1.336805000 | -3.312152000 |
| 1 | 5.358802000 | -1.374118000 | -3.407435000 |
| 1 | 6.187864000 | 0.152318000 | -3.104230000 |
| 6 | 6.181503000 | -2.694949000 | -1.108205000 |
| 1 | 6.150941000 | -2.907687000 | -0.037735000 |
| 1 | 5.336714000 | -3.204237000 | -1.573471000 |
| 1 | 7.097550000 | -3.130089000 | -1.515092000 |
| 6 | 7.405957000 | -0.557411000 | -0.737505000 |
| 1 | 8.295039000 | -1.011021000 | -1.179654000 |
| 1 | 7.464182000 | 0.518407000 | -0.913289000 |
| 1 | 7.449236000 | -0.731806000 | 0.339249000 |
| 6 | 3.718280000 | 2.053010000 | 1.822921000 |
| 6 | 3.024802000 | 3.332203000 | 1.306603000 |
| 1 | 3.531826000 | 3.714321000 | 0.417977000 |
| 1 | 1.981569000 | 3.153176000 | 1.053959000 |
| 1 | 3.059135000 | 4.109729000 | 2.073588000 |

| | | | |
|---|-------------|-------------|-------------|
| 6 | 3.003911000 | 1.547957000 | 3.095114000 |
| 1 | 1.959815000 | 1.307692000 | 2.904411000 |
| 1 | 3.495683000 | 0.654116000 | 3.484958000 |
| 1 | 3.038459000 | 2.316184000 | 3.871403000 |
| 6 | 5.156607000 | 2.427515000 | 2.213447000 |
| 1 | 5.127422000 | 3.200226000 | 2.983771000 |
| 1 | 5.705578000 | 1.577134000 | 2.622215000 |
| 1 | 5.720364000 | 2.827475000 | 1.368578000 |

Complex 1

| | | | |
|----|--------------|--------------|--------------|
| 32 | 0.000000000 | 0.000000000 | 0.000029000 |
| 8 | -1.276642000 | -1.339202000 | 0.000028000 |
| 8 | 1.306165000 | -1.311137000 | 0.000026000 |
| 7 | 0.000000000 | 0.000000000 | 2.184694000 |
| 6 | -0.682080000 | -2.565552000 | 0.000018000 |
| 6 | 0.724149000 | -2.544243000 | 0.000013000 |
| 6 | 1.461145000 | -3.712754000 | -0.000008000 |
| 1 | 2.540994000 | -3.638763000 | -0.000011000 |
| 6 | 0.806222000 | -4.949247000 | -0.000030000 |
| 6 | -0.588155000 | -4.948219000 | -0.000026000 |
| 1 | -1.100261000 | -5.895277000 | -0.000042000 |
| 6 | -1.371187000 | -3.781722000 | 0.000004000 |
| 6 | 1.636384000 | -6.243703000 | -0.000057000 |
| 6 | 2.530653000 | -6.285800000 | -1.256970000 |
| 1 | 3.132041000 | -7.198505000 | -1.268174000 |
| 1 | 3.214184000 | -5.436587000 | -1.295024000 |
| 1 | 1.924521000 | -6.267589000 | -2.165070000 |
| 6 | 2.530657000 | -6.285849000 | 1.256851000 |
| 1 | 1.924528000 | -6.267675000 | 2.164954000 |
| 1 | 3.214187000 | -5.436637000 | 1.294938000 |
| 1 | 3.132046000 | -7.198554000 | 1.268018000 |
| 6 | 0.761526000 | -7.506084000 | -0.000081000 |
| 1 | 1.398897000 | -8.392712000 | -0.000101000 |
| 1 | 0.123865000 | -7.558971000 | -0.884499000 |
| 1 | 0.123870000 | -7.559008000 | 0.884338000 |
| 6 | -2.908657000 | -3.833176000 | 0.000002000 |
| 6 | -3.456421000 | -3.130119000 | -1.260624000 |
| 1 | -3.097647000 | -3.627264000 | -2.164791000 |
| 1 | -3.149895000 | -2.086489000 | -1.295218000 |
| 1 | -4.548988000 | -3.167055000 | -1.267600000 |
| 6 | -3.456422000 | -3.130470000 | 1.260822000 |
| 1 | -3.149912000 | -2.086845000 | 1.295701000 |
| 1 | -3.097636000 | -3.627857000 | 2.164851000 |
| 1 | -4.548989000 | -3.167423000 | 1.267796000 |
| 6 | -3.446034000 | -5.272948000 | -0.000195000 |
| 1 | -4.537659000 | -5.248762000 | -0.000172000 |

| | | | |
|---|--------------|--------------|--------------|
| 1 | -3.129618000 | -5.828644000 | 0.884522000 |
| 1 | -3.129651000 | -5.828391000 | -0.885082000 |
| 6 | 1.100551000 | -0.355602000 | 2.855268000 |
| 1 | 1.950724000 | -0.638905000 | 2.250583000 |
| 6 | 1.144592000 | -0.369303000 | 4.237801000 |
| 1 | 2.047690000 | -0.662063000 | 4.753133000 |
| 6 | 0.000000000 | 0.000000000 | 4.946137000 |
| 6 | -1.144592000 | 0.369303000 | 4.237801000 |
| 1 | -2.047690000 | 0.662063000 | 4.753133000 |
| 6 | -1.100551000 | 0.355602000 | 2.855268000 |
| 1 | -1.950724000 | 0.638905000 | 2.250583000 |
| 8 | 1.276642000 | 1.339202000 | 0.000028000 |
| 8 | -1.306165000 | 1.311137000 | 0.000026000 |
| 7 | 0.000000000 | 0.000000000 | -2.184640000 |
| 6 | 0.682080000 | 2.565552000 | 0.000018000 |
| 6 | -0.724149000 | 2.544243000 | 0.000013000 |
| 6 | -1.461145000 | 3.712754000 | -0.000008000 |
| 1 | -2.540994000 | 3.638763000 | -0.000011000 |
| 6 | -0.806222000 | 4.949247000 | -0.000030000 |
| 6 | 0.588155000 | 4.948219000 | -0.000026000 |
| 1 | 1.100261000 | 5.895277000 | -0.000042000 |
| 6 | 1.371187000 | 3.781722000 | 0.000004000 |
| 6 | -1.636384000 | 6.243703000 | -0.000057000 |
| 6 | -2.530657000 | 6.285849000 | 1.256851000 |
| 1 | -3.132046000 | 7.198554000 | 1.268018000 |
| 1 | -3.214187000 | 5.436637000 | 1.294938000 |
| 1 | -1.924528000 | 6.267675000 | 2.164954000 |
| 6 | -2.530653000 | 6.285800000 | -1.256970000 |
| 1 | -1.924521000 | 6.267589000 | -2.165070000 |
| 1 | -3.214184000 | 5.436587000 | -1.295024000 |
| 1 | -3.132041000 | 7.198505000 | -1.268174000 |
| 6 | -0.761526000 | 7.506084000 | -0.000081000 |
| 1 | -1.398897000 | 8.392712000 | -0.000101000 |
| 1 | -0.123870000 | 7.559008000 | 0.884338000 |
| 1 | -0.123865000 | 7.558971000 | -0.884499000 |
| 6 | 2.908657000 | 3.833176000 | 0.000002000 |
| 6 | 3.456422000 | 3.130470000 | 1.260822000 |
| 1 | 3.097636000 | 3.627857000 | 2.164851000 |
| 1 | 3.149912000 | 2.086845000 | 1.295701000 |
| 1 | 4.548989000 | 3.167423000 | 1.267796000 |
| 6 | 3.456421000 | 3.130119000 | -1.260624000 |
| 1 | 3.149895000 | 2.086489000 | -1.295218000 |
| 1 | 3.097647000 | 3.627264000 | -2.164791000 |
| 1 | 4.548988000 | 3.167055000 | -1.267600000 |
| 6 | 3.446034000 | 5.272948000 | -0.000195000 |
| 1 | 4.537659000 | 5.248762000 | -0.000172000 |

| | | | |
|---|--------------|--------------|--------------|
| 1 | 3.129651000 | 5.828391000 | -0.885082000 |
| 1 | 3.129618000 | 5.828644000 | 0.884522000 |
| 6 | -1.100555000 | 0.355592000 | -2.855215000 |
| 1 | -1.950730000 | 0.638886000 | -2.250529000 |
| 6 | -1.144595000 | 0.369293000 | -4.237747000 |
| 1 | -2.047695000 | 0.662044000 | -4.753079000 |
| 6 | 0.000000000 | 0.000000000 | -4.946083000 |
| 6 | 1.144595000 | -0.369293000 | -4.237747000 |
| 1 | 2.047695000 | -0.662044000 | -4.753079000 |
| 6 | 1.100555000 | -0.355592000 | -2.855215000 |
| 1 | 1.950730000 | -0.638886000 | -2.250529000 |
| 6 | 0.000000000 | 0.000000000 | -6.377313000 |
| 7 | 0.000000000 | 0.000000000 | -7.528703000 |
| 6 | 0.000000000 | 0.000000000 | 6.377368000 |
| 7 | 0.000000000 | 0.000000000 | 7.528757000 |

Complex 2

| | | | |
|----|--------------|--------------|--------------|
| 32 | 0.000000000 | 0.000000000 | 0.000000000 |
| 8 | 1.218250000 | -0.779246000 | 1.152560000 |
| 8 | 1.421566000 | 0.665437000 | -0.978433000 |
| 7 | -0.001514000 | 1.813406000 | 1.228910000 |
| 6 | 2.493423000 | -0.506855000 | 0.754582000 |
| 6 | 2.598195000 | 0.280069000 | -0.405918000 |
| 6 | 3.827720000 | 0.635871000 | -0.925593000 |
| 1 | 3.850687000 | 1.245471000 | -1.819601000 |
| 6 | 5.000430000 | 0.209307000 | -0.292800000 |
| 6 | 4.874519000 | -0.570573000 | 0.856307000 |
| 1 | 5.771912000 | -0.902861000 | 1.349656000 |
| 6 | 3.642740000 | -0.951345000 | 1.414398000 |
| 6 | 6.363968000 | 0.612723000 | -0.878321000 |
| 6 | 6.488039000 | 0.076785000 | -2.320116000 |
| 1 | 7.450751000 | 0.361698000 | -2.752335000 |
| 1 | 5.703428000 | 0.471816000 | -2.966725000 |
| 1 | 6.417712000 | -1.012876000 | -2.336466000 |
| 6 | 6.483445000 | 2.151059000 | -0.899888000 |
| 1 | 6.409979000 | 2.560262000 | 0.109742000 |
| 1 | 5.698427000 | 2.609466000 | -1.502520000 |
| 1 | 7.446054000 | 2.453987000 | -1.319924000 |
| 6 | 7.542855000 | 0.057874000 | -0.065108000 |
| 1 | 8.482959000 | 0.372291000 | -0.523030000 |
| 1 | 7.539286000 | -1.033407000 | -0.035991000 |
| 1 | 7.537662000 | 0.426972000 | 0.962187000 |
| 6 | 3.555984000 | -1.812727000 | 2.686019000 |
| 6 | 2.809168000 | -3.128252000 | 2.378554000 |
| 1 | 3.338156000 | -3.701377000 | 1.613701000 |
| 1 | 1.797163000 | -2.935654000 | 2.028023000 |

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| 1 | 2.747503000 | -3.746060000 | 3.278201000 |
| 6 | 2.804284000 | -1.040125000 | 3.791352000 |
| 1 | 1.792062000 | -0.790183000 | 3.479383000 |
| 1 | 3.329749000 | -0.114946000 | 4.039297000 |
| 1 | 2.743280000 | -1.646225000 | 4.699108000 |
| 6 | 4.941796000 | -2.182666000 | 3.237901000 |
| 1 | 4.819608000 | -2.791179000 | 4.136198000 |
| 1 | 5.522015000 | -1.300332000 | 3.514607000 |
| 1 | 5.525140000 | -2.765841000 | 2.522882000 |
| 6 | 0.449312000 | 2.959926000 | 0.722790000 |
| 1 | 0.808828000 | 2.928077000 | -0.296497000 |
| 6 | 0.463034000 | 4.133570000 | 1.475707000 |
| 6 | -0.008173000 | 4.094479000 | 2.790909000 |
| 1 | -0.006308000 | 4.992966000 | 3.393055000 |
| 6 | -0.471639000 | 2.892843000 | 3.297945000 |
| 1 | -0.845201000 | 2.821126000 | 4.309467000 |
| 6 | -0.454461000 | 1.768850000 | 2.486889000 |
| 1 | -0.810543000 | 0.804754000 | 2.822717000 |
| 8 | -1.218250000 | 0.779246000 | -1.152560000 |
| 8 | -1.421566000 | -0.665437000 | 0.978433000 |
| 7 | 0.001514000 | -1.813406000 | -1.228910000 |
| 6 | -2.493423000 | 0.506855000 | -0.754582000 |
| 6 | -2.598195000 | -0.280069000 | 0.405918000 |
| 6 | -3.827720000 | -0.635871000 | 0.925593000 |
| 1 | -3.850687000 | -1.245471000 | 1.819601000 |
| 6 | -5.000430000 | -0.209307000 | 0.292800000 |
| 6 | -4.874519000 | 0.570573000 | -0.856307000 |
| 1 | -5.771912000 | 0.902861000 | -1.349656000 |
| 6 | -3.642740000 | 0.951345000 | -1.414398000 |
| 6 | -6.363968000 | -0.612723000 | 0.878321000 |
| 6 | -6.488039000 | -0.076785000 | 2.320116000 |
| 1 | -7.450751000 | -0.361698000 | 2.752335000 |
| 1 | -5.703428000 | -0.471816000 | 2.966725000 |
| 1 | -6.417712000 | 1.012876000 | 2.336466000 |
| 6 | -6.483445000 | -2.151059000 | 0.899888000 |
| 1 | -6.409979000 | -2.560262000 | -0.109742000 |
| 1 | -5.698427000 | -2.609466000 | 1.502520000 |
| 1 | -7.446054000 | -2.453987000 | 1.319924000 |
| 6 | -7.542855000 | -0.057874000 | 0.065108000 |
| 1 | -8.482959000 | -0.372291000 | 0.523030000 |
| 1 | -7.539286000 | 1.033407000 | 0.035991000 |
| 1 | -7.537662000 | -0.426972000 | -0.962187000 |
| 6 | -3.555984000 | 1.812727000 | -2.686019000 |
| 6 | -2.809168000 | 3.128252000 | -2.378554000 |
| 1 | -3.338156000 | 3.701377000 | -1.613701000 |
| 1 | -1.797163000 | 2.935654000 | -2.028023000 |

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| 1 | -2.747503000 | 3.746060000 | -3.278201000 |
| 6 | -2.804284000 | 1.040125000 | -3.791352000 |
| 1 | -1.792062000 | 0.790183000 | -3.479383000 |
| 1 | -3.329749000 | 0.114946000 | -4.039297000 |
| 1 | -2.743280000 | 1.646225000 | -4.699108000 |
| 6 | -4.941796000 | 2.182666000 | -3.237901000 |
| 1 | -4.819608000 | 2.791179000 | -4.136198000 |
| 1 | -5.522015000 | 1.300332000 | -3.514607000 |
| 1 | -5.525140000 | 2.765841000 | -2.522882000 |
| 6 | -0.449312000 | -2.959926000 | -0.722790000 |
| 1 | -0.808828000 | -2.928077000 | 0.296497000 |
| 6 | -0.463034000 | -4.133570000 | -1.475707000 |
| 6 | 0.008173000 | -4.094479000 | -2.790909000 |
| 1 | 0.006308000 | -4.992966000 | -3.393055000 |
| 6 | 0.471639000 | -2.892843000 | -3.297945000 |
| 1 | 0.845201000 | -2.821126000 | -4.309467000 |
| 6 | 0.454461000 | -1.768850000 | -2.486889000 |
| 1 | 0.810543000 | -0.804754000 | -2.822717000 |
| 6 | 0.953592000 | 5.347381000 | 0.903362000 |
| 7 | 1.346147000 | 6.330754000 | 0.450493000 |
| 6 | -0.953592000 | -5.347381000 | -0.903362000 |
| 7 | -1.346147000 | -6.330754000 | -0.450493000 |

Complex 3

| | | | |
|----|--------------|--------------|--------------|
| 32 | 0.000000000 | 0.000032000 | 0.000004000 |
| 8 | -1.345683000 | 0.134747000 | -1.271167000 |
| 8 | -1.314604000 | -0.139494000 | 1.300624000 |
| 7 | -0.001256000 | 2.156135000 | 0.229416000 |
| 6 | -2.567921000 | 0.071541000 | -0.677133000 |
| 6 | -2.544469000 | -0.078040000 | 0.722580000 |
| 6 | -3.713663000 | -0.156598000 | 1.454790000 |
| 1 | -3.638066000 | -0.271650000 | 2.528483000 |
| 6 | -4.951469000 | -0.086754000 | 0.805569000 |
| 6 | -4.952819000 | 0.062102000 | -0.580375000 |
| 1 | -5.900331000 | 0.117142000 | -1.088779000 |
| 6 | -3.785963000 | 0.145326000 | -1.359222000 |
| 6 | -6.244433000 | -0.175921000 | 1.633422000 |
| 6 | -6.286769000 | -1.522595000 | 2.385819000 |
| 1 | -7.197891000 | -1.598502000 | 2.985409000 |
| 1 | -5.435004000 | -1.635910000 | 3.057642000 |
| 1 | -6.271089000 | -2.358908000 | 1.683832000 |
| 6 | -6.284350000 | 0.975903000 | 2.659627000 |
| 1 | -6.266003000 | 1.944391000 | 2.155497000 |
| 1 | -5.433173000 | 0.939010000 | 3.340663000 |
| 1 | -7.195949000 | 0.922351000 | 3.260880000 |
| 6 | -7.508764000 | -0.079553000 | 0.766708000 |

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| 1 | -8.394482000 | -0.147855000 | 1.402028000 |
| 1 | -7.563430000 | -0.889203000 | 0.036561000 |
| 1 | -7.561044000 | 0.868840000 | 0.228687000 |
| 6 | -3.838583000 | 0.309590000 | -2.887969000 |
| 6 | -3.136966000 | -0.885681000 | -3.567990000 |
| 1 | -3.636344000 | -1.822281000 | -3.309318000 |
| 1 | -2.094523000 | -0.955429000 | -3.263987000 |
| 1 | -3.171811000 | -0.774383000 | -4.655257000 |
| 6 | -3.134615000 | 1.620779000 | -3.298543000 |
| 1 | -2.092334000 | 1.622597000 | -2.986084000 |
| 1 | -3.632752000 | 2.481954000 | -2.847160000 |
| 1 | -3.168795000 | 1.742842000 | -4.384676000 |
| 6 | -5.278424000 | 0.368252000 | -3.422208000 |
| 1 | -5.254317000 | 0.484667000 | -4.507798000 |
| 1 | -5.833309000 | 1.214568000 | -3.012717000 |
| 1 | -5.834829000 | -0.544726000 | -3.201476000 |
| 6 | -0.307909000 | 2.706347000 | 1.409418000 |
| 1 | -0.553737000 | 2.012953000 | 2.201373000 |
| 6 | -0.317945000 | 4.078853000 | 1.594579000 |
| 1 | -0.571125000 | 4.487139000 | 2.563035000 |
| 6 | -0.002002000 | 4.902129000 | 0.522140000 |
| 1 | -0.002276000 | 5.978565000 | 0.636882000 |
| 6 | 0.314248000 | 4.323600000 | -0.699763000 |
| 1 | 0.567216000 | 4.927001000 | -1.560360000 |
| 6 | 0.305036000 | 2.942906000 | -0.808090000 |
| 1 | 0.551498000 | 2.432272000 | -1.728363000 |
| 8 | 1.345685000 | -0.134683000 | 1.271175000 |
| 8 | 1.314604000 | 0.139555000 | -1.300618000 |
| 7 | 0.001256000 | -2.156076000 | -0.229410000 |
| 6 | 2.567922000 | -0.071521000 | 0.677135000 |
| 6 | 2.544470000 | 0.078058000 | -0.722578000 |
| 6 | 3.713666000 | 0.156573000 | -1.454791000 |
| 1 | 3.638070000 | 0.271627000 | -2.528484000 |
| 6 | 4.951471000 | 0.086691000 | -0.805573000 |
| 6 | 4.952821000 | -0.062157000 | 0.580372000 |
| 1 | 5.900332000 | -0.117221000 | 1.088777000 |
| 6 | 3.785963000 | -0.145343000 | 1.359219000 |
| 6 | 6.244436000 | 0.175821000 | -1.633429000 |
| 6 | 6.286792000 | 1.522481000 | -2.385851000 |
| 1 | 7.197912000 | 1.598361000 | -2.985446000 |
| 1 | 5.435026000 | 1.635797000 | -3.057673000 |
| 1 | 6.271128000 | 2.358807000 | -1.683879000 |
| 6 | 6.284335000 | -0.976022000 | -2.659612000 |
| 1 | 6.265969000 | -1.944501000 | -2.155465000 |
| 1 | 5.433160000 | -0.939126000 | -3.340651000 |
| 1 | 7.195936000 | -0.922498000 | -3.260864000 |

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| 6 | 7.508766000 | 0.079450000 | -0.766714000 |
| 1 | 8.394485000 | 0.147726000 | -1.402036000 |
| 1 | 7.563445000 | 0.889113000 | -0.036582000 |
| 1 | 7.561031000 | -0.868934000 | -0.228675000 |
| 6 | 3.838578000 | -0.309594000 | 2.887966000 |
| 6 | 3.136996000 | 0.885704000 | 3.567977000 |
| 1 | 3.636404000 | 1.822287000 | 3.309301000 |
| 1 | 2.094558000 | 0.955481000 | 3.263967000 |
| 1 | 3.171832000 | 0.774413000 | 4.655245000 |
| 6 | 3.134574000 | -1.620761000 | 3.298549000 |
| 1 | 2.092295000 | -1.622551000 | 2.986084000 |
| 1 | 3.632690000 | -2.481953000 | 2.847175000 |
| 1 | 3.168744000 | -1.742816000 | 4.384683000 |
| 6 | 5.278419000 | -0.368291000 | 3.422199000 |
| 1 | 5.254313000 | -0.484716000 | 4.507789000 |
| 1 | 5.833283000 | -1.214615000 | 3.012697000 |
| 1 | 5.834840000 | 0.544678000 | 3.201473000 |
| 6 | 0.307922000 | -2.706289000 | -1.409409000 |
| 1 | 0.553759000 | -2.012895000 | -2.201360000 |
| 6 | 0.317960000 | -4.078795000 | -1.594569000 |
| 1 | 0.571151000 | -4.487082000 | -2.563022000 |
| 6 | 0.002003000 | -4.902071000 | -0.522134000 |
| 1 | 0.002276000 | -5.978507000 | -0.636877000 |
| 6 | -0.314262000 | -4.323542000 | 0.699764000 |
| 1 | -0.567242000 | -4.926942000 | 1.560358000 |
| 6 | -0.305049000 | -2.942848000 | 0.808092000 |
| 1 | -0.551522000 | -2.432212000 | 1.728362000 |

Complex 4

| | | | |
|----|--------------|--------------|--------------|
| 32 | 0.000012000 | -0.000017000 | 0.000025000 |
| 8 | 1.325763000 | 1.029446000 | 0.775735000 |
| 8 | 1.311962000 | -0.942745000 | -0.873183000 |
| 7 | -0.123799000 | 1.394939000 | -1.770349000 |
| 6 | 2.559274000 | 0.591719000 | 0.388931000 |
| 6 | 2.542587000 | -0.483905000 | -0.515016000 |
| 6 | 3.709905000 | -1.040690000 | -0.999435000 |
| 1 | 3.633894000 | -1.872492000 | -1.687128000 |
| 6 | 4.944156000 | -0.526962000 | -0.588316000 |
| 6 | 4.940631000 | 0.538787000 | 0.311052000 |
| 1 | 5.886955000 | 0.937859000 | 0.633760000 |
| 6 | 3.773843000 | 1.127727000 | 0.827600000 |
| 6 | 6.240118000 | -1.152337000 | -1.130680000 |
| 6 | 6.303796000 | -2.640572000 | -0.727531000 |
| 1 | 7.215967000 | -3.103070000 | -1.113850000 |
| 1 | 5.453890000 | -3.201570000 | -1.117762000 |
| 1 | 6.302965000 | -2.747673000 | 0.359233000 |

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| 6 | 6.262797000 | -1.045511000 | -2.669904000 |
| 1 | 6.227356000 | -0.000996000 | -2.986652000 |
| 1 | 5.414756000 | -1.560521000 | -3.122719000 |
| 1 | 7.176768000 | -1.491634000 | -3.070765000 |
| 6 | 7.500812000 | -0.460907000 | -0.590775000 |
| 1 | 8.388420000 | -0.940811000 | -1.008418000 |
| 1 | 7.569458000 | -0.531271000 | 0.496422000 |
| 1 | 7.535588000 | 0.594665000 | -0.867112000 |
| 6 | 3.830369000 | 2.300659000 | 1.821435000 |
| 6 | 3.124718000 | 1.909245000 | 3.137406000 |
| 1 | 3.610675000 | 1.043082000 | 3.593097000 |
| 1 | 2.077434000 | 1.670148000 | 2.965092000 |
| 1 | 3.172360000 | 2.736853000 | 3.849964000 |
| 6 | 3.133627000 | 3.536021000 | 1.214398000 |
| 1 | 2.085562000 | 3.339308000 | 1.002248000 |
| 1 | 3.626628000 | 3.837446000 | 0.287082000 |
| 1 | 3.184090000 | 4.377525000 | 1.910313000 |
| 6 | 5.272240000 | 2.702167000 | 2.171286000 |
| 1 | 5.250320000 | 3.532108000 | 2.880459000 |
| 1 | 5.829375000 | 3.035417000 | 1.293676000 |
| 1 | 5.825148000 | 1.884394000 | 2.637777000 |
| 6 | 0.032065000 | 0.788106000 | -2.949911000 |
| 6 | -0.044710000 | 1.464769000 | -4.158373000 |
| 1 | 0.089743000 | 0.921916000 | -5.083289000 |
| 6 | -0.294160000 | 2.827577000 | -4.146255000 |
| 1 | -0.362047000 | 3.389322000 | -5.068581000 |
| 6 | -0.455155000 | 3.466255000 | -2.926654000 |
| 1 | -0.649201000 | 4.527101000 | -2.862100000 |
| 6 | -0.363326000 | 2.718671000 | -1.753671000 |
| 8 | -1.325734000 | -1.029465000 | -0.775704000 |
| 8 | -1.311941000 | 0.942714000 | 0.873230000 |
| 7 | 0.123804000 | -1.394939000 | 1.770378000 |
| 6 | -2.559247000 | -0.591692000 | -0.388961000 |
| 6 | -2.542565000 | 0.483918000 | 0.515003000 |
| 6 | -3.709887000 | 1.040717000 | 0.999398000 |
| 1 | -3.633880000 | 1.872508000 | 1.687104000 |
| 6 | -4.944135000 | 0.526990000 | 0.588266000 |
| 6 | -4.940603000 | -0.538762000 | -0.311100000 |
| 1 | -5.886925000 | -0.937839000 | -0.633806000 |
| 6 | -3.773812000 | -1.127681000 | -0.827663000 |
| 6 | -6.240101000 | 1.152355000 | 1.130634000 |
| 6 | -6.303812000 | 2.640579000 | 0.727451000 |
| 1 | -7.215989000 | 3.103068000 | 1.113768000 |
| 1 | -5.453914000 | 3.201605000 | 1.117661000 |
| 1 | -6.302994000 | 2.747656000 | -0.359315000 |
| 6 | -6.262753000 | 1.045565000 | 2.669860000 |

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| 1 | -6.227296000 | 0.001057000 | 2.986632000 |
| 1 | -5.414708000 | 1.560593000 | 3.122648000 |
| 1 | -7.176721000 | 1.491689000 | 3.070727000 |
| 6 | -7.500790000 | 0.460890000 | 0.590763000 |
| 1 | -8.388400000 | 0.940802000 | 1.008393000 |
| 1 | -7.569443000 | 0.531208000 | -0.496436000 |
| 1 | -7.535555000 | -0.594671000 | 0.867145000 |
| 6 | -3.830325000 | -2.300651000 | -1.821454000 |
| 6 | -3.125473000 | -1.908996000 | -3.137782000 |
| 1 | -3.611980000 | -1.043020000 | -3.593242000 |
| 1 | -2.078192000 | -1.669514000 | -2.965999000 |
| 1 | -3.173173000 | -2.736631000 | -3.850303000 |
| 6 | -3.132766000 | -3.535693000 | -1.214705000 |
| 1 | -2.084692000 | -3.338503000 | -1.003024000 |
| 1 | -3.625216000 | -3.837320000 | -0.287162000 |
| 1 | -3.183160000 | -4.377233000 | -1.910582000 |
| 6 | -5.272195000 | -2.702771000 | -2.170606000 |
| 1 | -5.250266000 | -3.532655000 | -2.879845000 |
| 1 | -5.828745000 | -3.036329000 | -1.292742000 |
| 1 | -5.825695000 | -1.885207000 | -2.636761000 |
| 6 | -0.032018000 | -0.788086000 | 2.949936000 |
| 6 | 0.044730000 | -1.464746000 | 4.158401000 |
| 1 | -0.089682000 | -0.921879000 | 5.083315000 |
| 6 | 0.294096000 | -2.827569000 | 4.146290000 |
| 1 | 0.361954000 | -3.389313000 | 5.068619000 |
| 6 | 0.455037000 | -3.466268000 | 2.926691000 |
| 1 | 0.649009000 | -4.527127000 | 2.862143000 |
| 6 | 0.363246000 | -2.718687000 | 1.753704000 |
| 6 | -0.525476000 | 3.421655000 | -0.511353000 |
| 7 | -0.663795000 | 4.123783000 | 0.389653000 |
| 6 | 0.525317000 | -3.421688000 | 0.511386000 |
| 7 | 0.663549000 | -4.123831000 | -0.389622000 |
| 1 | 0.232113000 | -0.272798000 | -2.903151000 |
| 1 | -0.232016000 | 0.272825000 | 2.903160000 |

Complex 5

| | | | |
|----|--------------|--------------|--------------|
| 32 | 0.000005000 | 0.000007000 | 0.000079000 |
| 8 | -1.304785000 | -1.301646000 | 0.001513000 |
| 8 | -1.318816000 | 1.249241000 | -0.001178000 |
| 7 | -0.000261000 | -0.002212000 | -2.423525000 |
| 6 | -2.551738000 | -0.738914000 | 0.000907000 |
| 6 | -2.548302000 | 0.663177000 | -0.000585000 |
| 6 | -3.715300000 | 1.400450000 | -0.001390000 |
| 1 | -3.640842000 | 2.479407000 | -0.002537000 |
| 6 | -4.944098000 | 0.734258000 | -0.000667000 |
| 6 | -4.930570000 | -0.660865000 | 0.000846000 |

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| 1 | -5.874231000 | -1.178680000 | 0.001424000 |
| 6 | -3.761773000 | -1.441176000 | 0.001682000 |
| 6 | -6.245764000 | 1.552833000 | -0.001583000 |
| 6 | -6.293644000 | 2.448333000 | 1.254217000 |
| 1 | -7.210321000 | 3.043745000 | 1.263785000 |
| 1 | -5.448709000 | 3.136676000 | 1.292235000 |
| 1 | -6.272828000 | 1.842972000 | 2.162948000 |
| 6 | -6.293803000 | 2.445199000 | -1.259607000 |
| 1 | -6.273129000 | 1.837573000 | -2.166828000 |
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| 1 | -7.210464000 | 3.040614000 | -1.270535000 |
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| 6 | -3.118259000 | -3.527351000 | 1.262577000 |
| 1 | -3.601348000 | -3.150528000 | 2.167660000 |
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| 1 | -5.817401000 | -3.191093000 | 0.888552000 |
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| 6 | 0.210580000 | -1.131121000 | -3.121650000 |
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| | | | |
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| 1 | 3.176435000 | 4.620838000 | 1.271083000 |
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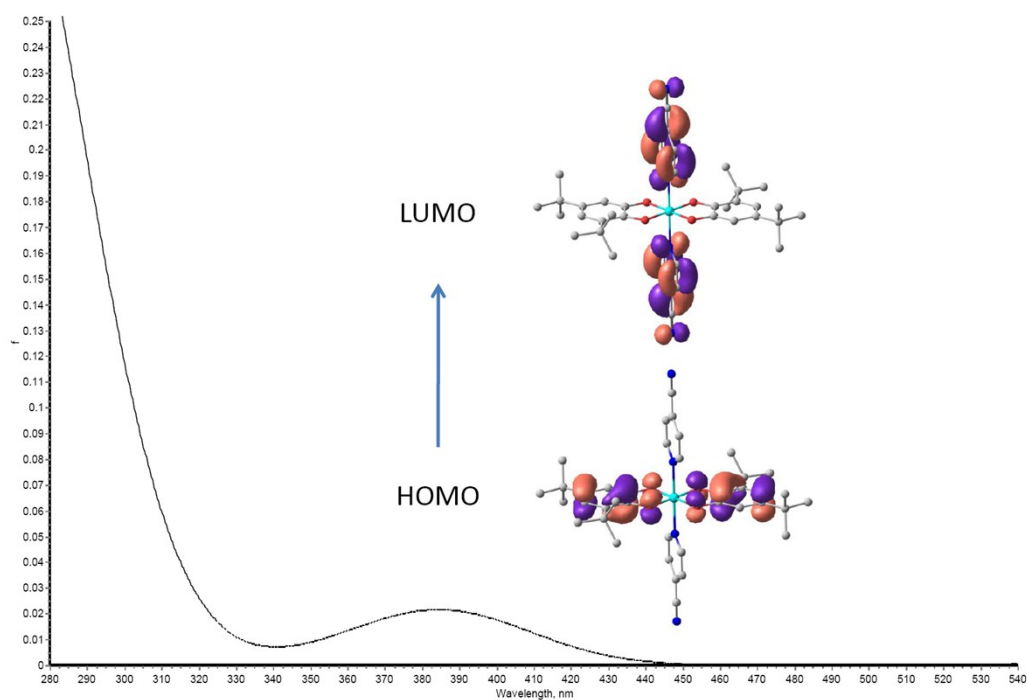


Figure S1. Electronic spectrum of **1** calculated by TD-DFT method (B3LYP/def2tzvp) with taking into account the non-specific solvation (SMD, solvent – toluene) and the shapes of molecular orbitals that dominate the long wavelength transitions in **1**, according to DFT B3LYP/def2tzvp calculations (cutoff=0.04 a.u.).