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Supplementary Material

Interaction of Triplet Excited States of Ketones with Nucleophilic Groups: (π,π^*) and (n,π^*) versus (σ^*,π^*) States. Substituent-Induced State Switching in Triplet Ketones

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Phenalenone 1, singlet ground state, optimized geometry (M05-2X/SDD)

6	0.550341000	-1.030057000	0.000000000
6	2.276529000	1.195014000	0.000000000
6	0.000000000	0.283674000	0.000000000
6	1.927736000	-1.208199000	0.000000000
6	2.796461000	-0.089358000	0.000000000
6	0.869437000	1.409577000	0.000000000
1	3.867585000	-0.243111000	0.000000000
1	2.937667000	2.054456000	0.000000000
6	0.308275000	2.721153000	0.000000000
1	0.973380000	3.577167000	0.000000000
6	-1.063182000	2.898686000	0.000000000
1	-1.483924000	3.895607000	0.000000000
6	-1.928162000	1.772911000	0.000000000
1	-3.002074000	1.921898000	0.000000000
6	-1.415008000	0.482563000	0.000000000
6	-0.346479000	-2.216591000	0.000000000
6	-1.795999000	-1.952249000	0.000000000
1	-2.438717000	-2.823241000	0.000000000
6	-2.286484000	-0.688584000	0.000000000
1	-3.357807000	-0.518180000	0.000000000
8	0.103467000	-3.389558000	0.000000000
1	2.315362000	-2.219363000	0.000000000

E(HF): -575.3006659

Phenalenone 1, singlet ground state, optimized geometry (M06/SDD)

6	0.542932000	-1.034741000	0.000000000
6	2.281505000	1.184908000	0.000000000
6	0.000000000	0.281730000	0.000000000
6	1.923195000	-1.215868000	0.000000000
6	2.795999000	-0.103857000	0.000000000
6	0.876923000	1.406440000	0.000000000
1	3.869401000	-0.262561000	0.000000000
1	2.947468000	2.044996000	0.000000000
6	0.322378000	2.719228000	0.000000000
1	0.995722000	3.573255000	0.000000000
6	-1.050474000	2.904800000	0.000000000
1	-1.466409000	3.906960000	0.000000000
6	-1.919446000	1.786108000	0.000000000
1	-2.996476000	1.938655000	0.000000000
6	-1.413864000	0.488367000	0.000000000
6	-0.357571000	-2.218470000	0.000000000
6	-1.801750000	-1.942053000	0.000000000
1	-2.451555000	-2.811939000	0.000000000
6	-2.288056000	-0.672697000	0.000000000
1	-3.361927000	-0.494382000	0.000000000
8	0.086013000	-3.395623000	0.000000000
1	2.305051000	-2.233371000	0.000000000

E(HF): -574.9385907

Phenalenone 1, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.537387000	-1.040437000	0.000000000
6	2.285928000	1.176332000	0.000000000
6	0.000000000	0.279685000	0.000000000
6	1.920569000	-1.223043000	0.000000000
6	2.797222000	-0.115403000	0.000000000
6	0.881963000	1.400793000	0.000000000
1	3.869411000	-0.277347000	0.000000000
1	2.954377000	2.033440000	0.000000000
6	0.334047000	2.717089000	0.000000000
1	1.011310000	3.567128000	0.000000000
6	-1.039141000	2.910368000	0.000000000
1	-1.449755000	3.913905000	0.000000000
6	-1.913326000	1.796310000	0.000000000
1	-2.988927000	1.953575000	0.000000000
6	-1.411884000	0.494475000	0.000000000
6	-0.369227000	-2.212900000	0.000000000
6	-1.805901000	-1.933413000	0.000000000
1	-2.467552000	-2.794471000	0.000000000
6	-2.289807000	-0.659406000	0.000000000
1	-3.362598000	-0.480171000	0.000000000
8	0.069491000	-3.402733000	0.000000000
1	2.310819000	-2.236901000	0.000000000

E(HF): -574.9506444

Phenalenone 1, singlet ground state, optimized geometry (M06/cc-pVTZ)

6	0.553216000	-1.019446000	0.000000000
6	2.246322000	1.197191000	0.000000000
6	0.000000000	0.278137000	0.000000000
6	1.919128000	-1.178504000	0.000000000
6	2.768515000	-0.068982000	0.000000000
6	0.854471000	1.403559000	0.000000000
1	3.840725000	-0.213630000	0.000000000
1	2.899617000	2.062194000	0.000000000
6	0.285772000	2.695776000	0.000000000
1	0.946729000	3.554588000	0.000000000
6	-1.070109000	2.861173000	0.000000000
1	-1.497489000	3.854920000	0.000000000
6	-1.915601000	1.743159000	0.000000000
1	-2.990927000	1.880357000	0.000000000
6	-1.404283000	0.466339000	0.000000000
6	-0.328452000	-2.212012000	0.000000000
6	-1.767102000	-1.944181000	0.000000000
1	-2.410887000	-2.814081000	0.000000000
6	-2.256201000	-0.697363000	0.000000000
1	-3.328249000	-0.528245000	0.000000000
8	0.114139000	-3.344741000	0.000000000
1	2.313309000	-2.187244000	0.000000000

E(HF): -575.1957189

Phenalenone 1, lowest triplet state, optimized geometry (M05-2X/SDD)

6	0.519374000	-1.045056000	0.000000000
6	2.290437000	1.149358000	0.000000000
6	0.000000000	0.268393000	0.000000000
6	1.932997000	-1.257335000	0.000000000
6	2.794091000	-0.168343000	0.000000000
6	0.897514000	1.389432000	0.000000000
1	3.864695000	-0.328504000	0.000000000
1	2.971845000	1.991718000	0.000000000
6	0.358387000	2.705005000	0.000000000
1	1.033102000	3.552046000	0.000000000
6	-1.045667000	2.916013000	0.000000000
1	-1.427702000	3.928898000	0.000000000
6	-1.921399000	1.851201000	0.000000000
1	-2.992311000	2.011438000	0.000000000
6	-1.423545000	0.486920000	0.000000000
6	-0.395814000	-2.163538000	0.000000000
6	-1.787477000	-1.920766000	0.000000000
1	-2.443716000	-2.781960000	0.000000000
6	-2.296583000	-0.608420000	0.000000000
1	-3.366054000	-0.439767000	0.000000000
8	0.066080000	-3.409503000	0.000000000
1	2.297624000	-2.275026000	0.000000000

E(HF): -575.2329879

Phenalenone 1, lowest triplet state, optimized geometry (M06/SDD)

6	0.529010000	-1.042043000	0.000000000
6	2.286001000	1.164782000	0.000000000
6	0.000000000	0.267890000	0.000000000
6	1.942446000	-1.243098000	0.000000000
6	2.798829000	-0.148238000	0.000000000
6	0.889387000	1.395026000	0.000000000
1	3.873352000	-0.302157000	0.000000000
1	2.960889000	2.017515000	0.000000000
6	0.341828000	2.707039000	0.000000000
1	1.016042000	3.560294000	0.000000000
6	-1.064273000	2.910219000	0.000000000
1	-1.453369000	3.923617000	0.000000000
6	-1.933415000	1.838734000	0.000000000
1	-3.009678000	1.989994000	0.000000000
6	-1.427530000	0.479543000	0.000000000
6	-0.377685000	-2.180679000	0.000000000
6	-1.782463000	-1.931441000	0.000000000
1	-2.435808000	-2.799373000	0.000000000
6	-2.294900000	-0.624226000	0.000000000
1	-3.368471000	-0.456378000	0.000000000
8	0.082773000	-3.403866000	0.000000000
1	2.311451000	-2.263634000	0.000000000

E(HF): -574.8750207

Phenalenone 1, lowest triplet state, optimized geometry (M06/SDD, solvated by DMF)

6	0.545550000	-1.038201000	0.000000000
6	2.274516000	1.195471000	0.000000000
6	0.000000000	0.265607000	0.000000000
6	1.961247000	-1.218305000	0.000000000
6	2.804065000	-0.110980000	0.000000000
6	0.874287000	1.404352000	0.000000000
1	3.880169000	-0.250674000	0.000000000
1	2.937520000	2.056470000	0.000000000
6	0.309530000	2.710592000	0.000000000
1	0.971983000	3.572231000	0.000000000
6	-1.101219000	2.896570000	0.000000000
1	-1.501522000	3.904798000	0.000000000
6	-1.956737000	1.814728000	0.000000000
1	-3.034163000	1.951406000	0.000000000
6	-1.432175000	0.462125000	0.000000000
6	-0.351786000	-2.187549000	0.000000000
6	-1.763739000	-1.949834000	0.000000000
1	-2.414892000	-2.819497000	0.000000000
6	-2.290032000	-0.651418000	0.000000000
1	-3.364413000	-0.495538000	0.000000000
8	0.116217000	-3.406069000	0.000000000
1	2.354548000	-2.229585000	0.000000000

E(HF): -574.8855365

Phenalenone 1, lowest triplet state, optimized geometry (M06/cc-pVTZ)

6	0.549094000	-1.021119000	0.000000000
6	2.242775000	1.192549000	0.000000000
6	0.000000000	0.260263000	0.000000000
6	1.951058000	-1.191051000	0.000000000
6	2.775167000	-0.094557000	0.000000000
6	0.858480000	1.396343000	0.000000000
1	3.849430000	-0.226432000	0.000000000
1	2.897445000	2.055940000	0.000000000
6	0.287216000	2.682047000	0.000000000
1	0.941584000	3.545316000	0.000000000
6	-1.112207000	2.856592000	0.000000000
1	-1.517559000	3.860083000	0.000000000
6	-1.947962000	1.788353000	0.000000000
1	-3.022947000	1.918388000	0.000000000
6	-1.424147000	0.445120000	0.000000000
6	-0.327748000	-2.186328000	0.000000000
6	-1.734563000	-1.944359000	0.000000000
1	-2.374346000	-2.817693000	0.000000000
6	-2.258868000	-0.662276000	0.000000000
1	-3.331752000	-0.511000000	0.000000000
8	0.133776000	-3.344167000	0.000000000
1	2.338163000	-2.200717000	0.000000000

E(HF): -575.1270203

9-Fluorophenalenone 2, singlet ground state, optimized geometry (M05-2X/SDD)

6	0.002149000	-0.932919000	0.000000000
6	-2.456021000	0.506247000	0.000000000
6	0.000000000	0.501285000	0.000000000
6	-1.232607000	-1.565039000	0.000000000
6	-2.462095000	-0.872544000	0.000000000
6	-1.226490000	1.224246000	0.000000000
1	-3.377231000	-1.448389000	0.000000000
1	-3.389223000	1.056207000	0.000000000
6	-1.207393000	2.648538000	0.000000000
1	-2.149128000	3.184791000	0.000000000
6	-0.007622000	3.335678000	0.000000000
1	0.004099000	4.417438000	0.000000000
6	1.214180000	2.618610000	0.000000000
1	2.153587000	3.159548000	0.000000000
6	1.230269000	1.228881000	0.000000000
6	1.293845000	-1.678273000	0.000000000
6	2.521260000	-0.860637000	0.000000000
1	3.448400000	-1.419019000	0.000000000
6	2.487443000	0.491394000	0.000000000
1	3.408291000	1.064272000	0.000000000
8	1.370815000	-2.928704000	0.000000000
9	-1.334091000	-2.939782000	0.000000000

E(HF): -674.5274873

9-Fluorophenalenone 2, singlet ground state, optimized geometry (M06/SDD)

6	0.009420000	-0.934755000	0.000000000
6	-2.457646000	0.496893000	0.000000000
6	0.000000000	0.498606000	0.000000000
6	-1.228230000	-1.573052000	0.000000000
6	-2.458480000	-0.883403000	0.000000000
6	-1.232571000	1.219134000	0.000000000
1	-3.374128000	-1.464092000	0.000000000
1	-3.395046000	1.046642000	0.000000000
6	-1.218810000	2.642217000	0.000000000
1	-2.167168000	3.173976000	0.000000000
6	-0.020756000	3.336657000	0.000000000
1	-0.014894000	4.421388000	0.000000000
6	1.201781000	2.626610000	0.000000000
1	2.143020000	3.171498000	0.000000000
6	1.226822000	1.233042000	0.000000000
6	1.303738000	-1.675947000	0.000000000
6	2.522154000	-0.849906000	0.000000000
1	3.455310000	-1.404832000	0.000000000
6	2.482544000	0.505780000	0.000000000
1	3.402693000	1.086728000	0.000000000
8	1.385713000	-2.927688000	0.000000000
9	-1.323922000	-2.940117000	0.000000000

E(HF): -674.1432421

9-Fluorophenalenone 2, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.017334000	-0.935481000	0.000000000
6	-2.459113000	0.486431000	0.000000000
6	0.000000000	0.498522000	0.000000000
6	-1.222789000	-1.573142000	0.000000000
6	-2.455267000	-0.896225000	0.000000000
6	-1.236825000	1.211614000	0.000000000
1	-3.371305000	-1.475402000	0.000000000
1	-3.398623000	1.030626000	0.000000000
6	-1.231058000	2.635669000	0.000000000
1	-2.181474000	3.162077000	0.000000000
6	-0.035981000	3.337581000	0.000000000
1	-0.036337000	4.421555000	0.000000000
6	1.190382000	2.634852000	0.000000000
1	2.127776000	3.184787000	0.000000000
6	1.221479000	1.239143000	0.000000000
6	1.311657000	-1.664251000	0.000000000
6	2.521389000	-0.840120000	0.000000000
1	3.462366000	-1.381699000	0.000000000
6	2.477313000	0.519268000	0.000000000
1	3.396534000	1.099984000	0.000000000
8	1.399875000	-2.926801000	0.000000000
9	-1.309896000	-2.950077000	0.000000000

E(HF): -674.1589296

9-Fluorophenalenone 2, singlet ground state, optimized geometry (M06/cc-pVTZ)

6	-0.000323000	-0.929605000	0.000000000
6	-2.428977000	0.503440000	0.000000000
6	0.000000000	0.489488000	0.000000000
6	-1.228506000	-1.560006000	0.000000000
6	-2.438630000	-0.858810000	0.000000000
6	-1.214088000	1.214340000	0.000000000
1	-3.357573000	-1.428742000	0.000000000
1	-3.360078000	1.057433000	0.000000000
6	-1.186005000	2.623138000	0.000000000
1	-2.127889000	3.158983000	0.000000000
6	0.001371000	3.299254000	0.000000000
1	0.016002000	4.380659000	0.000000000
6	1.203956000	2.586030000	0.000000000
1	2.147580000	3.119486000	0.000000000
6	1.221645000	1.208822000	0.000000000
6	1.281353000	-1.680345000	0.000000000
6	2.494792000	-0.861077000	0.000000000
1	3.424858000	-1.414299000	0.000000000
6	2.460520000	0.475687000	0.000000000
1	3.380466000	1.051194000	0.000000000
8	1.346526000	-2.892798000	0.000000000
9	-1.322025000	-2.871607000	0.000000000

E(HF): -674.4344293

9-Fluorophenalenone 2, lowest triplet excited state, optimized geometry (M05-2X/SDD)

6	0.029680000	-0.931513000	0.000000000
6	-2.457328000	0.466476000	0.000000000
6	0.000000000	0.489605000	0.000000000
6	-1.229188000	-1.604486000	0.000000000
6	-2.438142000	-0.937223000	0.000000000
6	-1.249977000	1.198726000	0.000000000
1	-3.351304000	-1.516785000	0.000000000
1	-3.402032000	0.994490000	0.000000000
6	-1.248584000	2.621754000	0.000000000
1	-2.195851000	3.146063000	0.000000000
6	-0.034745000	3.350396000	0.000000000
1	-0.063820000	4.432261000	0.000000000
6	1.176648000	2.691499000	0.000000000
1	2.109551000	3.240935000	0.000000000
6	1.231354000	1.241405000	0.000000000
6	1.309897000	-1.604475000	0.000000000
6	2.490042000	-0.835217000	0.000000000
1	3.425784000	-1.379500000	0.000000000
6	2.457398000	0.572341000	0.000000000
1	3.379173000	1.139895000	0.000000000
8	1.423107000	-2.935581000	0.000000000
9	-1.278743000	-2.987604000	0.000000000

E(HF): -674.4582149

9-Fluorophenalenone 2, lowest triplet excited state, optimized geometry (M06/SDD)

6	0.025899000	-0.934898000	0.000000000
6	-2.459062000	0.470506000	0.000000000
6	0.000000000	0.485973000	0.000000000
6	-1.235422000	-1.605026000	0.000000000
6	-2.445167000	-0.931472000	0.000000000
6	-1.247504000	1.199441000	0.000000000
1	-3.362175000	-1.510437000	0.000000000
1	-3.403455000	1.007274000	0.000000000
6	-1.242842000	2.622274000	0.000000000
1	-2.194292000	3.148413000	0.000000000
6	-0.026512000	3.350830000	0.000000000
1	-0.054449000	4.435668000	0.000000000
6	1.183064000	2.689235000	0.000000000
1	2.122288000	3.235739000	0.000000000
6	1.234934000	1.239594000	0.000000000
6	1.310744000	-1.625028000	0.000000000
6	2.497995000	-0.835538000	0.000000000
1	3.436320000	-1.382858000	0.000000000
6	2.462447000	0.568179000	0.000000000
1	3.385043000	1.141603000	0.000000000
8	1.417431000	-2.928114000	0.000000000
9	-1.291129000	-2.979435000	0.000000000

E(HF): -674.0779375

9-Fluorophenalenone 2, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

6	0.010355000	-0.928607000	0.000000000
6	-2.430062000	0.478634000	0.000000000
6	0.000000000	0.472577000	0.000000000
6	-1.242854000	-1.591582000	0.000000000
6	-2.429868000	-0.907140000	0.000000000
6	-1.229380000	1.193505000	0.000000000
1	-3.350706000	-1.474265000	0.000000000
1	-3.366534000	1.022346000	0.000000000
6	-1.207262000	2.601243000	0.000000000
1	-2.149846000	3.134761000	0.000000000
6	0.007384000	3.313120000	0.000000000
1	-0.013048000	4.395060000	0.000000000
6	1.192034000	2.654905000	0.000000000
1	2.132697000	3.190818000	0.000000000
6	1.236202000	1.213078000	0.000000000
6	1.287809000	-1.642965000	0.000000000
6	2.472874000	-0.846697000	0.000000000
1	3.406328000	-1.394878000	0.000000000
6	2.442574000	0.537882000	0.000000000
1	3.364838000	1.106194000	0.000000000
8	1.371379000	-2.884611000	0.000000000
9	-1.294843000	-2.910095000	0.000000000

E(HF): -674.3628799

9-Fluorophenalenone 2, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

6	0.010355000	-0.928607000	0.000000000
6	-2.430062000	0.478634000	0.000000000
6	0.000000000	0.472577000	0.000000000
6	-1.242854000	-1.591582000	0.000000000
6	-2.429868000	-0.907140000	0.000000000
6	-1.229380000	1.193505000	0.000000000
1	-3.350706000	-1.474265000	0.000000000
1	-3.366534000	1.022346000	0.000000000
6	-1.207262000	2.601243000	0.000000000
1	-2.149846000	3.134761000	0.000000000
6	0.007384000	3.313120000	0.000000000
1	-0.013048000	4.395060000	0.000000000
6	1.192034000	2.654905000	0.000000000
1	2.132697000	3.190818000	0.000000000
6	1.236202000	1.213078000	0.000000000
6	1.287809000	-1.642965000	0.000000000
6	2.472874000	-0.846697000	0.000000000
1	3.406328000	-1.394878000	0.000000000
6	2.442574000	0.537882000	0.000000000
1	3.364838000	1.106194000	0.000000000
8	1.371379000	-2.884611000	0.000000000
9	-1.294843000	-2.910095000	0.000000000

E(HF): -674.3628799

9-Chlorophenalenone 3, singlet ground state, optimized geometry (M05-2X/SDD)

6	0.000000000	0.673812000	0.000000000
6	-2.187129000	-1.150002000	0.000000000
6	0.231460000	-0.746258000	0.000000000
6	-1.321726000	1.112860000	0.000000000
6	-2.413607000	0.208505000	0.000000000
6	-0.860124000	-1.659896000	0.000000000
1	-3.418534000	0.607704000	0.000000000
1	-3.021324000	-1.841323000	0.000000000
6	-0.617555000	-3.063339000	0.000000000
1	-1.464760000	-3.739302000	0.000000000
6	0.674513000	-3.554063000	0.000000000
1	0.857334000	-4.620309000	0.000000000
6	1.764904000	-2.650932000	0.000000000
1	2.779078000	-3.033701000	0.000000000
6	1.560338000	-1.276078000	0.000000000
6	1.176802000	1.597726000	0.000000000
6	2.515253000	0.979574000	0.000000000
1	3.342876000	1.676893000	0.000000000
6	2.691868000	-0.359696000	0.000000000
1	3.689047000	-0.785573000	0.000000000
8	1.076942000	2.846719000	0.000000000
17	-1.804073000	2.840505000	0.000000000

E(HF): -1034.8410258

9-Chlorophenalenone 3, singlet ground state, optimized geometry (M06/SDD)

6	0.000000000	0.676704000	0.000000000
6	-2.179937000	-1.165312000	0.000000000
6	0.237679000	-0.741970000	0.000000000
6	-1.330973000	1.101694000	0.000000000
6	-2.416795000	0.193566000	0.000000000
6	-0.851076000	-1.665296000	0.000000000
1	-3.427004000	0.588284000	0.000000000
1	-3.010812000	-1.866031000	0.000000000
6	-0.599814000	-3.065881000	0.000000000
1	-1.447210000	-3.747179000	0.000000000
6	0.696718000	-3.550813000	0.000000000
1	0.885126000	-4.619003000	0.000000000
6	1.779905000	-2.643341000	0.000000000
1	2.800361000	-3.019534000	0.000000000
6	1.569460000	-1.265290000	0.000000000
6	1.171289000	1.609771000	0.000000000
6	2.507345000	0.994279000	0.000000000
1	3.334974000	1.696883000	0.000000000
6	2.691798000	-0.347734000	0.000000000
1	3.693755000	-0.772058000	0.000000000
8	1.065200000	2.859595000	0.000000000
17	-1.823788000	2.828212000	0.000000000

E(HF): -1034.4726465

9-Chlorophenalenone 3, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.000000000	0.679280000	0.000000000
6	-2.168610000	-1.183454000	0.000000000
6	0.246585000	-0.738916000	0.000000000
6	-1.338936000	1.085930000	0.000000000
6	-2.418286000	0.175743000	0.000000000
6	-0.836038000	-1.669599000	0.000000000
1	-3.433294000	0.556441000	0.000000000
1	-2.993611000	-1.889616000	0.000000000
6	-0.575457000	-3.069763000	0.000000000
1	-1.417798000	-3.755997000	0.000000000
6	0.724944000	-3.546498000	0.000000000
1	0.920585000	-4.612596000	0.000000000
6	1.802066000	-2.631773000	0.000000000
1	2.824153000	-3.001171000	0.000000000
6	1.580609000	-1.253533000	0.000000000
6	1.163482000	1.614198000	0.000000000
6	2.497982000	1.013309000	0.000000000
1	3.327386000	1.713796000	0.000000000
6	2.694096000	-0.330441000	0.000000000
1	3.699716000	-0.743579000	0.000000000
8	1.048174000	2.873096000	0.000000000
17	-1.855715000	2.816533000	0.000000000

E(HF): -1034.4865395

9-Chlorophenalenone 3, singlet ground state, optimized geometry (M06/cc-pVTZ)

6	0.000000000	0.676641000	0.000000000
6	-2.171120000	-1.125373000	0.000000000
6	0.223201000	-0.729620000	0.000000000
6	-1.313830000	1.115167000	0.000000000
6	-2.392275000	0.217241000	0.000000000
6	-0.861606000	-1.636622000	0.000000000
1	-3.395145000	0.620835000	0.000000000
1	-3.005638000	-1.816491000	0.000000000
6	-0.620702000	-3.024915000	0.000000000
1	-1.471592000	-3.695798000	0.000000000
6	0.654539000	-3.513623000	0.000000000
1	0.834155000	-4.580092000	0.000000000
6	1.732332000	-2.623903000	0.000000000
1	2.747052000	-3.005013000	0.000000000
6	1.539391000	-1.260190000	0.000000000
6	1.172815000	1.598176000	0.000000000
6	2.492876000	0.967627000	0.000000000
1	3.327887000	1.655781000	0.000000000
6	2.658867000	-0.357449000	0.000000000
1	3.652945000	-0.792218000	0.000000000
8	1.076357000	2.808272000	0.000000000
17	-1.763968000	2.783993000	0.000000000

E(HF): -1034.7908041

9-Chlorophenalenone 3, lowest triplet excited state, optimized geometry (M05-2X/SDD)

6	0.000000000	0.675467000	0.000000000
6	-2.153123000	-1.199538000	0.000000000
6	0.254683000	-0.727968000	0.000000000
6	-1.371600000	1.096988000	0.000000000
6	-2.411402000	0.177513000	0.000000000
6	-0.825630000	-1.675033000	0.000000000
1	-3.430447000	0.540616000	0.000000000
1	-2.975308000	-1.903742000	0.000000000
6	-0.547801000	-3.070247000	0.000000000
1	-1.376888000	-3.766664000	0.000000000
6	0.783847000	-3.551007000	0.000000000
1	0.966739000	-4.617566000	0.000000000
6	1.839146000	-2.665655000	0.000000000
1	2.862904000	-3.018268000	0.000000000
6	1.608084000	-1.231990000	0.000000000
6	1.142038000	1.571206000	0.000000000
6	2.447852000	1.038174000	0.000000000
1	3.260208000	1.753662000	0.000000000
6	2.686715000	-0.346667000	0.000000000
1	3.699132000	-0.729377000	0.000000000
8	1.024153000	2.898193000	0.000000000
17	-1.877436000	2.824019000	0.000000000

E(HF): -1034.7718884

9-Chlorophenalenone 3, lowest triplet excited state, optimized geometry (M06/SDD)

6	0.000000000	0.678204000	0.000000000
6	-2.158446000	-1.195631000	0.000000000
6	0.252417000	-0.725634000	0.000000000
6	-1.372139000	1.097167000	0.000000000
6	-2.417431000	0.179807000	0.000000000
6	-0.828802000	-1.671981000	0.000000000
1	-3.438310000	0.547043000	0.000000000
1	-2.981261000	-1.905130000	0.000000000
6	-0.553766000	-3.066952000	0.000000000
1	-1.389368000	-3.762682000	0.000000000
6	0.778272000	-3.552213000	0.000000000
1	0.958599000	-4.622172000	0.000000000
6	1.835115000	-2.668626000	0.000000000
1	2.862795000	-3.021836000	0.000000000
6	1.607309000	-1.235424000	0.000000000
6	1.146548000	1.587018000	0.000000000
6	2.460525000	1.030837000	0.000000000
1	3.277861000	1.746368000	0.000000000
6	2.690624000	-0.351282000	0.000000000
1	3.703425000	-0.743829000	0.000000000
8	1.032437000	2.887906000	0.000000000
17	-1.876153000	2.825131000	0.000000000

E(HF): -1034.4077041

9-Chlorophenalenone 3, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

6	0.000000000	0.681032000	0.000000000
6	-2.159248000	-1.199015000	0.000000000
6	0.252338000	-0.723302000	0.000000000
6	-1.372001000	1.090087000	0.000000000
6	-2.420268000	0.176587000	0.000000000
6	-0.827601000	-1.669633000	0.000000000
1	-3.442969000	0.538086000	0.000000000
1	-2.980306000	-1.909100000	0.000000000
6	-0.551046000	-3.066542000	0.000000000
1	-1.385507000	-3.762605000	0.000000000
6	0.782655000	-3.552128000	0.000000000
1	0.962006000	-4.621438000	0.000000000
6	1.839075000	-2.668575000	0.000000000
1	2.866354000	-3.020335000	0.000000000
6	1.609206000	-1.235067000	0.000000000
6	1.148626000	1.590001000	0.000000000
6	2.465979000	1.027376000	0.000000000
1	3.290496000	1.734614000	0.000000000
6	2.695276000	-0.352253000	0.000000000
1	3.707174000	-0.744109000	0.000000000
8	1.038196000	2.888740000	0.000000000
17	-1.888280000	2.828444000	0.000000000

E(HF): -1034.4208056

9-Chlorophenalenone 3, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

6	0.000000000	0.676362000	0.000000000
6	-2.156102000	-1.144347000	0.000000000
6	0.234110000	-0.709645000	0.000000000
6	-1.355183000	1.118213000	0.000000000
6	-2.395276000	0.216241000	0.000000000
6	-0.848248000	-1.637155000	0.000000000
1	-3.407713000	0.596277000	0.000000000
1	-2.984230000	-1.842216000	0.000000000
6	-0.589231000	-3.018341000	0.000000000
1	-1.429808000	-3.701439000	0.000000000
6	0.727665000	-3.517602000	0.000000000
1	0.891307000	-4.587115000	0.000000000
6	1.779048000	-2.664895000	0.000000000
1	2.798486000	-3.029495000	0.000000000
6	1.576402000	-1.236851000	0.000000000
6	1.154874000	1.581301000	0.000000000
6	2.455462000	0.989822000	0.000000000
1	3.282295000	1.688447000	0.000000000
6	2.657879000	-0.376645000	0.000000000
1	3.660690000	-0.786221000	0.000000000
8	1.056023000	2.820997000	0.000000000
17	-1.806330000	2.790297000	0.000000000

E(HF): -1034.7202025

9-Bromophenalenone 4, singlet ground state, optimized geometry (M05-2X/SDD)

6	-0.097898000	0.344015000	-0.000002000
6	0.587135000	-2.418050000	0.000002000
6	1.281837000	-0.067486000	0.000000000
6	-1.076286000	-0.649959000	0.000002000
6	-0.733662000	-2.028386000	0.000006000
6	1.626178000	-1.448748000	0.000001000
1	-1.526417000	-2.763539000	0.000009000
1	0.843401000	-3.470954000	0.000005000
6	2.994242000	-1.845325000	-0.000003000
1	3.230648000	-2.903084000	-0.000004000
6	4.000764000	-0.898356000	-0.000007000
1	5.039765000	-1.200403000	-0.000011000
6	3.666087000	0.477443000	0.000000000
1	4.454338000	1.221668000	-0.000002000
6	2.340580000	0.895331000	0.000002000
6	-0.408693000	1.807900000	-0.000004000
6	0.731632000	2.740994000	0.000004000
1	0.466012000	3.790243000	0.000013000
6	2.013134000	2.313982000	0.000006000
1	2.832816000	3.023810000	0.000018000
8	-1.575384000	2.265339000	-0.000010000
35	-2.979651000	-0.318874000	0.000000000

E(HF): -588.0296473

9-Bromophenalenone 4, singlet ground state, optimized geometry (M06/SDD)

6	0.098760000	0.349333000	-0.000003000
6	-0.588232000	-2.417947000	0.000004000
6	-1.279620000	-0.064541000	-0.000001000
6	1.077429000	-0.652032000	0.000000000
6	0.734869000	-2.028681000	0.000003000
6	-1.625669000	-1.449142000	0.000002000
1	1.529427000	-2.767389000	0.000004000
1	-0.848247000	-3.473431000	0.000006000
6	-2.992113000	-1.845282000	0.000004000
1	-3.226923000	-2.906926000	0.000006000
6	-4.002198000	-0.898525000	0.000004000
1	-5.043277000	-1.203091000	0.000005000
6	-3.669065000	0.474337000	0.000002000
1	-4.458197000	1.222806000	0.000003000
6	-2.340235000	0.896649000	0.000000000
6	0.410788000	1.813699000	-0.000009000
6	-0.731899000	2.738655000	-0.000001000
1	-0.468039000	3.791725000	0.000002000
6	-2.016788000	2.309243000	0.000001000
1	-2.841107000	3.019487000	0.000004000
8	1.578393000	2.273842000	0.000003000
35	2.979230000	-0.320815000	-0.000002000

E(HF): -587.6742081

9-Bromophenalenone 4, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.096193000	0.359627000	0.000000000
6	-0.578742000	-2.415998000	0.000002000
6	-1.280831000	-0.063943000	0.000001000
6	1.076021000	-0.644240000	0.000000000
6	0.744896000	-2.020714000	0.000001000
6	-1.618178000	-1.451196000	0.000002000
1	1.538201000	-2.759690000	0.000001000
1	-0.832794000	-3.471920000	0.000003000
6	-2.983412000	-1.856571000	0.000004000
1	-3.211251000	-2.918985000	0.000005000
6	-4.000079000	-0.916024000	0.000004000
1	-5.038521000	-1.226808000	0.000004000
6	-3.675904000	0.459286000	0.000002000
1	-4.468844000	1.202586000	0.000002000
6	-2.347879000	0.889212000	0.000001000
6	0.392676000	1.822657000	-0.000001000
6	-0.749222000	2.737661000	-0.000002000
1	-0.500937000	3.794524000	-0.000003000
6	-2.035088000	2.301323000	-0.000001000
1	-2.861588000	3.007719000	-0.000001000
8	1.564761000	2.297362000	-0.000002000
35	2.988999000	-0.320365000	-0.000002000

E(HF): -587.6875444

9-Bromophenalenone 4, singlet ground state, optimized geometry (M06/cc-pVTZ)

6	0.104828000	0.346287000	0.000000000
6	-0.568089000	-2.392076000	0.000002000
6	-1.258669000	-0.066459000	0.000001000
6	1.075476000	-0.641610000	0.000000000
6	0.736568000	-2.003848000	0.000001000
6	-1.600154000	-1.438351000	0.000002000
1	1.532470000	-2.735541000	0.000001000
1	-0.824754000	-3.444866000	0.000003000
6	-2.954114000	-1.829119000	0.000003000
1	-3.185242000	-2.887696000	0.000004000
6	-3.951426000	-0.896302000	0.000003000
1	-4.989117000	-1.201036000	0.000004000
6	-3.622776000	0.462130000	0.000002000
1	-4.409067000	1.208217000	0.000002000
6	-2.311988000	0.884886000	0.000001000
6	0.416269000	1.805004000	-0.000002000
6	-0.726674000	2.716841000	-0.000001000
1	-0.472307000	3.768505000	-0.000002000
6	-1.990895000	2.286512000	0.000000000
1	-2.816646000	2.990269000	0.000000000
8	1.547082000	2.247298000	-0.000004000
35	2.934225000	-0.316560000	-0.000002000

E(HF): -3148.6967635

9-Bromophenalenone 4, lowest triplet excited state, optimized geometry (M05-2X/SDD)

6	0.000000000	0.322774000	0.000000000
6	-0.074804000	-2.518240000	0.000000000
6	1.222958000	-0.428411000	0.000000000
6	-1.225257000	-0.392910000	0.000000000
6	-1.262504000	-1.789763000	0.000000000
6	1.185065000	-1.858396000	0.000000000
1	-2.216174000	-2.299773000	0.000000000
1	-0.105452000	-3.600505000	0.000000000
6	2.404148000	-2.586212000	0.000000000
1	2.367715000	-3.668969000	0.000000000
6	3.632691000	-1.920794000	0.000000000
1	4.553266000	-2.490245000	0.000000000
6	3.679697000	-0.522923000	0.000000000
1	4.632515000	-0.007451000	0.000000000
6	2.485482000	0.241550000	0.000000000
6	0.089877000	1.745430000	0.000000000
6	1.334629000	2.402706000	0.000000000
1	1.353235000	3.484195000	0.000000000
6	2.510217000	1.665359000	0.000000000
1	3.464403000	2.177169000	0.000000000
8	-1.028098000	2.548638000	0.000000000
35	-2.906226000	0.567299000	0.000000000

E(HF): -587.9621457

9-Bromophenalenone 4, lowest triplet excited state, optimized geometry (M06/SDD)

6	0.000000000	0.314399000	0.000000000
6	-0.077198000	-2.526724000	0.000000000
6	1.221261000	-0.434778000	0.000000000
6	-1.222995000	-0.403413000	0.000000000
6	-1.268121000	-1.800246000	0.000000000
6	1.182625000	-1.866313000	0.000000000
1	-2.224999000	-2.312124000	0.000000000
1	-0.104426000	-3.613098000	0.000000000
6	2.404219000	-2.590982000	0.000000000
1	2.368485000	-3.677696000	0.000000000
6	3.631702000	-1.922182000	0.000000000
1	4.556065000	-2.491261000	0.000000000
6	3.677182000	-0.523462000	0.000000000
1	4.631811000	-0.002885000	0.000000000
6	2.481997000	0.239723000	0.000000000
6	0.071044000	1.742288000	0.000000000
6	1.321170000	2.401066000	0.000000000
1	1.334087000	3.485646000	0.000000000
6	2.497431000	1.663879000	0.000000000
1	3.454156000	2.179848000	0.000000000
8	-1.048603000	2.514136000	0.000000000
35	-2.889950000	0.587399000	0.000000000

E(HF): -587.6088715

9-Bromophenalenone 4, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

6	0.000000000	0.376080000	0.000000000
6	-0.019426000	-2.484279000	0.000000000
6	1.220707000	-0.364140000	0.000000000
6	-1.223380000	-0.374835000	0.000000000
6	-1.222317000	-1.768781000	0.000000000
6	1.215451000	-1.800004000	0.000000000
1	-2.165562000	-2.304965000	0.000000000
1	-0.032306000	-3.569884000	0.000000000
6	2.443970000	-2.519212000	0.000000000
1	2.412101000	-3.605406000	0.000000000
6	3.692093000	-1.843092000	0.000000000
1	4.611694000	-2.417496000	0.000000000
6	3.730233000	-0.466792000	0.000000000
1	4.674020000	0.070195000	0.000000000
6	2.504416000	0.311377000	0.000000000
6	0.086681000	1.838977000	0.000000000
6	1.381465000	2.452569000	0.000000000
1	1.397411000	3.538724000	0.000000000
6	2.565735000	1.709695000	0.000000000
1	3.530332000	2.206816000	0.000000000
8	-0.957157000	2.618545000	0.000000000
35	-3.000692000	0.420808000	0.000000000

E(HF): -587.6775967

9-Bromophenalenone 4, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

6	0.000000000	0.312271000	0.000000000
6	-0.150205000	-2.492998000	0.000000000
6	1.191098000	-0.457449000	0.000000000
6	-1.230321000	-0.365112000	0.000000000
6	-1.306616000	-1.745993000	0.000000000
6	1.116766000	-1.875340000	0.000000000
1	-2.273993000	-2.229737000	0.000000000
1	-0.205537000	-3.574619000	0.000000000
6	2.309555000	-2.617986000	0.000000000
1	2.247295000	-3.699565000	0.000000000
6	3.537733000	-1.986193000	0.000000000
1	4.444861000	-2.576501000	0.000000000
6	3.618011000	-0.607117000	0.000000000
1	4.581849000	-0.112177000	0.000000000
6	2.456267000	0.180255000	0.000000000
6	0.092433000	1.729168000	0.000000000
6	1.353439000	2.345411000	0.000000000
1	1.391581000	3.425547000	0.000000000
6	2.496030000	1.589008000	0.000000000
1	3.460558000	2.082906000	0.000000000
8	-0.970749000	2.489590000	0.000000000
35	-2.822450000	0.649139000	0.000000000

E(HF): -3148.6208283

9-Iodophenalenone 5, singlet ground state, optimized geometry (M05-2X/SDD)

6	0.353926000	0.368532000	-0.000002000
6	0.964629000	-2.406804000	0.000004000
6	1.722801000	-0.077662000	-0.000001000
6	-0.658504000	-0.593023000	-0.000006000
6	-0.345517000	-1.981126000	0.000005000
6	2.030144000	-1.467232000	-0.000001000
1	-1.151076000	-2.702230000	0.000006000
1	1.190857000	-3.466621000	0.000004000
6	3.386580000	-1.900906000	-0.000002000
1	3.593978000	-2.964679000	-0.000003000
6	4.418534000	-0.981367000	-0.000002000
1	5.448840000	-1.311719000	-0.000001000
6	4.121182000	0.402879000	-0.000002000
1	4.929247000	1.125534000	-0.000001000
6	2.807065000	0.856484000	0.000001000
6	0.085130000	1.840126000	-0.000004000
6	1.247314000	2.744000000	0.000008000
1	1.009740000	3.799844000	0.000023000
6	2.517414000	2.283000000	0.000002000
1	3.355541000	2.971081000	0.000010000
8	-1.071532000	2.324852000	-0.000008000
53	-2.749227000	-0.199461000	0.000001000

E(HF): -586.0687882

9-Iodophenalenone 5, singlet ground state, optimized geometry (M06/SDD)

6	0.000000000	0.512537000	0.000000000
6	2.361780000	-1.075252000	0.000000000
6	1.298211000	1.132865000	0.000000000
6	-0.064895000	-0.887277000	0.000000000
6	1.118397000	-1.674087000	0.000000000
6	2.483432000	0.338724000	0.000000000
1	1.034544000	-2.756123000	0.000000000
1	3.261666000	-1.685305000	0.000000000
6	3.762217000	0.961914000	0.000000000
1	4.648773000	0.332340000	0.000000000
6	3.875369000	2.342002000	0.000000000
1	4.851685000	2.814731000	0.000000000
6	2.707108000	3.136290000	0.000000000
1	2.790211000	4.220768000	0.000000000
6	1.438415000	2.557296000	0.000000000
6	-1.211810000	1.389833000	0.000000000
6	-0.990129000	2.841920000	0.000000000
1	-1.892911000	3.444747000	0.000000000
6	0.250532000	3.386696000	0.000000000
1	0.384705000	4.466507000	0.000000000
8	-2.384855000	0.941016000	0.000000000
53	-1.852294000	-2.040501000	0.000000000

E(HF): -585.7171559

9-Iodophenalenone 5, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.000000000	0.522029000	0.000000000
6	2.346888000	-1.095545000	0.000000000
6	1.307710000	1.125141000	0.000000000
6	-0.075761000	-0.879945000	0.000000000
6	1.094772000	-1.681435000	0.000000000
6	2.482894000	0.315796000	0.000000000
1	1.004696000	-2.762474000	0.000000000
1	3.237817000	-1.717010000	0.000000000
6	3.771194000	0.922322000	0.000000000
1	4.648905000	0.281772000	0.000000000
6	3.902808000	2.301418000	0.000000000
1	4.884520000	2.761024000	0.000000000
6	2.744966000	3.110931000	0.000000000
1	2.842483000	4.193430000	0.000000000
6	1.467719000	2.546746000	0.000000000
6	-1.193867000	1.416412000	0.000000000
6	-0.956011000	2.859289000	0.000000000
1	-1.844948000	3.482516000	0.000000000
6	0.293879000	3.390551000	0.000000000
1	0.438736000	4.468058000	0.000000000
8	-2.381745000	0.980980000	0.000000000
53	-1.873234000	-2.031649000	0.000000000

E(HF): -585.7299909

9-Iodophenalenone 5, lowest triplet excited state, optimized geometry (M05-2X/SDD)

6	0.000000000	0.454814000	0.000000000
6	2.529071000	-0.831410000	0.000000000
6	1.199373000	1.238475000	0.000000000
6	0.115444000	-0.958461000	0.000000000
6	1.361625000	-1.593852000	0.000000000
6	2.474622000	0.591008000	0.000000000
1	1.422955000	-2.674088000	0.000000000
1	3.493540000	-1.323716000	0.000000000
6	3.652361000	1.383987000	0.000000000
1	4.617175000	0.891251000	0.000000000
6	3.571856000	2.779241000	0.000000000
1	4.479261000	3.369793000	0.000000000
6	2.327616000	3.419238000	0.000000000
1	2.269053000	4.501150000	0.000000000
6	1.127576000	2.665319000	0.000000000
6	-1.257148000	1.128033000	0.000000000
6	-1.320850000	2.537061000	0.000000000
1	-2.293339000	3.010236000	0.000000000
6	-0.154646000	3.288394000	0.000000000
1	-0.213941000	4.369869000	0.000000000
8	-2.445187000	0.443826000	0.000000000
53	-1.659898000	-2.118984000	0.000000000

E(HF): -586.002658

9-Iodophenalenone 5, lowest triplet excited state, optimized geometry (M06/SDD)

6	0.000000000	0.456743000	0.000000000
6	2.528447000	-0.838030000	0.000000000
6	1.201757000	1.235450000	0.000000000
6	0.115536000	-0.957734000	0.000000000
6	1.359045000	-1.599822000	0.000000000
6	2.476654000	0.583981000	0.000000000
1	1.416870000	-2.684065000	0.000000000
1	3.496529000	-1.332073000	0.000000000
6	3.656550000	1.374130000	0.000000000
1	4.622116000	0.874034000	0.000000000
6	3.580263000	2.770282000	0.000000000
1	4.492155000	3.359327000	0.000000000
6	2.337238000	3.413566000	0.000000000
1	2.279205000	4.499413000	0.000000000
6	1.133857000	2.663598000	0.000000000
6	-1.262766000	1.128981000	0.000000000
6	-1.316931000	2.542752000	0.000000000
1	-2.291498000	3.019075000	0.000000000
6	-0.146739000	3.288625000	0.000000000
1	-0.200491000	4.374503000	0.000000000
8	-2.437071000	0.449100000	0.000000000
53	-1.665958000	-2.114682000	0.000000000

E(HF): -585.6547299

9-Iodophenalenone 5, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

6	0.000000000	0.454768000	0.000000000
6	2.535623000	-0.827485000	0.000000000
6	1.196960000	1.240460000	0.000000000
6	0.123115000	-0.959426000	0.000000000
6	1.369629000	-1.596673000	0.000000000
6	2.475637000	0.595051000	0.000000000
1	1.435345000	-2.679962000	0.000000000
1	3.505599000	-1.316859000	0.000000000
6	3.651815000	1.392583000	0.000000000
1	4.620128000	0.898760000	0.000000000
6	3.566575000	2.789513000	0.000000000
1	4.474777000	3.383680000	0.000000000
6	2.319266000	3.427119000	0.000000000
1	2.255482000	4.512284000	0.000000000
6	1.119534000	2.668865000	0.000000000
6	-1.267710000	1.117049000	0.000000000
6	-1.331870000	2.530385000	0.000000000
1	-2.307585000	3.004871000	0.000000000
6	-0.165600000	3.285994000	0.000000000
1	-0.227798000	4.371010000	0.000000000
8	-2.436452000	0.421886000	0.000000000
53	-1.657022000	-2.118077000	0.000000000

E(HF): -585.6627654

9-Methoxyphenalenone 6, singlet ground state, optimized geometry (M05-2X/SDD)

6	0.550366000	0.406203000	0.000000000
6	0.038537000	-2.389537000	0.000000000
6	-0.795486000	-0.087815000	0.000000000
6	1.602694000	-0.525967000	0.000001000
6	1.334747000	-1.927553000	0.000001000
6	-1.059697000	-1.487968000	0.000000000
1	2.153582000	-2.632956000	0.000001000
1	-0.157297000	-3.455817000	0.000001000
6	-2.399611000	-1.966511000	-0.000001000
1	-2.571812000	-3.036946000	-0.000001000
6	-3.463224000	-1.082655000	-0.000001000
1	-4.482010000	-1.447042000	-0.000002000
6	-3.210745000	0.310030000	-0.000002000
1	-4.042215000	1.006078000	-0.000002000
6	-1.912704000	0.808604000	-0.000001000
6	0.789813000	1.875577000	0.000000000
6	-0.409196000	2.739081000	-0.000001000
1	-0.204386000	3.802275000	-0.000001000
6	-1.665866000	2.242160000	-0.000001000
1	-2.524062000	2.905521000	-0.000002000
8	1.922900000	2.416703000	0.000000000
8	2.888435000	-0.060195000	0.000001000
6	4.008427000	-0.984866000	0.000002000
1	4.887314000	-0.347875000	0.000003000
1	4.000939000	-1.608997000	0.897613000
1	4.000941000	-1.608998000	-0.897608000

E(HF): -689.78005

9-Methoxyphenalenone 6, singlet ground state, optimized geometry (M06/SDD)

6	-0.551336000	0.405786000	0.000004000
6	-0.028997000	-2.391253000	0.000007000
6	0.794097000	-0.084131000	0.000002000
6	-1.604133000	-0.535287000	0.000007000
6	-1.329160000	-1.934202000	0.000008000
6	1.064808000	-1.486955000	0.000002000
1	-2.147470000	-2.646277000	0.000011000
1	0.173391000	-3.459922000	0.000009000
6	2.405218000	-1.959290000	-0.000003000
1	2.580103000	-3.032865000	-0.000002000
6	3.468297000	-1.070553000	-0.000008000
1	4.490671000	-1.433434000	-0.000014000
6	3.211530000	0.318416000	-0.000006000
1	4.041754000	1.021457000	-0.000009000
6	1.908649000	0.816086000	-0.000001000
6	-0.798881000	1.874592000	0.000001000
6	0.397166000	2.736743000	0.000007000
1	0.189750000	3.802877000	0.000011000
6	1.659185000	2.242646000	0.000004000
1	2.519682000	2.909231000	0.000004000
8	-1.937049000	2.408670000	-0.000008000
8	-2.883442000	-0.067681000	0.000003000
6	-3.997723000	-0.984375000	-0.000013000
1	-4.882224000	-0.348806000	-0.000025000
1	-3.997006000	-1.614764000	-0.898642000
1	-3.997034000	-1.614759000	0.898621000

E(HF): -689.3733506

9-Methoxyphenalenone 6, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

6	0.551235000	0.419409000	0.000000000
6	0.049272000	-2.385900000	0.000001000
6	-0.793250000	-0.083701000	0.000000000
6	1.612045000	-0.520414000	0.000001000
6	1.345891000	-1.920179000	0.000001000
6	-1.051553000	-1.488384000	0.000000000
1	2.165936000	-2.628489000	0.000002000
1	-0.143457000	-3.455330000	0.000001000
6	-2.386345000	-1.974382000	-0.000001000
1	-2.549747000	-3.049005000	-0.000001000
6	-3.461280000	-1.096046000	-0.000002000
1	-4.478836000	-1.470176000	-0.000002000
6	-3.218747000	0.293500000	-0.000002000
1	-4.054827000	0.988552000	-0.000002000
6	-1.916636000	0.803089000	-0.000001000
6	0.775236000	1.884126000	0.000001000
6	-0.421297000	2.732970000	-0.000001000
1	-0.233547000	3.802913000	-0.000001000
6	-1.682793000	2.228272000	-0.000002000
1	-2.546226000	2.889568000	-0.000002000
8	1.915798000	2.441669000	0.000000000
8	2.893052000	-0.056300000	0.000002000
6	4.010067000	-0.987673000	0.000002000
1	4.900162000	-0.360642000	0.000003000
1	3.999335000	-1.614227000	0.898197000
1	3.999336000	-1.614227000	-0.898193000

E(HF): -689.3923073

9-Methoxyphenalenone 6, singlet ground state, optimized geometry (M06/cc-pVTZ)

6	0.549901000	0.401639000	0.000001000
6	0.038350000	-2.363951000	0.000000000
6	-0.780626000	-0.085348000	0.000000000
6	1.597465000	-0.526533000	0.000001000
6	1.322507000	-1.910163000	0.000001000
6	-1.048809000	-1.475074000	0.000000000
1	2.136790000	-2.619435000	0.000001000
1	-0.158519000	-3.429948000	0.000000000
6	-2.377258000	-1.940613000	-0.000001000
1	-2.548898000	-3.010840000	-0.000001000
6	-3.426444000	-1.064625000	-0.000002000
1	-4.445563000	-1.426656000	-0.000002000
6	-3.172034000	0.309390000	-0.000002000
1	-3.998722000	1.010866000	-0.000002000
6	-1.886863000	0.806188000	-0.000001000
6	0.796683000	1.864533000	0.000003000
6	-0.396389000	2.714817000	-0.000001000
1	-0.198207000	3.778878000	-0.000003000
6	-1.638304000	2.221188000	-0.000002000
1	-2.499081000	2.882152000	-0.000003000
8	1.902460000	2.371989000	-0.000001000
8	2.846077000	-0.067897000	0.000002000
6	3.928081000	-0.963741000	0.000002000
1	4.824441000	-0.349747000	0.000003000
1	3.930945000	-1.597124000	0.891502000
1	3.930947000	-1.597123000	-0.891499000

E(HF): -689.690019

9-Methoxyphenalenone 6, lowest triplet excited state, optimized geometry (M05-2X/SDD)

6	0.542483000	0.416700000	-0.000007000
6	0.036025000	-2.388430000	-0.000027000
6	-0.791702000	-0.078071000	-0.000002000
6	1.625654000	-0.548064000	0.000001000
6	1.355601000	-1.915281000	-0.000017000
6	-1.056220000	-1.494339000	-0.000013000
1	2.167263000	-2.629261000	-0.000016000
1	-0.153393000	-3.454778000	-0.000039000
6	-2.393495000	-1.963634000	-0.000012000
1	-2.574096000	-3.031553000	-0.000022000
6	-3.484228000	-1.058976000	0.000006000
1	-4.496034000	-1.444259000	0.000008000
6	-3.261590000	0.300440000	0.000017000
1	-4.087144000	1.001320000	0.000030000
6	-1.912392000	0.829486000	0.000014000
6	0.741535000	1.849597000	-0.000015000
6	-0.382588000	2.705951000	0.000013000
1	-0.176641000	3.768909000	0.000014000
6	-1.692214000	2.211857000	0.000026000
1	-2.536479000	2.889739000	0.000044000
8	1.945331000	2.435535000	-0.000071000
8	2.906366000	-0.050863000	0.000043000
6	4.024734000	-0.973271000	0.000034000
1	4.907593000	-0.341413000	0.000060000
1	4.012855000	-1.599959000	0.896672000
1	4.012875000	-1.599917000	-0.896635000

E(HF): -689.710634

9-Methoxyphenalenone 6, lowest triplet excited state, optimized geometry (M06/SDD)

6	-0.545088000	0.411246000	-0.011366000
6	-0.036462000	-2.391463000	-0.058163000
6	0.788229000	-0.079764000	-0.001059000
6	-1.627467000	-0.553256000	0.005109000
6	-1.356368000	-1.923211000	-0.037927000
6	1.055152000	-1.495061000	-0.026019000
1	-2.170370000	-2.640400000	-0.041987000
1	0.159857000	-3.460376000	-0.085979000
6	2.393302000	-1.962212000	-0.023039000
1	2.573947000	-3.034222000	-0.047805000
6	3.484049000	-1.056112000	0.010520000
1	4.498897000	-1.441540000	0.014735000
6	3.259329000	0.303784000	0.036552000
1	4.085280000	1.009662000	0.061388000
6	1.910942000	0.830853000	0.028794000
6	-0.759530000	1.855389000	-0.034525000
6	0.383143000	2.711809000	0.029993000
1	0.176042000	3.778195000	0.028504000
6	1.687738000	2.215462000	0.055414000
1	2.537528000	2.891567000	0.092187000
8	-1.934935000	2.419161000	-0.153201000
8	-2.897574000	-0.050794000	0.087554000
6	-4.015683000	-0.958202000	0.073872000
1	-4.899598000	-0.324115000	0.130069000
1	-4.039765000	-1.546036000	-0.853613000
1	-3.989467000	-1.635243000	0.938737000

E(HF): -689.3076838

9-Methoxyphenalenone 6, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

6	0.546650000	0.421004000	0.000001000
6	0.060921000	-2.389650000	0.000001000
6	-0.782637000	-0.083795000	0.000000000
6	1.636469000	-0.534883000	0.000001000
6	1.375322000	-1.908145000	0.000001000
6	-1.037174000	-1.501053000	0.000000000
1	2.193250000	-2.619758000	0.000001000
1	-0.123897000	-3.460148000	0.000001000
6	-2.371506000	-1.983908000	-0.000001000
1	-2.539945000	-3.057580000	-0.000001000
6	-3.475016000	-1.088838000	-0.000002000
1	-4.484262000	-1.486792000	-0.000003000
6	-3.265582000	0.272968000	-0.000002000
1	-4.098380000	0.970096000	-0.000003000
6	-1.921393000	0.814456000	-0.000001000
6	0.738215000	1.873673000	0.000002000
6	-0.423754000	2.714696000	-0.000001000
1	-0.239187000	3.785343000	-0.000002000
6	-1.720834000	2.203499000	-0.000002000
1	-2.578968000	2.868277000	-0.000003000
8	1.905200000	2.459996000	0.000001000
8	2.915417000	-0.033806000	0.000001000
6	4.030709000	-0.959023000	0.000002000
1	4.923624000	-0.335318000	0.000002000
1	4.020247000	-1.589825000	0.896873000
1	4.020248000	-1.589825000	-0.896870000

E(HF): -689.3232905

9-Methoxyphenalenone 6, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

6	0.541766000	0.406645000	0.000000000
6	0.056352000	-2.364991000	0.000001000
6	-0.770182000	-0.082628000	0.000000000
6	1.626654000	-0.541169000	0.000001000
6	1.360906000	-1.895426000	0.000001000
6	-1.030448000	-1.488481000	0.000000000
1	2.174176000	-2.606073000	0.000002000
1	-0.131532000	-3.431904000	0.000001000
6	-2.353303000	-1.952804000	-0.000001000
1	-2.528796000	-3.021642000	-0.000001000
6	-3.441175000	-1.057435000	-0.000002000
1	-4.450145000	-1.449239000	-0.000002000
6	-3.230688000	0.280998000	-0.000002000
1	-4.057416000	0.980006000	-0.000003000
6	-1.894429000	0.817089000	-0.000001000
6	0.759591000	1.856546000	0.000000000
6	-0.402017000	2.691927000	-0.000001000
1	-0.207419000	3.756759000	-0.000001000
6	-1.682320000	2.187783000	-0.000002000
1	-2.538097000	2.852382000	-0.000002000
8	1.885563000	2.387469000	0.000001000
8	2.865439000	-0.042729000	0.000001000
6	3.953902000	-0.925817000	0.000002000
1	4.847339000	-0.307377000	0.000002000
1	3.958106000	-1.562121000	0.890599000
1	3.958107000	-1.562122000	-0.890594000

E(HF): -689.618913

9-Methylthiophenalenone 7, singlet ground state, optimized geometry (M05-2X/SDD)

1	-4.372943000	0.794382000	0.000002000
6	-3.502968000	0.147199000	0.000001000
6	-2.233634000	0.718235000	0.000001000
6	-2.562410000	-2.081893000	0.000000000
6	-1.072261000	-0.118366000	0.000000000
6	-3.674219000	-1.256884000	0.000001000
6	-1.253084000	-1.528408000	-0.000001000
6	0.244512000	0.446587000	-0.000003000
1	-4.670864000	-1.678121000	0.000002000
1	-0.220332000	-3.432380000	-0.000001000
1	-2.675856000	-3.160086000	0.000000000
6	1.370655000	-0.398222000	-0.000001000
6	1.167581000	-1.811450000	-0.000003000
1	2.015065000	-2.479989000	-0.000003000
6	-0.096425000	-2.355190000	-0.000002000
6	-2.065746000	2.163140000	0.000002000
1	-2.958434000	2.779106000	0.000001000
6	-0.836607000	2.729950000	0.000001000
1	-0.687565000	3.801912000	-0.000001000
6	0.388175000	1.918490000	-0.000001000
8	1.518101000	2.477386000	-0.000001000
16	3.048681000	0.279815000	0.000000000
6	4.079191000	-1.282052000	0.000005000
1	3.912278000	-1.874693000	-0.897915000
1	3.912278000	-1.874689000	0.897929000
1	5.106105000	-0.918376000	0.000005000

E(HF): -1012.7334396

9-Methylthiophenalenone 7, singlet ground state, optimized geometry (M06/SDD)

1	4.376201000	0.805599000	0.000003000
6	3.506372000	0.152287000	0.000002000
6	2.232562000	0.724309000	0.000000000
6	2.567126000	-2.076863000	0.000000000
6	1.072941000	-0.114730000	0.000000000
6	3.679901000	-1.248465000	0.000001000
6	1.257736000	-1.528040000	0.000000000
6	-0.243053000	0.447779000	0.000000000
1	4.679577000	-1.669829000	0.000001000
1	0.234144000	-3.437151000	-0.000004000
1	2.681679000	-3.158452000	0.000000000
6	-1.368297000	-0.406316000	-0.000001000
6	-1.163139000	-1.816576000	-0.000002000
1	-2.012800000	-2.489349000	-0.000004000
6	0.104676000	-2.357071000	-0.000003000
6	2.061757000	2.162255000	0.000000000
1	2.956584000	2.781624000	0.000002000
6	0.826950000	2.727309000	0.000000000
1	0.676015000	3.802375000	0.000001000
6	-0.394587000	1.918078000	-0.000001000
8	-1.529432000	2.473660000	-0.000002000
16	-3.046707000	0.278711000	-0.000001000
6	-4.084459000	-1.285127000	0.000004000
1	-3.917368000	-1.879645000	0.901198000
1	-3.917379000	-1.879647000	-0.901190000
1	-5.112800000	-0.917165000	0.000011000

E(HF): -1012.3417213

9-Methylthiophenalenone 7, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

1	4.385738000	0.780188000	0.000006000
6	3.511718000	0.133701000	0.000004000
6	2.239204000	0.714535000	0.000002000
6	2.554159000	-2.087770000	0.000000000
6	1.073027000	-0.113892000	-0.000001000
6	3.674688000	-1.267669000	0.000002000
6	1.248385000	-1.528621000	-0.000002000
6	-0.241616000	0.458770000	-0.000001000
1	4.670333000	-1.696635000	0.000004000
1	0.216227000	-3.433785000	-0.000008000
1	2.660086000	-3.169422000	-0.000002000
6	-1.369025000	-0.397590000	-0.000002000
6	-1.173582000	-1.807367000	-0.000005000
1	-2.024437000	-2.477461000	-0.000008000
6	0.092920000	-2.353995000	-0.000005000
6	2.080823000	2.150715000	0.000003000
1	2.977435000	2.765976000	0.000006000
6	0.846607000	2.724184000	0.000001000
1	0.713628000	3.801900000	0.000002000
6	-0.376532000	1.927093000	-0.000002000
8	-1.511957000	2.502552000	-0.000006000
16	-3.053962000	0.275861000	-0.000001000
6	-4.101847000	-1.278359000	0.000011000
1	-3.932900000	-1.871058000	0.900601000
1	-3.932921000	-1.871060000	-0.900583000
1	-5.127704000	-0.905244000	0.000022000

E(HF): -1012.3572855

9-Methylthiophenalenone 7, singlet ground state, optimized geometry (M06/cc-pVTZ)

1	4.323074000	0.817966000	0.000000000
6	3.460349000	0.161409000	0.000000000
6	2.200657000	0.724263000	0.000002000
6	2.546065000	-2.046167000	-0.000002000
6	1.054891000	-0.113372000	0.000001000
6	3.639919000	-1.222852000	-0.000002000
6	1.245733000	-1.512773000	0.000000000
6	-0.249420000	0.437886000	0.000003000
1	4.638713000	-1.637776000	-0.000005000
1	0.235860000	-3.410624000	-0.000011000
1	2.664430000	-3.123501000	-0.000004000
6	-1.363697000	-0.410387000	0.000009000
6	-1.150734000	-1.807317000	-0.000001000
1	-1.992684000	-2.481773000	-0.000010000
6	0.104019000	-2.334451000	-0.000004000
6	2.020075000	2.148819000	0.000006000
1	2.910731000	2.768565000	0.000011000
6	0.801450000	2.703476000	0.000005000
1	0.652806000	3.775303000	0.000008000
6	-0.412840000	1.897694000	-0.000002000
8	-1.517172000	2.424818000	-0.000015000
16	-2.987623000	0.257350000	-0.000003000
6	-4.015902000	-1.239215000	0.000008000
1	-3.870433000	-1.843010000	0.894520000
1	-3.870434000	-1.843026000	-0.894492000
1	-5.036113000	-0.860349000	0.000009000

E(HF): -1012.6808164

9-Methylthiophenalenone 7, lowest triplet excited state, optimized geometry (M05-2X/SDD)

1	-4.051439000	1.635482000	0.280439000
6	-3.359160000	0.806152000	0.195086000
6	-1.974537000	1.070117000	0.066138000
6	-2.953367000	-1.594239000	0.102364000
6	-1.072144000	-0.030638000	-0.045032000
6	-3.832943000	-0.512718000	0.211782000
6	-1.556485000	-1.376092000	-0.027769000
6	0.323873000	0.209755000	-0.177820000
1	-4.895581000	-0.696541000	0.310146000
1	-0.990607000	-3.467816000	-0.140397000
1	-3.331096000	-2.609765000	0.115557000
6	1.213931000	-0.882968000	-0.275045000
6	0.745134000	-2.201840000	-0.268758000
1	1.442627000	-3.025112000	-0.362842000
6	-0.622821000	-2.449040000	-0.144955000
6	-1.437197000	2.395436000	0.042514000
1	-2.117871000	3.234621000	0.124987000
6	-0.075071000	2.629471000	-0.089088000
1	0.321306000	3.635696000	-0.112478000
6	0.828974000	1.547337000	-0.207502000
8	2.159788000	1.762240000	-0.340786000
16	2.978294000	-0.479288000	-0.439561000
6	3.450298000	-0.323256000	1.365503000
1	3.376137000	-1.301187000	1.836792000
1	2.772977000	0.390640000	1.826338000
1	4.471633000	0.049790000	1.396208000

E(HF): -1012.673096

9-Methylthiophenalenone 7, lowest triplet excited state, optimized geometry (M06/SDD)

1	-4.082122000	1.579435000	0.286451000
6	-3.376439000	0.756725000	0.197875000
6	-1.995302000	1.046938000	0.069311000
6	-2.925789000	-1.632009000	0.097304000
6	-1.067410000	-0.033758000	-0.046326000
6	-3.828275000	-0.569144000	0.210713000
6	-1.532790000	-1.387635000	-0.032724000
6	0.327142000	0.231763000	-0.178477000
1	-4.889980000	-0.773964000	0.309332000
1	-0.944281000	-3.473435000	-0.148118000
1	-3.280717000	-2.659862000	0.107340000
6	1.232925000	-0.854079000	-0.281157000
6	0.777356000	-2.179184000	-0.275695000
1	1.491673000	-2.992526000	-0.371152000
6	-0.587174000	-2.446719000	-0.151920000
6	-1.491231000	2.381426000	0.050031000
1	-2.194388000	3.206667000	0.134844000
6	-0.134125000	2.646757000	-0.080769000
1	0.242644000	3.664048000	-0.100308000
6	0.796466000	1.585408000	-0.200440000
8	2.111708000	1.857168000	-0.327005000
16	3.007521000	-0.475119000	-0.447769000
6	3.467327000	-0.351867000	1.369114000
1	3.258858000	-1.309079000	1.851289000
1	2.877233000	0.450717000	1.814002000
1	4.531006000	-0.115190000	1.415612000

E(HF): -1012.2809902

9-Methylthiophenalenone 7, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

1	-4.090507000	1.565765000	0.298543000
6	-3.381488000	0.746998000	0.204424000
6	-2.000373000	1.043210000	0.073958000
6	-2.920096000	-1.642161000	0.092662000
6	-1.068151000	-0.034210000	-0.048346000
6	-3.827205000	-0.582200000	0.212282000
6	-1.527266000	-1.391024000	-0.038771000
6	0.325187000	0.237993000	-0.180955000
1	-4.887476000	-0.792026000	0.312415000
1	-0.927404000	-3.474733000	-0.157568000
1	-3.271022000	-2.670973000	0.099496000
6	1.234523000	-0.844407000	-0.289847000
6	0.787599000	-2.172630000	-0.286248000
1	1.504120000	-2.983903000	-0.376866000
6	-0.576733000	-2.446299000	-0.161984000
6	-1.501532000	2.380273000	0.060280000
1	-2.206371000	3.202718000	0.152919000
6	-0.143587000	2.650243000	-0.072851000
1	0.224514000	3.671168000	-0.086069000
6	0.790788000	1.592920000	-0.200373000
8	2.107002000	1.864362000	-0.337448000
16	3.007403000	-0.452571000	-0.442257000
6	3.474082000	-0.385155000	1.375380000
1	3.331107000	-1.378102000	1.804706000
1	2.833461000	0.350571000	1.863778000
1	4.520633000	-0.085557000	1.426673000

E(HF): -1012.2906609

9-Methylthiophenalenone 7, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

1	-4.033028000	1.581227000	0.285302000
6	-3.332037000	0.759672000	0.195432000
6	-1.965536000	1.045451000	0.069130000
6	-2.895780000	-1.604081000	0.093536000
6	-1.053454000	-0.031421000	-0.047266000
6	-3.781566000	-0.547920000	0.205888000
6	-1.517287000	-1.372749000	-0.034155000
6	0.326095000	0.226673000	-0.176876000
1	-4.840950000	-0.747743000	0.303780000
1	-0.931807000	-3.444093000	-0.145928000
1	-3.255670000	-2.626032000	0.103026000
6	1.225917000	-0.846843000	-0.279824000
6	0.770437000	-2.160973000	-0.272023000
1	1.480993000	-2.973678000	-0.362624000
6	-0.575401000	-2.421140000	-0.151282000
6	-1.447148000	2.360369000	0.053478000
1	-2.141689000	3.188157000	0.141700000
6	-0.106644000	2.615095000	-0.073093000
1	0.273595000	3.627549000	-0.087218000
6	0.819333000	1.560743000	-0.200145000
8	2.087525000	1.786818000	-0.329605000
16	2.933535000	-0.448544000	-0.423790000
6	3.413170000	-0.364114000	1.321074000
1	3.262546000	-1.340171000	1.779112000
1	2.804912000	0.390784000	1.814182000
1	4.463748000	-0.086414000	1.362914000

E(HF): -1012.6111521

9-Dimethylaminophenalenone 8, singlet ground state, optimized geometry (M05-2X/SDD)

1	-4.193177000	1.223468000	0.271362000
6	-3.414838000	0.472463000	0.190701000
6	-2.084038000	0.885564000	0.098521000
6	-2.754813000	-1.845098000	0.038792000
6	-1.033745000	-0.080347000	0.006485000
6	-3.758994000	-0.893263000	0.166961000
6	-1.396753000	-1.455948000	-0.042572000
6	0.344062000	0.324025000	-0.060989000
1	-4.796215000	-1.193673000	0.235995000
1	-0.627847000	-3.471329000	-0.285732000
1	-3.000874000	-2.900422000	-0.003015000
6	1.357537000	-0.677326000	-0.050807000
6	0.960386000	-2.056745000	-0.218416000
1	1.721031000	-2.821374000	-0.286384000
6	-0.357401000	-2.424199000	-0.203585000
6	-1.743028000	2.295261000	0.072301000
1	-2.543653000	3.018508000	0.185246000
6	-0.466646000	2.700758000	-0.130886000
1	-0.194270000	3.745818000	-0.208868000
6	0.638144000	1.746495000	-0.312976000
8	1.757986000	2.175765000	-0.724500000
7	2.683441000	-0.418651000	0.171785000
6	3.154891000	0.699512000	0.992210000
1	3.510443000	1.527517000	0.378794000
1	3.951009000	0.327416000	1.644771000
1	2.340088000	1.071264000	1.615016000
6	3.719185000	-1.382744000	-0.212042000
1	3.482006000	-1.846464000	-1.169811000
1	3.861084000	-2.164319000	0.544845000
1	4.658703000	-0.842432000	-0.330899000

E(HF): -709.2220642

9-Dimethylaminophenalenone 8, singlet ground state, optimized geometry (M06/SDD)

1	-4.198069000	1.223494000	0.270414000
6	-3.418136000	0.469030000	0.189558000
6	-2.085186000	0.886268000	0.098278000
6	-2.754092000	-1.846873000	0.036334000
6	-1.032197000	-0.078740000	0.006650000
6	-3.760677000	-0.895470000	0.164450000
6	-1.396024000	-1.457727000	-0.043470000
6	0.344191000	0.326692000	-0.060319000
1	-4.800284000	-1.198312000	0.232436000
1	-0.632378000	-3.474487000	-0.282696000
1	-2.997811000	-2.906281000	-0.007184000
6	1.357956000	-0.680288000	-0.048531000
6	0.960613000	-2.055526000	-0.214801000
1	1.724278000	-2.823700000	-0.275009000
6	-0.359521000	-2.424190000	-0.203132000
6	-1.748569000	2.291157000	0.075729000
1	-2.555131000	3.013585000	0.187429000
6	-0.469021000	2.700137000	-0.125000000
1	-0.198996000	3.749254000	-0.204220000
6	0.637514000	1.753521000	-0.312448000
8	1.753551000	2.184759000	-0.733375000
7	2.688599000	-0.424743000	0.180440000
6	3.158586000	0.691849000	0.998064000
1	3.472297000	1.541814000	0.382758000
1	3.988610000	0.336291000	1.622313000
1	2.354895000	1.038492000	1.655738000
6	3.725120000	-1.375248000	-0.222826000
1	3.474346000	-1.847398000	-1.177049000
1	3.895137000	-2.158403000	0.532049000
1	4.661169000	-0.826767000	-0.364281000

E(HF): -708.7893404

9-Dimethylaminophenalenone 8, singlet ground state, optimized geometry (M06/SDD, solvated by DMF)

1	-4.201229000	1.198435000	0.324666000
6	-3.418290000	0.450385000	0.223593000
6	-2.085993000	0.877442000	0.114999000
6	-2.735639000	-1.859829000	0.036949000
6	-1.028415000	-0.079032000	-0.000476000
6	-3.749738000	-0.915063000	0.190335000
6	-1.382728000	-1.460584000	-0.057922000
6	0.345680000	0.336214000	-0.082789000
1	-4.785147000	-1.227435000	0.270748000
1	-0.607874000	-3.469462000	-0.341765000
1	-2.973185000	-2.919629000	-0.015190000
6	1.368739000	-0.670315000	-0.073383000
6	0.977370000	-2.045575000	-0.268865000
1	1.740609000	-2.810221000	-0.354692000
6	-0.340700000	-2.419738000	-0.247423000
6	-1.757651000	2.281621000	0.099489000
1	-2.562466000	3.001345000	0.232772000
6	-0.479873000	2.696676000	-0.122487000
1	-0.225267000	3.750601000	-0.195417000
6	0.621943000	1.757198000	-0.339959000
8	1.731952000	2.198283000	-0.796149000
7	2.687046000	-0.409528000	0.184514000
6	3.127754000	0.717303000	1.007728000
1	3.470153000	1.558522000	0.396709000
1	3.935551000	0.369332000	1.661050000
1	2.302447000	1.071811000	1.633283000
6	3.734569000	-1.390836000	-0.128440000
1	3.548562000	-1.870787000	-1.092566000
1	3.821183000	-2.162930000	0.648145000
1	4.689564000	-0.864358000	-0.198246000

E(HF): -708.8035122

9-Dimethylaminophenalenone 8, singlet ground state, optimized geometry (M06/cc-pVTZ)

1	-4.159971000	1.205952000	0.258528000
6	-3.382165000	0.454475000	0.180567000
6	-2.067868000	0.873393000	0.095273000
6	-2.725464000	-1.832537000	0.035147000
6	-1.020762000	-0.081065000	0.009315000
6	-3.720163000	-0.896085000	0.155108000
6	-1.379196000	-1.447829000	-0.038140000
6	0.340985000	0.323468000	-0.055246000
1	-4.756590000	-1.198629000	0.217812000
1	-0.613071000	-3.447336000	-0.255142000
1	-2.963807000	-2.889251000	-0.007768000
6	1.347175000	-0.668567000	-0.049498000
6	0.955827000	-2.029564000	-0.200502000
1	1.716494000	-2.794896000	-0.253483000
6	-0.347796000	-2.398282000	-0.186320000
6	-1.735488000	2.267848000	0.072956000
1	-2.544327000	2.983351000	0.180357000
6	-0.476266000	2.678957000	-0.118432000
1	-0.215891000	3.726956000	-0.193843000
6	0.631726000	1.746343000	-0.308301000
8	1.712239000	2.160354000	-0.709430000
7	2.666738000	-0.399830000	0.140538000
6	3.136454000	0.668374000	0.993202000
1	3.545880000	1.502704000	0.423191000
1	3.902397000	0.261401000	1.659700000
1	2.322200000	1.049520000	1.606024000
6	3.688815000	-1.346917000	-0.236687000
1	3.429179000	-1.857352000	-1.162247000
1	3.881832000	-2.097238000	0.540564000
1	4.615714000	-0.801263000	-0.412683000

E(HF): -709.1073199

9-Dimethylaminophenalenone 8, lowest triplet excited state, optimized geometry (M05-2X/SDD)

1	4.141540000	1.528623000	0.000001000
6	3.413137000	0.726179000	0.000000000
6	2.032167000	1.038242000	0.000000000
6	2.918991000	-1.666739000	0.000000000
6	1.094780000	-0.038016000	0.000000000
6	3.837695000	-0.611178000	0.000000000
6	1.522711000	-1.401922000	0.000000000
6	-0.290426000	0.249108000	0.000000000
1	4.898440000	-0.830866000	0.000000000
1	0.855278000	-3.466570000	-0.000001000
1	3.265970000	-2.693254000	0.000000000
6	-1.240909000	-0.788774000	0.000000000
6	-0.832904000	-2.128119000	-0.000001000
1	-1.569338000	-2.923902000	-0.000001000
6	0.533320000	-2.432106000	-0.000001000
6	1.521632000	2.376167000	0.000000000
1	2.227530000	3.198783000	0.000000000
6	0.156527000	2.649272000	0.000000000
1	-0.206577000	3.668540000	-0.000001000
6	-0.784248000	1.590585000	-0.000001000
8	-2.117662000	1.769206000	-0.000001000
7	-2.609440000	-0.344725000	0.000000000
6	-3.365664000	-0.419311000	-1.253515000
1	-4.182944000	0.300990000	-1.213187000
1	-3.767663000	-1.428051000	-1.413491000
1	-2.705570000	-0.156142000	-2.078185000
6	-3.365662000	-0.419310000	1.253517000
1	-2.705567000	-0.156138000	2.078185000
1	-3.767659000	-1.428051000	1.413496000
1	-4.182943000	0.300990000	1.213189000

E(HF): -709.1596339

9-Dimethylaminophenalenone 8, lowest triplet excited state, optimized geometry (M06/SDD)

1	-4.152690000	1.505685000	0.000001000
6	-3.419124000	0.702657000	0.000002000
6	-2.039353000	1.026351000	0.000000000
6	-2.904629000	-1.682401000	0.000002000
6	-1.087496000	-0.038611000	0.000001000
6	-3.835395000	-0.636300000	0.000003000
6	-1.510770000	-1.406081000	0.000001000
6	0.297895000	0.260229000	-0.000002000
1	-4.897016000	-0.865905000	0.000004000
1	-0.843589000	-3.471755000	-0.000005000
1	-3.239017000	-2.717241000	0.000003000
6	1.252496000	-0.781550000	-0.000003000
6	0.843678000	-2.122974000	-0.000002000
1	1.591899000	-2.913432000	-0.000001000
6	-0.520705000	-2.433416000	-0.000002000
6	-1.548739000	2.368228000	-0.000003000
1	-2.269604000	3.183101000	-0.000002000
6	-0.187369000	2.658412000	-0.000008000
1	0.166587000	3.684417000	-0.000013000
6	0.773025000	1.613462000	-0.000008000
8	2.091201000	1.834688000	-0.000014000
7	2.627149000	-0.377480000	0.000002000
6	3.372980000	-0.422090000	1.253260000
1	4.200501000	0.293076000	1.206142000
1	3.773340000	-1.430304000	1.450686000
1	2.709488000	-0.134034000	2.072913000
6	3.373009000	-0.422136000	-1.253235000
1	2.709547000	-0.134082000	-2.072913000
1	3.773353000	-1.430361000	-1.450632000
1	4.200547000	0.293011000	-1.206112000

E(HF): -708.7269324

9-Dimethylaminophenalenone 8, lowest triplet excited state, optimized geometry (M06/SDD, solvated by DMF)

1	4.171342000	1.471035000	0.000000000
6	3.429378000	0.675999000	0.000000000
6	2.051603000	1.014467000	0.000000000
6	2.888127000	-1.705013000	0.000000000
6	1.085463000	-0.040073000	0.000000000
6	3.831294000	-0.668377000	0.000000000
6	1.496131000	-1.412831000	0.000000000
6	-0.297859000	0.275666000	0.000000000
1	4.890103000	-0.909761000	0.000000000
1	0.806973000	-3.472950000	0.000000000
1	3.210541000	-2.743300000	0.000000000
6	-1.257972000	-0.761382000	0.000000000
6	-0.864938000	-2.107850000	0.000000000
1	-1.620536000	-2.889941000	0.000001000
6	0.496363000	-2.431333000	0.000000000
6	1.578043000	2.363115000	-0.000001000
1	2.308932000	3.168834000	-0.000001000
6	0.218847000	2.667420000	-0.000001000
1	-0.118046000	3.700137000	-0.000001000
6	-0.761882000	1.636743000	-0.000001000
8	-2.071729000	1.871985000	-0.000001000
7	-2.637136000	-0.367364000	0.000001000
6	-3.380390000	-0.426877000	-1.256908000
1	-4.249658000	0.233185000	-1.196991000
1	-3.721868000	-1.454045000	-1.455397000
1	-2.731694000	-0.101723000	-2.073692000
6	-3.380389000	-0.426877000	1.256910000
1	-2.731693000	-0.101724000	2.073693000
1	-3.721866000	-1.454046000	1.455399000
1	-4.249657000	0.233184000	1.196994000

E(HF): -708.7394829

9-Dimethylaminophenalenone 8, lowest triplet excited state, optimized geometry (M06/cc-pVTZ)

1	-4.135303000	1.448726000	0.000002000
6	-3.393722000	0.658462000	0.000002000
6	-2.033486000	1.001326000	0.000001000
6	-2.853408000	-1.690167000	0.000002000
6	-1.075466000	-0.041111000	0.000000000
6	-3.785723000	-0.668563000	0.000002000
6	-1.477136000	-1.402849000	0.000001000
6	0.293766000	0.273455000	0.000000000
1	-4.840794000	-0.911719000	0.000003000
1	-0.785870000	-3.442818000	0.000000000
1	-3.172784000	-2.725616000	0.000002000
6	1.250624000	-0.747451000	0.000000000
6	0.862316000	-2.078552000	0.000000000
1	1.618348000	-2.856523000	0.000000000
6	-0.480164000	-2.403524000	0.000000000
6	-1.559541000	2.332937000	0.000000000
1	-2.288222000	3.135973000	0.000000000
6	-0.220727000	2.639997000	-0.000002000
1	0.116022000	3.667989000	-0.000003000
6	0.754610000	1.622878000	-0.000002000
8	2.021460000	1.856736000	-0.000005000
7	2.605897000	-0.333204000	0.000001000
6	3.346486000	-0.427794000	1.229329000
1	4.204873000	0.243413000	1.188627000
1	3.703611000	-1.452366000	1.402122000
1	2.704590000	-0.133570000	2.057658000
6	3.346486000	-0.427788000	-1.229327000
1	2.704591000	-0.133560000	-2.057655000
1	3.703611000	-1.452359000	-1.402126000
1	4.204873000	0.243419000	-1.188622000

E(HF): -709.0359988

2-Iodobenzophenone 9, lowest triplet excited state, optimized geometry (M06/SDD)

6	-1.456084000	0.813392000	-0.017798000
6	-0.343319000	3.342462000	-0.330354000
6	-0.034871000	0.909361000	-0.104185000
6	-2.292361000	1.927290000	-0.051017000
6	-1.737893000	3.210476000	-0.191692000
6	0.486156000	2.226767000	-0.295900000
1	-3.369303000	1.808035000	0.025001000
1	-2.385145000	4.080827000	-0.212613000
1	1.553761000	2.345537000	-0.453244000
1	0.093370000	4.325173000	-0.480412000
6	0.808795000	-0.245403000	-0.068713000
8	0.281270000	-1.502391000	-0.066983000
6	2.276049000	-0.262824000	-0.022379000
6	5.095079000	-0.412518000	0.109934000
6	2.977220000	-1.291913000	-0.694643000
6	3.011308000	0.666679000	0.750639000
6	4.406221000	0.595906000	0.803801000
6	4.371738000	-1.360161000	-0.631078000
1	2.415262000	-2.020995000	-1.270843000
1	2.486971000	1.415620000	1.337806000
1	4.956682000	1.317018000	1.401041000
1	4.895988000	-2.149905000	-1.160921000
1	6.178574000	-0.465234000	0.156926000
53	-2.348765000	-1.119887000	0.106668000

E(HF): -586.8172077

4-Iodo-2-butanone 10, lowest triplet excited state, optimized geometry (M06/SDD)

6	3.582602000	-0.335015000	0.036936000
1	3.808252000	-0.526082000	1.098950000
1	4.140096000	0.553720000	-0.278648000
1	3.944107000	-1.192527000	-0.539239000
6	2.106935000	-0.112988000	-0.202464000
6	1.447376000	1.138916000	0.333501000
1	1.286507000	1.069145000	1.425406000
1	2.131663000	1.981832000	0.160990000
6	0.121055000	1.443723000	-0.353703000
1	0.221769000	1.479689000	-1.440329000
1	-0.349271000	2.353431000	0.026159000
8	1.374648000	-1.271988000	-0.128105000
53	-1.315625000	-0.157568000	0.031810000

E(HF): -242.946648

Iodoacetone 11, lowest triplet excited state, optimized geometry (M06/SDD)

6	-2.260771000	0.023006000	-0.009828000
8	-1.272954000	-0.791742000	-0.011543000
6	-2.056213000	1.438752000	-0.002572000
1	-1.042076000	1.834684000	0.010316000
1	-2.898032000	2.126057000	-0.005119000
53	1.396861000	-0.020511000	0.001095000
6	-3.662741000	-0.539524000	0.005309000
1	-3.963525000	-0.738692000	1.040350000
1	-3.683205000	-1.488638000	-0.534843000
1	-4.384815000	0.154228000	-0.433865000

E(HF): -203.7119524

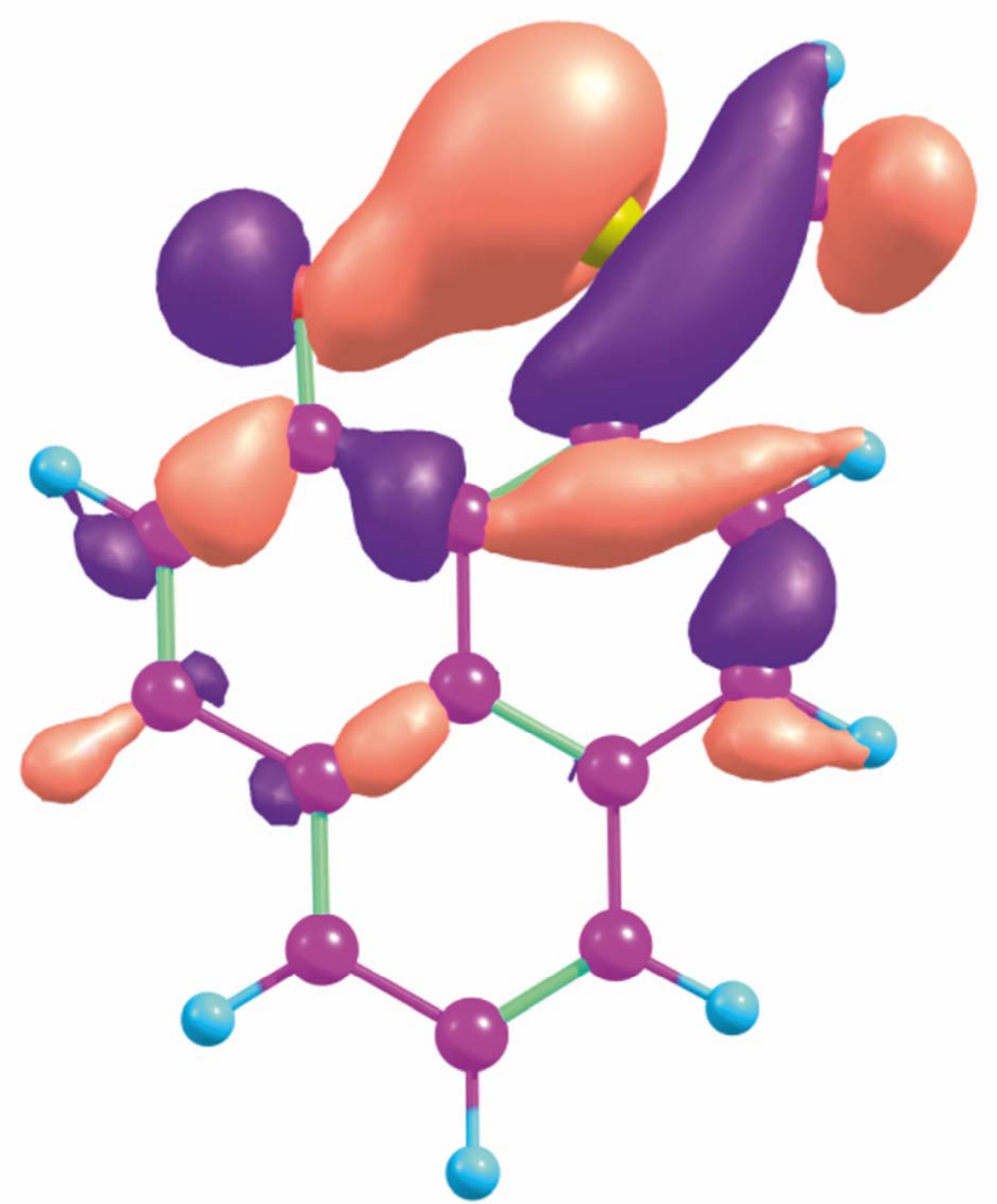

Figure S1: HOMO-6 of **7 (singlet ground state) showing the binding S-O interaction (M052X/SDD)**