Supporting Information

**Impact of Electronically Excited State Hydrogen Bonding on Luminescent Covalent Organic Framework: A TD-DFT investigation**

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Geometry coordinates of PPy-COF in the S0 state

C -9.32647600 1.21125500 0.00000000

C -7.92284200 1.23707000 0.00000000

C -7.17411200 2.46514400 0.00000000

H -9.87389800 2.15069300 0.00000000

H -7.72398600 3.40327200 0.00000000

C 5.71433300 7.46564800 0.00000000

C 5.03369000 6.23784500 0.00000000

C 5.72175800 4.97480700 0.00000000

H 6.80158900 7.46877800 0.00000000

H 6.80911400 4.98101900 0.00000000

C 3.61749100. -8.67888200 0.00000000

C 2.89210500 -7.47691900 0.00000000

C 1.45412100 -7.44390600 0.00000000

H 3.07842900 -9.62313400 0.00000000

H 0.91734100 -8.38959500 0.00000000

C -3.66446700 -1.20746300 0.00000000

C -5.06538100 -1.23574600 0.00000000

C -5.81293800 -2.46464900 0.00000000

H -3.11899800 -2.14794200 0.00000000

H -5.26173800 -3.40193300 0.00000000

C 0.78502600 3.77622100 0.00000000

C 1.46222500 5.00295400 0.00000000

C 0.77284100 6.26545500 0.00000000

H -0.30217500 3.77547500 0.00000000

H -0.31447100 6.25768200 0.00000000

C 2.87539700 -2.56690400 0.00000000

C 3.60158800 -3.76526900 0.00000000

C 5.03965700 -3.79686100 0.00000000

H 3.41615000 -1.62373000 0.00000000

H 5.57504900 -2.85045300 0.00000000

C 0.78502600 -3.77622100 0.00000000

C 1.46222500 -5.00295400 0.00000000

C 0.77284100 -6.26545500 0.00000000

H -0.30217500 -3.77547500 0.00000000

H -0.31447100 -6.25768200 0.00000000

C 2.87539700 2.56690400 0.00000000

C 3.60158800 3.76526900 0.00000000

C 5.03965700 3.79686100 0.00000000

H 3.41615000 1.62373000 0.00000000

H 5.57504900 2.85045300 0.00000000

C -3.66446700 1.20746300 0.00000000

C -5.06538100 1.23574600 0.00000000

C -5.81293800 2.46464900 0.00000000

H -3.11899800 2.14794200 0.00000000

H -5.26173800 3.40193300 0.00000000

C 5.71433300 -7.46564800 0.00000000

C 5.03369000 -6.23784500 0.00000000

C 5.72175800 -4.97480700 0.00000000

H 6.80158900 -7.46877800 0.00000000

H 6.80911400 -4.98101900 0.00000000

C 3.61749100 8.67888200 0.00000000

C 2.89210500 7.47691900 0.00000000

C 1.45412100 7.44390600 0.00000000

H 3.07842900 9.62313400 0.00000000

H 0.91734100 8.38959500 0.00000000

C -9.32647600 -1.21125500 0.00000000

C -7.92284200 -1.23707100 0.00000000

C -7.17411200 -2.46514400 0.00000000

H -9.87389800 -2.15069300 0.00000000

H -7.72398600 -3.40327200 0.00000000

C -10.01659300 0.00000000 0.00000000

C -7.20799400 0.00000000 0.00000000

C 5.01152000 8.66953100 0.00000000

C 3.60494400 6.23866100 0.00000000

C 5.01152000 -8.66953100 0.00000000

C 3.60494400 -6.23866100 0.00000000

B -1.39394200 0.00000000 0.00000000

C -2.94692100 0.00000000 0.00000000

C -5.78221100 0.00000000 0.00000000

B 0.69398100 1.20559800 0.00000000

C 1.47094400 2.55049400 0.00000000

C 2.89087500 5.00453600 0.00000000

B 0.69398100 -1.20559800 0.00000000

C 1.47094400 -2.55049400 0.00000000

C 2.89087500 -5.00453600 0.00000000

O -0.68909500 1.19015200 0.00000000

O 1.37214400 0.00000000 0.00000000

O -0.68909500 -1.19015200 0.00000000

H -11.10329400 0.00000000 0.00000000

H 5.55573600 -9.61012800 0.00000000

H 5.55573600 9.61012800 0.00000000

Geometry coordinates of PPy-COF-HCHO complex in the S0 state

B -0.29022 -1.24344 -0.05121

C -1.12065 -2.53662 -0.06036

O 1.11982 -1.20956 -0.02637

C - 0.53464 -3.81203 -0.00609

C -2.52094 -2.42405 -0.12151

O -0.95336 -0.0001 -0.06287

B 1.85208 -0.00023 -0.01958

C -1.32017 -4.97437 -0.00773

H 0.54613 -3.89709 0.03923

C -3.34411 -3.55504 -0.12949

H -2.97803 -1.44336 -0.16203

B -0.29012 1.24318 -0.05124

C 3.38978 -0.00032 -0.00632

O 1.11993 1.20919 -0.02648

C -2.74477 -4.85024 -0.07056

C -0.75015 -6.29689 0.05188

C -4.78019 -3.44758 -0.19475

C -1.1203 2.53651 -0.06035

C 4.09983 1.21223 -0.00281

C 4.09952 -1.21306 -0.00268

C -3.56903 -6.01383 -0.07451

C -1.53579 -7.40784 0.04952

H 0.32993 -6.38556 0.0988

C -5.56491 -4.55888 -0.20029

H -5.19799 -2.44706 -0.2438

C -0.53378 3.81169 -0.00619

C -2.52065 2.42447 -0.12144

C 5.50072 1.23783 0.00391

H 3.54554 2.1444 -0.00689

C 5.50041 -1.23902 0.00406

H 3.54499 -2.14508 -0.00668

C -2.97263 -7.31187 -0.01401

C -4.9922 -5.88173 -0.14011

H -1.09228 -8.39673 0.09484

H -6.64517 -4.47362 -0.2535

C -1.31883 4.97435 -0.0078

H 0.54703 3.8963 0.03905

C -3.34333 3.55581 -0.12947

H -2.97816 1.44395 -0.16184

C 6.21701 -0.00069 0.00717

C 6.25108 2.46822 0.00631

C 6.25044 -2.46961 0.00662

C -3.80445 -8.44361 -0.01954

C -5.78125 -7.04387 -0.14387

C -2.74348 4.85079 -0.07056

C -0.74828 6.29664 0.05178

C -4.77945 3.44898 -0.19476

C 7.64391 -0.00088 0.01235

C 7.61126 2.4679 0.01138

H 5.69893 3.40177 0.00336

C 7.61062 -2.46966 0.0117

H 5.69803 -3.40302 0.0038

C -5.19071 -8.30606 -0.08414

H -3.35612 -9.43007 0.02617

H -6.86052 -6.94967 -0.19471

C -3.56726 6.01471 -0.07449

C -1.53346 7.4079 0.04945

H 0.33184 6.38486 0.09865

C -5.56374 4.56059 -0.20028

H -5.1977 2.44865 -0.24397

C 8.35981 -1.23875 0.01463

C 8.36014 1.2368 0.01447

H 8.16354 3.40147 0.01273

H 8.16265 -3.40336 0.01319

H -5.81689 -9.19073 -0.08847

C -4.99049 5.8832 -0.14003

C -2.97034 7.31251 -0.014

H -1.08955 8.39661 0.09476

H -6.64403 4.47576 -0.25355

C 9.76414 -1.21331 0.01907

C 9.76446 1.21099 0.0189

C -5.77908 7.04567 -0.14371

C -3.80169 8.44458 -0.01948

C 10.45361 -0.00125 0.02115

H 10.30984 -2.15052 0.02056

H 10.31041 2.14806 0.02027

C -5.18801 8.30762 -0.084

H -6.85838 6.9519 -0.19452

H -3.35296 9.43085 0.02623

H 11.53741 -0.00139 0.02431

H -5.81383 9.19254 -0.08829

C -5.15016 0.00121 1.5308

H -5.2682 0.93214 2.10393

H -5.27519 -0.92881 2.10394

O -4.89228 0.00024 0.32141

Geometry coordinates of PPy-COF in the S1 state

C -9.37393000 -1.20929700 0.00000000

C -7.96017100 -1.23916300 0.00000000

C -7.21746100 -2.45481600 0.00000000

H -9.91620000 -2.15171300 0.00000000

H -7.75678100 -3.39869700 0.00000000

C 5.73869700 -7.45294100 0.00000000

C 5.05323300 -6.22739700 0.00000000

C 5.73545000 -4.96148200 0.00000000

H 6.82609600 -7.45147700 0.00000000

H 6.82296300 -4.96275900 0.00000000

C 3.64650900 8.67405500 0.00000000

C 2.91654700 7.47523200 0.00000000

C 1.47818100 7.44709300 0.00000000

H 3.11106800 9.62051100 0.00000000

H 0.94485300 8.39490700 0.00000000

C -3.68734500 1.20721500 0.00000000

C -5.09165600 1.23617500 0.00000000

C -5.83610600 2.45228200 0.00000000

H -3.14965100 2.15248700 0.00000000

H -5.29532300 3.39538000 0.00000000

C 0.79494500 -3.78116600 0.00000000

C 1.47631100 -5.00517100 0.00000000

C 0.79286300 -6.27093700 0.00000000

H -0.29245500 -3.78477900 0.00000000

H -0.29469300 -6.26768400 0.00000000

C 2.87832200 2.56417300 0.00000000

C 3.60971400 3.75972000 0.00000000

C 5.04791900 3.78629400 0.00000000

H 3.41511500 1.61872800 0.00000000

H 5.57961200 2.83769400 0.00000000

C 0.79494500 3.78116600 0.00000000

C 1.47631100 5.00517100 0.00000000

C 0.79286300 6.27093700 0.00000000

H -0.29245500 3.78477900 0.00000000

H -0.29469300 6.26768400 0.00000000

C 2.87832200 -2.56417300 0.00000000

C 3.60971400 -3.75972000 0.00000000

C 5.04791900 -3.78629400 0.00000000

H 3.41511400 -1.61872800 0.00000000

H 5.57961200 -2.83769400 0.00000000

C -3.68734500 -1.20721500 0.00000000

C -5.09165600 -1.23617500 0.00000000

C -5.83610600 -2.45228200 0.00000000

H -3.14965100 -2.15248700 0.00000000

H -5.29532300 -3.39537900 0.00000000

C 5.73869700 7.45294100 0.00000000

C 5.05323300 6.22739700 0.00000000

C 5.73545000 4.96148200 0.00000000

H 6.82609600 7.45147700 0.00000000

H 6.82296300 4.96275900 0.00000000

C 3.64650900 -8.67405500 0.00000000

C 2.91654700 -7.47523200 0.00000000

C 1.47818100 -7.44709300 0.00000000

H 3.11106800 -9.62051100 0.00000000

H 0.94485300 -8.39490700 0.00000000

C -9.37393000 1.20929700 0.00000000

C -7.96017100 1.23916300 0.00000000

C -7.21746100 2.45481600 0.00000000

H -9.91620000 2.15171300 0.00000000

H -7.75678100 3.39869700 0.00000000

C -10.0776970 0.00000000 0.00000000

C -7.23128500 0.00000000 0.00000000

C 5.04100700 -8.65955900 0.00000000

C 3.62411900 -6.23347300 0.00000000

C 5.04100700 8.65955900 0.00000000

C 3.62411900 6.23347300 0.00000000

B -1.40138000 0.00000000 0.00000000

C -2.93348400 0.00000000 0.00000000

C -5.83068400 0.00000000 0.00000000

C 0.68884700 -1.20692100 0.00000000

C 1.47321800 -2.55091100 0.00000000

C 2.90544000 -5.00251600 0.00000000

B 0.68884700 1.20692100 0.00000000

C 1.47321800 2.55091100 0.00000000

C 2.90544000 5.00251600 0.00000000

O -0.68670300 -1.19926100 0.00000000

O 1.37381000 0.00000000 0.00000000

O -0.68670300 1.19926100 0.00000000

H -11.16260200 0.00000000 0.00000000

H 5.58889100 9.59815500 0.00000000

H 5.58889100 -9.59815500 0.00000000

Geometry coordinates of PPy-COF-HCHO complex in the S1 state

B 0.27916100 1.19948800 0.16473700

C 1.20208300 2.46898900 0.10999000

O -1.09300600 1.28030000 0.10816400

C 0.72772300 3.76381300 -0.10459400

C 2.58960300 2.27383800 0.24581000

O 0.89941500 -0.00934600 0.23291600

B -1.84553800 0.10265800 0.11229400

C 1.60319400 4.88334300 -0.20849800

H -0.34239600 3.93161400 -0.20321300

C 3.50242700 3.35558200 0.14075400

H 3.00634100 1.28986400 0.43996900

B 0.19205100 -1.20334100 0.17423200

C -3.39615000 0.17349800 0.09055200

O -1.19385600 -1.11114100 0.13075200

C 3.00460500 4.66748300 -0.09104900

C 1.13175100 6.20300700 -0.43521200

C 4.89744600 3.12119900 0.25471200

C 0.97033200 -2.53098800 0.11459500

C -4.16127200 -1.00459300 0.08257900

C -4.06460200 1.40869500 0.07910700

C 3.90751500 5.75115600 -0.20585300

C 2.01041400 7.26376800 -0.54401900

H 0.06247700 6.37316800 -0.52461000

C 5.77642000 4.19057600 0.13502200

H 5.21428900 2.08752700 0.43986200

C 0.32254100 -3.76899800 -0.04262700

C 2.37742600 -2.49539500 0.17400800

C -5.56207400 -0.97616600 0.06275200

H -3.65301100 -1.96539100 0.09252700

C - 5.46305200 1.49358500 0.05986300

H -3.48277400 2.32721800 0.08668600

C 3.41486200 7.06655500 -0.43421200

C 5.31072700 5.51333800 -0.09255300

H 1.63195200 8.26716800 -0.71756300

H 6.84558000 4.02011500 0.22072100

C 1.04223600 -4.96564900 -0.15032100

H -0.76403300 -3.80291400 -0.08825400

C 3.13676400 -3.66758000 0.06270600

H 2.90724400 -1.55503400 0.31589300

C -6.22870600 0.28735800 0.05090600

C -6.35771400 -2.17451400 0.05391200

C -6.16127900 2.75110100 0.04869200

C 4.34293400 8.13482300 -0.54539700

C 6.19416300 6.61752900 -0.21261400

C 2.47057000 -4.91884900 -0.10294400

C 0.40298700 -6.24411600 -0.31421400

C 4.57471900 -3.63503700 0.10408800

C -7.65318500 0.34440500 0.03065000

C -7.71766100 -2.12038700 0.03431000

H -5.84431700 -3.13278600 0.06364400

C -7.52121200 2.80606100 0.02930500

H -5.57354600 3.66606000 0.05675000

C 5.71215700 7.90654100 -0.43517700

H 3.97056000 9.14057700 -0.71921700

H 7.26300000 6.44440900 -0.12735100

C 3.23112800 -6.11851700 -0.22087900

C 1.12918700 -7.39026600 -0.42474800

H -0.68377400 -6.27586600 -0.34834700

C 5.29766600 -4.78303700 -0.01174500

H 5.05273700 -2.66848600 0.23383300

C -8.31827800 1.60884700 0.01935900

C -8.41647500 -0.86332900 0.02188600

H -8.30444600 -3.03574900 0.02803400

H -8.03330500 3.76533200 0.02139400

H 6.40699900 8.73527900 -0.52287600

C 4.65871000 -6.06209900 -0.17623600

C 2.56749300 -7.37357700 -0.38345900

H 0.62935300 -8.34844000 -0.54773700

H 6.38413100 -4.75222600 0.02284900

C -9.72160400 1.63916900 -0.00061700

C -9.81787600 -0.78145800 0.00180800

C 5.38491900 -7.25862000 -0.29446200

C 3.33813600 -8.54108900 -0.49680100

C -10.45921900 0.45622600 -0.00928500

H -10.23113600 2.59964300 -0.00905500

H -10.40209800 -1.69835300 -0.00478700

C 4.73056800 -8.47934200 -0.45212200

H 6.47117300 -7.22273600 -0.26032700

H 2.83716900 -9.49846400 -0.61980800

H -11.54492300 0.49931200 -0.02461000

H 5.31220000 -9.39340100 -0.54081800

C 5.42704300 -0.25616800 1.99769400

H 5.33576800 -1.31459800 2.29254600

H 6.40895800 0.16608900 2.27766400

O 4.85881300 0.14178600 0.86783700

Geometry coordinates of PPy-COF complex in the T1 state

C 1.22250000 -9.33103400 0.00000000

C 1.24831700 -7.92738000 0.00000000

C 2.47640800 -7.17867600 0.00000000

H 2.16196600 -9.87836700 0.00000000

H 3.41452300 -7.72853600 0.00000000

C 7.47874200 5.70751600 0.00000000

C 6.25053100 5.02761900 0.00000000

C 4.98785200 5.71621800 0.00000000

H 7.48255200 6.79478300 0.00000000

H 4.99431900 6.80359600 0.00000000

C -8.74404900 3.64827800 0.00000000

C -7.50468700 2.89656400 0.00000000

C -7.47880400 1.50137600 0.00000000

H -9.68298900 3.10175300 0.00000000

H -8.41556100 0.94976900 0.00000000

C -1.19631700 -3.66894900 0.00000000

C -1.22458400 -5.06993900 0.00000000

C -2.45351200 -5.81747900 0.00000000

H -2.13685000 -3.12362100 0.00000000

H -3.39080900 -5.26632700 0.00000000

C 3.78654500 0.78035000 0.00000000

C 5.01367800 1.45677500 0.00000000

C 6.27576600 0.76687100 0.00000000

H 3.78505500 -0.30683700 0.00000000

H 6.26778400 -0.32045000 0.00000000

C -2.55488300 2.86825000 0.00000000

C -3.79064000 3.62049000 0.00000000

C -3.81484700 5.01618600 0.00000000

H -1.61721400 3.41671000 0.00000000

H -2.87740600 5.56643500 0.00000000

C -3.76169900 0.77714700 0.00000000

C -5.03127200 1.47078100 0.00000000

C -6.25184100 0.79346700 0.00000000

H -3.76746000 -0.30912800 0.00000000

H -6.25926600 -0.29350700 0.00000000

C 2.57822300 2.87135100 0.00000000

C 3.77705300 3.59677500 0.00000000

C 3.80950500 5.03474900 0.00000000

H 1.63552600 3.41291600 0.00000000

H 2.86345100 5.57075800 0.00000000

C 1.21873700 -3.66896900 0.00000000

C 1.24700600 -5.06994400 0.00000000

C 2.47593000 -5.81747700 0.00000000

H 2.15929300 -3.12367100 0.00000000

H 3.41322800 -5.26632100 0.00000000

C -7.53355000 5.74578900 0.00000000

C -6.26261800 5.04877600 0.00000000

C -5.04164300 5.72438300 0.00000000

H -7.53010700 6.83220000 0.00000000

H -5.03270200 6.81144500 0.00000000

C 8.69082700 3.60999100 0.00000000

C 7.48847200 2.88535700 0.00000000

C 7.45458700 1.44751700 0.00000000

H 9.63474800 3.07038200 0.00000000

H 8.39993200 0.91015700 0.00000000

C -1.20006400 -9.33103100 0.00000000

C -1.22588500 -7.92737800 0.00000000

C -2.45397200 -7.17868200 0.00000000

H -2.13953200 -9.87836300 0.00000000

H -3.39208400 -7.72854800 0.00000000

C 0.01121600 -10.02111800 0.00000000

C 0.01121600 -7.21256700 0.00000000

C 8.68231100 5.00404400 0.00000000

C 6.25048200 3.59877700 0.00000000

C -8.73323000 5.04008500 0.00000000

C -6.26367200 3.61487200 0.00000000

B 0.01124300 -1.39854200 0.00000000

C 0.01121600 -2.95148800 0.00000000

C 0.01120900 -5.78677500 0.00000000

B 1.21649200 0.68985400 0.00000000

C 2.56113500 1.46685300 0.00000000

C 5.01613400 2.88549700 0.00000000

B -1.19424200 0.68918500 0.00000000

C -2.54070100 1.46627300 0.00000000

C -5.03278200 2.90450200 0.00000000

O 1.20129800 -0.69333900 0.00000000

O 0.01050600 1.36806100 0.00000000

O -1.17926700 -0.69354500 0.00000000

H 0.01121200 -11.1078140 0.00000000

H -9.67464600 5.5833860 0.00000000

H 9.62319400 5.5477460 0.00000000

Geometry coordinates of PPy-COF-HCHO complex in the T1 state

B 0.39165700 1.20657400 -0.10356700

C 1.19068200 2.53741800 -0.10366500

O -0.99174900 1.19219600 -0.07490000

C 0.54446400 3.78274300 -0.04048000

C 2.59434800 2.50888700 -0.15944100

O 1.06555800 0.00014900 -0.12232900

B -1.69375600 -0.00013400 -0.06431000

C 1.26199500 4.98695800 -0.02829800

H -0.54166300 3.81658300 0.00174500

C 3.35826400 3.68313600 -0.15024500

H 3.10755200 1.55291900 -0.21333200

B 0.39190200 -1.20641000 -0.10357200

C -3.24846800 -0.00029800 -0.03862400

O -0.99150300 -1.19232300 -0.07485300

C 2.68937800 4.94299800 -0.08268900

C 0.61705200 6.27102400 0.03831700

C 4.79610900 3.66242700 -0.20479400

C 1.19120800 -2.53709000 -0.10373700

C -3.96113200 -1.20757500 -0.02685300

C -3.96139000 1.20682500 -0.02679800

C 3.44484700 6.15187700 -0.06976800

C 1.33787000 7.42585800 0.05062400

H -0.46920900 6.29971400 0.07896400

C 5.51632700 4.81790800 -0.19197800

H 5.29037400 2.69509300 -0.25881600

C 0.54528500 -3.78254200 -0.04006700

C 2.59484700 -2.50826300 -0.16005300

C -5.40744700 -1.24157100 -0.00253900

H -3.42273500 -2.15101500 -0.03659500

C -5.40771300 1.24050900 -0.00247800

H -3.42319500 2.15038100 -0.03649800

C 2.77529700 7.41221300 -0.00264100

C 4.87204900 6.10261800 -0.12440800

H 0.83390900 8.38813500 0.10110200

H 6.60264500 4.78966000 -0.23562700

C 1.26308400 -4.98659800 -0.02789000

H -0.54081900 -3.81661100 0.00256300

C 3.35902000 -3.68234600 -0.15091300

H 3.10781400 -1.55219100 -0.21436000

C -6.12523800 -0.00060800 0.00974400

C -6.12573100 -2.43846300 0.00937100

C -6.12625400 2.43724700 0.00949400

C 3.54091100 8.58891400 0.00872800

C 5.59350500 7.30703200 -0.11056100

C 2.69043700 -4.94233900 -0.08282500

C 0.61844800 -6.27079100 0.03924900

C 4.79684000 -3.66133700 -0.20602800

C -7.54645900 -0.00076100 0.03378300

C -7.54207300 -2.43873900 0.03337000

H -5.58841500 -3.38329400 -0.00017800

C -7.54259700 2.43721800 0.03349500

H -5.58914100 3.38219400 -0.00000700

C 4.93289600 8.53294500 -0.04477900

H 3.03518300 9.55011300 0.05945300

H 6.67953000 7.27455800 -0.15275200

C 3.44617700 -6.15104900 -0.06992000

C 1.33952300 -7.42546500 0.05154400

H -0.46779200 -6.29971100 0.08030800

C 5.51731900 -4.81665700 -0.19322100

H 5.29086700 -2.69390600 -0.26048700

C -8.26204500 1.24165000 0.04583400

C -8.26177800 -1.24332600 0.04577000

H -8.07790500 -3.38455400 0.04212400

H -8.07863100 3.38291700 0.04229900

H 5.50891400 9.45443300 -0.03554300

C 4.87334700 -6.10149100 -0.12511000

C 2.77692700 -7.41151700 -0.00226000

H 0.83579200 -8.38784000 0.10242500

H 6.60361300 -4.78818200 -0.23730300

C -9.71132500 1.20989400 0.07034700

C -9.71106500 -1.21188300 0.07028400

C 5.59507200 -7.30574400 -0.11126400

C 3.54280300 -8.58804700 0.00908600

C -10.39727900 -0.00106800 0.08191900

H -10.25151400 2.15245900 0.07936500

H -10.25105200 -2.15456400 0.07925300

C 4.93475600 -8.53178700 -0.04495700

H 6.68107300 -7.27304300 -0.15387300

H 3.03730500 -9.54934600 0.06021500

H -11.48411200 -0.00118500 0.10021100

H 5.51097800 -9.45314700 -0.03573100

C 5.33799500 -0.00091400 1.60069700

H 5.35977100 -0.94108500 2.18557500

H 5.36120500 0.93814200 2.18731300

O 5.29070800 0.00023500 0.39098200

Summary of NPA of PPy-COF in the S0 state

C 1 -0.21147

C 2 -0.04910

C 3 -0.20777

H 4 0.23521

H 5 0.23666

C 6 -0.21145

C 7 -0.04911

C 8 -0.20775

H 9 0.23521

H 10 0.23666

C 11 -0.21146

C 12 -0.04910

C 13 -0.20778

H 14 0.23521

H 15 0.23667

C 16 -0.15368

C 17 -0.06017

C 18 -0.20079

H 19 0.23919

H 20 0.23710

C 21 -0.15372

C 22 -0.06015

C 23 -0.20080

H 24 0.23917

H 25 0.23709

C 26 -0.15370

C 27 -0.06016

C 28 -0.20081

H 29 0.23919

H 30 0.23710

C 31 -0.15372

C 32 -0.06015

C 33 -0.20080

H 34 0.23917

H 35 0.23709

C 36 -0.15370

C 37 -0.06016

C 38 -0.20081

H 39 0.23919

H 40 0.23710

C 41 -0.15368

C 42 -0.06017

C 43 -0.20079

H 44 0.23919

H 45 0.23710

C 46 -0.21145

C 47 -0.04911

C 48 -0.20775

H 49 0.23521

H 50 0.23666

C 51 -0.21146

C 52 -0.04910

C 53 -0.20778

H 54 0.23521

H 55 0.23667

C 56 -0.21147

C 57 -0.04910

C 58 -0.20777

H 59 0.23521

H 60 0.23666

C 61 -0.22701

C 62 -0.01422

C 63 -0.22702

C 64 -0.01421

C 65 -0.22702

C 66 -0.01421

B 67 1.19314

C 68 -0.42876

C 69 0.00238

B 70 1.19320

C 71 -0.42871

C 72 0.00238

B 73 1.19320

C 74 -0.42871

C 75 0.00238

O 76 -0.89542

O 77 -0.89553

O 78 -0.89542

H 79 0.23952

H 80 0.23951

H 81 0.23951

Summary of NPA of PPy-COF-HCHO complex in the S0 state

B 1 1.19206

C 2 -0.43032

O 3 -0.89494

C 4 -0.15478

C 5 -0.15521

O 6 -0.89586

B 7 1.19286

C 8 -0.06099

H 9 0.23811

C 10 -0.06062

H 11 0.24702

B 12 1.19206

C 13 -0.42858

O 14 -0.89494

C 15 0.00141

C 16 -0.20102

C 17 -0.20402

C 18 -0.43031

C 19 -0.15374

C 20 -0.15373

C 21 -0.01460

C 22 -0.20876

H 23 0.23667

C 24 -0.21059

H 25 0.24548

C 26 -0.15478

C 27 -0.15522

C 28 -0.06031

H 29 0.23955

C 30 -0.06031

H 31 0.23955

C 32 -0.04926

C 33 -0.04883

H 34 0.23621

H 35 0.23545

C 36 -0.06098

H 37 0.23811

C 38 -0.06062

H 39 0.24702

C 40 0.00222

C 41 -0.20069

C 42 -0.20069

C 43 -0.21268

C 44 -0.21265

C 45 0.00140

C 46 -0.20102

C 47 -0.20405

C 48 -0.01421

C 49 -0.20805

H 50 0.23712

C 51 -0.20805

H 52 0.23713

C 53 -0.22753

H 54 0.23474

H 55 0.23464

C 56 -0.01460

C 57 -0.20876

H 58 0.23667

C 59 -0.21058

H 60 0.24547

C 61 -0.04911

C 62 -0.04912

H 63 0.23654

H 64 0.23654

H 65 0.23896

C 66 -0.04884

C 67 -0.04926

H 68 0.23621

H 69 0.23545

C 70 -0.21168

C 71 -0.21168

C 72 -0.21265

C 73 -0.21268

C 74 -0.22716

H 75 0.23510

H 76 0.23510

C 77 -0.22753

H 78 0.23464

H 79 0.23474

H 80 0.23938

H 81 0.23896

C 82 0.24260

H 83 0.14667

H 84 0.14665

O 85 -0.52185

Summary of NPA of HCHO in the S0 state

C 1 0.22491

H 2 0.13578

H 3 0.13578

O 4 -0.49647

Summary of NPA of PPy-COF-HCHO complex in the S1 state

B 1 1.18592

C 2 -0.42541

O 3 -0.89076

C 4 -0.15676

C 5 -0.14790

O 6 -0.89428

B 7 1.19347

C 8 -0.06246

H 9 0.23445

C 10 -0.06285

H 11 0.25063

B 12 1.19596

C 13 -0.42991

O 14 -0.89652

C 15 -0.00484

C 16 -0.20151

C 17 -0.19981

C 18 -0.43654

C 19 -0.15381

C 20 -0.15283

C 21 -0.01385

C 22 -0.20974

H 23 0.23562

C 24 -0.21691

H 25 0.25329

C 26 -0.15254

C 27 -0.15152

C 28 -0.06063

H 29 0.23906

C 30 -0.06042

H 31 0.24135

C 32 -0.05323

C 33 -0.05178

H 34 0.23504

H 35 0.23028

C 36 -0.06076

H 37 0.23910

C 38 -0.06087

H 39 0.25232

C 40 0.00226

C 41 -0.20068

C 42 -0.20036

C 43 -0.21208

C 44 -0.21142

C 45 0.00165

C 46 -0.20064

C 47 -0.20377

C 48 -0.01427

C 49 -0.20838

H 50 0.23675

C 51 -0.20826

H 52 0.23774

C 53 -0.23424

H 54 0.23234

H 55 0.23151

C 56 -0.01319

C 57 -0.20826

H 58 0.23764

C 59 -0.20927

H 60 0.23405

C 61 -0.04903

C 62 -0.04911

H 63 0.23626

H 64 0.23657

H 65 0.23770

C 66 -0.04945

C 67 -0.04931

H 68 0.23696

H 69 0.23456

C 70 -0.21180

C 71 -0.21198

C 72 -0.21208

C 73 -0.21101

C 74 -0.22727

H 75 0.23508

H 76 0.23486

C 77 -0.22731

H 78 0.23469

H 79 0.23571

H 80 0.23922

H 81 0.23975

C 82 0.18908

H 83 0.17566

H 84 0.17381

O 85 -0.50869