Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLIMENTARY INFORMATION FILE

Donors Contribute More than Acceptors to increase the Two-Photon Activity - A Case study with Cyclopenta[b]naphthalene Based Molecules

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Contents:

1) Optimized Coordinates of All the systems in Gas, CH_2Cl_2 and n-C_6H_{12} solvents

Optimized Coordinates of molecule A in Gas phase

C	3.18101700	-0.76167700	-0.05258300
C	1.96502600	-1.43875400	-0.07013400
C	0.72432200	-0.75734300	-0.04933700
C	0.69623500	0.67353800	-0.02027200
C	1.94536800	1.34651700	-0.02840900
C	3.13613700	0.66675500	-0.04628200
H	-0.48406500	-2.55681500	-0.10116300
H	1.93540500	-2.51942400	-0.10134900
C	-0.50677400	-1.47147200	-0.06867300
C	-0.56115000	1.35521100	0.02495300
H	1.96640700	2.42947400	-0.04671600
C	-1.73096000	0.62641000	0.01370500
C	-1.69661100	-0.79360000	-0.04817200
C	-3.17124700	1.10281000	-0.01769200
H	-3.37668200	1.95135000	0.63914200
C	-3.10493900	-1.34507400	-0.10421300
H	-3.23711400	-2.24561400	0.50075100
C	-3.97266900	-0.15958500	0.37808900
H	-4.06962700	-0.20039700	1.46742900
H	-3.43197700	1.42430900	-1.03420800
H	-4.98011700	-0.17013900	-0.04275900
H	-3.35850000	-1.61255700	-1.13802300
C	-0.59068600	2.86473800	0.07372900
O	-0.28360300	3.53654800	-0.88901100
C	-0.95973900	3.50098800	1.39913300
H	-0.12817100	3.34325100	2.09586700
H	-1.12333100	4.57118100	1.27097500
H	-1.83576900	3.02817400	1.84742800
H	4.05356600	1.23807400	-0.06311900
N	4.40222600	-1.42994300	-0.02726600
C	4.41266000	-2.86823200	-0.23679000
H	5.43210200	-3.23661200	-0.12571500
H	3.79692800	-3.37245700	0.51248800
H	4.04489300	-3.15787200	-1.23332700
C	5.62169400	-0.71045400	-0.36877300
H	6.46979400	-1.38560100	-0.25829100
H	5.61911900	-0.32636200	-1.39975700
H	5.78729600	0.12922700	0.30974200

Optimized Coordinates of molecule B in Gas phase

C	1.88055600	-0.75891500	-0.16666000
C	0.65208300	-1.39207900	-0.01014600
C	-0.53930800	-0.66577700	0.22627300
C	-0.52348100	0.76650400	0.29523500
C	0.74029100	1.39226000	0.11842200
C	1.88413900	0.66752800	-0.10274700
H	-1.77196500	-2.43953600	0.32843700

H	0.57244100	-2.46937700	-0.06144100
C	-1.76961500	-1.35610600	0.39280600
C	-1.75712200	1.46431800	0.55019800
H	0.79703900	2.46882000	0.14580700
C	-2.92272900	0.73078900	0.72193400
C	-2.93521100	-0.67416200	0.63479600
C	-1.84658000	2.96048100	0.61886300
O	-0.95328600	3.69328300	0.22849900
C	-3.10979900	3.59312700	1.19361200
H	-3.37979600	3.16468600	2.16146700
H	-2.92680300	4.66095800	1.30200300
H	-3.95833300	3.45306000	0.51735700
H	2.81046100	1.21045200	-0.23103700
N	3.06203900	-1.46415200	-0.35851500
C	2.98944400	-2.89645500	-0.59438300
H	3.99990000	-3.29948800	-0.65464500
H	2.48340300	-3.39939700	0.23383100
H	2.45865500	-3.14976100	-1.52494700
C	4.24224700	-0.77126600	-0.85794800
H	5.06664800	-1.48110000	-0.91734100
H	4.09068200	-0.33487300	-1.85593500
H	4.55049700	0.02598700	-0.17789500
H	-3.86874300	-1.21059900	0.76136100
H	-3.85716100	1.23955200	0.91576700

Optimized Coordinates of molecule C in Gas phase

C	1.50079100	-0.63362700	0.06242600
C	1.50809900	0.76953900	0.17075700
H	0.21315000	-2.37309700	0.25218700
C	0.28276600	-1.29771500	0.33920900
C	0.37080600	1.47949200	0.56320900
C	-0.81941000	0.79972800	0.84957200
C	-0.84587200	-0.58669600	0.72844200
C	0.48158700	2.97465500	0.65567000
O	1.52449100	3.54354300	0.38832800
C	-0.73471600	3.77204200	1.09125500
H	-1.06898600	3.46258700	2.08558700
H	-0.47179500	4.82840900	1.10938600
H	-1.56964400	3.61692900	0.40186600
N	2.64437700	-1.33731800	-0.28945900
C	2.53724600	-2.74572300	-0.63436300
H	3.53212800	-3.13432700	-0.84825200
H	2.13314100	-3.32527300	0.20024200
H	1.90151800	-2.92272100	-1.51491700
C	3.80173400	-0.60928500	-0.78851300
H	4.61641700	-1.31294400	-0.95604300
H	3.59893800	-0.08201200	-1.73219400
H	4.14680500	0.12504400	-0.05663400
H	-1.76185900	-1.12905900	0.93602300
H	-1.71148000	1.33188400	1.15224300
H	2.39419900	1.34818400	-0.04525500

Optimized Coordinates of molecule D in Gas phase

C	3.19064600	-0.76477100	-0.07951700
C	1.96739400	-1.42953000	-0.08640600
C	0.73602500	-0.73517700	-0.04901600
C	0.71871600	0.69707100	-0.00637100
C	1.97297300	1.35909400	-0.02431800
C	3.15372400	0.66296600	-0.06570100
H	-0.46795100	-2.53419500	-0.07278400
H	1.92479900	-2.50923800	-0.12525400
C	-0.49589500	-1.44881800	-0.05843800
C	-0.55699100	1.34232400	-0.00006000
H	2.00869800	2.43825100	0.00464300
C	-1.73826600	0.63666100	-0.03064800
C	-1.69180000	-0.78233600	-0.04726300
C	-3.17621900	1.10642100	-0.02470900
H	-3.34875900	1.97072100	0.61872500
C	-3.09709800	-1.34417500	-0.06065500
H	-3.20674900	-2.23341200	0.56457300
C	-3.95692900	-0.15291300	0.41927200
H	-4.02686700	-0.17173400	1.51099400
H	-3.46109100	1.41567100	-1.03642000
H	-4.97393900	-0.17606300	0.02344900
H	-3.37121000	-1.63341600	-1.08315800
H	4.07523500	1.22763300	-0.08439700
N	4.40169800	-1.44116400	-0.07430900
C	4.40256800	-2.88147500	-0.27030300
H	5.42195500	-3.25342400	-0.17529500
H	3.79806000	-3.37721400	0.49419300
H	4.01617200	-3.17653200	-1.25753600
C	5.63448600	-0.72474500	-0.37201600
H	6.47249200	-1.41413800	-0.27690100
H	5.64943400	-0.30354400	-1.38763900
H	5.80074600	0.08732200	0.33965900
N	-0.64488700	2.81165600	0.05689100
O	-1.50207700	3.35324700	-0.63435800
O	0.12263700	3.41557500	0.79991100

Optimized Coordinates of molecule E in Gas phase

C	3.18195000	-0.76112000	-0.06971700
C	1.96522600	-1.43996400	-0.09520600
C	0.72637100	-0.75742100	-0.07357200
C	0.70521600	0.67096400	-0.03846600
C	1.94710700	1.34870300	-0.03004500
C	3.13754400	0.66778700	-0.04872700
H	-0.48806700	-2.55205400	-0.11176500
H	1.93658400	-2.52034300	-0.13026800
C	-0.50935800	-1.46649900	-0.08758800
C	-0.55767300	1.34966400	-0.01506300
H	1.95699400	2.43272700	-0.01226500
C	-1.73580600	0.62642100	-0.02468300
C	-1.70203600	-0.79012700	-0.06326700
C	-3.16330100	1.11994800	-0.01082800

H	-3.31696200	1.97066100	0.65667800
C	-3.11473800	-1.33461100	-0.08344200
H	-3.23822300	-2.22732500	0.53441600
C	-3.96459200	-0.13718000	0.40656200
H	-4.04256400	-0.17006800	1.49724300
H	-3.45138600	1.45196300	-1.01663100
H	-4.97901600	-0.14392700	0.00369900
H	-3.39151000	-1.61226800	-1.10840600
H	4.05581200	1.23783900	-0.04667300
N	4.39983700	-1.42801400	-0.04905800
C	4.41503100	-2.86661400	-0.25684900
H	5.43659600	-3.23058600	-0.15437500
H	3.80726000	-3.37399600	0.49733400
H	4.04105100	-3.15696600	-1.25033100
C	5.62906400	-0.70046700	-0.33398600
H	6.47193300	-1.38329700	-0.23437600
H	5.64916500	-0.27506100	-1.34790500
H	5.78331900	0.11019400	0.38202900
C	-0.60098000	2.77751400	0.02375900
N	-0.64227100	3.93332000	0.05423400

Optimized Coordinates of molecule F in Gas phase

C	3.19409600	-0.68459200	0.00393600
C	2.00397500	-1.38605400	-0.03068800
C	0.75245000	-0.72359600	-0.02454400
C	0.71137700	0.70853500	0.02000000
C	1.95067100	1.40307200	0.04890400
C	3.14815700	0.73504500	0.04514100
H	-0.43353200	-2.53513300	-0.11354400
H	2.01672000	-2.47165400	-0.06301500
C	-0.46907900	-1.45057400	-0.07164000
C	-0.55499200	1.37461800	0.04929100
H	1.95428700	2.48623400	0.05357300
C	-1.71617800	0.63326100	0.00816000
C	-1.66639100	-0.78526100	-0.06634400
C	-3.16043900	1.09557600	-0.04507100
H	-3.38618500	1.93528000	0.61631800
C	-3.06736400	-1.35076700	-0.15296600
H	-3.20074300	-2.25776500	0.44191300
C	-3.95641500	-0.17861000	0.32305700
H	-4.07473900	-0.23078600	1.40975200
H	-3.40511000	1.42496700	-1.06298300
H	-4.95505700	-0.19525500	-0.11793200
H	-3.29856600	-1.61225800	-1.19349600
C	-0.60451900	2.88354900	0.11263800
O	-0.29650700	3.56762000	-0.84093800
C	-0.99679800	3.50155800	1.43967900
H	-0.17386100	3.34356000	2.14651900
H	-1.16883400	4.57148000	1.32100600
H	-1.87458700	3.01568300	1.87037000
H	4.07829300	1.29402900	0.07055200
N	4.43141900	-1.33087300	0.05551800

H	4.44032400	-2.28621500	-0.27025700
H	5.21579800	-0.80122400	-0.29537200

Optimized Coordinates of molecule G in Gas phase

C	3.03136800	-0.86175100	-0.51761700
C	1.82734100	-1.52823400	-0.41577100
C	0.61153000	-0.82344300	-0.27731500
C	0.62794200	0.61068700	-0.23482000
C	1.88163600	1.25983700	-0.34746800
C	3.05555000	0.55263300	-0.48534200
H	-0.63903300	-2.59340800	-0.22717800
H	1.82445700	-2.61179000	-0.44733100
C	-0.63338000	-1.50855000	-0.18534000
C	-0.60600700	1.32160300	-0.06424900
H	1.92317900	2.34201900	-0.34937600
C	-1.78719200	0.62046900	0.02505800
C	-1.79669500	-0.80164300	-0.05038100
C	-3.21195000	1.13088500	0.13216800
H	-3.33345400	1.98154100	0.80648600
C	-3.21798200	-1.31567400	0.02352400
H	-3.31558300	-2.21969400	0.62955500
C	-4.00332800	-0.11374500	0.59709900
H	-3.99354800	-0.16194800	1.69036500
H	-3.55761400	1.46305000	-0.85509000
H	-5.04697900	-0.09498200	0.27725300
H	-3.57550900	-1.56383300	-0.98390100
C	-0.59404800	2.83096500	0.00434300
O	-0.34621700	3.50707300	-0.97212500
C	-0.83864200	3.45766500	1.36255900
H	0.04737500	3.27877600	1.98300800
H	-0.99353100	4.53181700	1.25960600
H	-1.68047300	2.99430900	1.88053500
H	3.98867000	1.09212400	-0.57564500
O	4.14906800	-1.63701100	-0.65014900
C	5.41586300	-1.00425100	-0.77229400
H	5.65499300	-0.40733700	0.11456400
H	6.14099500	-1.81105100	-0.86670400
H	5.46469500	-0.37001100	-1.66397000

Optimized Coordinates of molecule A in CH2Cl2 solvent

C	3.18369000	-0.76621800	-0.05345600
C	1.96414000	-1.44178600	-0.08257300
C	0.72387600	-0.75878700	-0.05825600
C	0.69608000	0.67280100	-0.01927000
C	1.94713800	1.34397200	-0.01079300
C	3.13852600	0.66381800	-0.03043700
C	-0.50893800	-1.47300600	-0.07897000
C	-0.56322700	1.35351800	0.02551500
C	-1.73448000	0.62586700	0.01631600
C	-1.69929200	-0.79521800	-0.04926300
C	-3.17531100	1.10114900	-0.00465000
C	-3.10796300	-1.34658200	-0.09637700

C	-3.97203200	-0.16267600	0.39564600
C	-0.59781600	2.86176100	0.05965000
C	-0.95740300	3.51770100	1.37123700
C	4.41307000	-2.87134400	-0.26461200
C	5.62821700	-0.70984800	-0.34132900
H	-0.48655300	-2.55809700	-0.11657100
H	1.93383500	-2.52215500	-0.12159800
H	1.97286900	2.42724600	-0.00272500
H	-3.37595600	1.94871500	0.65420300
H	-3.23389700	-2.24922200	0.50614700
H	-4.06033400	-0.20480200	1.48549400
H	-3.44398400	1.42082400	-1.01957100
H	-4.98169000	-0.17270200	-0.01882200
H	-3.36821000	-1.61020700	-1.12923400
H	-0.11477900	3.38178000	2.05930400
H	-1.13726300	4.58362600	1.23108800
H	-1.82064600	3.04041800	1.83836300
H	4.05618900	1.23488900	-0.03099700
H	5.43159800	-3.23996500	-0.15301200
H	3.79083500	-3.39079800	0.46813800
H	4.05446400	-3.13796900	-1.26981600
H	6.47255500	-1.38772000	-0.22556600
H	5.63998500	-0.31622600	-1.36773400
H	5.78272900	0.12193600	0.34863300
N	4.40039700	-1.43415300	-0.02833900
O	-0.30395300	3.51803000	-0.92436400

Optimized Coordinates of molecule B in CH2Cl2 solvent

C	1.87367000	-0.75674400	-0.16974000
C	0.64349400	-1.39429600	-0.01865800
C	-0.55234600	-0.67126500	0.20469400
C	-0.54343000	0.76214400	0.25940800
C	0.72047000	1.39161500	0.09607200
C	1.87114900	0.67223900	-0.10937100
C	-1.78272100	-1.36364400	0.37651100
C	-1.78001300	1.45599500	0.50602300
C	-2.94345200	0.72389800	0.69743800
C	-2.94984000	-0.68279300	0.61943400
C	-1.87875500	2.94984800	0.52522000
C	-3.03979200	3.59358400	1.26465100
C	2.99105000	-2.89089200	-0.58989800
C	4.24933500	-0.75704500	-0.81285700
H	-1.78293800	-2.44722000	0.31847300
H	0.56995000	-2.47235500	-0.05991500
H	0.77869500	2.46868900	0.12276200
H	-3.19597300	3.14859800	2.24907600
H	-2.83516400	4.65850800	1.36610400
H	-3.96665600	3.47524300	0.69534100
H	2.79735500	1.21760200	-0.22693700
H	4.00364600	-3.28649900	-0.64865200
H	2.48318700	-3.40091300	0.23249600
H	2.46634200	-3.13879000	-1.52402000

H	5.07344300	-1.46703100	-0.85922800
H	4.11931800	-0.31377400	-1.80980600
H	4.54021400	0.03415700	-0.11870800
H	-3.88109600	-1.22129500	0.75225100
H	-3.87877800	1.23262600	0.88874600
N	3.05477300	-1.45585900	-0.34892100
O	-1.06454500	3.66443100	-0.04496100

Optimized Coordinates of molecule C in CH2Cl2 solvent

C	1.50573500	-0.63222300	0.06118700
C	1.51344300	0.77294000	0.16999100
C	0.28383500	-1.29364600	0.33771400
C	0.37550400	1.48490800	0.56313800
C	-0.81672400	0.80641200	0.84959300
C	-0.84382800	-0.58077600	0.72735300
C	0.47663900	2.97740100	0.65797200
C	-0.74008100	3.76745400	1.09242800
C	2.53490400	-2.74904200	-0.63226500
C	3.80595700	-0.61310800	-0.79025500
H	0.21213400	-2.36867800	0.24977300
H	-1.07154600	3.45511500	2.08643600
H	-0.48911600	4.82675900	1.11129400
H	-1.57453000	3.60466800	0.40476700
H	3.52909500	-3.13797100	-0.84522500
H	2.12791500	-3.32662800	0.20147600
H	1.90032600	-2.92111800	-1.51327900
H	4.61586300	-1.32049200	-0.96051800
H	3.60061200	-0.08732200	-1.73359800
H	4.15661800	0.11999800	-0.05986800
H	-1.76054400	-1.12197500	0.93419800
H	-1.70851100	1.33835200	1.15241400
H	2.40423900	1.34333100	-0.04698700
N	2.64488100	-1.33705700	-0.28784000
O	1.52161300	3.55493400	0.39087400

Optimized Coordinates of molecule D in CH2Cl2 solvent

C	3.19382300	-0.76501900	-0.08793200
C	1.96609200	-1.42788400	-0.09071600
C	0.73693500	-0.73079500	-0.05277000
C	0.72009500	0.70216200	-0.01216000
C	1.97545000	1.36156800	-0.04422800
C	3.15666900	0.66431500	-0.08684800
C	-0.49650000	-1.44451200	-0.06190100
C	-0.55886500	1.34601200	-0.00390900
C	-1.74263900	0.64008400	-0.03873400
C	-1.69366400	-0.77931000	-0.05511400
C	-3.18214000	1.10487600	-0.02263300
C	-3.09715700	-1.34444000	-0.06386200
C	-3.95686000	-0.15707600	0.42387000
C	4.40070200	-2.88503900	-0.26697000
C	5.64019400	-0.72602400	-0.35798100
H	-0.46858700	-2.52964500	-0.07221800

H	1.92150500	-2.50742100	-0.12787900
H	2.01711800	2.44102200	-0.03321000
H	-3.35381300	1.96689300	0.62421600
H	-3.19992300	-2.23586300	0.55842100
H	-4.02037200	-0.17726400	1.51572700
H	-3.47634900	1.40961500	-1.03321500
H	-4.97482300	-0.18079100	0.03171300
H	-3.37395900	-1.62986400	-1.08630000
H	4.07805400	1.22834700	-0.12012700
H	5.41968600	-3.25466400	-0.16725500
H	3.79242200	-3.37770400	0.49596000
H	4.01886500	-3.18058900	-1.25462600
H	6.47368600	-1.41754600	-0.24797400
H	5.66938300	-0.31027000	-1.37450300
H	5.79562600	0.08822200	0.35308300
N	4.39892600	-1.44070400	-0.07836900
N	-0.64621700	2.80748100	0.07248900
O	-1.50877800	3.36849500	-0.60133500
O	0.12714500	3.40993000	0.81612500

Optimized Coordinates of molecule E in CH2Cl2 solvent

C	3.18554100	-0.76214700	-0.07384300
C	1.96474300	-1.43927700	-0.09819700
C	0.72753700	-0.75411300	-0.07529700
C	0.70715600	0.67506900	-0.04116700
C	1.95058600	1.35067400	-0.03622900
C	3.14119200	0.66845400	-0.05601800
C	-0.50990500	-1.46310300	-0.08722000
C	-0.55894200	1.35084000	-0.01596800
C	-1.73948200	0.62885600	-0.02292200
C	-1.70395100	-0.78821700	-0.06154000
C	-3.16771500	1.11962300	-0.00747600
C	-3.11546400	-1.33487500	-0.07964900
C	-3.96696000	-0.13892100	0.40986300
C	4.41413700	-2.86944000	-0.26344000
C	5.63431300	-0.70120300	-0.32226000
C	-0.60490900	2.77683600	0.02083100
H	-0.48855900	-2.54843600	-0.11104300
H	1.93435600	-2.51952000	-0.13233000
H	1.96691600	2.43479200	-0.02109700
H	-3.32415000	1.96857400	0.66176500
H	-3.23514000	-2.22719200	0.53868000
H	-4.04638800	-0.17124100	1.50027200
H	-3.45624400	1.44933500	-1.01370900
H	-4.97958000	-0.14616900	0.00369400
H	-3.39121400	-1.61304600	-1.10430100
H	4.05972900	1.23790300	-0.05799800
H	5.43509100	-3.23226700	-0.15834300
H	3.80216300	-3.37950400	0.48488600
H	4.04519000	-3.15265400	-1.25977100
H	6.47336100	-1.38629900	-0.21385000
H	5.66381800	-0.27803800	-1.33591200

H	5.78102500	0.10939700	0.39474800
N	4.39827600	-1.42841700	-0.05177500
N	-0.64895100	3.93352400	0.04907900

Optimized Coordinates of molecule F in CH2Cl2 solvent

C	3.19724800	-0.68840000	0.00510900
C	2.00437100	-1.38808400	-0.04274100
C	0.75315100	-0.72356300	-0.03390800
C	0.71241900	0.70878400	0.02376400
C	1.95332900	1.40103100	0.07065200
C	3.15140800	0.73221700	0.06421700
C	-0.46950500	-1.45086100	-0.08639200
C	-0.55603900	1.37375400	0.05285600
C	-1.71843400	0.63329100	0.00985200
C	-1.66763500	-0.78603400	-0.07225600
C	-3.16346400	1.09421100	-0.03405900
C	-3.06883700	-1.35148300	-0.15387600
C	-3.95527900	-0.18248300	0.33385900
C	-0.61036700	2.88137300	0.10645200
C	-0.99542300	3.51493000	1.42150100
H	-0.43362800	-2.53494300	-0.13664100
H	2.01618600	-2.47291500	-0.08761500
H	1.96133200	2.48398600	0.10221900
H	-3.38586100	1.93112500	0.63123400
H	-3.19665300	-2.26219600	0.43587800
H	-4.06658700	-0.23893100	1.42090500
H	-3.41425700	1.42422800	-1.05017400
H	-4.95557700	-0.19752400	-0.10242600
H	-3.30507500	-1.60623000	-1.19466900
H	-0.16719800	3.36860800	2.12464700
H	-1.17508700	4.58256700	1.29518000
H	-1.86713700	3.02868000	1.86322900
H	4.08151900	1.28998300	0.10237000
H	4.44175200	-2.28506800	-0.28997000
H	5.21847600	-0.80311300	-0.28453600
N	4.43197100	-1.33664900	0.05872700
O	-0.31344600	3.55315900	-0.86585300

Optimized Coordinates of molecule G in CH2Cl2 solvent

C	1.82465900	-1.53092800	-0.43370500
C	0.60917500	-0.82449900	-0.28891700
C	0.62882100	0.60923800	-0.23092000
C	1.88654300	1.25557400	-0.32354400
C	3.06017600	0.54800100	-0.46645400
C	-0.63691300	-1.50965300	-0.20166500
C	-0.60652400	1.31979200	-0.05961900
C	-1.78931000	0.61997500	0.02899100
C	-1.79958700	-0.80269500	-0.05554900
C	-3.21329600	1.12975500	0.14673400
C	-3.22056200	-1.31611900	0.02332100
C	-4.00151400	-0.11763400	0.60918200
C	-0.59989300	2.82818500	-0.00304900

C	-0.84050400	3.47329300	1.34051000
C	5.42310800	-1.00331600	-0.77120500
H	-0.64390800	-2.59395800	-0.25341600
H	1.81414600	-2.61432200	-0.47741600
H	1.93693600	2.33709100	-0.29349000
H	-3.33029000	1.97636300	0.82610000
H	-3.31352300	-2.22453800	0.62281800
H	-3.98561500	-0.17158900	1.70189900
H	-3.56446300	1.46477400	-0.83747000
H	-5.04594200	-0.09619500	0.29351600
H	-3.58279500	-1.55629100	-0.98406800
H	0.06094800	3.32786100	1.94750400
H	-1.02517700	4.54142500	1.22622200
H	-1.65981000	2.99610300	1.88050300
H	3.99560800	1.08598300	-0.53688000
H	5.65486300	-0.42234400	0.12631900
H	6.14704500	-1.80913000	-0.87567600
H	5.47130000	-0.35646600	-1.65209100
O	-0.36111500	3.48990700	-0.99791100
O	4.14902900	-1.64035900	-0.66359200

Optimized Coordinates of molecule A in C6H12

C	3.18074400	-0.76192200	-0.05289200
C	1.96356700	-1.43905700	-0.07489100
C	0.72263100	-0.75780100	-0.05443600
C	0.69409900	0.67343300	-0.02333200
C	1.94356400	1.34641200	-0.02551300
C	3.13502000	0.66723700	-0.04241700
C	-0.50899600	-1.47242300	-0.07370500
C	-0.56418200	1.35396500	0.02022700
C	-1.73428200	0.62555300	0.01035300
C	-1.69930000	-0.79491800	-0.05088700
C	-3.17455900	1.10183000	-0.01527500
C	-3.10790000	-1.34623800	-0.10203200
C	-3.97378600	-0.16089400	0.38399500
C	-0.59795100	2.86296800	0.06532000
C	-0.94375100	3.50248900	1.39249400
C	4.41269400	-2.86756800	-0.24448300
C	5.62340000	-0.70748700	-0.35470600
H	-0.48610200	-2.55773100	-0.10652100
H	1.93458400	-2.51966900	-0.10783000
H	1.96591100	2.42968600	-0.03518300
H	-3.37649200	1.95034700	0.64259100
H	-3.23738500	-2.24716400	0.50268500
H	-4.06639600	-0.20152900	1.47365500
H	-3.43975300	1.42248400	-1.03079400
H	-4.98242700	-0.17158900	-0.03354800
H	-3.36477900	-1.61266200	-1.13516500
H	-0.10327400	3.34163600	2.07765100
H	-1.10719600	4.57304900	1.26800400
H	-1.81467000	3.03135900	1.85243900
H	4.05232100	1.23882000	-0.05380300

H	5.43195000	-3.23517600	-0.13229300
H	3.79442400	-3.37764700	0.49848500
H	4.04932900	-3.14908600	-1.24447200
H	6.47016900	-1.38305400	-0.23963900
H	5.62803700	-0.32102800	-1.38437900
H	5.78288800	0.12994900	0.32769300
N	4.40028600	-1.42931300	-0.02577700
O	-0.31597500	3.53131000	-0.91022300

Optimized Coordinates of molecule B in C6H12

C	1.87825100	-0.75827400	-0.16826900
C	0.64888500	-1.39265000	-0.01265700
C	-0.54415700	-0.66706000	0.21730200
C	-0.53109900	0.76588100	0.27860600
C	0.73275300	1.39246500	0.10507700
C	1.87923500	0.66935000	-0.10881200
C	-1.77455800	-1.35796700	0.38625900
C	-1.76580100	1.46237400	0.53035200
C	-2.93065300	0.72936300	0.71038200
C	-2.94092900	-0.67624700	0.62752700
C	-1.85947000	2.95764800	0.58011900
C	-3.08411100	3.59150200	1.22679800
C	2.98994100	-2.89492900	-0.59155000
C	4.24626600	-0.76668700	-0.83832000
H	-1.77607500	-2.44150300	0.32522900
H	0.57159400	-2.47032900	-0.05804500
H	0.79020200	2.46921200	0.12824200
H	-3.30833700	3.15109300	2.20051400
H	-2.89319900	4.65773000	1.33841800
H	-3.96543400	3.46370400	0.59124300
H	2.80532900	1.21294600	-0.23523300
H	4.00114000	-3.29515500	-0.65140600
H	2.48333300	-3.40068700	0.23445300
H	2.46146400	-3.14576200	-1.52349600
H	5.07077900	-1.47652800	-0.88940500
H	4.10503400	-0.32967400	-1.83707600
H	4.54624700	0.02944100	-0.15349600
H	-3.87366100	-1.21336900	0.75641800
H	-3.86541700	1.23818500	0.90306000
N	3.05930900	-1.46135200	-0.35384600
O	-0.99626700	3.68604200	0.11464200

Optimized Coordinates of molecule C in C6H12

C	1.50311100	-0.63289700	0.06168400
C	1.51059300	0.77120300	0.17053300
C	0.28339600	-1.29573700	0.33846100
C	0.37325000	1.48201600	0.56358900
C	-0.81800600	0.80280100	0.84983800
C	-0.84479400	-0.58390200	0.72806500
C	0.47981400	2.97581600	0.65787500
C	-0.73751900	3.76975800	1.09098100
C	2.53591100	-2.74720800	-0.63312600

C	3.80361000	-0.61090300	-0.78999800
H	0.21295900	-2.37097800	0.25110100
H	-1.07195000	3.45873700	2.08460600
H	-0.48035900	4.82752400	1.11011800
H	-1.57089200	3.61113200	0.40075300
H	3.53037200	-3.13598700	-0.84704000
H	2.13125600	-3.32549800	0.20173400
H	1.90012300	-2.92234600	-1.51338800
H	4.61561800	-1.31656100	-0.95982200
H	3.59918300	-0.08354600	-1.73294300
H	4.15215300	0.12203900	-0.05845100
H	-1.76107100	-1.12581100	0.93540000
H	-1.70984000	1.33488200	1.15287700
H	2.39882900	1.34596900	-0.04585400
N	2.64442600	-1.33698500	-0.28917900
O	1.52425500	3.54872200	0.39295800

Optimized Coordinates of molecule D in C6H12

C	1.50311100	-0.63289700	0.06168400
C	1.51059300	0.77120300	0.17053300
C	0.28339600	-1.29573700	0.33846100
C	0.37325000	1.48201600	0.56358900
C	-0.81800600	0.80280100	0.84983800
C	-0.84479400	-0.58390200	0.72806500
C	0.47981400	2.97581600	0.65787500
C	-0.73751900	3.76975800	1.09098100
C	2.53591100	-2.74720800	-0.63312600
C	3.80361000	-0.61090300	-0.78999800
H	0.21295900	-2.37097800	0.25110100
H	-1.07195000	3.45873700	2.08460600
H	-0.48035900	4.82752400	1.11011800
H	-1.57089200	3.61113200	0.40075300
H	3.53037200	-3.13598700	-0.84704000
H	2.13125600	-3.32549800	0.20173400
H	1.90012300	-2.92234600	-1.51338800
H	4.61561800	-1.31656100	-0.95982200
H	3.59918300	-0.08354600	-1.73294300
H	4.15215300	0.12203900	-0.05845100
H	-1.76107100	-1.12581100	0.93540000
H	-1.70984000	1.33488200	1.15287700
H	2.39882900	1.34596900	-0.04585400
N	2.64442600	-1.33698500	-0.28917900
O	1.52425500	3.54872200	0.39295800

Optimized Coordinates of molecule E in C6H12

C	3.18360300	-0.76189800	-0.07093700
C	1.96503700	-1.43985800	-0.09609700
C	0.72697400	-0.75605800	-0.07394500
C	0.70624400	0.67267800	-0.03923400
C	1.94884400	1.34936700	-0.03196100
C	3.13919900	0.66776600	-0.05096700
C	-0.50961500	-1.46485600	-0.08729600

C	-0.55805300	1.34997600	-0.01524300
C	-1.73745900	0.62757500	-0.02380100
C	-1.70293400	-0.78916700	-0.06253700
C	-3.16529000	1.11993900	-0.00934100
C	-3.11513800	-1.33461200	-0.08225800
C	-3.96578100	-0.13790100	0.40758900
C	4.41506000	-2.86795400	-0.25881000
C	5.63102400	-0.70045900	-0.33051500
C	-0.60261300	2.77706700	0.02240200
H	-0.48855900	-2.55034900	-0.11139900
H	1.93580100	-2.52016600	-0.13080700
H	1.96183100	2.43340700	-0.01499000
H	-3.32034500	1.96956000	0.65925200
H	-3.23718000	-2.22721500	0.53568000
H	-4.04459900	-0.17072800	1.49810900
H	-3.45339700	1.45142000	-1.01520800
H	-4.97932000	-0.14470200	0.00303700
H	-3.39120200	-1.61223200	-1.10723700
H	4.05770100	1.23733400	-0.05002300
H	5.43620600	-3.23139200	-0.15372700
H	3.80469600	-3.37617100	0.49238100
H	4.04451200	-3.15544300	-1.25394000
H	6.47243500	-1.38432400	-0.22930700
H	5.65286500	-0.27551700	-1.34411000
H	5.78354400	0.10960700	0.38624400
N	4.39924600	-1.42816200	-0.04974700
N	-0.64576400	3.93326300	0.05120600

Optimized Coordinates of molecule F in C6H12

C	3.19402900	-0.68301800	0.00770800
C	2.00335300	-1.38477500	-0.03242600
C	0.75130000	-0.72271500	-0.02767700
C	0.70933500	0.70955200	0.01999400
C	1.94861500	1.40433500	0.05653100
C	3.14701500	0.73716600	0.05401600
C	-0.47013600	-1.45083400	-0.07700100
C	-0.55823600	1.37396300	0.04618800
C	-1.71928100	0.63241700	0.00421000
C	-1.66827400	-0.78648800	-0.07054200
C	-3.16379000	1.09396400	-0.04467500
C	-3.06922600	-1.35241800	-0.15452100
C	-3.95759000	-0.18116500	0.32500500
C	-0.61265600	2.88238700	0.10639100
C	-0.97974600	3.50332800	1.43632000
H	-0.43368200	-2.53528100	-0.12015700
H	2.01681700	-2.47010900	-0.06817000
H	1.95315300	2.48764000	0.07067200
H	-3.38723600	1.93300400	0.61823500
H	-3.20024500	-2.26028100	0.43929200
H	-4.07293400	-0.23398900	1.41192300
H	-3.41173200	1.42312300	-1.06175600
H	-4.95691500	-0.19806900	-0.11400600

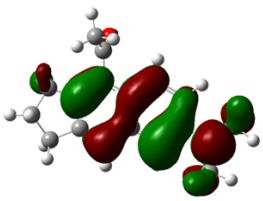
H	-3.30229700	-1.61217200	-1.19494000
H	-0.15113300	3.33458100	2.13378700
H	-1.14417800	4.57496100	1.32326600
H	-1.85745700	3.02431600	1.87503600
H	4.07664600	1.29655300	0.08440200
H	4.44036400	-2.28189600	-0.27368400
H	5.21552600	-0.79824100	-0.28705600
N	4.43073900	-1.32942200	0.06206900
O	-0.33247700	3.56303000	-0.86089700

Optimized Coordinates of molecule G in C6H12

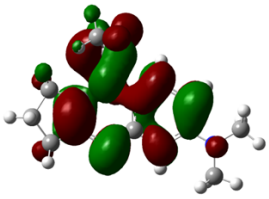
C	3.03139200	-0.86320300	-0.51756200
C	1.82615300	-1.52918600	-0.42058700
C	0.61023400	-0.82390900	-0.28052300
C	0.62766500	0.61010000	-0.23276000
C	1.88284700	1.25832800	-0.33725500
C	3.05687600	0.55119300	-0.47640200
C	-0.63511700	-1.50918400	-0.19076800
C	-0.60707700	1.32061100	-0.06349300
C	-1.78881100	0.62002100	0.02559800
C	-1.79841300	-0.80235900	-0.05252200
C	-3.21314800	1.13040600	0.13682300
C	-3.21967900	-1.31603000	0.02263500
C	-4.00359700	-0.11529400	0.60043600
C	-0.59829900	2.82957500	0.00023900
C	-0.83378400	3.46234400	1.35432000
C	5.41856000	-1.00216500	-0.77226000
H	-0.64108300	-2.59385300	-0.23615800
H	1.82026200	-2.61272000	-0.45657200
H	1.92791400	2.34040600	-0.32739500
H	-3.33252500	1.97929200	0.81353400
H	-3.31593100	-2.22167100	0.62618900
H	-3.99221600	-0.16575200	1.69350600
H	-3.56074100	1.46416500	-0.84910200
H	-5.04729600	-0.09546800	0.28142400
H	-3.57832300	-1.56103200	-0.98502600
H	0.06008300	3.29306000	1.96617500
H	-0.99858900	4.53476400	1.24969800
H	-1.66608300	2.99408100	1.88288800
H	3.99084000	1.09017000	-0.55932600
H	5.65539500	-0.40960900	0.11733700
H	6.14371700	-1.80815600	-0.86998800
H	5.46495800	-0.36493100	-1.66115800
O	-0.36192600	3.50068900	-0.98526900
O	4.14924100	-1.63758400	-0.65262300

2) Solvent phase orbital pictures of all the systems

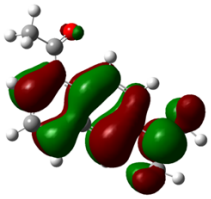
In CH_2Cl_2 solvent:



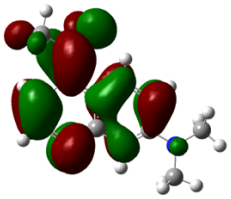
A-HOMO



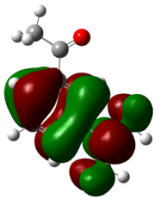
A-LUMO



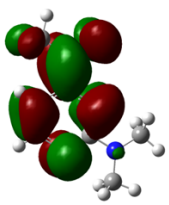
B-HOMO



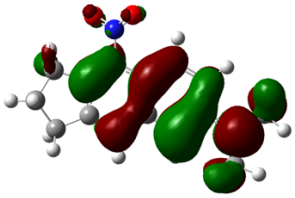
B-LUMO



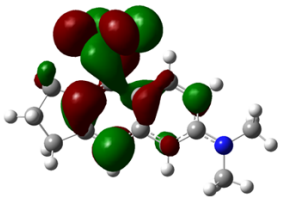
C-HOMO



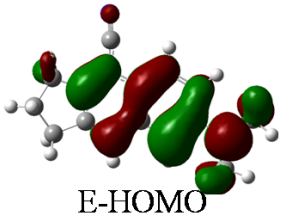
C-LUMO



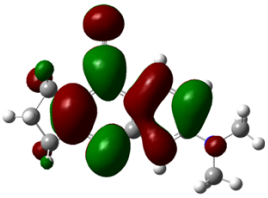
D-HOMO



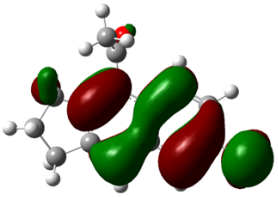
D-LUMO



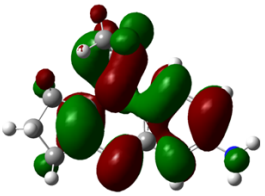
E-HOMO



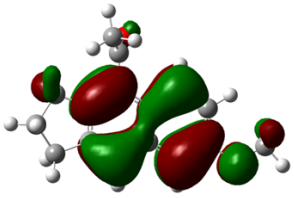
E-LUMO



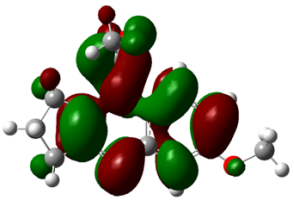
F-HOMO



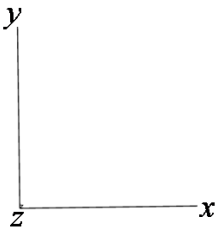
F-LUMO



G-HOMO



G-LUMO



In n-C_6H_{12} solvent: