Supporting Information for

Harnessing Greenhouse Gases Absorption by Doped Fullerenes with Externally Oriented Electric Field

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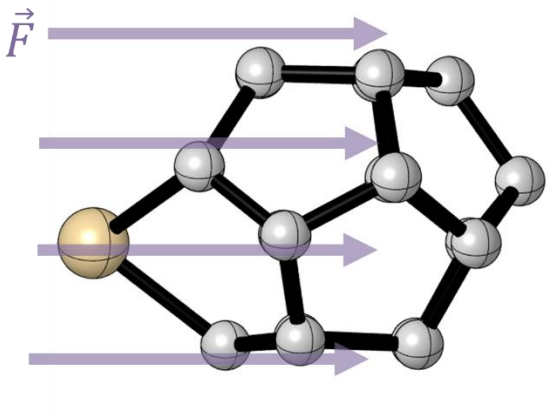


Figure S1. Orientation of the electric field vector with respect to the $C_{19}Si$ cage.

Table S 1. Optimized coordinates for C_{20} and $C_{19}Si$ fullerenes at theoretical levels ωB97XD/6-31G(d) and ωB97XD/6-311+G(d,p). Electic field F in atomic units and Total energies in hartree.

ωB97XD/6-31G(d)			**ωB97XD/6-311+G(d,p)**		
C_{20}					
$F = 0.000$ $Energy = -761.177568$			$F = 0.000$ $Energy = -761.327563$		
C	1.96817100	-0.00013300 -0.69597200	C	1.96549500	-0.00012400 -0.69506900
C	1.17416600	-1.17719400 -1.11374100	C	1.17269000	-1.17611700 -1.11335400
C	1.96818000	0.00019900 0.69595700	C	1.96550400	0.00019000 0.69505300
C	1.17417700	-1.17663900 1.11421000	C	1.17268800	-1.17556800 1.11383100
C	0.76585100	-1.94678400 0.00041000	C	0.76534100	-1.94358200 0.00041000
C	1.17413600	1.17723200 1.11373200	C	1.17266000	1.17615500 1.11334400
C	-0.00000400	0.71876000 1.80649800	C	-0.00000400	0.71793600 1.80537200
C	0.00002100	-0.71792800 1.80682100	C	0.00002000	-0.71709800 1.80568900
C	0.76578600	1.94680900 -0.00041700	C	0.76527500	1.94360700 -0.00041600
C	-0.76585100	1.94678400 -0.00041000	C	-0.76534100	1.94358200 -0.00041000
C	-1.17416600	1.17719400 1.11374100	C	-1.17269000	1.17611700 1.11335400
C	1.17412600	1.17667800 -1.11422100	C	1.17263900	1.17560800 -1.11384100
C	-0.00002100	0.71792800 -1.80682100	C	-0.00002000	0.71709800 -1.80568900
C	-1.17417700	1.17663900 -1.11421000	C	-1.17268800	1.17556800 -1.11383100
C	0.00000400	-0.71876000 -1.80649800	C	0.00000400	-0.71793600 -1.80537200
C	-1.17413600	-1.17723200 -1.11373200	C	-1.17266000	-1.17615500 -1.11334400
C	-1.96818000	-0.00019900 -0.69595700	C	-1.96550400	-0.00019000 -0.69505300
C	-1.96817000	0.00013300 0.69597200	C	-1.96549500	0.00012400 0.69506900
C	-1.17412600	-1.17667800 1.11422100	C	-1.17263900	-1.17560800 1.11384100
C	-0.76578600	-1.94680900 0.00041700	C	-0.76527500	-1.94360700 0.00041600
$C_{19}Si$					
$F = 0.000\ a.u.$ $Energy = -1012.776536$			$F = 0.000\ a.u.$ $Energy = -1012.776536$		
C	0.91421500	-1.35551500 1.29928900	C	0.91350600	-1.84301600 0.34754400
C	-0.46189100	-1.63458100 0.89484300	C	-0.46149100	-1.85569100 -0.14347700
C	0.91450100	-0.06538400 1.87665100	C	0.91394900	-1.07876600 1.53446200
C	-0.46174800	0.42245100 1.81454000	C	-0.46096700	-0.63649900 1.74873400
C	-1.34175300	-0.58521000 1.30795100	C	-1.33934700	-1.20253900 0.77463600
C	1.74935900	0.76130800 1.05169500	C	1.74766000	0.06292500 1.29723800

C	0.91452400	1.80318500	0.52415000	C	0.91405800	1.22253600	1.42223800
C	-0.46154200	1.59262900	0.96830600	C	-0.46085100	0.80361500	1.67892200
C	2.40815000	0.00005600	-0.00001200	C	2.40412100	-0.00015800	-0.00004700
C	1.74933200	0.53028200	-1.18500300	C	1.74775700	1.09179100	-0.70348400
C	0.91451600	1.65802200	-0.88145600	C	0.91411000	1.86820400	0.16696600
C	1.74918000	-1.29269300	0.13354700	C	1.74732600	-1.15578700	-0.59420500
C	0.91418900	-1.59240900	-0.99460900	C	0.91351100	-0.78957200	-1.70099700
C	0.91484500	-0.44771000	-1.82373900	C	0.91405500	0.62050800	-1.77010800
C	-0.46181500	-1.78319500	-0.54180800	C	-0.46143000	-1.19624900	-1.42584500
C	-1.34137600	-0.84011300	-1.16072200	C	-1.33919400	-0.06934500	-1.42861400
C	-0.46141100	0.04244100	-1.86261100	C	-0.46083400	1.05213400	-1.53507800
C	-0.46148600	1.36092700	-1.27331800	C	-0.46078800	1.83309200	-0.32315800
C	-1.34103000	1.42507400	-0.14712300	C	-1.33885800	1.27204300	0.65410100
Si	-2.72089700	0.00018600	-0.00024400	Si	-2.71984000	0.00033200	0.00007400

Table S2. Optimized coordinates for the dimers formed by pure and doped fullerenes and CO, CO_2 and N_2 gases in each of the studied field values. Electic field F in atomic units and BSSE-corrected adsorption energies in electron-volts.

ωB97XD/6-31G(d)				**ωB97XD/6-311+G(d,p)**			
C_{20}-CO							
$F = 0.000$ $E_{ads}(BSSE) = -0.04027087$				$F = 0.000$ $E_{ads}(BSSE) = -0.04215341$			
O	3.34694300	-1.80506800	0.01811600	O	3.31257900	-1.80409600	-0.00638300
C	2.84804700	-0.78483600	0.01561800	C	2.81785900	-0.79251200	-0.01452300
C	7.10590900	1.54087900	-1.04107100	C	7.10338800	1.53702400	-1.03496000
C	8.15189300	0.88878000	-1.78265500	C	8.14497600	0.88517100	-1.78004600
C	7.68118100	2.17225900	0.08656100	C	7.68248900	2.16892800	0.08883400
C	9.18190700	1.87216300	0.04331300	C	9.18249800	1.87070500	0.03835600
C	9.40715300	1.08075200	-1.10748700	C	9.40199500	1.07971400	-1.11231000
C	7.15262400	1.45547100	1.18492300	C	7.16149800	1.45667800	1.19085900
C	8.22795100	0.74904100	1.82827900	C	8.23985000	0.75204300	1.82799100
C	9.45442200	0.99510700	1.11853300	C	9.46152700	0.99890800	1.11321900
C	6.13412700	0.47380400	0.74935500	C	6.14309600	0.47282300	0.76014300
C	6.68897000	-0.85068600	1.10429100	C	6.70056200	-0.84895500	1.11459200
C	7.94490600	-0.65854600	1.77880900	C	7.95835300	-0.65429300	1.78176100
C	6.10467400	0.52802400	-0.64163500	C	6.10638300	0.52492400	-0.62850900
C	6.64176400	-0.76501000	-1.12208600	C	6.64108600	-0.76808600	-1.11135600
C	6.91461300	-1.64107000	-0.04664800	C	6.92053300	-1.63887000	-0.03623700
C	7.86888600	-0.51885300	-1.83116300	C	7.86347500	-0.52121200	-1.82547600
C	8.94380100	-1.22584200	-1.18837800	C	8.94131100	-1.22636600	-1.18876800
C	8.41492500	-1.94243400	-0.08994000	C	8.42004700	-1.93856800	-0.08673800
C	8.99049600	-1.31120700	1.03774600	C	8.99942000	-1.30661200	1.03706300
C	9.99192700	-0.29814000	0.63786700	C	9.99668100	-0.29435500	0.63014900
C	9.96248900	-0.24398100	-0.75235100	C	9.96000400	-0.24238700	-0.75766300
C_{20}-C0₂							
$F = 0.000$ $E_{ads}(BSSE) = -0.06556463$				$F = 0.000$ $E_{ads}(BSSE) = -0.07502922$			
C	0.58561400	0.04675200	-0.41514800	C	0.62769000	0.12142600	-0.49236200
O	0.65222200	-0.11126900	0.73682800	O	0.75707800	-0.23508500	0.60113400
O	0.51242700	0.20215400	-1.56707300	O	0.49117600	0.47711300	-1.58391000

C	5.09326500	1.57819800	-0.99626800	C	5.00397000	1.52753400	-1.00164100
C	5.80464400	0.60183500	-1.77425100	C	5.71549600	0.55341100	-1.78089600
C	5.95372500	2.06216100	0.02663500	C	5.90262700	2.05078800	0.04246900
C	7.27627200	1.30785900	-0.11891200	C	7.16704700	1.29046200	-0.10866300
C	7.12118600	0.42514100	-1.21987300	C	7.03427400	0.40510400	-1.23268600
C	5.35427900	1.61579500	1.21969700	C	5.35171100	1.66819300	1.26010000
C	6.22410900	0.63410500	1.81685000	C	6.27427100	0.67467200	1.83967500
C	7.38779700	0.45057200	0.99445500	C	7.42958600	0.51335000	1.03799800
C	4.04978100	0.96293300	0.93543900	C	4.11288600	0.91728400	0.94599300
C	4.20411500	-0.43844000	1.34568000	C	4.27788600	-0.44201700	1.38186500
C	5.51978100	-0.61591700	1.89887700	C	5.59670100	-0.58935000	1.92711900
C	3.87380900	0.96468100	-0.44627600	C	3.85687900	0.91448400	-0.44060900
C	3.93751600	-0.46425400	-0.86908600	C	3.88001800	-0.55067700	-0.89125700
C	4.04882400	-1.32110100	0.24313600	C	4.14760100	-1.32531200	0.25607900
C	5.10192200	-0.64775400	-1.69253700	C	5.03865800	-0.70987900	-1.69043600
C	5.97097300	-1.62925700	-1.09523500	C	5.96079200	-1.70393100	-1.11290200
C	5.37045100	-2.07664900	0.09669500	C	5.40990900	-2.08744500	0.10441900
C	6.23055200	-1.59222600	1.12033500	C	6.30910300	-1.56572100	1.14991700
C	7.44906800	-0.97744000	0.57078000	C	7.45273600	-0.94965300	0.58800900
C	7.27766900	-0.97788200	-0.81074600	C	7.20190500	-0.95475800	-0.79940900

C_{20}-N_2

$F = 0.000$ $E_{ads}(BSSE) = -0.04191301$				$F = 0.000$ $E_{ads}(BSSE) = -0.04214772$			
N	0.58478100	-1.97944200	-0.13254500	N	0.41249400	-1.57070000	-0.52204300
N	0.22177400	-0.96292700	0.08912200	N	0.26623900	-1.40781400	0.54810000
C	4.40572800	1.54579000	-1.08795800	C	4.42922300	1.53961000	-1.11932400
C	5.43565800	0.83559500	-1.79713600	C	5.46409300	0.81720000	-1.80600800
C	4.99058300	2.18474400	0.03067400	C	5.00261600	2.18398500	-0.00206400
C	6.48036700	1.83084800	0.01615600	C	6.49079500	1.82649200	0.00383600
C	6.68852900	0.99870000	-1.10939100	C	6.70972700	0.98594100	-1.10919600
C	4.42075000	1.52060900	1.14085000	C	4.41997700	1.53416600	1.10964100
C	5.46059400	0.79227800	1.81698700	C	5.44849600	0.81164400	1.80531900
C	6.70466700	0.97306900	1.11750000	C	6.69886200	0.98085900	1.11758200
C	3.37182400	0.56522500	0.71648000	C	3.37393700	0.58001300	0.68591700
C	3.87209800	-0.76789100	1.11391300	C	3.86402300	-0.75134700	1.10645200
C	5.12541800	-0.60470100	1.80109900	C	5.10978200	-0.58293000	1.80343500
C	3.36178600	0.58242300	-0.67534600	C	3.37963000	0.58144200	-0.70384900
C	3.85604200	-0.74219700	-1.11333800	C	3.87486400	-0.74622700	-1.12013500
C	4.08070600	-1.59950600	-0.01180600	C	4.08258200	-1.59213100	-0.00644600
C	5.10045000	-0.56139500	-1.81229800	C	5.12527800	-0.57739200	-1.80795000
C	6.13996400	-1.29024100	-1.13648600	C	6.15336100	-1.30002500	-1.11208200
C	5.56995800	-1.95434700	-0.02629900	C	5.57063700	-1.95000100	-0.00048500
C	6.15504600	-1.31547200	1.09238600	C	6.14420400	-1.30545700	1.11664600
C	7.19898300	-0.35211500	0.67951700	C	7.19418600	-0.34733900	0.70102400
C	7.18908200	-0.33498300	-0.71208300	C	7.19978200	-0.34592700	-0.68837000

C_{19}Si-CO

$F = 0.000$ $E_{ads}(BSSE) = -0.70264080$				$F = 0.000$ $E_{ads}(BSSE) = -0.73799673$			
O	2.01502800	-0.01037600	-0.00025500	O	2.01053700	-0.01993600	0.00877900
C	3.14119300	-0.01035200	0.00416500	C	3.12664200	-0.01236700	0.02139200
C	8.18173800	-1.37815000	1.29081900	C	8.18322500	-1.37772500	1.29143500
C	6.84077900	-1.70008500	0.93491700	C	6.84358000	-1.69783900	0.93565400

C	8.17811900	-0.09251600	1.86489000	C	8.18137600	-0.09268300	1.86216600
C	6.80722200	0.39724100	1.83179100	C	6.81098700	0.39819100	1.83171700
C	5.91034300	-0.66680100	1.53729200	C	5.91495700	-0.66098500	1.53607100
C	8.99384900	0.72449500	0.99628100	C	8.99552200	0.72393400	0.99540100
C	8.17088900	1.80029200	0.49388800	C	8.17432400	1.79810700	0.49239500
C	6.80234500	1.60888300	0.95395200	C	6.80639800	1.60939900	0.95402600
C	9.61024300	-0.02434200	-0.04136000	C	9.60982200	-0.02548100	-0.04224800
C	9.11370900	0.54602200	-1.28538900	C	9.10965000	0.54232300	-1.28439600
C	8.17025500	1.65582400	-0.90653600	C	8.17203800	1.65651400	-0.90645900
C	9.12023000	-1.38623300	0.11429200	C	9.11686600	-1.38546600	0.11186300
C	8.26240700	-1.59477900	-0.96999200	C	8.26108300	-1.59574600	-0.97082300
C	8.25819600	-0.42346100	-1.81759800	C	8.25698200	-0.42505000	-1.81896400
C	6.87070400	-1.78477600	-0.50104900	C	6.87091900	-1.78145600	-0.49872700
C	6.00349900	-0.89551100	-1.22489600	C	6.00500400	-0.89019800	-1.21777000
C	6.86375400	0.07422800	-1.84728800	C	6.86434500	0.07480800	-1.84356300
C	6.82876700	1.41163900	-1.31889100	C	6.83209500	1.41154400	-1.31692500
C	5.90151500	1.65588400	-0.14531800	C	5.90626700	1.65429600	-0.14124800
Si	5.14268300	0.04177400	0.07515100	Si	5.13484700	0.04471700	0.07762900

$C_{19}Si\text{-}CO_2$

$F = 0.000$ $E_{ads}(BSSE) = -0.06827564$			$F = 0.000$ $E_{ads}(BSSE) = -0.07742641$		
C	-0.44956200	-0.05900700	-0.12760900	C	-0.26804500	0.10709200	-0.28998600
O	-0.69772900	-0.29614200	0.98521300	O	-0.72140800	-0.26570200	0.70588900
O	-0.23344200	0.17451900	-1.24866500	O	0.15830400	0.48185700	-1.29904000
C	6.95651900	-1.39165200	1.20360200	C	7.08254700	-1.35536100	1.17685600
C	5.52910600	-1.60788700	0.97902400	C	5.65973000	-1.65581400	1.04510600
C	7.08667300	-0.11025000	1.78487900	C	7.17426400	-0.06525500	1.74238100
C	5.73615500	0.43500500	1.90584000	C	5.80598000	0.40172800	1.94720700
C	4.75618300	-0.52928900	1.51216500	C	4.86247400	-0.61993900	1.62105500
C	7.84214900	0.69165400	0.86452200	C	7.82108900	0.77204600	0.77491700
C	6.99122600	1.77351300	0.45643700	C	6.88483500	1.79718600	0.41622100
C	5.67653800	1.61417000	1.07390900	C	5.62487100	1.56727700	1.11727600
C	8.32581500	-0.08312500	-0.26933200	C	8.27189400	0.01677100	-0.38435100
C	7.54225300	0.48848700	-1.35497200	C	7.39241900	0.53430600	-1.42203700
C	6.80285500	1.64594700	-0.93827400	C	6.61619600	1.64827200	-0.96124400
C	7.63523200	-1.34799300	-0.06046100	C	7.67486700	-1.28516600	-0.12697700
C	6.64947800	-1.59964100	-1.07311900	C	6.64351700	-1.59856800	-1.07253100
C	6.59135100	-0.44600400	-1.88696900	C	6.46652700	-0.45779200	-1.88468700
C	5.33676700	-1.73861600	-0.44664800	C	5.38498800	-1.80811300	-0.36252400
C	4.42566000	-0.75366400	-0.94110000	C	4.39019800	-0.88153200	-0.80064200
C	5.24358400	0.10120100	-1.74461100	C	5.10254400	0.01168200	-1.65813800
C	5.37630000	1.41081300	-1.15002200	C	5.19598100	1.32945500	-1.08041300
C	4.65373100	1.49959200	0.08104700	C	4.55108300	1.38501600	0.19297500
Si	3.25102100	0.12812000	0.39547000	Si	3.25300600	-0.05969500	0.60301100

$C_{19}Si\text{-}N_2$

$F = 0.000$ $E_{ads}(BSSE) = -0.01722895$				$F = 0.000$ $E_{ads}(BSSE) = -0.04477245$			
N	-2.66042400	-0.12112300	-0.02744200	N	-1.31609500	0.56939400	-1.66307200
N	-2.14664100	-0.25597700	-0.99254600	N	-0.23966900	0.72589600	-1.56415600
C	5.53073000	-1.36769300	1.24568000	C	5.74786800	-1.18227700	1.30374800
C	4.09734300	-1.57680900	1.05314900	C	4.33401400	-1.46336600	1.53817700
C	5.68206700	-0.07708100	1.80067100	C	5.93814000	0.19077800	1.56973700

C	4.33835200	0.48106700	1.93782900	C	4.63730400	0.72654000	1.96223900
C	3.34315600	-0.48192200	1.58018500	C	3.66086400	-0.31237300	2.05081100
C	6.42540400	0.70185800	0.85109100	C	6.35139800	0.80283600	0.34089700
C	5.57471300	1.78272700	0.43998300	C	5.34476700	1.76237500	-0.00784900
C	4.27128100	1.64500600	1.08598500	C	4.26593400	1.70954600	0.97492200
C	6.88079900	-0.09735900	-0.27775000	C	6.55701300	-0.17846700	-0.71437700
C	6.07996500	0.46064600	-1.35813400	C	5.46879700	0.14834600	-1.62411100
C	5.35780100	1.63132100	-0.94812300	C	4.79136400	1.35203200	-1.23982000
C	6.18465500	-1.35272900	-0.03199400	C	6.04810400	-1.38695800	-0.08325700
C	5.17699400	-1.61481300	-1.02003200	C	4.84410600	-1.85219100	-0.70766000
C	5.11145100	-0.47579400	-1.85367500	C	4.48101200	-0.88953800	-1.67391600
C	3.87583900	-1.73200000	-0.36550900	C	3.76858400	-1.88183100	0.27963700
C	2.96229100	-0.74824200	-0.85875100	C	2.68904100	-1.03210800	-0.11287400
C	3.77089700	0.08462400	-1.69453100	C	3.18925600	-0.34676000	-1.26185100
C	3.92542600	1.40358300	-1.12726900	C	3.38348800	1.05537400	-0.99033300
C	3.22787600	1.51957900	0.11602500	C	3.02269400	1.37758100	0.35379000
Si	1.81656300	0.16712900	0.48402400	Si	1.85855400	0.08117100	1.30818500

C_{19}Si-CO

$F = 0.001$ $E_{ads}(BSSE) = -0.74916933$				$F = 0.001$ $E_{ads}(BSSE) = -0.78821735$			
O	1.99978300	-0.01200700	-0.00168200	O	2.00507900	-0.01622700	0.01401400
C	3.12640300	-0.00644800	0.00977500	C	3.12040700	-0.00712700	0.02868000
C	8.18551700	-1.37801600	1.28937700	C	8.18555300	-1.37796100	1.29035100
C	6.84233700	-1.69669200	0.93882600	C	6.84434900	-1.69531900	0.93850200
C	8.18666000	-0.09188400	1.86270000	C	8.18727300	-0.09223700	1.86004800
C	6.81531800	0.40070300	1.83327400	C	6.81642400	0.40056400	1.83261800
C	5.91679600	-0.65941800	1.54123300	C	5.91936800	-0.65558200	1.53917900
C	8.99970500	0.72205600	0.99011600	C	8.99929700	0.72197000	0.99030500
C	8.17919200	1.79968800	0.48930800	C	8.18023800	1.79709100	0.48809100
C	6.81044300	1.61202500	0.95347400	C	6.81183100	1.61169500	0.95292900
C	9.61209200	-0.03030800	-0.04917600	C	9.61099800	-0.03032900	-0.04887700
C	9.11234600	0.53936300	-1.29160900	C	9.10854000	0.53679800	-1.29015700
C	8.17371300	1.65290600	-0.91112000	C	8.17438100	1.65352000	-0.91075600
C	9.12022900	-1.39116600	0.10979300	C	9.11572100	-1.38892800	0.10793500
C	8.25638500	-1.59804700	-0.97128800	C	8.25565500	-1.59886100	-0.97262600
C	8.25204300	-0.42901100	-1.82046500	C	8.25155200	-0.42988300	-1.82150600
C	6.86582500	-1.78403700	-0.49663300	C	6.86653000	-1.78101700	-0.49566700
C	5.99899400	-0.89117800	-1.21569900	C	6.00071000	-0.88754200	-1.21121400
C	6.85888800	0.07305400	-1.84523700	C	6.85993700	0.07344300	-1.84235400
C	6.83032100	1.41092800	-1.31767200	C	6.83286200	1.41050300	-1.31680800
C	5.90760900	1.65800800	-0.14157100	C	5.91070800	1.65522600	-0.13886500
Si	5.13686400	0.04838600	0.08314200	Si	5.13005000	0.04910800	0.08358400

C_{19}Si-CO_2

$F = 0.001$ $E_{ads}(BSSE) = -0.08110533$				$F = 0.001$ $E_{ads}(BSSE) = -0.08655367$			
C	0.29581300	0.39203400	-0.74958400	C	-4.78429600	-0.42291500	-0.00002200
O	-0.66453900	0.12557900	-0.15065000	O	-5.66717600	0.32066100	-0.00040100
O	1.25049100	0.66396800	-1.36292000	O	-3.90664200	-1.18018700	0.00035200
C	7.32425600	-1.27519600	1.03703200	C	2.43400700	1.19711100	0.70601000
C	5.93969600	-1.72597800	1.16341700	C	1.09506300	1.60211300	1.12571600
C	7.37972300	0.02537000	1.58855500	C	2.43388100	1.19714000	-0.70624400
C	6.02786500	0.34651800	2.04196300	C	1.09486200	1.60215800	-1.12569600

C	5.15270100	-0.77336400	1.88341600	C	0.29187500	1.96058600	0.00008900
C	7.74682900	0.91511500	0.52412000	C	2.67324900	-0.15250200	-1.12569600
C	6.65723200	1.83381000	0.35137000	C	1.51508100	-0.57552300	-1.85771500
C	5.57572900	1.47809800	1.26723000	C	0.52002900	0.49295000	-1.84565400
C	8.06223500	0.20063900	-0.70515400	C	2.95690500	-1.03119100	-0.00020900
C	6.95487700	0.61010100	-1.55953100	C	1.77614900	-1.88460700	-0.00012100
C	6.15982900	1.64165000	-0.95726300	C	0.95286400	-1.66076300	-1.15175300
C	7.65888400	-1.15419200	-0.35331900	C	2.67345000	-0.15254700	1.12536500
C	6.51189600	-1.58768200	-1.09938900	C	1.51541100	-0.57559700	1.85757300
C	6.06977900	-0.47948700	-1.85663000	C	0.95306900	-1.66080900	1.15166700
C	5.43120200	-1.92110800	-0.17405300	C	0.52035700	0.49287600	1.84573200
C	4.27880200	-1.10955100	-0.41609700	C	-0.69603600	0.05388600	1.23857500
C	4.72580300	-0.15472200	-1.38219900	C	-0.37734300	-1.23830900	0.72025000
C	4.78199800	1.17257100	-0.81942100	C	-0.37747100	-1.23828000	-0.72008100
C	4.37578500	1.17253800	0.55146200	C	-0.69625600	0.05393600	-1.23829700
Si	3.33097900	-0.39695900	1.17797100	Si	-1.58989700	1.32271000	0.00024500

$C_{19}Si\text{-}N_2$

$F = 0.001$				$F = 0.001$			
$E_{ads}(BSSE) = -0.04514641$				$E_{ads}(BSSE) = -0.04598611$			
N	-1.31510200	1.05683100	-1.32379700	N	-5.37064000	-0.63226000	-0.11732600
N	-0.29099500	0.65716800	-1.39524700	N	-4.31001800	-0.69445300	0.13647900
C	5.88944400	-1.14395200	1.17613500	C	2.32574400	0.97064100	0.56838900
C	4.52012600	-1.60758400	1.39184400	C	1.08579800	1.60432000	1.00930200
C	5.92197600	0.21696400	1.55676500	C	2.25937900	0.88581100	-0.83949100
C	4.57203000	0.56154900	1.99842400	C	0.98007000	1.46919500	-1.23526900
C	3.72298200	-0.58939600	2.00282200	C	0.29412100	2.01446900	-0.10694200
C	6.24347800	0.97265100	0.37972300	C	2.26936400	-0.50728700	-1.17720900
C	5.12654100	1.83563900	0.11853400	C	1.02696300	-0.78719400	-1.83603100
C	4.07390600	1.57409400	1.09781800	C	0.20901800	0.42253400	-1.85810200
C	6.55184200	0.11495200	-0.75644200	C	2.46717100	-1.35025800	-0.00670600
C	5.41635000	0.38601900	-1.62896000	C	1.17098700	-2.00737200	0.09386100
C	4.60722700	1.46680400	-1.14289600	C	0.33883200	-1.72716300	-1.03907300
C	6.19186400	-1.19318300	-0.22595700	C	2.37494000	-0.37210800	1.06789600
C	5.04130600	-1.74518700	-0.88290400	C	1.20131900	-0.56413600	1.86875600
C	4.55432300	-0.75309100	-1.76372000	C	0.44682600	-1.58903200	1.25794800
C	3.98909000	-1.98311800	0.10304200	C	0.38222900	0.64423900	1.82258200
C	2.81057500	-1.23578100	-0.21126400	C	-0.91425400	0.36520800	1.29027300
C	3.21268700	-0.40241400	-1.30176600	C	-0.82104000	-0.99016500	0.84867900
C	3.24567900	0.98675700	-0.91324800	C	-0.88871800	-1.07664200	-0.58733300
C	2.86742300	1.15057900	0.45624800	C	-1.03041900	0.21657600	-1.17718100
Si	1.87378800	-0.35030200	1.30371400	Si	-1.66467000	1.68265500	0.00570200

$C_{19}Si\text{-}CO$

$F = 0.005$				$F = 0.005$			
$E_{ads}(BSSE) = -0.95684190$				$E_{ads}(BSSE) = -1.00925177$			
O	1.97416600	0.03725900	-0.02547300	O	1.97940500	0.02780700	-0.01109300
C	3.09787900	0.04225200	0.00046800	C	3.09172700	0.04023200	0.01880800
C	8.17257100	-1.38106500	1.28549900	C	8.17245300	-1.38135500	1.28655100
C	6.82584300	-1.68061900	0.93336700	C	6.82726900	-1.67842200	0.93335000
C	8.18676800	-0.09636500	1.86358100	C	8.18744000	-0.09685100	1.86046700
C	6.81631600	0.40944900	1.83425700	C	6.81715000	0.40999300	1.83416000
C	5.91159600	-0.63408000	1.53486300	C	5.91372800	-0.62876500	1.53313700
C	9.00422600	0.71080000	0.99299600	C	9.00433200	0.71064500	0.99351000

C	8.20134500	1.79857600	0.49398100	C	8.20348100	1.79560400	0.49307100
C	6.82538400	1.62561400	0.95533300	C	6.82740100	1.62640700	0.95536000
C	9.61391500	-0.04749200	-0.05082300	C	9.61316800	-0.04842700	-0.05131200
C	9.12214900	0.53048300	-1.29244700	C	9.11868200	0.52719900	-1.29182200
C	8.19602700	1.65304300	-0.90715700	C	8.19798800	1.65364500	-0.90678500
C	9.10561100	-1.40149900	0.10432000	C	9.10036800	-1.39948600	0.10210600
C	8.23615900	-1.59659000	-0.97895800	C	8.23425000	-1.59773200	-0.98078200
C	8.24543700	-0.42799300	-1.82206200	C	8.24418900	-0.42940400	-1.82374800
C	6.84397400	-1.76701800	-0.50166100	C	6.84370200	-1.76307700	-0.50036800
C	5.98854000	-0.85768400	-1.20999900	C	5.98975200	-0.85279000	-1.20510300
C	6.85830700	0.09230700	-1.84483900	C	6.85923200	0.09338400	-1.84155800
C	6.84945400	1.42717700	-1.31243200	C	6.85307500	1.42734600	-1.31104300
C	5.92946100	1.67716200	-0.13564200	C	5.93415700	1.67524300	-0.13242400
Si	5.11337300	0.08274800	0.08423300	Si	5.10555300	0.08526700	0.08546400

$C_{19}Si\text{-}CO_2$

$F = 0.005$ $E_{ads}(BSSE) = -0.08494219$				$F = 0.005$ $E_{ads}(BSSE) = -0.09138179$			
C	0.32708100	0.45075200	-0.85467000	C	0.30080200	0.47149500	-0.85094400
O	-0.74916700	0.24831900	-0.47170700	O	-0.78330300	0.30851100	-0.49972000
O	1.41181700	0.65407600	-1.24127000	O	1.39542200	0.63560300	-1.20517100
C	7.37530300	-1.28206700	0.97269100	C	7.38519000	-1.27325800	0.97407900
C	6.00364900	-1.76369800	1.13139800	C	6.01746400	-1.76407600	1.13165800
C	7.42338000	0.00544100	1.55977300	C	7.42417500	0.01382300	1.55924900
C	6.07987500	0.28503800	2.06534900	C	6.07893200	0.28489000	2.06238800
C	5.21973600	-0.84612100	1.89973200	C	5.22728700	-0.85116400	1.89642000
C	7.73572600	0.93129300	0.50983800	C	7.73215800	0.94148800	0.51166900
C	6.62262600	1.83086800	0.39823500	C	6.61286600	1.83055400	0.39572800
C	5.57908700	1.42578800	1.33824900	C	5.57212800	1.41945500	1.33492100
C	8.02770000	0.25802500	-0.75107600	C	8.02562600	0.26701400	-0.74772300
C	6.87911400	0.66828600	-1.55705800	C	6.87785000	0.66966800	-1.55837000
C	6.08527900	1.66318700	-0.89811600	C	6.07828600	1.65785200	-0.89957100
C	7.65949700	-1.11535600	-0.42318200	C	7.67087800	-1.10989000	-0.42023200
C	6.49688100	-1.55072500	-1.14332200	C	6.51189500	-1.54988800	-1.14008500
C	6.00745400	-0.43044600	-1.85266000	C	6.01600600	-0.43533700	-1.85128500
C	5.45422600	-1.93076000	-0.19183600	C	5.47178500	-1.93610000	-0.18984600
C	4.27769300	-1.13545200	-0.36818100	C	4.29174200	-1.14895100	-0.36848100
C	4.67232000	-0.14729400	-1.32438300	C	4.67961700	-0.16066800	-1.32501000
C	4.72087000	1.16161300	-0.72788000	C	4.71857500	1.14665200	-0.73063000
C	4.36117700	1.11101600	0.65562700	C	4.35910600	1.09389600	0.65143700
Si	3.35653700	-0.49203400	1.27477000	Si	3.36337400	-0.51181900	1.26983900

$C_{19}Si\text{-}N_2$

$F = 0.005$ $E_{ads}(BSSE) = -0.05377844$				$F = 0.005$ $E_{ads}(BSSE) = -0.05636742$			
N	-1.32195000	0.90194600	-1.47271000	N	-1.32775300	0.87494400	-1.48440400
N	-0.24969700	0.68184500	-1.34816100	N	-0.26102300	0.69182300	-1.33755900
C	5.88013300	-1.17120100	1.15892300	C	5.87753900	-1.17285600	1.15726300
C	4.50333900	-1.61059600	1.38401100	C	4.50047800	-1.60921400	1.38135500
C	5.94130000	0.18757900	1.55051900	C	5.94146100	0.18415600	1.54941700
C	4.60081900	0.55256000	2.00702900	C	4.60243600	0.55176600	2.00550600
C	3.72850600	-0.58160900	2.00679000	C	3.72876900	-0.57947400	2.00342600
C	6.26392400	0.94625300	0.37652100	C	6.26668400	0.94435500	0.37902200
C	5.16044200	1.83067900	0.13207200	C	5.16480600	1.82800900	0.13333500

C	4.11217900	1.57910400	1.11955900	C	4.11692200	1.57815200	1.12011300
C	6.54967000	0.09192600	-0.77122000	C	6.54657900	0.08867700	-0.76864500
C	5.40575600	0.39069700	-1.63105800	C	5.40619300	0.39122800	-1.63154500
C	4.62203300	1.47993500	-1.12699600	C	4.62656100	1.47988000	-1.12479100
C	6.16716300	-1.21456800	-0.24570700	C	6.16520600	-1.21867200	-0.24551600
C	5.00025800	-1.73912700	-0.89591600	C	4.99732200	-1.73661200	-0.89598500
C	4.52283400	-0.73066500	-1.76347800	C	4.52282300	-0.72784600	-1.76216500
C	3.95299800	-1.96446500	0.09909600	C	3.95056700	-1.96044100	0.09833500
C	2.78476800	-1.19110400	-0.19406200	C	2.78590100	-1.18392200	-0.19386200
C	3.19076400	-0.35925300	-1.28497100	C	3.19241700	-0.35363000	-1.28383000
C	3.25284100	1.02280200	-0.88693500	C	3.25728100	1.02533600	-0.88559200
C	2.89139800	1.17856000	0.48864400	C	2.89716600	1.17987500	0.48893100
Si	1.86706300	-0.30530100	1.33691800	Si	1.86820500	-0.29953500	1.33605800

C_{19}Si-CO

$F = 0.010$ $E_{ads}(BSSE) = -1.26088602$				$F = 0.010$ $E_{ads}(BSSE) = -1.32802545$			
O	1.94882700	-0.02443100	-0.01647800	O	1.95599700	-0.02593500	0.00455300
C	3.06987600	-0.01053700	0.01228300	C	3.06579600	-0.00796000	0.02853600
C	8.19175900	-1.38011600	1.30854900	C	8.20031700	-1.37791900	1.28911100
C	6.84930400	-1.67015400	0.93821400	C	6.85759600	-1.68726600	0.93584500
C	8.19355300	-0.08778500	1.87785400	C	8.19800000	-0.09123100	1.86040500
C	6.81899100	0.39648800	1.83676100	C	6.81523700	0.39754900	1.83441500
C	5.91834300	-0.66014200	1.55065900	C	5.93264200	-0.64483900	1.52640400
C	9.00590600	0.72430900	0.99745100	C	9.00102900	0.72542200	0.99538700
C	8.20209900	1.79249400	0.48630100	C	8.19148200	1.79727700	0.48933100
C	6.81724400	1.60983800	0.95359200	C	6.81093800	1.61489200	0.95043000
C	9.62699800	-0.02463100	-0.05436000	C	9.62476600	-0.03298600	-0.05197800
C	9.16432800	0.55302700	-1.32861100	C	9.12110600	0.53315200	-1.29224600
C	8.20275900	1.62550100	-0.91187800	C	8.18988200	1.65274900	-0.91094000
C	9.08893600	-1.34990100	0.10571700	C	9.12832100	-1.39068700	0.10399600
C	8.24847100	-1.60132100	-0.99556400	C	8.25677500	-1.59832200	-0.97963600
C	8.25347500	-0.41959900	-1.80615000	C	8.25293100	-0.43683200	-1.82329300
C	6.86024400	-1.77390200	-0.50648600	C	6.86821400	-1.77896900	-0.49553200
C	5.99643700	-0.88098700	-1.20052600	C	6.00546400	-0.87173500	-1.19045100
C	6.85913000	0.08081000	-1.85112200	C	6.86201000	0.07348500	-1.84059500
C	6.84711700	1.40385100	-1.32181300	C	6.84696900	1.40607600	-1.30994600
C	5.93738600	1.61686400	-0.13362000	C	5.92457000	1.64093000	-0.13304500
Si	5.08628500	0.02922400	0.09809200	Si	5.07742800	0.05205000	0.08665200

C_{19}Si-CO_2

$F = 0.010$ $E_{ads}(BSSE) = -0.10993079$				$F = 0.010$ $E_{ads}(BSSE) = -0.12354919$			
C	0.27117300	0.53068500	-0.95472800	C	0.28395900	0.61706600	-0.93352700
O	-0.88470100	0.52655700	-0.91370700	O	-0.85715100	0.73365700	-0.93228800
O	1.44377200	0.53612200	-0.99831000	O	1.44542800	0.50391400	-0.93712200
C	7.45390500	-1.25189700	0.93438500	C	7.48386300	-1.21288500	0.94499900
C	6.10211900	-1.77145700	1.14691700	C	6.14778100	-1.77209700	1.15557200
C	7.48689800	0.04081800	1.51837000	C	7.47363100	0.08364800	1.51862000
C	6.15433800	0.28143300	2.07391500	C	6.13216300	0.28635200	2.06660400
C	5.31829200	-0.87268000	1.93877200	C	5.33390300	-0.89310300	1.93656900
C	7.72905600	0.97175600	0.45562400	C	7.69262000	1.01565000	0.45391100
C	6.58534100	1.83672100	0.38478000	C	6.52141800	1.83924500	0.36891700
C	5.59105800	1.40158100	1.36490100	C	5.53840900	1.38105400	1.34815700

C	7.99665500	0.30411200	-0.81758500	C	7.98140000	0.34451800	-0.81301700
C	6.79865600	0.67832200	-1.57953300	C	6.77801000	0.67724000	-1.58655500
C	6.00285600	1.64717300	-0.88922900	C	5.95177200	1.62411800	-0.90486400
C	7.67711300	-1.08038200	-0.47093900	C	7.70854900	-1.04817400	-0.45937300
C	6.49959400	-1.55022000	-1.14435100	C	6.54759800	-1.55483300	-1.13275000
C	5.94996400	-0.44600500	-1.83418400	C	5.96811000	-0.47479700	-1.83334400
C	5.50581000	-1.95613100	-0.15089300	C	5.56427300	-1.98389700	-0.14094900
C	4.29853600	-1.19501400	-0.27727200	C	4.33611800	-1.26004800	-0.27711700
C	4.62610500	-0.20117800	-1.25434700	C	4.63560800	-0.26611400	-1.26084600
C	4.65925600	1.10615300	-0.66415800	C	4.62575500	1.04274700	-0.68175100
C	4.35561400	1.04371300	0.73338400	C	4.31937100	0.97958900	0.71414300
Si	3.40645100	-0.58043300	1.39850900	Si	3.41527400	-0.66310000	1.38633500

C_{19}Si-N_2

$F = 0.010$ $E_{ads}(BSSE) = -0.07166555$				$F = 0.010$ $E_{ads}(BSSE) = -0.07659200$			
N	-1.26616900	0.80685300	-1.54125200	N	-1.26724600	0.80628400	-1.52147400
N	-0.20408800	0.65325200	-1.29151400	N	-0.21188800	0.65604400	-1.28266800
C	5.87099400	-1.18491500	1.14733100	C	5.86792600	-1.18344900	1.14908200
C	4.48883800	-1.60970000	1.37624500	C	4.48560300	-1.60788500	1.37378700
C	5.94846900	0.17372300	1.54606300	C	5.94400900	0.17427200	1.54699000
C	4.61179600	0.54954700	2.00889200	C	4.60650100	0.55021500	2.00535800
C	3.72441200	-0.57402800	2.00258300	C	3.72027400	-0.57245800	1.99629300
C	6.27207400	0.93394900	0.37427300	C	6.27229400	0.93592600	0.37927000
C	5.17606000	1.82984700	0.13798900	C	5.17559200	1.82736800	0.13722200
C	4.12914300	1.58240700	1.12893800	C	4.12710800	1.58052200	1.12500800
C	6.54947100	0.08196500	-0.78157400	C	6.54791400	0.08117700	-0.77499700
C	5.39750000	0.39694400	-1.63534900	C	5.40108000	0.39665700	-1.63624300
C	4.62793800	1.48854800	-1.12001000	C	4.63198700	1.48627200	-1.12105600
C	6.15028000	-1.22450400	-0.25784000	C	6.15208900	-1.22723300	-0.25338300
C	4.97441000	-1.73196500	-0.90523200	C	4.97745900	-1.73033400	-0.90347800
C	4.50342500	-0.71365800	-1.76484800	C	4.50958200	-0.71392200	-1.76439100
C	3.92878300	-1.94962500	0.09438100	C	3.93030200	-1.94772000	0.09293800
C	2.76599100	-1.16061500	-0.18522700	C	2.77008900	-1.15810900	-0.18952300
C	3.17510100	-0.33100100	-1.27800200	C	3.18071400	-0.33069800	-1.28171400
C	3.25299200	1.04447600	-0.87518000	C	3.25719600	1.04181900	-0.88025900
C	2.89994600	1.19256700	0.50442100	C	2.90140900	1.18907000	0.49736100
Si	1.84917300	-0.27807000	1.35378100	Si	1.84654500	-0.27782100	1.34474600

C_{19}Si-CO

$F = 0.015$ $E_{ads}(BSSE) = -1.60888130$				$F = 0.015$ $E_{ads}(BSSE) = -1.69386335$			
O	1.91954500	-0.01286000	0.00018700	O	1.92700900	-0.02083000	0.01198100
C	3.03892700	-0.00811300	0.02064100	C	3.03498500	-0.00583200	0.03150900
C	8.19503700	-1.37817300	1.32130700	C	8.20964800	-1.37828400	1.28856400
C	6.84495900	-1.64676800	0.93330700	C	6.86551100	-1.68339400	0.93183200
C	8.19605300	-0.08275000	1.89186100	C	8.20193300	-0.09072500	1.85864400
C	6.82490500	0.39398500	1.83331000	C	6.81212400	0.39537100	1.83313000
C	5.91599800	-0.67108000	1.54832400	C	5.93809100	-0.64139400	1.51459000
C	9.01740200	0.73367900	1.00970500	C	9.00311700	0.72951000	1.00052600
C	8.21823300	1.79172200	0.48731600	C	8.19481500	1.79636200	0.48959700
C	6.82533700	1.60084500	0.95432500	C	6.80757500	1.61446200	0.94778500
C	9.64121500	-0.01069500	-0.04652800	C	9.63446900	-0.03216500	-0.05092500
C	9.20335100	0.57381000	-1.34913000	C	9.12890900	0.53314500	-1.29107400

C	8.22717400	1.60400200	-0.90927800	C	8.19825800	1.65406200	-0.91137400
C	9.05788000	-1.30813100	0.11235300	C	9.13946600	-1.39234300	0.10429300
C	8.24046500	-1.59401200	-1.00789200	C	8.26071900	-1.59656800	-0.98148800
C	8.25274400	-0.40926800	-1.79399400	C	8.25642300	-0.44013600	-1.82318500
C	6.84883700	-1.77162000	-0.52237300	C	6.87162900	-1.78035200	-0.49711800
C	5.98790200	-0.89156800	-1.20973200	C	6.01053200	-0.86548800	-1.18168700
C	6.86054300	0.07822900	-1.86772600	C	6.86493800	0.07166000	-1.84192900
C	6.85729300	1.38530400	-1.32343800	C	6.85425400	1.40078200	-1.30627300
C	5.95950800	1.57230800	-0.13712400	C	5.92879900	1.63050600	-0.13347500
Si	5.05415900	0.00005400	0.09344200	Si	5.04426400	0.05055200	0.08348300
$C_{19}Si\text{-}CO_2$							
$F = 0.015$ $E_{ads}(BSSE) = -0.16062570$				$F = 0.015$ $E_{ads}(BSSE) = -0.19373070$			
C	0.29735800	0.52793600	-0.91562600	C	-4.83873800	-0.41781100	0.00001900
O	-0.85237700	0.58457000	-0.98263000	O	-5.98104900	-0.38178600	-0.00014700
O	1.47263100	0.47367500	-0.85278800	O	-3.66661500	-0.45570500	0.00018600
C	7.44603000	-1.23526300	0.96595600	C	2.60731400	0.93744500	0.71089600
C	6.08790300	-1.73200400	1.20336900	C	1.33686100	1.53737500	1.12564600
C	7.49373900	0.08119700	1.50145100	C	2.60712900	0.93722100	-0.71160500
C	6.16308400	0.35399500	2.05098300	C	1.33657600	1.53702900	-1.12622800
C	5.31186500	-0.79458100	1.95900500	C	0.58494000	2.00027200	-0.00026800
C	7.73809500	0.96798300	0.40305500	C	2.63587600	-0.43164600	-1.12937400
C	6.60051300	1.83880300	0.30284500	C	1.42097100	-0.67737900	-1.85422500
C	5.60608300	1.44814500	1.30224400	C	0.59829600	0.52977900	-1.83621500
C	8.00034400	0.25018400	-0.84844100	C	2.79388300	-1.35075700	-0.00002600
C	6.79415700	0.60657100	-1.61951900	C	1.47760400	-2.02002800	0.00024000
C	6.01061600	1.60400000	-0.96045500	C	0.70262400	-1.66260400	-1.14361100
C	7.66338900	-1.11926000	-0.44490700	C	2.63615600	-0.43130000	1.12907200
C	6.47718300	-1.60109200	-1.09469400	C	1.42143100	-0.67681400	1.85431200
C	5.93470400	-0.51785100	-1.82230400	C	0.70290600	-1.66225800	1.14416900
C	5.48362100	-1.95792200	-0.08146300	C	0.59875800	0.53034100	1.83613100
C	4.28047100	-1.18999700	-0.22720900	C	-0.67325200	0.29204400	1.21880100
C	4.61266800	-0.23952100	-1.24698200	C	-0.55655900	-1.04227900	0.71338200
C	4.66010400	1.08502200	-0.70909400	C	-0.55673700	-1.04249800	-0.71270400
C	4.36239000	1.07373700	0.69242200	C	-0.67356400	0.29166700	-1.21851600
Si	3.38329300	-0.50857900	1.42510900	Si	-1.41382400	1.68808100	0.00002100
$C_{19}Si\text{-}N_2$							
$F = 0.015$ $E_{ads}(BSSE) = -0.09723814$				$F = 0.015$ $E_{ads}(BSSE) = -0.11392979$			
N	-1.26164500	0.75148800	-1.46851600	N	-5.31090100	-0.74408500	0.00023300
N	-0.19483500	0.62199700	-1.22398300	N	-4.22618000	-0.61162400	-0.00024700
C	5.85253300	-1.19301800	1.15460500	C	2.27950300	0.97444900	0.71209100
C	4.46224100	-1.60549000	1.36629200	C	0.99749500	1.54849700	1.12720400
C	5.93638800	0.16728500	1.55653700	C	2.28007100	0.97522900	-0.70973900
C	4.59473000	0.55205900	2.00207700	C	0.99838300	1.54971900	-1.12522800
C	3.69509000	-0.56292200	1.97988400	C	0.23716600	1.99650200	0.00093200
C	6.27868000	0.92529100	0.38962100	C	2.33711100	-0.39263000	-1.12857900
C	5.19108100	1.82830600	0.13998700	C	1.12840500	-0.66217300	-1.85451700
C	4.12992500	1.58606400	1.11791100	C	0.28163000	0.52826900	-1.83667900
C	6.57000500	0.07168500	-0.76703000	C	2.51354500	-1.30937500	0.00002600
C	5.42242800	0.39662600	-1.63453900	C	1.21093300	-2.00472700	-0.00086300
C	4.65524500	1.49013800	-1.12461900	C	0.42961800	-1.66250600	-1.14514800

C	6.14763000	-1.23385400	-0.24611000	C	2.33622600	-0.39385700	1.12950000
C	4.97433800	-1.72914800	-0.90762200	C	1.12695100	-0.66418400	1.85417700
C	4.52171200	-0.70582600	-1.77107200	C	0.42872400	-1.66374400	1.14318900
C	3.91455700	-1.93786200	0.08011400	C	0.28018200	0.52627800	1.83697700
C	2.75939800	-1.13772800	-0.20840400	C	-0.98585400	0.26279500	1.21814700
C	3.18788000	-0.31350800	-1.29981200	C	-0.84213700	-1.06860500	0.71223000
C	3.27142200	1.05695300	-0.89638600	C	-0.84158500	-1.06783600	-0.71453600
C	2.90314200	1.20176400	0.48099300	C	-0.98488900	0.26411600	-1.21910800
Si	1.81459600	-0.25430100	1.31894100	Si	-1.75066400	1.64804700	-0.00002600

C_{19}Si-CO

$F = 0.020$ $E_{ads}(BSSE) = -1.98886525$				$F = 0.020$ $E_{ads}(BSSE) = -2.10539484$			
O	1.88954200	0.00012800	0.02114300	O	1.90102200	-0.01104400	0.02234300
C	3.00771700	-0.00457200	0.02868300	C	3.00793500	-0.00078600	0.03536300
C	8.19856400	-1.37220000	1.32653600	C	8.22171000	-1.37766500	1.28255300
C	6.83366300	-1.62894600	0.93039200	C	6.87463900	-1.68403200	0.92637900
C	8.20196000	-0.07674400	1.90312500	C	8.20635100	-0.09068500	1.85205500
C	6.83746600	0.39577700	1.83171400	C	6.80859700	0.39445000	1.83100000
C	5.91816200	-0.68091400	1.53482200	C	5.94628100	-0.63607100	1.49511900
C	9.03638600	0.74858300	1.02295600	C	9.00633800	0.73558300	1.00593700
C	8.23680900	1.79890100	0.49317200	C	8.19516900	1.79763900	0.49069500
C	6.83940000	1.58790000	0.95628300	C	6.80272300	1.61347900	0.94356100
C	9.65750300	0.00516800	-0.03393400	C	9.64581900	-0.03098600	-0.04797100
C	9.22829800	0.59456400	-1.35402000	C	9.12431300	0.53008700	-1.27813500
C	8.25093200	1.59378000	-0.90349100	C	8.20353100	1.66232100	-0.91174500
C	9.03338200	-1.27578200	0.12173900	C	9.16420600	-1.40606400	0.10654800
C	8.22934200	-1.57939500	-1.01099100	C	8.26644300	-1.59247700	-0.97692300
C	8.24730500	-0.40253400	-1.79178800	C	8.25874200	-0.44704500	-1.82490500
C	6.83214900	-1.77373200	-0.53944600	C	6.87694500	-1.78517800	-0.49707200
C	5.97629200	-0.90933400	-1.22594800	C	6.01505600	-0.86146700	-1.17556100
C	6.86395700	0.07006000	-1.89047700	C	6.86604600	0.06631300	-1.84223600
C	6.86713200	1.36014000	-1.31818000	C	6.85838200	1.39378700	-1.29808400
C	5.98082000	1.52679900	-0.14236600	C	5.92711300	1.62630800	-0.13635200
Si	5.02068600	-0.02874600	0.07893700	Si	5.01010800	0.05243600	0.07483300

C_{19}Si-CO_2

$F = 0.020$ $E_{ads}(BSSE) = -0.23431939$				$E_{ele} = 0.020$ $E_{ads}(BSSE) = -0.27245444$			
C	0.32322500	0.49300400	-0.83982400	C	0.33691300	0.49228500	-0.83160700
O	-0.82158300	0.55334000	-0.92393000	O	-0.79530900	0.56174200	-0.93425400
O	1.50299400	0.43517800	-0.76015000	O	1.51025000	0.42470900	-0.73249100
C	7.41995500	-1.24375000	0.98093600	C	7.41748500	-1.24178200	0.97985100
C	6.05023300	-1.72600300	1.19295000	C	6.04740300	-1.72423300	1.19081300
C	7.46952500	0.07549700	1.51841900	C	7.46553800	0.07713800	1.51671300
C	6.12785900	0.35845300	2.04098600	C	6.12284700	0.35902200	2.03773400
C	5.26409500	-0.78029600	1.92956000	C	5.26113100	-0.77959400	1.92606900
C	7.74082000	0.95898500	0.42511200	C	7.74047800	0.96407600	0.42907300
C	6.61066000	1.83732400	0.30200200	C	6.60553800	1.83425200	0.30013300
C	5.59336500	1.45315800	1.28180600	C	5.58947800	1.45034700	1.27924300
C	8.02837400	0.23869000	-0.82561800	C	8.02154800	0.23871700	-0.82204000
C	6.83073200	0.60557000	-1.61949300	C	6.82707900	0.60740900	-1.62406100
C	6.04317600	1.60527800	-0.97230300	C	6.04116100	1.60391900	-0.97410900
C	7.66388900	-1.13027400	-0.42450700	C	7.66490800	-1.13476300	-0.42383100

C	6.48356400	-1.59896000	-1.09544500	C	6.48192900	-1.59584800	-1.09384000
C	5.96517800	-0.51046100	-1.83247900	C	5.96513700	-0.50989300	-1.83272000
C	5.46725300	-1.94446600	-0.09981100	C	5.46696400	-1.94229200	-0.09933200
C	4.27096300	-1.16510600	-0.26438700	C	4.27201900	-1.16084000	-0.26348000
C	4.63142700	-0.22072000	-1.28307900	C	4.63122600	-0.21943000	-1.28480900
C	4.68030500	1.09939200	-0.74656200	C	4.67866400	1.09646400	-0.75037600
C	4.35507800	1.08572800	0.65089300	C	4.35337800	1.07910500	0.64656500
Si	3.32678100	-0.47981300	1.36525200	Si	3.32210000	-0.48076100	1.36108300

$C_{19}Si\text{-}N_2$

$F = 0.020$ $E_{ads}(BSSE) = -0.13186518$				$F = 0.020$ $E_{ads}(BSSE) = -0.14614638$			
N	-1.27155400	0.70522700	-1.37834600	N	-1.20947700	0.71534600	-1.37477400
N	-0.20053500	0.58927700	-1.14355600	N	-0.15333000	0.58537200	-1.12337000
C	5.83284100	-1.20001400	1.16501000	C	5.83016800	-1.19641300	1.16224000
C	4.43393100	-1.60039900	1.35539000	C	4.43188700	-1.59891700	1.35357100
C	5.92124400	0.16233300	1.56974100	C	5.91573500	0.16571300	1.56577400
C	4.57286200	0.55546900	1.99328700	C	4.56666600	0.55608500	1.98972100
C	3.66160000	-0.55112500	1.95335200	C	3.65877300	-0.55162200	1.95092900
C	6.28564200	0.91738200	0.40870900	C	6.28109800	0.92487500	0.40954800
C	5.20644700	1.82627500	0.14172100	C	5.19575100	1.82392800	0.13874400
C	4.12812100	1.58924800	1.10312300	C	4.12017600	1.58571900	1.10093500
C	6.59653000	0.06127500	-0.74769400	C	6.58505900	0.06417300	-0.74738800
C	5.45502200	0.39501200	-1.63258000	C	5.44534000	0.39690300	-1.63870300
C	4.68739300	1.48987800	-1.13084700	C	4.67827800	1.48771300	-1.13284000
C	6.14850300	-1.24333300	-0.22983200	C	6.14694000	-1.24596700	-0.23041800
C	4.97979500	-1.72690000	-0.90849100	C	4.97598900	-1.72392000	-0.90739200
C	4.54819200	-0.69964500	-1.77773800	C	4.54310900	-0.70001300	-1.77738100
C	3.90286200	-1.92628800	0.06396600	C	3.90190800	-1.92534500	0.06569200
C	2.75528700	-1.11620100	-0.23800600	C	2.75413500	-1.11534300	-0.23476500
C	3.20712700	-0.29810200	-1.32712300	C	3.20212400	-0.29971300	-1.32666900
C	3.29423800	1.06754400	-0.92375000	C	3.28645100	1.06198400	-0.92546000
C	2.90546400	1.20979900	0.45006600	C	2.89920800	1.20099800	0.44854700
Si	1.77552900	-0.23071300	1.27246600	Si	1.77055200	-0.23555800	1.27232700

$C_{19}Si\text{-}CO$

$F = 0.025$ $E_{ads}(BSSE) = -2.40028075$				$F = 0.025$ $E_{ads}(BSSE) = -2.57870530$			
O	1.85816900	-0.00376100	0.03338800	O	1.86113700	-0.01874700	0.06004300
C	2.97544400	-0.00582500	0.03322200	C	2.96684000	-0.00883200	0.05139700
C	8.20407300	-1.37330600	1.32777100	C	8.21102200	-1.38099200	1.31912800
C	6.83386500	-1.62468900	0.92907300	C	6.85409900	-1.63787900	0.92246500
C	8.20779500	-0.07616600	1.90537100	C	8.20274900	-0.08436100	1.87999800
C	6.83909300	0.39478400	1.82816800	C	6.81261200	0.38848900	1.82095100
C	5.92277500	-0.67575000	1.52215300	C	5.92300900	-0.65589800	1.51393200
C	9.03887500	0.74625500	1.02363700	C	9.02123800	0.73670900	1.02193000
C	8.24130900	1.79873300	0.49187000	C	8.21879100	1.78062900	0.48393000
C	6.83997800	1.58729400	0.95370000	C	6.81565900	1.60348500	0.94728200
C	9.67552400	0.00323900	-0.02800900	C	9.66935000	-0.01820000	-0.03577300
C	9.24468100	0.59704400	-1.35841800	C	9.22352100	0.56838400	-1.34508400
C	8.25895500	1.59186600	-0.90288600	C	8.24181200	1.61781800	-0.91149900
C	9.03374500	-1.27279500	0.12461800	C	9.07905100	-1.31963200	0.11570600
C	8.23214500	-1.57741100	-1.01143400	C	8.25222200	-1.58890500	-1.00516400
C	8.25384000	-0.40200400	-1.79048200	C	8.26894100	-0.41838400	-1.80024000

C	6.83091700	-1.77198800	-0.54169500	C	6.85521800	-1.77110600	-0.52293800
C	5.97926600	-0.90390900	-1.22108300	C	6.00893400	-0.86683800	-1.18752200
C	6.87098800	0.07009700	-1.89119700	C	6.88098900	0.07760300	-1.86728400
C	6.87451100	1.35810400	-1.31824000	C	6.88080700	1.38233300	-1.32119100
C	5.98541900	1.51652200	-0.14376100	C	5.96859500	1.55378800	-0.14166200
Si	4.98610100	-0.02743500	0.07309700	Si	4.97087100	0.00943600	0.07900000
$C_{19}Si\text{-}CO_2$							
$F = 0.025$ $E_{ads}(BSSE) = -0.33903162$				$F = 0.025$ $E_{ads}(BSSE) = -0.40174203$			
C	0.31320300	0.45154600	-0.73552100	C	0.30768200	0.43695200	-0.70366100
O	-0.82939200	0.50319000	-0.80162800	O	-0.82237100	0.49545200	-0.78429400
O	1.50139000	0.40247400	-0.67388700	O	1.49178700	0.38007900	-0.62617300
C	7.38570500	-1.25707400	1.00523500	C	7.37581900	-1.25673900	1.01137100
C	6.00062500	-1.71968700	1.17665200	C	5.98717900	-1.71439400	1.17441700
C	7.43587700	0.06409200	1.54700600	C	7.42591000	0.06483100	1.55050900
C	6.07849200	0.36082800	2.02763300	C	6.06530000	0.36615400	2.02117100
C	5.20034200	-0.76472400	1.88708600	C	5.18643200	-0.75627100	1.87668400
C	7.74911600	0.94424400	0.46400500	C	7.75471800	0.94714000	0.47642200
C	6.63033800	1.83286000	0.30668600	C	6.63311700	1.82803100	0.30245200
C	5.57822700	1.45716400	1.25400600	C	5.57495100	1.45799600	1.24267100
C	8.07547000	0.22180000	-0.78391600	C	8.07910900	0.21436000	-0.77058500
C	6.89566800	0.60451800	-1.61336900	C	6.90929400	0.60306900	-1.61923300
C	6.09995100	1.60791400	-0.98491000	C	6.11469800	1.60593200	-0.99297600
C	7.67185900	-1.14613300	-0.39084700	C	7.67601900	-1.15865900	-0.38053500
C	6.50280600	-1.59546600	-1.09514000	C	6.50502400	-1.59320200	-1.08969400
C	6.02190200	-0.49962200	-1.84654500	C	6.03598900	-0.49973600	-1.84930800
C	5.45192600	-1.92614300	-0.12926400	C	5.44839900	-1.91887200	-0.13114500
C	4.26685400	-1.13080300	-0.32565400	C	4.26881500	-1.11547700	-0.33601700
C	4.67223700	-0.19407100	-1.33880500	C	4.68376200	-0.18672700	-1.35406400
C	4.72108800	1.12041400	-0.80165300	C	4.73267400	1.12323900	-0.82152700
C	4.35074700	1.10238900	0.58755500	C	4.35244200	1.10188500	0.56580500
Si	3.25343100	-0.43996100	1.26560400	Si	3.24111400	-0.42529600	1.23803600
$C_{19}Si\text{-}N_2$							
$F = 0.025$ $E_{ads}(BSSE) = -0.17736559$				$F = 0.025$ $E_{ads}(BSSE) = -0.20140237$			
N	-1.33534300	0.66360200	-1.26486100	N	-1.29172000	0.66420600	-1.23049000
N	-0.25854600	0.55945800	-1.04850900	N	-0.22750900	0.54873500	-1.00363100
C	5.81248000	-1.20679300	1.18059600	C	5.80378000	-1.20446500	1.18191100
C	4.40407900	-1.59420200	1.34297900	C	4.39421500	-1.59196000	1.33867600
C	5.90395000	0.15796300	1.58773100	C	5.89234900	0.16007900	1.58782900
C	4.54684800	0.56000700	1.98188700	C	4.53304400	0.56175300	1.97606100
C	3.62402200	-0.53771600	1.92063500	C	3.61227900	-0.53568700	1.91087100
C	6.29681400	0.90886600	0.43464400	C	6.29568700	0.91614700	0.44407800
C	5.22744400	1.82302900	0.14416300	C	5.22106900	1.81891900	0.14215800
C	4.12693600	1.59235200	1.08309200	C	4.11802700	1.58939000	1.07597800
C	6.63499500	0.04887000	-0.71964200	C	6.63066700	0.04861000	-0.71065400
C	5.50308000	0.39107200	-1.62777100	C	5.50577200	0.39223400	-1.63346100
C	4.73220500	1.48751100	-1.13862500	C	4.73469800	1.48525500	-1.14303600
C	6.15611600	-1.25438900	-0.20591400	C	6.15685800	-1.26187100	-0.19965000
C	4.99508100	-1.72570500	-0.90687300	C	4.99489800	-1.72216600	-0.90455000
C	4.59001200	-0.69538600	-1.78484900	C	4.59588400	-0.69501600	-1.78680000
C	3.89601700	-1.91432400	0.04447400	C	3.89364100	-1.91081500	0.04160200

C	2.75751300	-1.09433800	-0.27774300	C	2.75808600	-1.08738600	-0.28542000
C	3.23967800	-0.28384600	-1.36275300	C	3.24398600	-0.28178100	-1.37307500
C	3.32882600	1.07707100	-0.96001700	C	3.33052100	1.07440600	-0.97270200
C	2.91128600	1.21780100	0.40787900	C	2.90687200	1.21074900	0.39408000
Si	1.73304800	-0.20490300	1.20834800	Si	1.72343800	-0.20333600	1.18909600

Table S3. Frontier orbital energies (in eV) for C_{20} and $C_{19}Si$ fullerenes. Percentual increase of the HOMO-LUMO gap, ΔE_{HL} is also shown.

B3LYP/6-31G(d)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-5.061	-3.111	1.949	
$C_{19}Si$	-5.610	-3.295	2.316	18.81%
B3LYP/6-311+G(d,p)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-5.537	-3,623	1.914	
$C_{19}Si$	-5.924	-3.050	2.219	15.92%
B3LYP/def2TVZP				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-5.443	-3.524	1.919	
$C_{19}Si$	-5.821	-3.615	2.206	14.96%
ωB97XD/6-31G(d)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-7.017	-1.560	5.458	
$C_{19}Si$	-7.537	-1.731	5.805	6.37%
ωB97XD /6-311+G(d,p)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-7.355	-1.960	5.395	
$C_{19}Si$	-7.765	-2.044	5.722	6.06%
ωB97XD /def2TVZP				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-7.246	-1.817	5.429	
$C_{19}Si$	-7.655	-1.927	5.727	5.49%
M06L/6-31G(d)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-4.464	-3.607	0.857	
$C_{19}Si$	-5.059	-3.730	1.329	55.10%
M06L/6-311+G(d,p)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-4.710	-3.847	0.862	
$C_{19}Si$	-5.198	-3.901	1.297	50.36%
M06L/def2TVZP				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-4,542	-3,652	0,890	
$C_{19}Si$	-5,049	-3,734	1,315	47.80%
M062X/6-31G(d)				

	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-6.310	-2.427	3.883	
$C_{19}Si$	-6.843	-2.589	4.254	9.57%
M062X/6-311+G(d,p)				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-6.310	-2.427	3.883	
$C_{19}Si$	-7.104	-2.923	4.181	7.68%
M062X/def2TVZP				
	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}	-6.540	-2.689	3.851	
$C_{19}Si$	-6.968	-2.779	4.188	8.76%

Table S4. Si-C bond lengths and Merz-Kollmann (MK) charges on the Si-atom and adjacent carbons.

XCF/basis set	Bond length (Å)			MK charges (e)			
	C1-Si	C2-Si	C3-Si	C1	C2	C3	Si
ωB97XD/6-31G(d)	1.98894	1.98900	1.98895	0.116	0.110	0.081	-0.222
ωB97XD/6-311+G(d,p)	1.98812	1.98799	1.98801	0.069	0.093	0.064	-0.162
ωB97XD/DF2TZVP	1.97993	1.97987	1.97976	0.053	0.108	0.107	-0.191
M062X/6-31G(d)	2.00155	2.00156	2.00131	0.047	0.047	0.061	-0.142
M062X/6-311+G(d,p)	2.00052	2.00063	2.00038	0.031	0.060	0.035	-0.092
M062X/6-311++G(d,p)	2.00052	2.00063	2.00038	0.031	0.060	0.035	-0.092
M062X/DF2TZVP	1.99038	1.99058	1.99057	0.085	0.090	0.028	-0.143
M06L/6-31G(d)	1.99147	1.99131	1.9914	0.032	0.082	0.075	-0.174
M06L/6-311+G(d,p)	1.99006	1.99000	1.98985	0.075	0.023	0.070	-0.142
M06L/DF2TZVP	1.98098	1.98094	1.98089	0.048	0.075	0.047	-0.159
B3LYP/6-31G(d)	2.00814	2.00839	2.00871	0.106	0.105	0.022	-0.222
B3LYP/6-311+G(d,p)	2.00745	2.00737	2.00734	0.054	0.044	0.031	-0.112
B3LYP/DF2TZVP	1.99733	1.9974	1.99736	0.072	0.048	0.051	-0.131

Table S5. Adsorption energies (in eV), E_{ads}, and adsorption energy with and without BSSE corrections, $E_{ads}\,(BSSE)$, for the dimers formed between C_{20} fullerenes with CO, CO_2 and N_2 molecules calculated with the theoretical levels ωB97XD /6-31G(d) and ωB97XD/6-311+G(d,p).

Molecules	ωB97XD/6-31G(d)			ωB97XD/6-311+G(d.p)		
	BSSE	E_{ads}	$E_{ads}(BSSE)$	BSSE	E_{ads}	$E_{ads}(BSSE)$
C_{20}-CO	0.040	-0.080	-0.040	0.023	-0.065	-0.042
C_{20}-CO_2	0.045	-0.110	-0.066	0.029	-0.104	-0.075
C_{20}-N_2	0.034	-0.076	-0.042	0.024	-0.066	-0.042

Table S6. Externally oriented electric field effect on the BSSE correction, adsorption energies, E_{ads}, and BSSE corrected, $E_{ads}(BSSE)$, for the interaction of C_{20} and $C_{19}Si$ fullerenes with the CO, CO_2 and N_2 molecules as obtained at the ωB97XD/6-31G(d) and ωB97XD/6-311+G(d,p) levels of theory. Adjusted adsorption energy, $E_{ads}(fit)$ and the R-squared coefficient of determination, R^2, are also presented. All energies in eV.

ωB97XD/6-31G(d)					ωB97XD/6-311+G(d.p)				
$C_{19}Si$-CO									
F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$	F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$
0.000	0.134	-0.837	-0.703	-0.650	0.000	0.049	-0.787	-0.738	-0.677
0.001	0.134	-0.884	-0.749	-0.717	0.001	0.049	-0.838	-0.788	-0.749
0.005	0.140	-1.097	-0.957	-0.987	0.005	0.050	-1.060	-1.009	-1.039
0.010	0.148	-1.409	-1.261	-1.323	0.010	0.052	-1.380	-1.328	-1.401
0.015	0.157	-1.766	-1.609	-1.660	0.015	0.052	-1.746	-1.694	-1.763
0.020	0.168	-2.157	-1.989	-1.997	0.020	0.054	-2.159	-2.105	-2.125
0.025	0.180	-2.581	-2.400	-2.334	0.025	0.053	-2.631	-2.579	-2.488
R^2	0.994				R^2	0.991			
$C_{19}Si$-CO_2									
F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$	F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$
0.000	0.027	-0.095	-0.068	-0.076	0.000	0.015	-0.092	-0.077	-0.083
0.001	0.040	-0.121	-0.081	-0.075	0.001	0.023	-0.109	-0.087	-0.082
0.005	0.045	-0.130	-0.085	-0.081	0.005	0.026	-0.118	-0.091	-0.09
0.010	0.052	-0.162	-0.110	-0.110	0.010	0.029	-0.153	-0.124	-0.125
0.015	0.062	-0.223	-0.161	-0.162	0.015	0.032	-0.225	-0.194	-0.189
0.020	0.076	-0.310	-0.234	-0.238	0.020	0.034	-0.307	-0.272	-0.280
0.025	0.093	-0.432	-0.339	-0.337	0.025	0.036	-0.438	-0.402	-0.399
R^2	0.998				R^2	0.998			
$C_{19}Si$-N_2									
F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$	F	BSSE	E_{ads}	$E_{ads}(BSSE)$	$E_{ads}(fit)$
0.000	0.134	-0.837	-0.017	-0.031	0.000	0.024	-0.069	-0.045	-0.044
0.001	0.134	-0.884	-0.045	-0.034	0.001	0.026	-0.072	-0.046	-0.046
0.005	0.140	-1.097	-0.054	-0.048	0.005	0.026	-0.082	-0.056	-0.057
0.010	0.148	-1.409	-0.072	-0.072	0.010	0.027	-0.104	-0.077	-0.078
0.015	0.157	-1.766	-0.097	-0.101	0.015	0.029	-0.143	-0.114	-0.109
0.020	0.168	-2.157	-0.132	-0.135	0.020	0.030	-0.177	-0.146	-0.150
0.025	0.180	-2.581	-0.177	-0.174	0.025	0.032	-0.233	-0.201	-0.200

R^2	0.980	R^2	0.998

Table S7. Energies (in eV) of the HOMO, E_H, LUMO, E_L and the gap between them, E_{HL}, calculated with the theoretical levels ωB97XD/6-31G(d) and ωB97XD/6-311+G(d,p), for the dimers.. The percentual change in the fullerene energy gap after adsorbing the gas, in relation to the fullerene energy gap before adsorption, is represented by ΔE_{HL} (in %). Positive values of ΔE_{HL} indicate an increase in the gap, negative values indicate a reduction.

Dimers	**ωB97XD /6-31G(d)**				**ωB97XD /6-311+G(d,p)**			
	$F = 0.000\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{20}-CO	-7.045	-1.580	5.465	0.130	-7.355	-1.957	5.397	0.050
C_{20}-CO_2	-7.072	-1.607	5.465	0.145	-7.405	-2.011	5.394	-0.020
C_{20}-N_2	-7.039	-1.579	5.461	0.060	-7.356	-1.958	5.397	0.050
Dimers	$F = 0.000\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-6.888	-2.256	4.632	-20.212	-7.188	-2.609	4.579	-19.966
C_{19}Si-CO_2	-7.516	-1.739	5.776	-0.497	-7.740	-2.055	5.684	-0.652
C_{19}Si-N_2	-7.534	-1.733	5.801	-0.080	-7.760	-2.048	5.712	-0.171
Dimers	$F = 0.001\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-7.257	-2.637	4.620	-20.418	-7.563	-2.981	4.581	-19.928
C_{19}Si-CO_2	-7.791	-2.031	5.760	-0.778	-7.759	-2.093	5.666	-0.975
C_{19}Si-N_2	-7.734	-1.949	5.785	-0.351	-7.766	-2.072	5.694	-0.485
Dimers	$F = 0.005\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-8.741	-4.125	4.616	-20.488	-9.067	-4.491	4.576	-20.023
C_{19}Si-CO_2	-8.889	-3.201	5.688	-2.030	-9.131	-3.543	5.588	-2.340
C_{19}Si-N_2	-8.522	-2.814	5.708	-1.683	-8.767	-3.154	5.613	-1.893
Dimers	$F = 0.010\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-10.589	-6.014	4.575	-21.192	-10.959	-6.416	4.543	-20.594
C_{19}Si-CO_2	-10.279	-4.673	5.605	-3.446	-10.556	-5.051	5.504	-3.794
C_{19}Si-N_2	-9.504	-3.896	5.607	-3.412	-9.783	-4.275	5.507	-3.748
Dimers	$F = 0.015\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-12.431	-7.920	4.511	-22,297	-12,869	-8,377	4,492	-21,498
C_{19}Si-CO_2	-11.657	-6.143	5.514	-5,016	-8,153	-2,720	5,433	-5,046
C_{19}Si-N_2	-10.485	-4.980	5.505	-5,166	-7,904	-2,479	5,425	-5,175
Dimers	$F = 0.020\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
C_{19}Si-CO	-14.298	-9.830	4.468	-23.033	-14.808	-10.373	4.435	-22.492
C_{19}Si-CO_2	-13.036	-7.607	5.429	-6.477	-13.433	-8.136	5.297	-7.414
C_{19}Si-N_2	-11.475	-6.065	5.410	-6.807	-11.869	-6.595	5.274	-7.815

Dimers	$F = 0.025\ a.u.$							
	E_H	E_L	E_{HL}	ΔE_{HL}	E_H	E_L	E_{HL}	ΔE_{HL}
$C_{19}Si$-CO	-16.191	-11.740	4.451	-23.326	-16.768	-12.492	4.276	-25.264
$C_{19}Si$-CO_2	-14.439	-9.066	5.373	-7.439	-14.956	-10.362	4.594	-19.703
$C_{19}Si$-N_2	-12.484	-7.155	5.330	-8.194	-12.996	-8.488	4.508	-21.212

Table S8. Topological parameters calculated using the Quantum Theory of Atoms in Molecules (QTAIM) with the theoretical level ωB97XD /6-31G(d). Results are presented for all dimers formed by C_{20} and $C_{19}Si$ fullerenes with adsorbed gas molecules. The results were obtained for all electric field values and are all presented in atomic units.

Dimers	**ωB97XD/6-31G(d)**							
	$F = 0.000\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
C_{20}-CO	1	C-C	3.704	1.239	6.475	2.451	-1.804	1.359
	2	C-O	2.760	1.132	5.118	2.317	-1.806	1.283
C_{20}-CO_2	1	C-O	2.926	1.225	4.988	2.563	-2.064	1.242
	2	C-O	2.458	1.122	4.738	2.331	-1.857	1.255
	3	C-O	2.441	1.094	4.170	2.317	-1.900	1.220
C_{20}-N_2	1	C-N	3.564	1.146	4.610	2.404	-1.943	1.237
	2	C-N	3.677	1.184	4.532	2.507	-2.054	1.221
$C_{19}Si$-CO	1	Si-C	18.256	13.592	-14.977	35.478	-36.976	0.959
	2	Si-C	16.693	13.265	-9.297	35.533	-37.084	0.958
	3	Si-C	18.351	13.593	-15.515	34.092	-35.022	0.973
	4	Si-C	16.969	35.720	137.366	75.564	-61.827	1.222
	5		16.968	35.240	133.473	74.753	-61.406	1.2174
	6		16.950	33.938	123.195	72.525	-60.205	1.2046
	7		15.970	27.519	79.730	60.825	-52.852	1.1509
$C_{19}Si$-CO_2	1	Si-O	3.623	1.257	4.928	2.649	-2.156	1.2285
	2	Si-O	3.906	1.301	8.257	2.428	-1.602	1.5155
$C_{19}Si$-N_2	1	Si-N	1.955	0.557	3.054	1.087	-0.782	1.391
Dimers	$F = 0.001\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
$C_{19}Si$-CO	1	Si-C	17.948	13.307	-14.384	34.705	-36.144	0.960
	2	Si-C	17.850	13.302	-13.867	34.641	-36.027	0.961
	3	Si-C	16.473	12.987	-9.191	33.387	-34.306	0.973
	4		16.504	33.454	122.812	71.355	-59.073	1.2079
	5		15.669	27.605	82.555	60.757	-52.501	1.1572
$C_{19}Si$-CO2	1	Si-O	5.278	1.743	2.901	4.068	-3.778	1.0768
$C_{19}Si$-N2	1	C-N	3.342	1.124	4.152	2.394	-1.979	1.210
	2	Si-N	3.464	1.027	3.293	2.239	-1.9010	1.172
Dimers	$F = 0.005\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
$C_{19}Si$-CO	1	Si-C	17.254	13.077	-11.884	33.881	-35.070	0.966
	2	Si-C	17.202	13.079	-11.575	33.856	-35.013	0.967

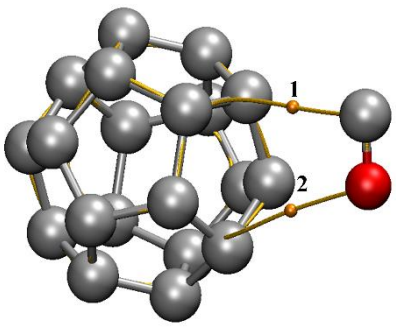
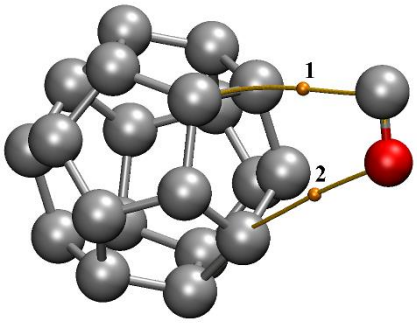
	3	Si-C	16.017	12.768	-7.9833	32.719	-33.517	0.976
	4	Si-C	16.011	34.688	136.235	73.099	-59.476	1.229
C_{19}Si-CO2	1	C-O	3.390	1.521	6.239	3.178	-0.624	5.093
	2	Si-O	5.740	1.932	2.848	4.545	-4.260	1.067
C_{19}Si-N2	1	C-N	3.624	1.192	4.301	2.551	-2.121	1.203
	2	Si-N	3.622	1.113	3.541	2.427	-2.072	1.171
Dimers	$F = 0.010\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
	1	Si-C	16.202	12.805	-7.832	32.795	-33.578	0.977
	2	Si-C	16.726	12.995	-9.367	33.423	-34.360	0.973
C_{19}Si-CO	3	Si-C	15.465	12.554	-5.991	31.985	-32.584	9.816
	4		15.313	28.936	96.422	62.697	-53.054	1.182
	5		14.762	26.454	80.775	58.058	-49.981	1.162
C_{19}Si-CO2	1		3.925	1.760	7.226	3.677	-2.955	1.245
	2		6.528	2.172	1.915	5.210	-5.048	1.038
C_{19}Si-N2	1	C-N	3.950	1.294	4.499	2.786	-2.336	1.193
	2	Si-N	4.064	1.292	3.853	2.845	-2.460	1.157
Dimers	$F = 0.015\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
C_{19}Si-CO	1	Si-C	66.488	24.612	-246.685	86.198	-110.866	0.778
C_{19}Si-CO_2	1	C-O	4.174	1.920	7.843	4.017	-7.843	5.121
	2	Si-O	8.587	2.718	-1.205	6.917	-7.037	0.983
C_{19}Si-N2	1	C-N	2.982	1.195	5.559	2.431	-1.876	1.2964
	2	Si-N	5.814	1.913	4.681	4.315	-3.846	1.1217
Dimers	$F = 0.020\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
C_{19}Si-CO	1	Si-C	75.218	18.519	-317.233	78.021	-109.74	0.711
C_{19}Si-CO2	1	Si-O	12.480	2.993	-2.139	7.696	-7.910	0.973
C_{19}Si-N2	1	Si-N	8.297	2.100	4.859	4.764	-4.278	1.114
Dimers	$F = 0.025\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP} \rvert$
C_{19}Si-CO	1	Si-C	77.475	17.822	-340.719	78.628	-112.699	0.698
C_{19}Si-CO2	1	Si-O	18.086	3.699	-10.581	10.306	-11.364	0.907
C_{19}Si-N2	1	Si-N	10.488	2.481	4.123	5.710	-53.776	1.0767

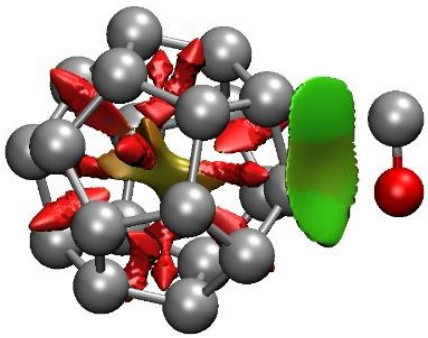
Table S9. Topological parameters calculated using the Quantum Theory of Atoms in Molecules (QTAIM) with the theoretical level ωB97XD /6-311+G(d,p). Results are presented for all dimers formed by C_{20} and $C_{19}Si$ fullerenes with adsorbed gas molecules. The results were obtained for all electric field values and are all presented in atomic units.

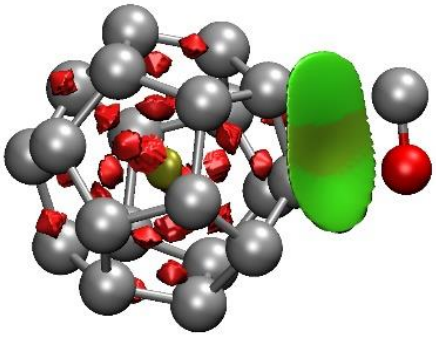
Dimers	**ωB97XD/6-311+G(d.p)**							
	$F = 0.000\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
C_{20}-CO	1	C-C	3.686	1.054	6.371	1.998	-1.361	1.468
	2	C-O	2.736	0.978	5.130	1.932	-1.419	1.361
C_{20}-CO_2	1	C-C	4.766	1.884	11.374	3.572	-2.434	1.467
C_{20}-N_2	1	C-N	2.866	0.962	5.162	1.888	-1.372	1.376
	2	C-N	2.635	0.872	4.617	1.718	-1.256	1.367
$C_{19}Si$-CO	1	Si-C	70.630	20.211	-276.945	78.223	-105.91	0.738
$C_{19}Si$-CO_2	1	Si-O	5.744	1.625	7.969	3.266	-2.470	1.323
$C_{19}Si$-N_2	1	C-N	3.078	1.026	5.654	2.000	-1.435	1.394
	2	Si-N	4.126	1.135	4.793	2.360	-1.880	1.255
Dimers	$F = 0.001\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si$-CO	1	Si-C	70.630	20.211	-276.945	78.223	-105.917	0.738
$C_{19}Si$-CO_2	1	Si-O	6.177	1.633	4.400	3.643	-3.203	1.137
$C_{19}Si$-N_2	1	C-N	3.665	1.215	6.606	2.376	-1.716	1.385
	2	Si-N	4.514	1.253	5.124	2.620	-2.107	1.243
Dimers	$F = 0.005\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si$-CO	1	Si-C	71.154	19.405	-285.140	77.027	-105.541	0.730
$C_{19}Si$-CO_2	1	C-O	3.922	1.523	8.174	2.990	-2.173	1.376
	2	Si-O	6.170	1.665	3.751	3.787	-3.412	1.110
$C_{19}Si$-N_2	1	C-N	3.408	1.135	6.285	2.208	-1.579	1.398
	2	Si-N	4.519	1.254	5.144	2.622	-2.107	1.244
Dimers	$F = 0.010\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si$-CO	1	Si-C	73.074	18.976	-303.144	77.755	-108.070	0.719
$C_{19}Si$-CO_2	1	C-O	4.963	1.969	10.203	3.902	-2.881	1.354
	2	Si-O	6.909	1.945	4.489	4.414	-3.965	1.113
$C_{19}Si$-N_2	1	C-N	3.812	1.279	7.106	2.487	-1.776	1.400
	2	Si-N	5.310	1.459	5.588	3.088	-2.529	1.221
Dimers	$F = 0.015\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si$-CO	1	Si-C	75.200	18.480	-323.587	78.559	-110.918	0.708
$C_{19}Si$-CO_2	1	C-O	5.041	2.053	11.121	4.020	-2.908	1.382

	2	Si-O	8.960	2.422	4.184	5.638	-5.219	1.080
	1	C-N	4.061	1.393	7.806	2.703	-1.922	1.406
$C_{19}Si\text{-}N_2$	2	Si-N	6.513	1.741	6.012	3.752	-3.150	1.191
Dimers	$F = 0.020\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si\text{-}CO$	1	Si-C	78.138	18.319	-349.540	80.751	-115.705	0.698
$C_{19}Si\text{-}CO_2$	1	Si-O	12.880	3.2435	2.4203	7.867	-7.625	1.032
	1	C-N	4.209	1.522	8.479	2.957	-2.109	1.402
$C_{19}Si\text{-}N_2$	2	Si-N	8.899	2.281	6.614	5.040	-4.379	1.151
Dimers	$F = 0.025\ a.u.$							
	BCP	Bond	$\rho_{BCP} \times 10^{-3}$	$\nabla^2\rho_{BCP} \times 10^{-2}$	$H_{BCP} \times 10^{-4}$	$G_{BCP} \times 10^{-3}$	$V_{BCP} \times 10^{-3}$	$\lvert G_{BCP}/V_{BCP}$
$C_{19}Si\text{-}CO$	1	Si-C	80.146	17.195	-373.751	80.364	-1.17.739	0.682
$C_{19}Si\text{-}CO_2$	1	Si-O	19.799	4.395	-4.569	11.445	-11.902	0.962
$C_{19}Si\text{-}N_2$	1	Si-N	11.871	28.437	6.329	6.476	-5.843	1.108

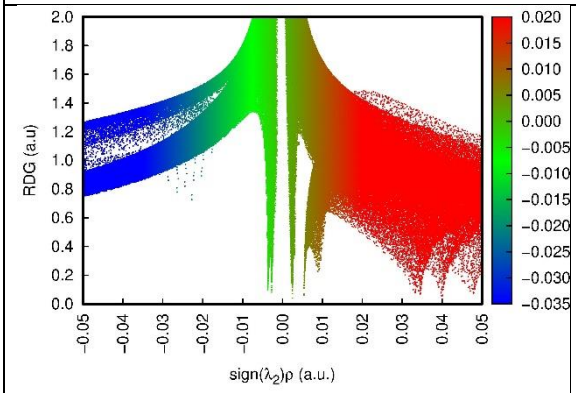
Table S10. Critical bond points, BCP, isosurfaces and scatter plots for the dimers formed by C_{20} and $C_{19}Si$ fullerenes with the adsorbed gas molecules. The results were obtained for all electric field values using both the theoretical level ωB97XD/6-31G(d) and ωB97XD/6-311+G(d,p).

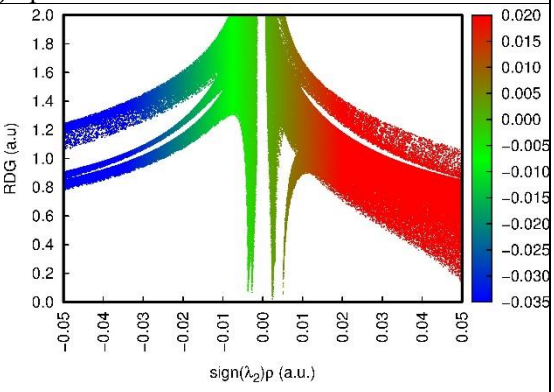
ωB97XD/6-31G(d)	**ωB97XD/6-311+G(d,p)**
C_{20}-CO $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.04027087\ eV$	**C_{20}-CO** $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.04215341\ eV$
QTAIM	
	
RDG	





Scatter graph

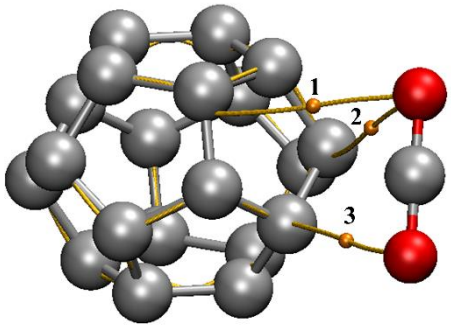


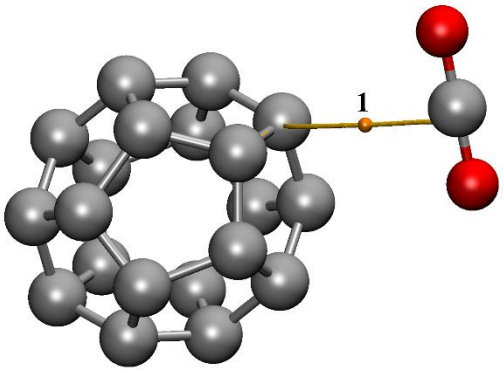


C_{20}-CO_2
$F = 0.000\ a.u.$
$E_{ads}(BSSE) = -0.06556463\ eV$

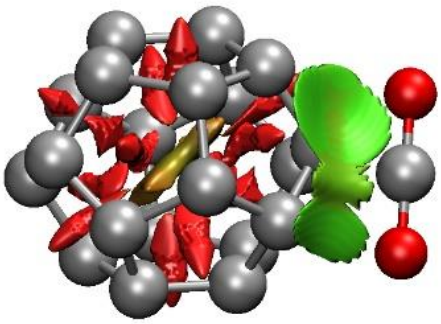
C_{20}-CO_2
$F = 0.000\ a.u.$
$E_{ads}(BSSE) = -0.07502922\ eV$

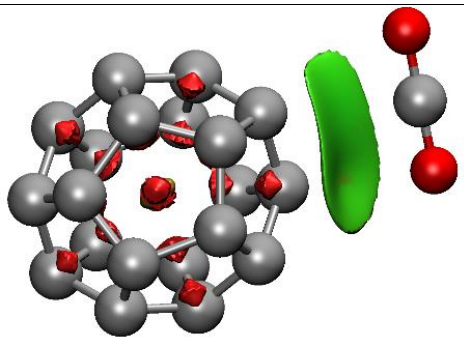
QTAIM



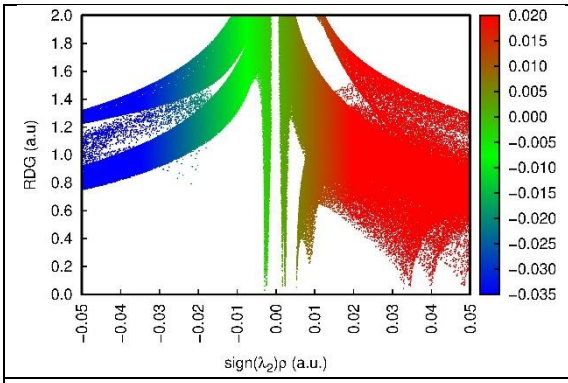
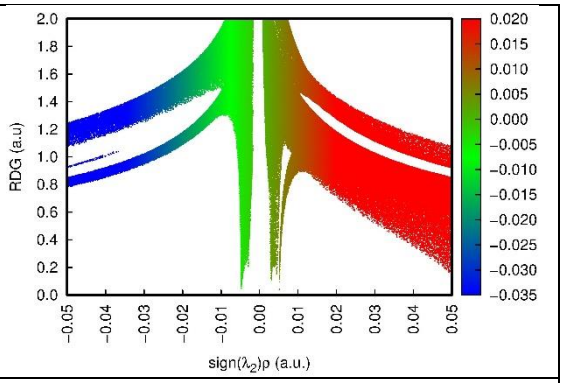
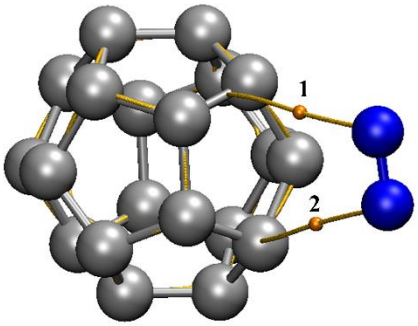
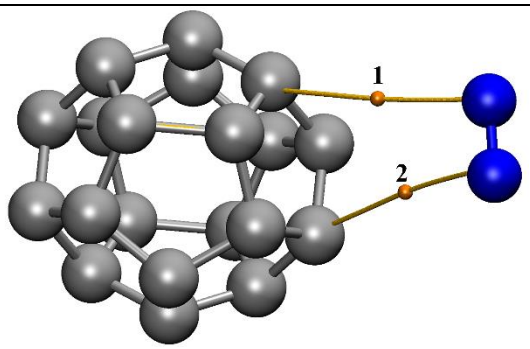
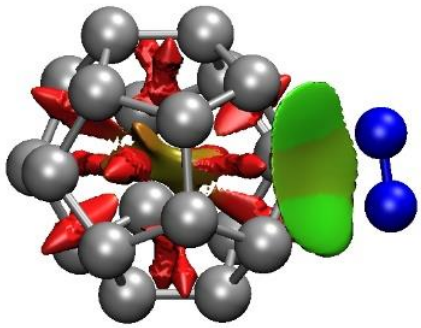
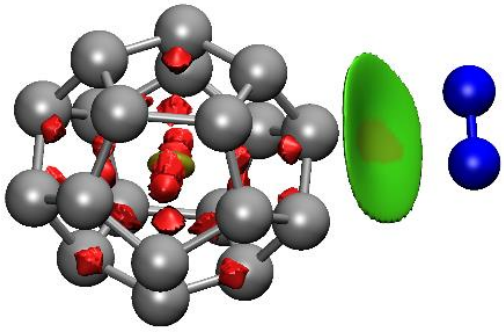
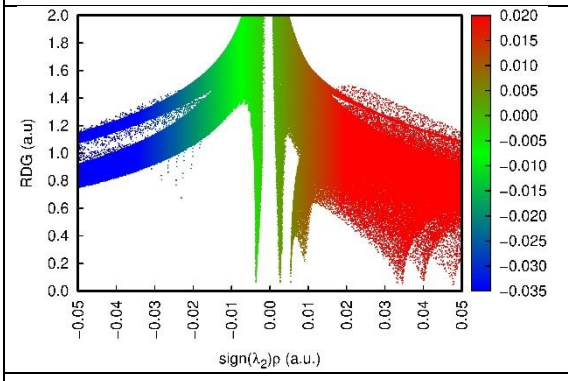
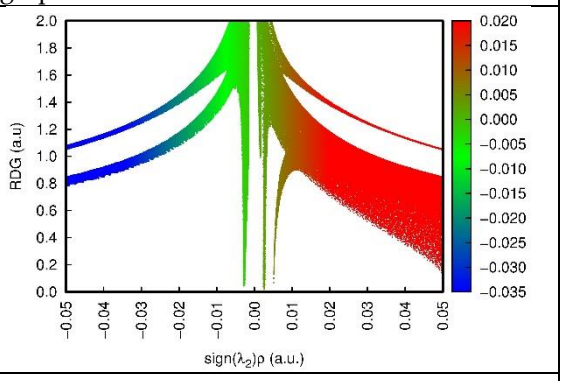


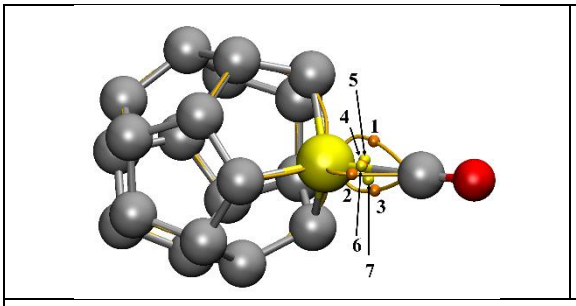
RDG

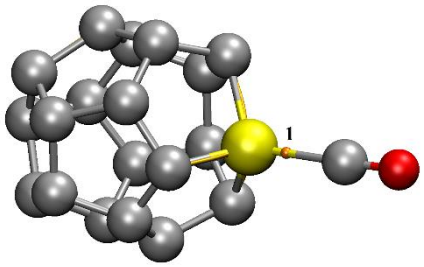




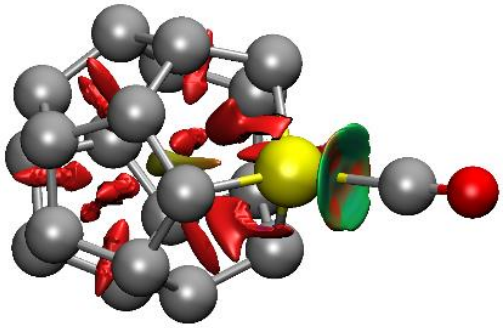
Scatter graph

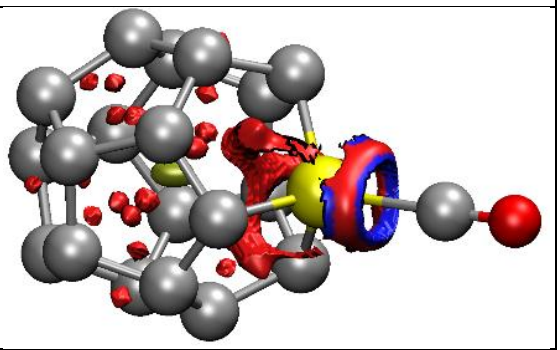
	
C_{20}-N_2 $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.04191301eV$	**C_{20}-N_2** $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.04214772\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
C_{19}Si-CO $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.70264080\ eV$	**C_{19}Si-CO** $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.73799673\ eV$
QTAIM	



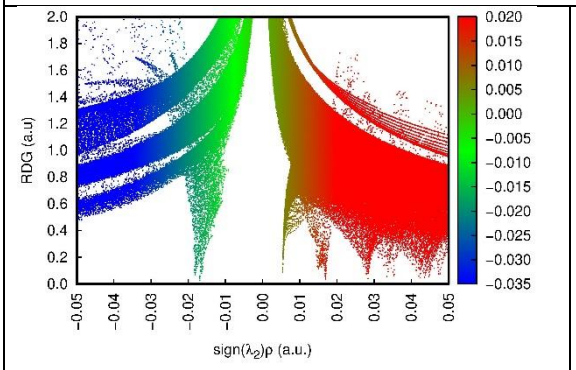


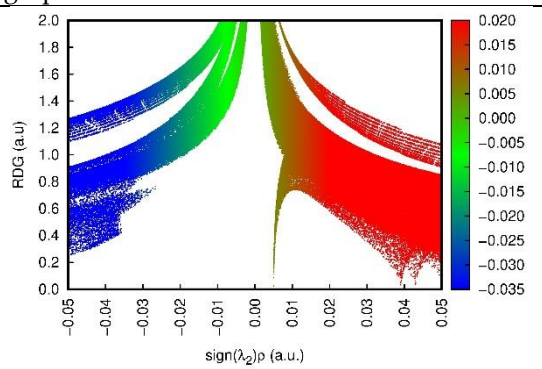
RDG





Scatter graph

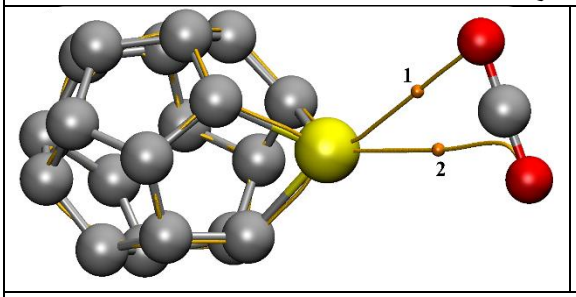


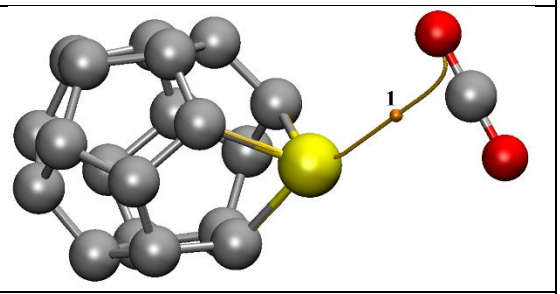


$C_{19}Si\text{-}CO_2$
$F = 0.000\ a.u.$
$E_{ads}(BSSE) = -0.06827564\ eV$

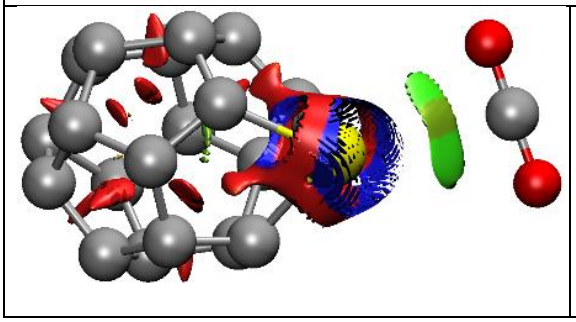
$C_{19}Si\text{-}CO_2$
$F = 0.000\ a.u.$
$E_{ads}(BSSE) = -0.07742641\ eV$

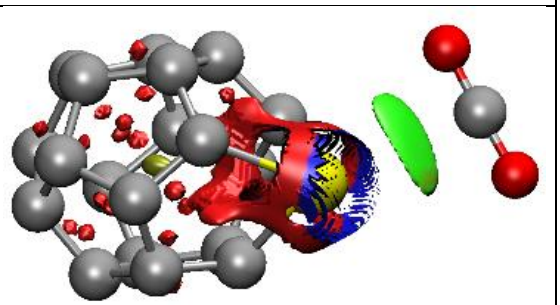
QTAIM

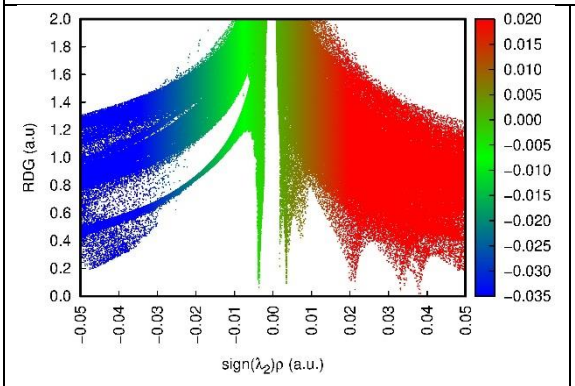
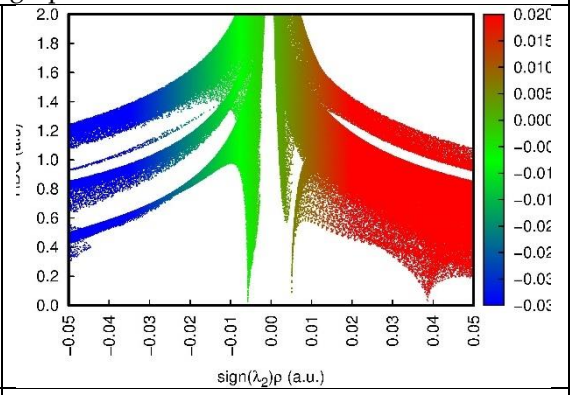
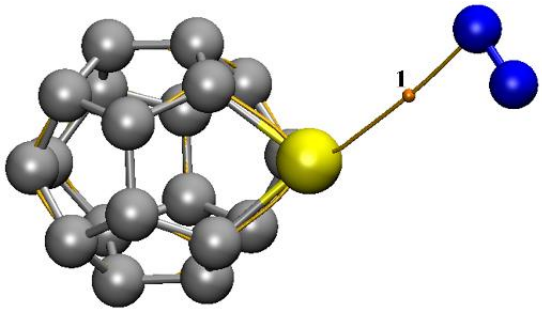
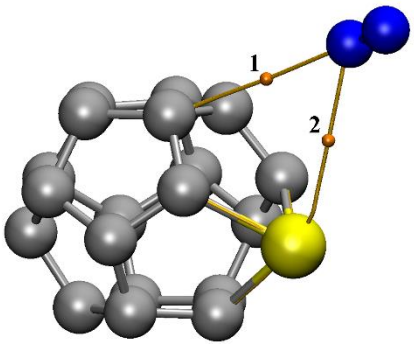
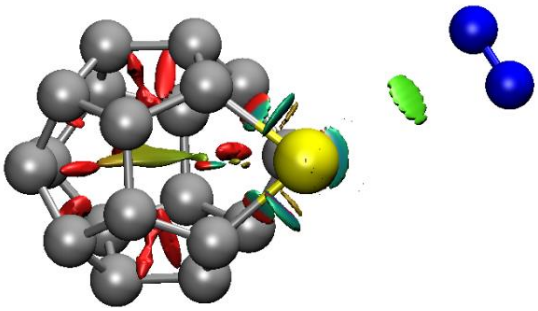
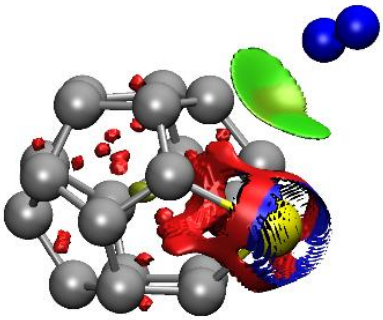
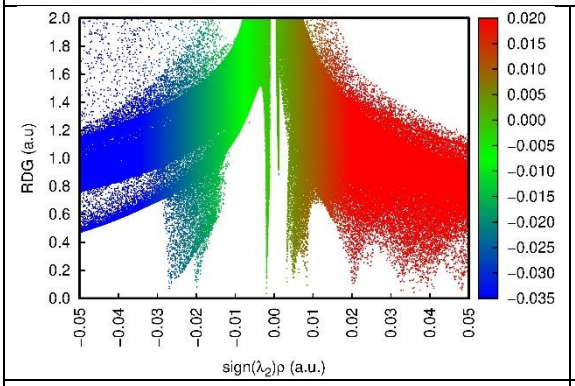
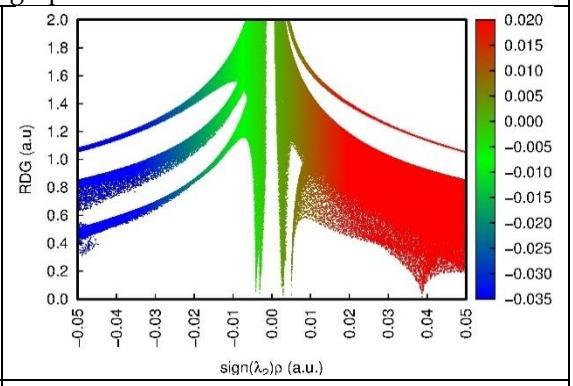




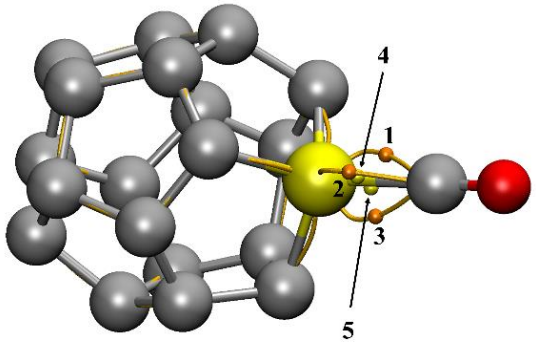
RDG

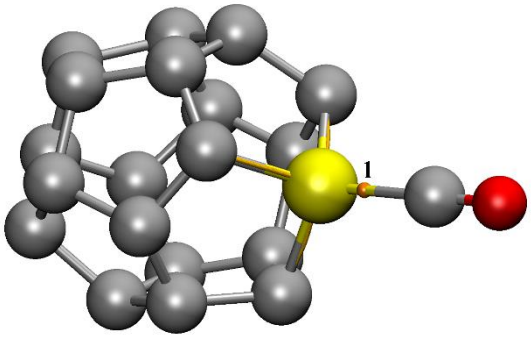




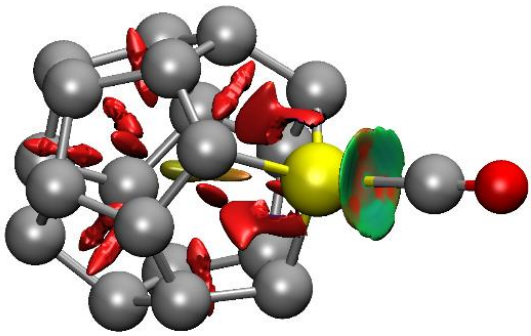
Scatter graph	
	
$C_{19}Si\text{-}N_2$ $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.01722895\ eV$	**$C_{19}Si\text{-}N_2$** $F = 0.000\ a.u.$ $E_{ads}(BSSE) = -0.04477245\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
$C_{19}Si\text{-}CO$ $F = 0.001\ a.u.$ $E_{ads}(BSSE) = -0.74916933\ eV$	**$C_{19}Si\text{-}CO$** $F = 0.001\ a.u.$ $E_{ads}(BSSE) = -0.78821735\ eV$

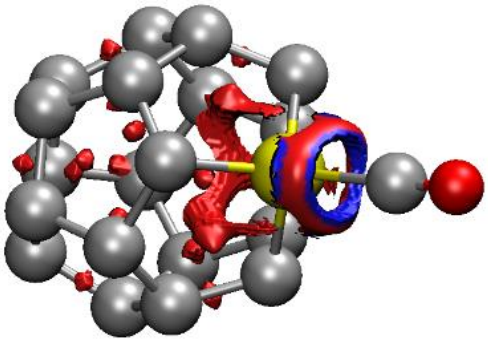
QTAIM



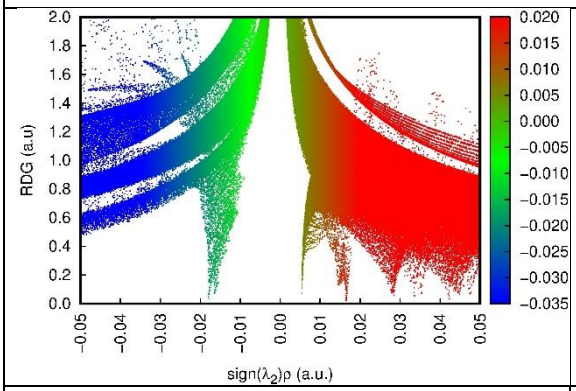


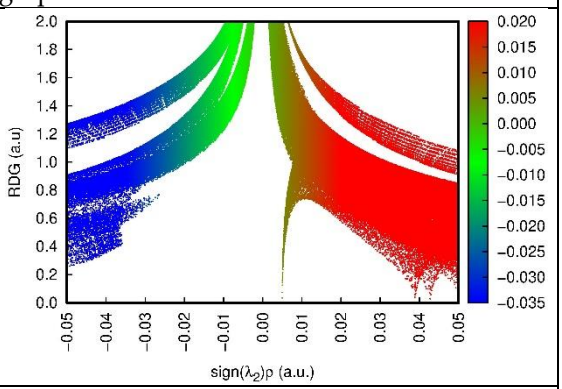
RDG





Scatter graph

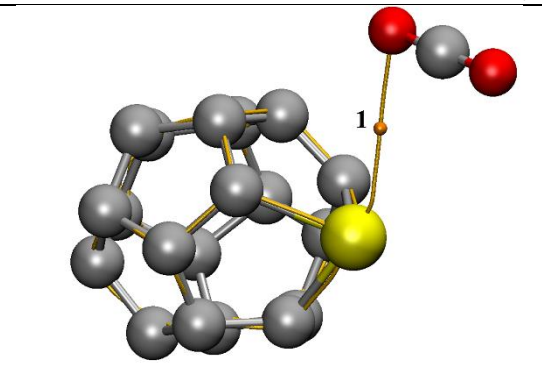


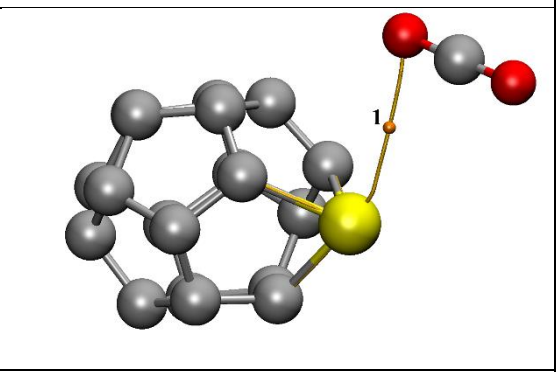


$C_{19}Si\text{-}CO_2$
$F = 0.001\ a.u.$
$E_{ads}(BSSE) = -0.08110533\ eV$

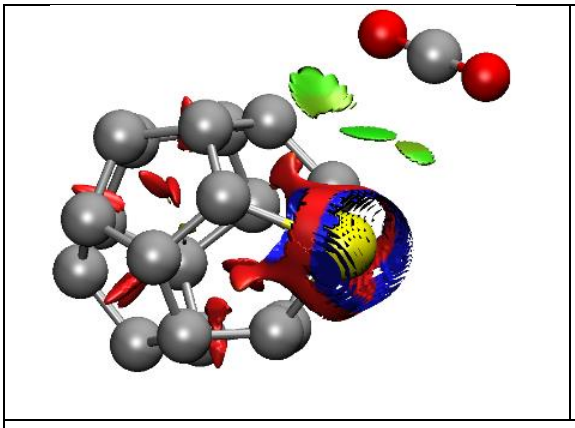
$C_{19}Si\text{-}CO_2$
$F = 0.001\ a.u.$
$E_{ads}(BSSE) = -0.08655367\ eV$

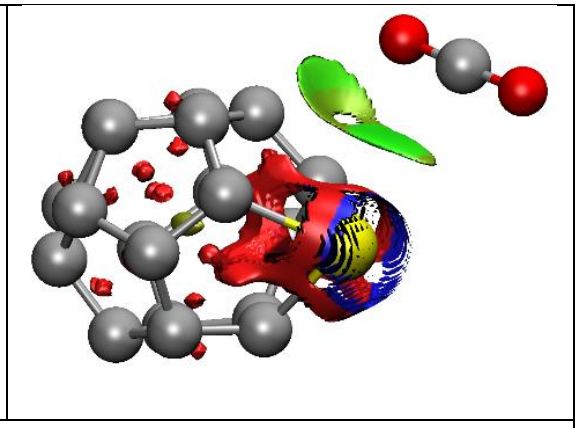
QTAIM



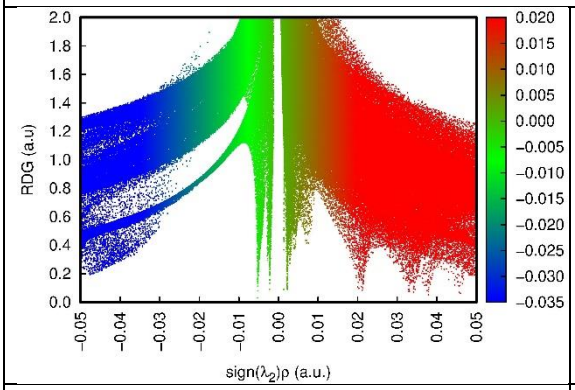


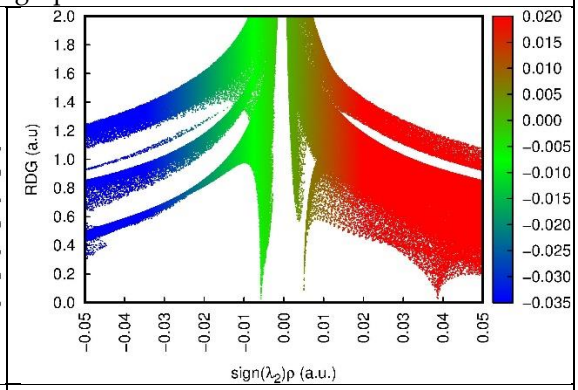
RDG





Scatter graph

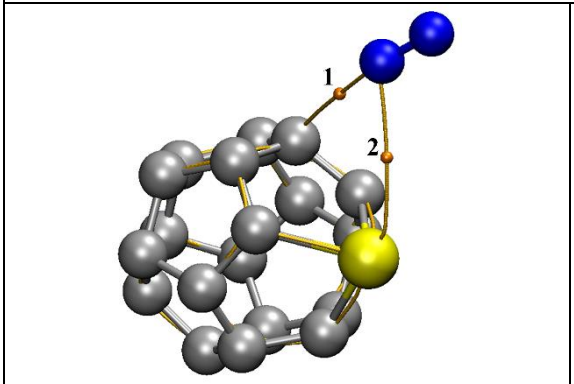


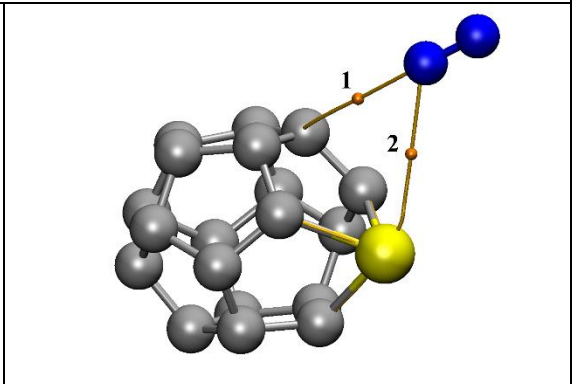


$C_{19}Si\text{-}N_2$
$F = 0.001\ a.u.$
$E_{ads}(BSSE) = -0.04514641\ eV$

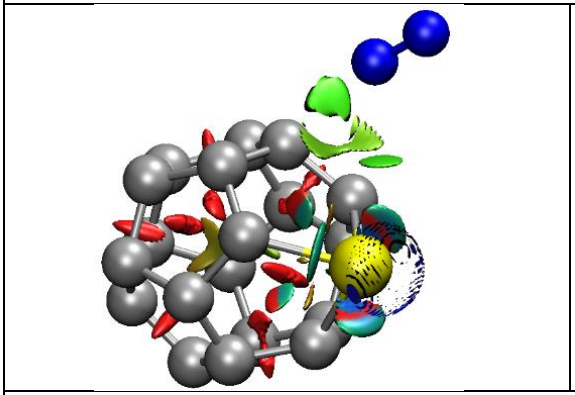
$C_{19}Si\text{-}N_2$
$F = 0.001\ a.u.$
$E_{ads}(BSSE) = -0.04598611\ eV$

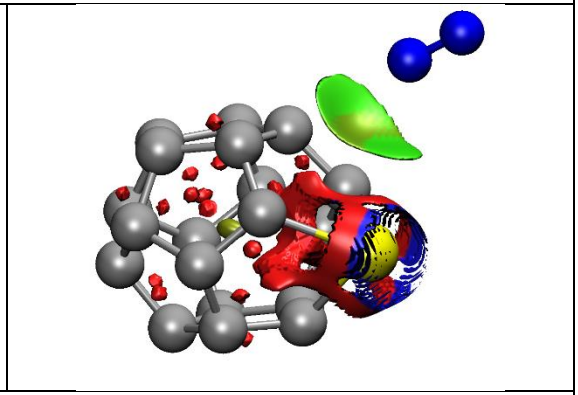
QTAIM



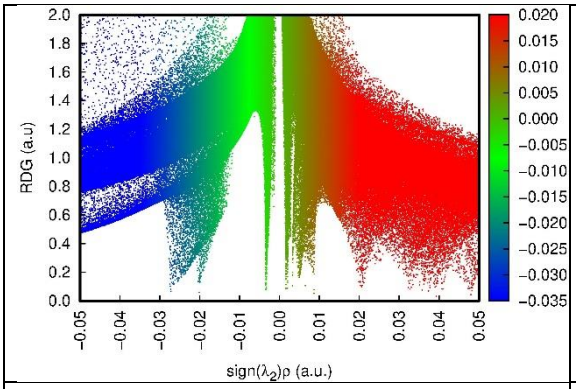
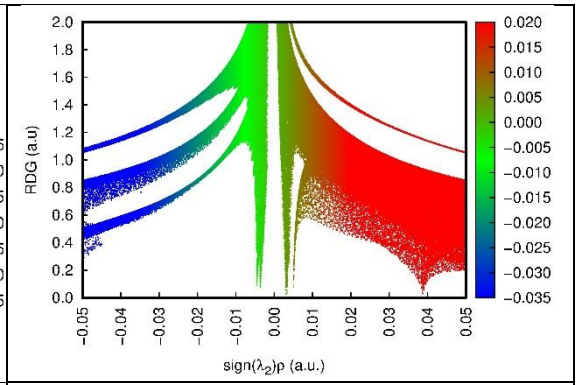
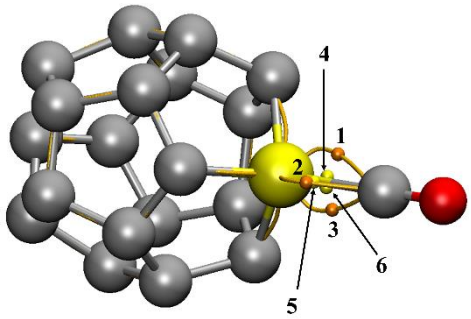
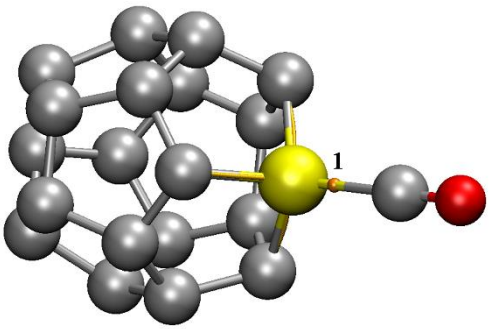
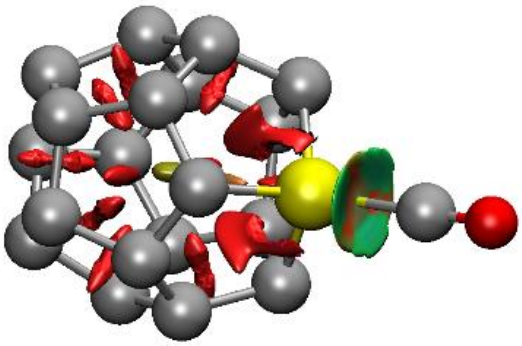
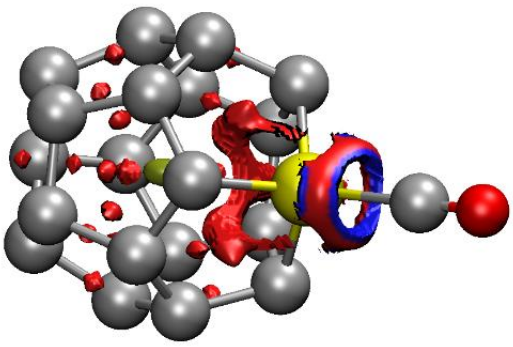
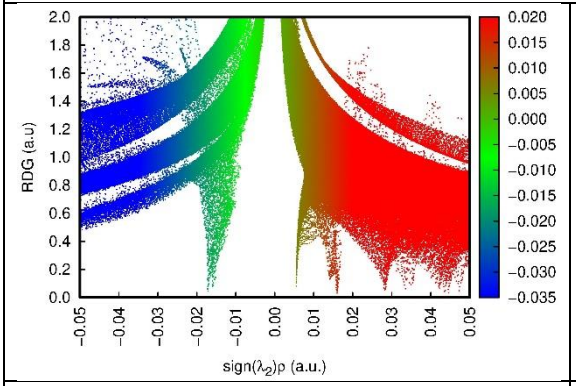
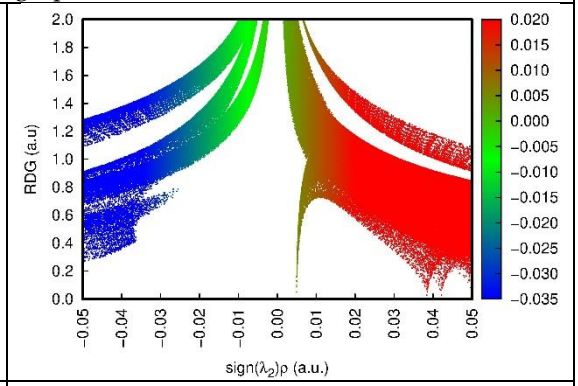


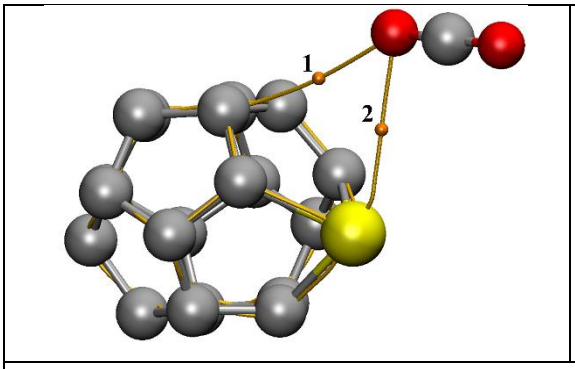
RDG

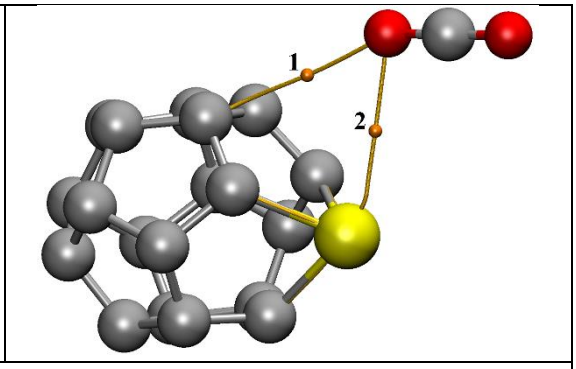




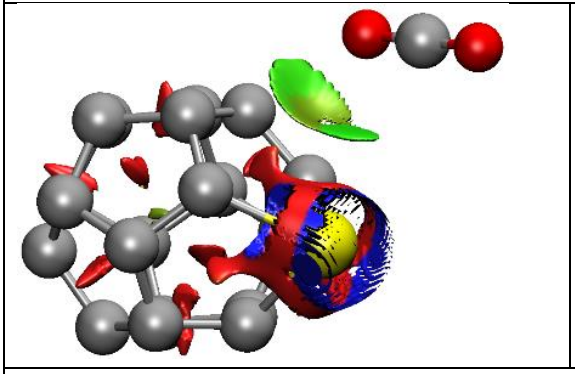
Scatter graph

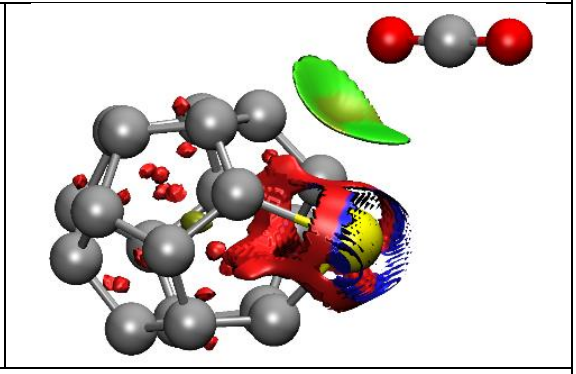
	
C_{19}Si-CO $F = 0.005\ a.u.$ $E_{ads}(BSSE) = -0.95684190\ eV$	**C_{19}Si-CO** $F = 0.005\ a.u.$ $E_{ads}(BSSE) = -1.00925177\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
C_{19}Si-CO_2 $F = 0.005\ a.u.$ $E_{ads}(BSSE) = -0.08494219\ eV$	**C_{19}Si-CO_2** $F = 0.005\ a.u.$ $E_{ads}(BSSE) = -0.09138179\ eV$
QTAIM	



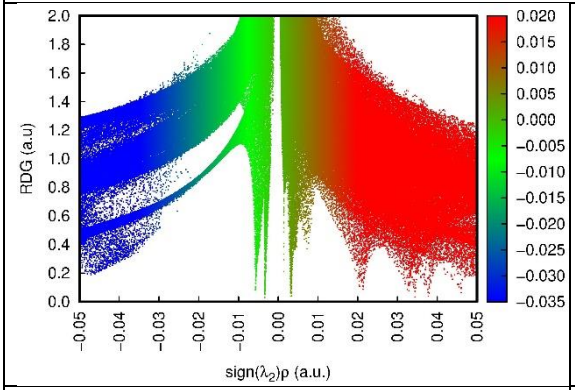


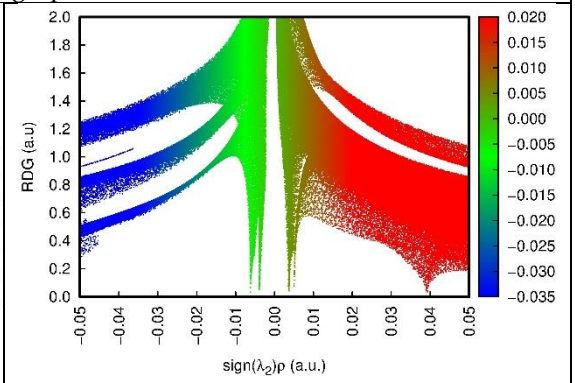
RDG





Scatter graph

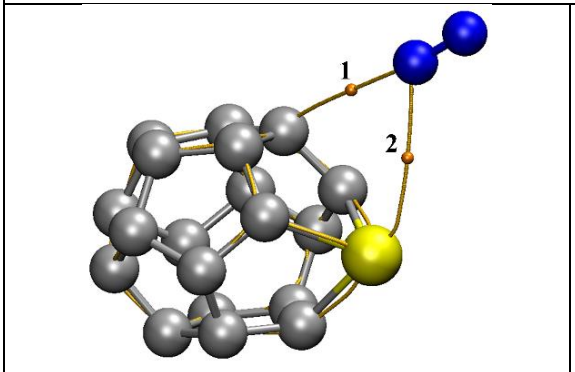


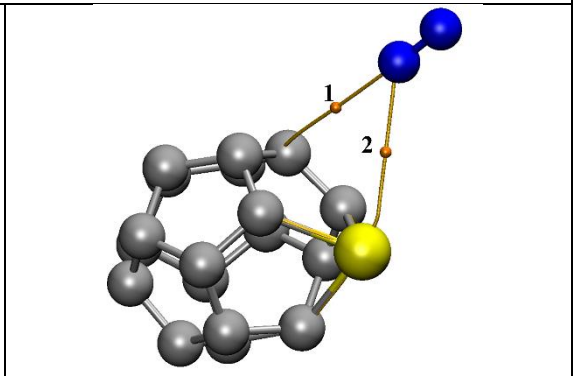


$C_{19}Si\text{-}N_2$
$F = 0.005\ a.u.$
$E_{ads}(BSSE) = -0.05377844\ eV$

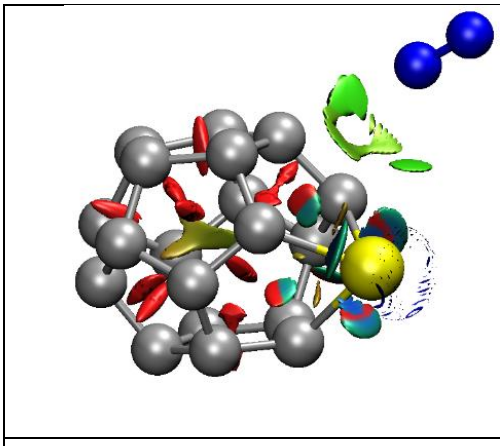
$C_{19}Si\text{-}N_2$
$F = 0.005\ a.u.$
$E_{ads}(BSSE) = -0.05636742\ eV$

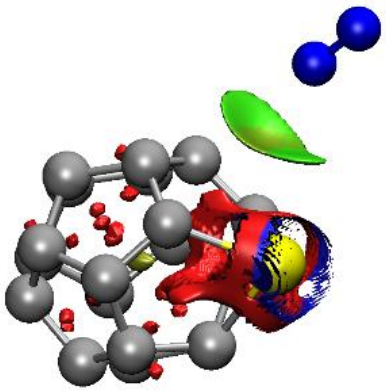
QTAIM



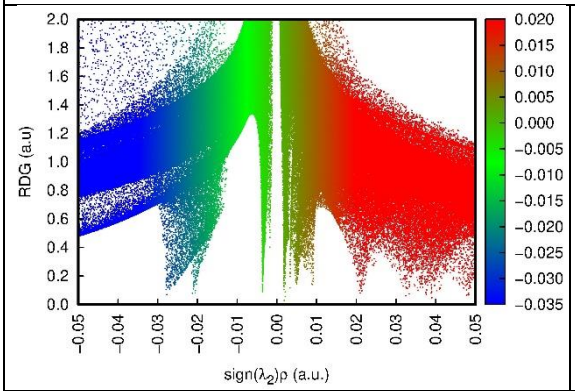


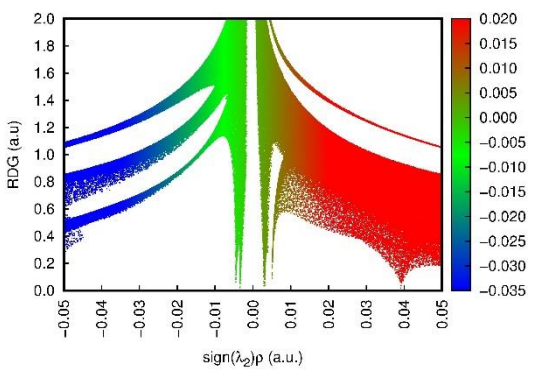
RDG





Scatter graph

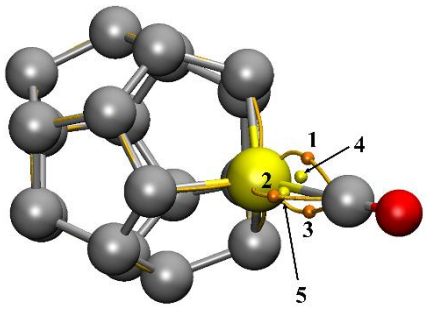


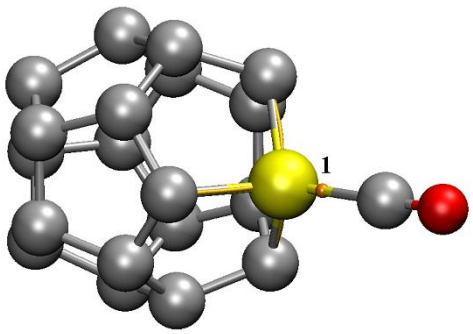


C_{19}Si-CO
$F = 0.010\ a.u.$
$E_{ads}(BSSE) = -1.26088602\ eV$

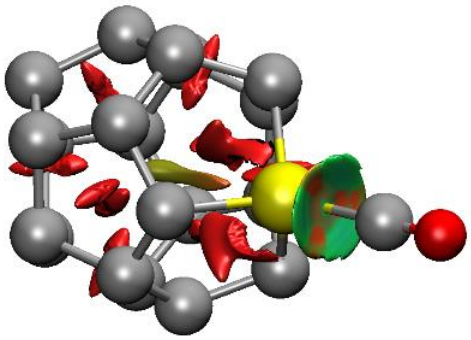
C_{19}Si-CO
$F = 0.010\ a.u.$
$E_{ads}(BSSE) = -1.32802545\ eV$

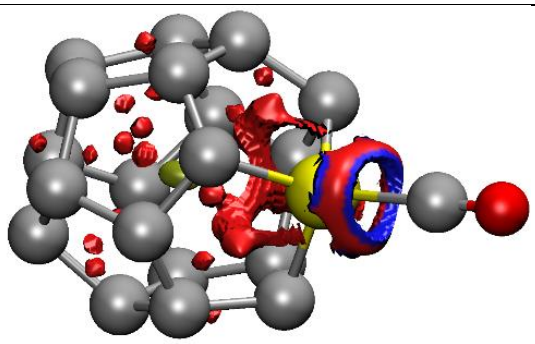
QTAIM



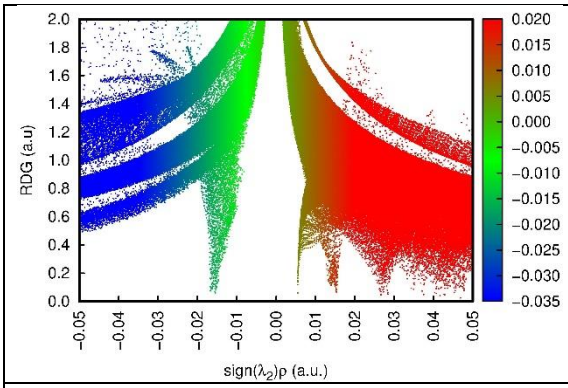


RDG

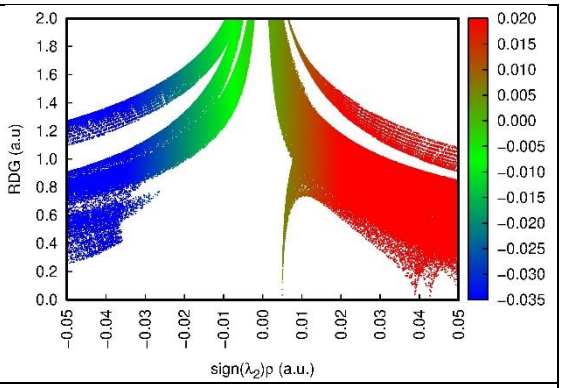




Scatter graph

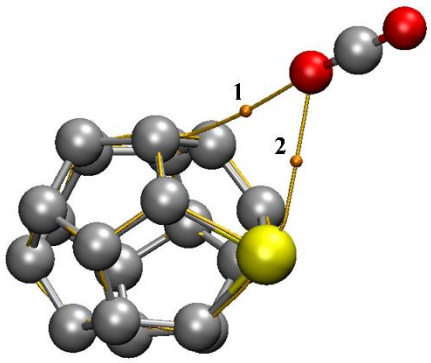


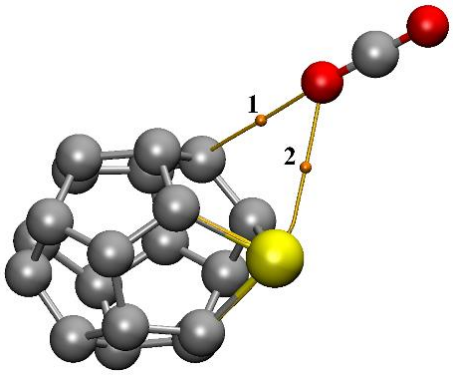
$C_{19}Si\text{-}CO_2$
$F = 0.010\ a.u.$
$E_{ads}(BSSE) = -0.10993079\ eV$



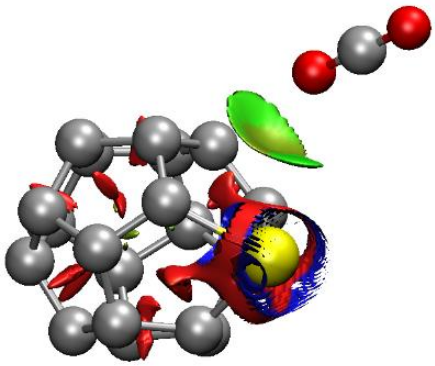
$C_{19}Si\text{-}CO_2$
$F = 0.010\ a.u.$
$E_{ads}(BSSE) = -0.12354919\ eV$

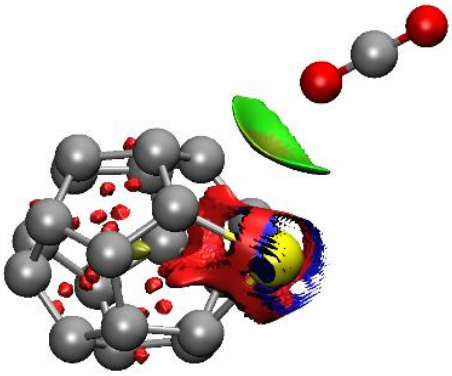
QTAIM



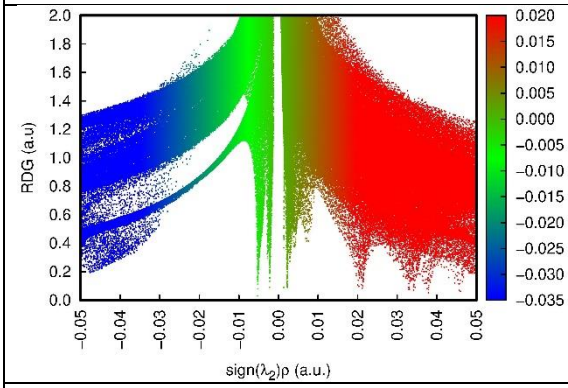


RDG

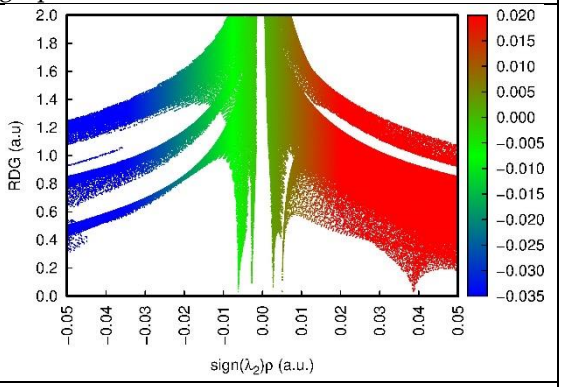




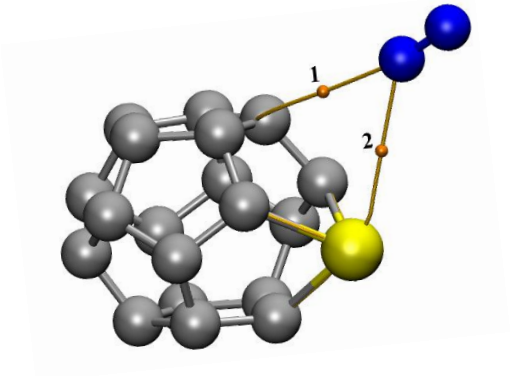
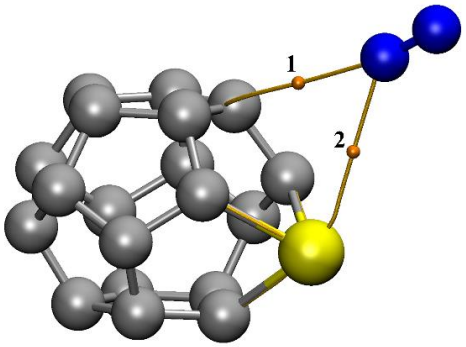
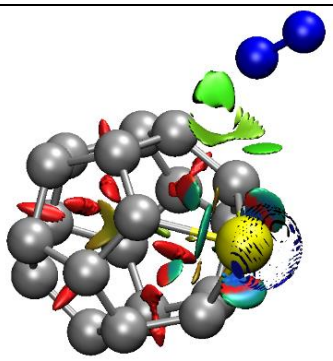
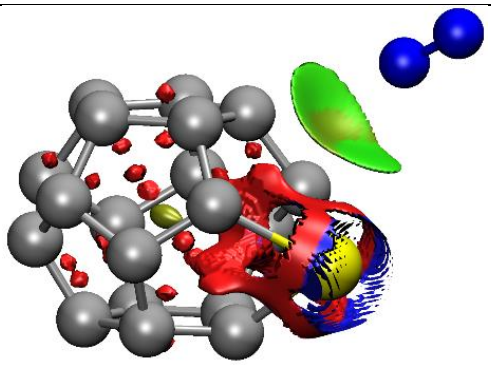
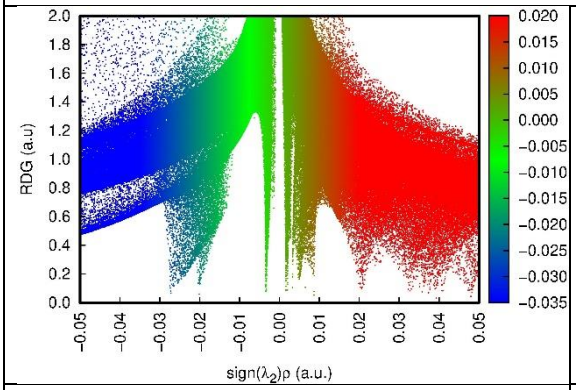
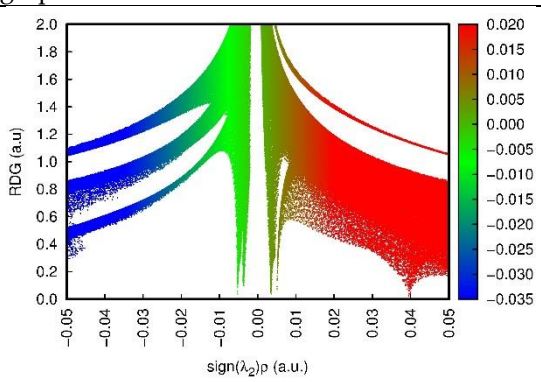
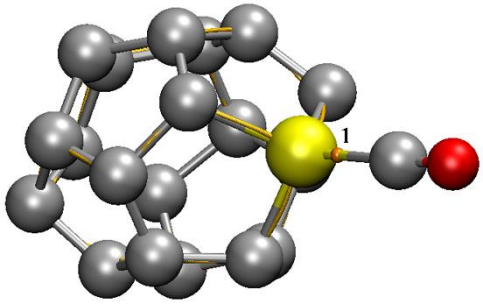
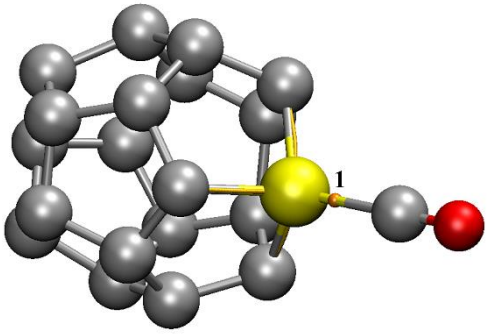
Scatter graph

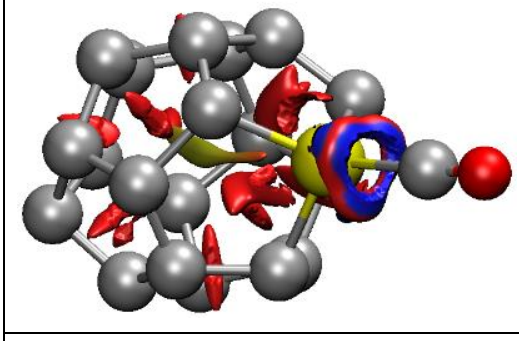


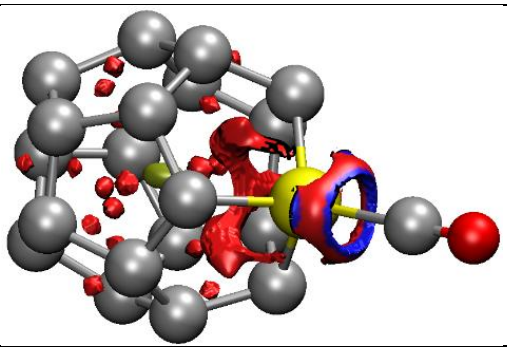
$C_{19}Si\text{-}N_2$
$F = 0.010\ a.u.$



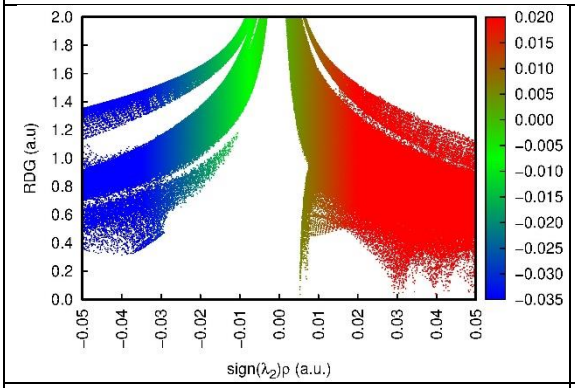
$C_{19}Si\text{-}N_2$
$F = 0.010\ a.u.$

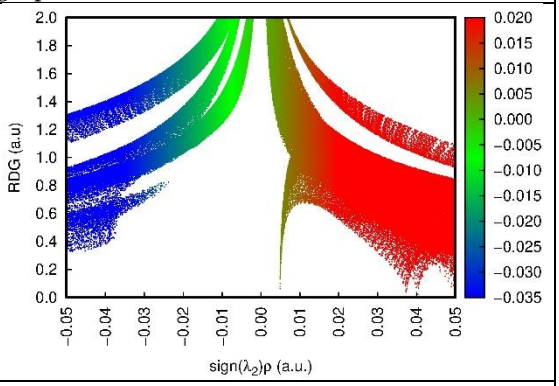
$E_{ads}(BSSE) = -0.07166555\ eV$	$E_{ads}(BSSE) = -0.07659200\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
C_{19}Si-CO $F = 0.015\ a.u.$ $E_{ads}(BSSE) = -1.60888130\ eV$	**C_{19}Si-CO** $F = 0.015\ a.u.$ $E_{ads}(BSSE) = -1.69386335\ eV$
QTAIM	
	
RDG	





Scatter graph

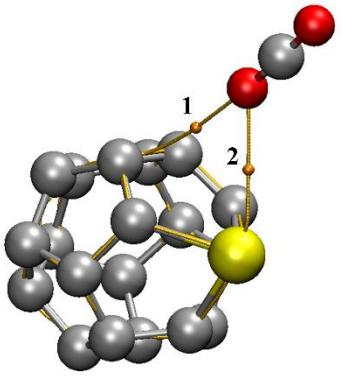


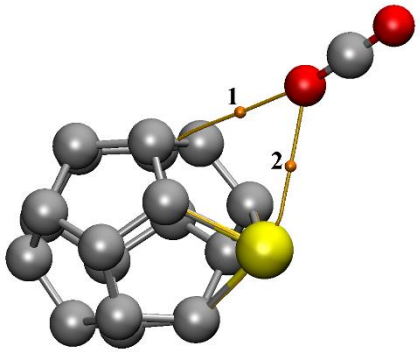


$C_{19}Si\text{-}CO_2$
$F = 0.015\ a.u.$
$E_{ads}(BSSE) = -0.16062570\ eV$

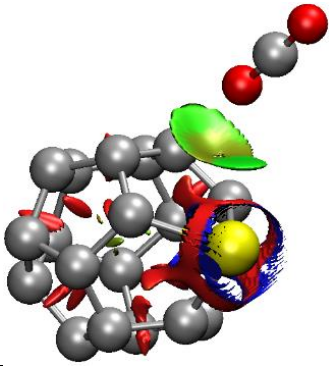
$C_{19}Si\text{-}CO_2$
$F = 0.015\ a.u.$
$E_{ads}(BSSE) = -0.19373070\ eV$

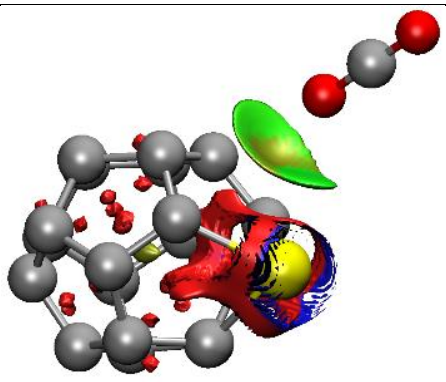
QTAIM



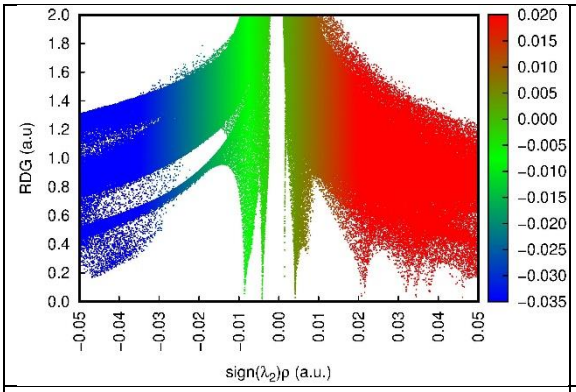
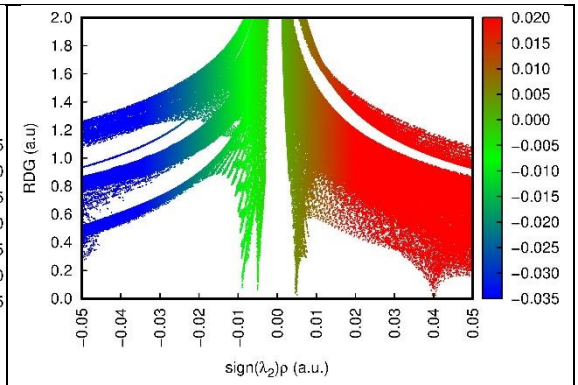
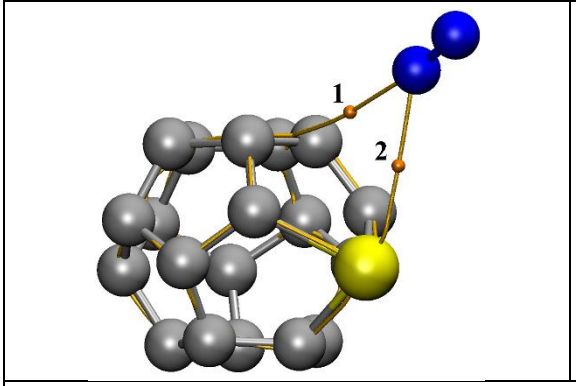
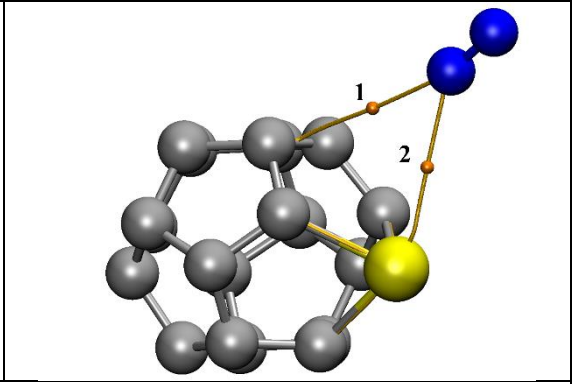
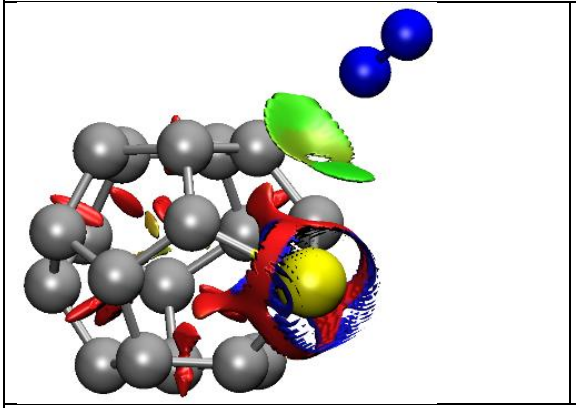
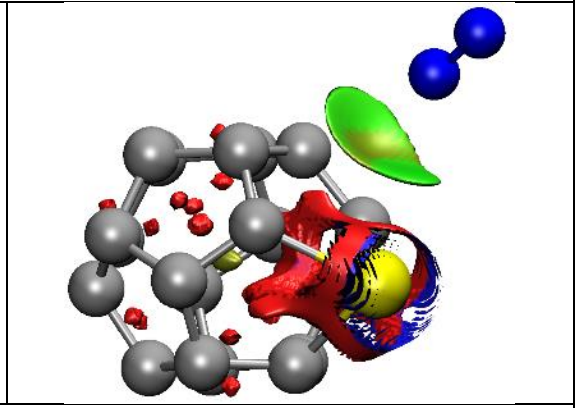
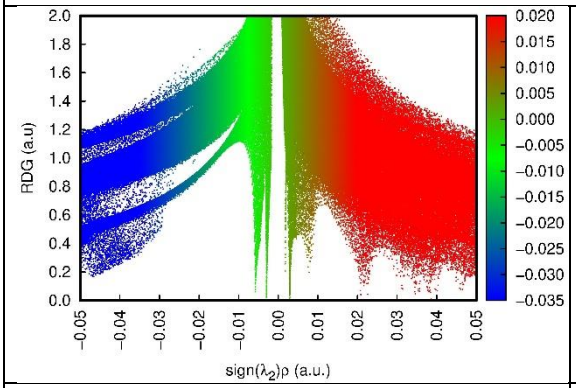
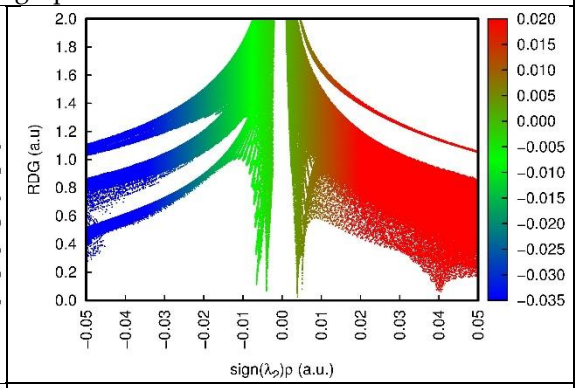


RDG

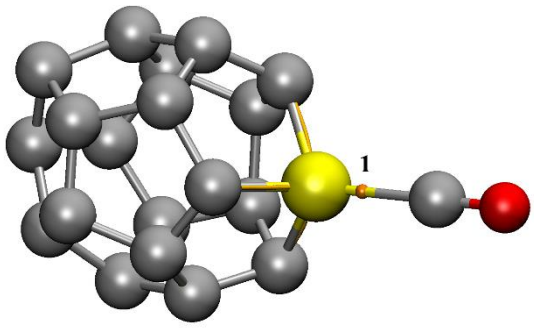


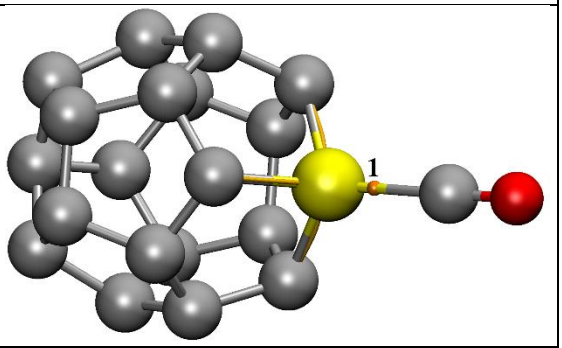


Scatter graph

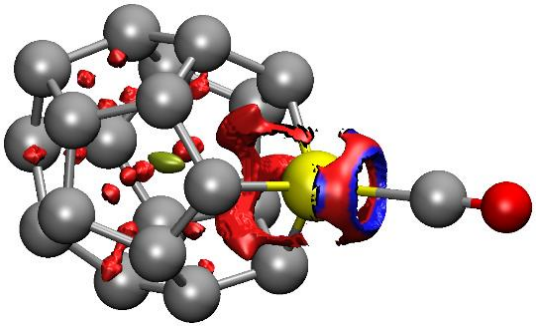
	
$C_{19}Si$-N_2 $F = 0.015\ a.u.$ $E_{ads}(BSSE) = -0.09723814\ eV$	**$C_{19}Si$-N_2** $F = 0.015\ a.u.$ $E_{ads}(BSSE) = -0.11392979\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
$C_{19}Si$-CO $F = 0.020\ a.u.$ $E_{ads}(BSSE) = -1.98886525\ eV$	**$C_{19}Si$-CO** $F = 0.020\ a.u.$ $E_{ads}(BSSE) = -2.10539484\ eV$

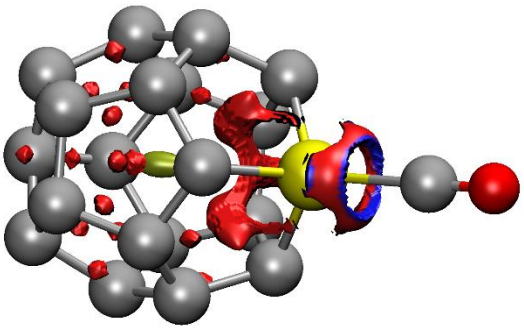
QTAIM



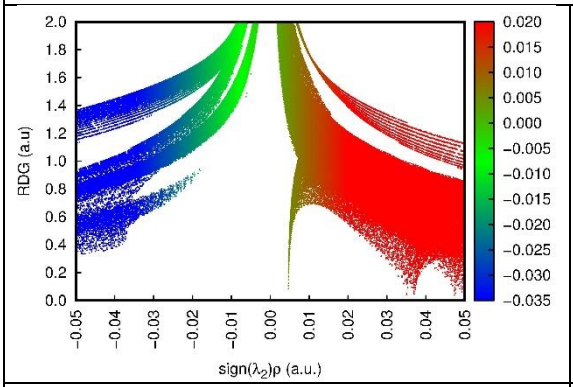


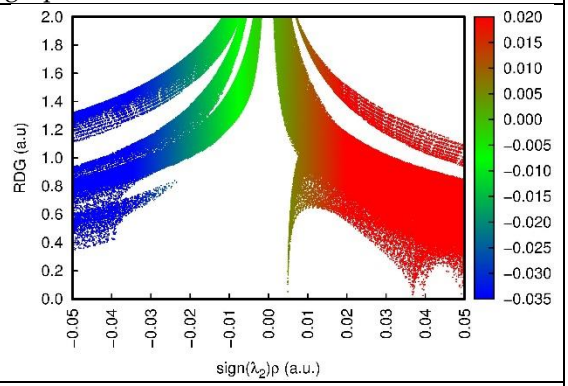
RDG





Scatter graph

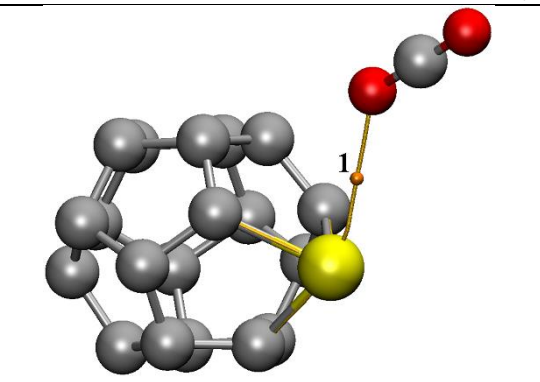


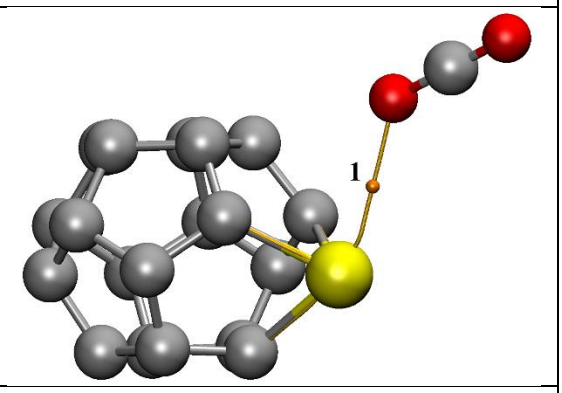


$C_{19}Si\text{-}CO_2$
$F = 0.020\ a.u.$
$E_{ads}(BSSE) = -0.23431939\ eV$

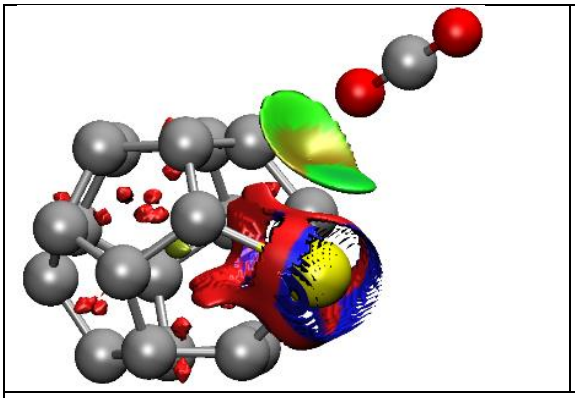
$C_{19}Si\text{-}CO_2$
$F = 0.020\ a.u.$
$E_{ads}(BSSE) = -0.27245444\ \ eV$

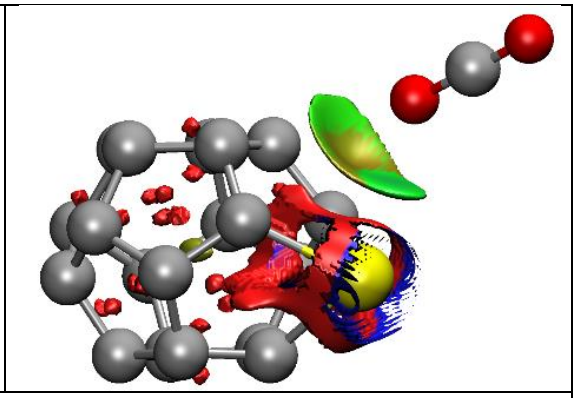
QTAIM



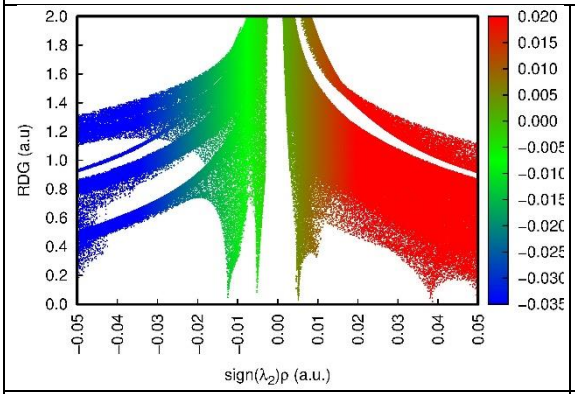


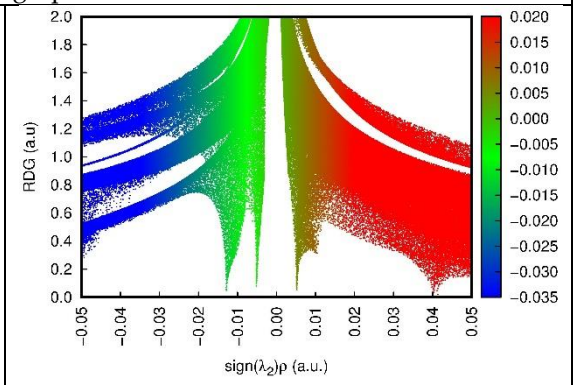
RDG





Scatter graph

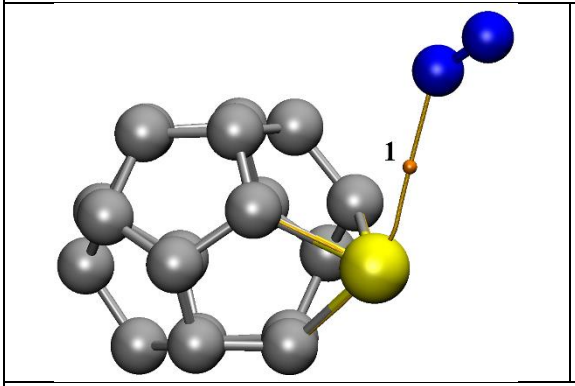


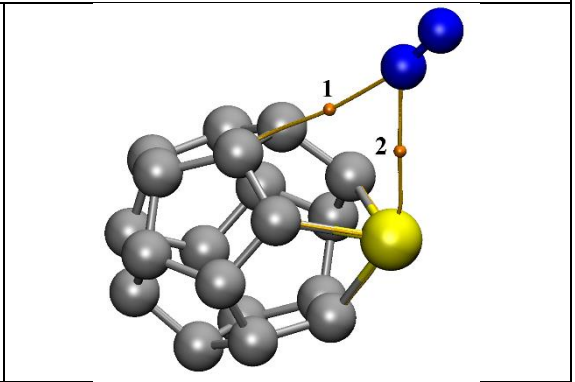


$C_{19}Si\text{-}N_2$
$F = 0.020\ a.u.$
$E_{ads}(BSSE) = -0.13186518\ eV$

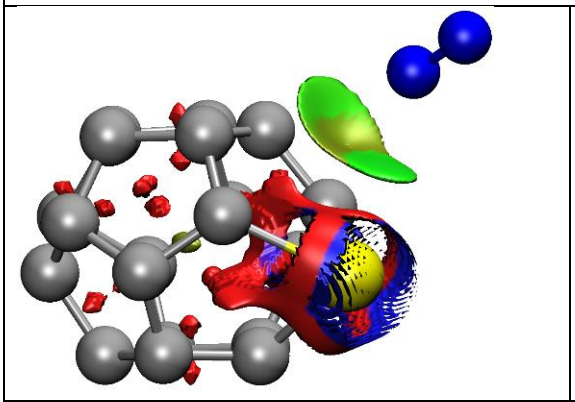
$C_{19}Si\text{-}N_2$
$F = 0.020\ a.u.$
$E_{ads}(BSSE) = -0.14614638\ eV$

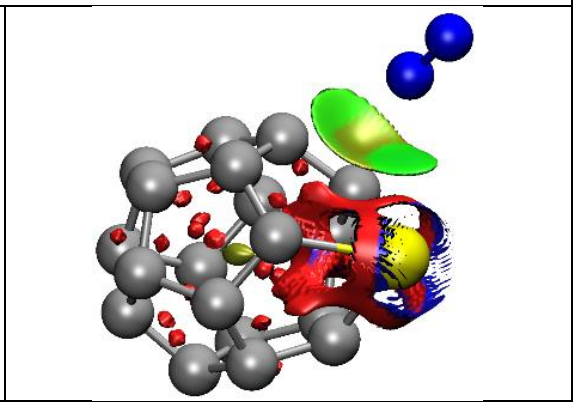
QTAIM



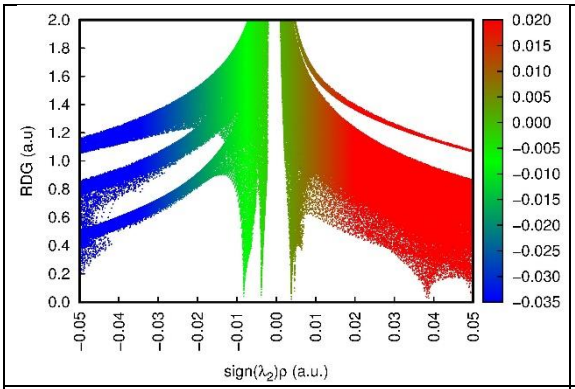
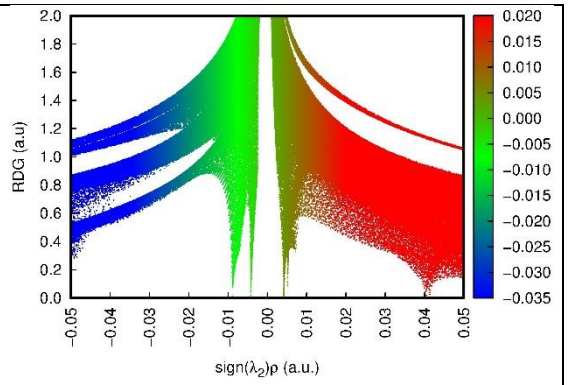
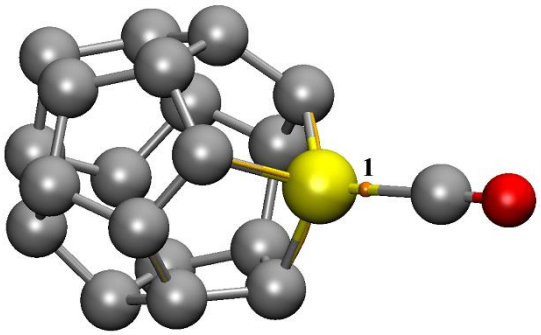
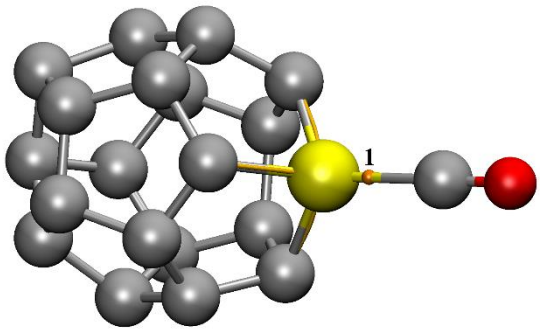
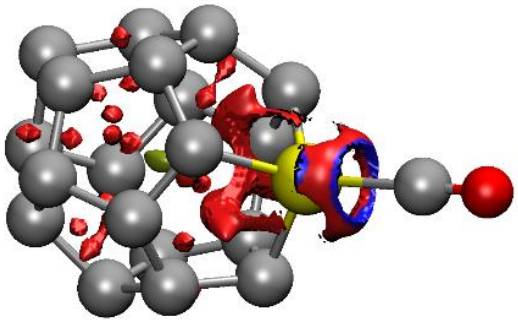
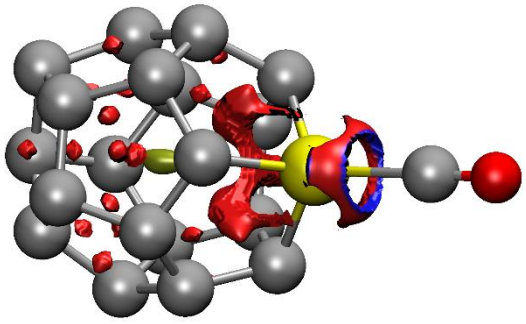
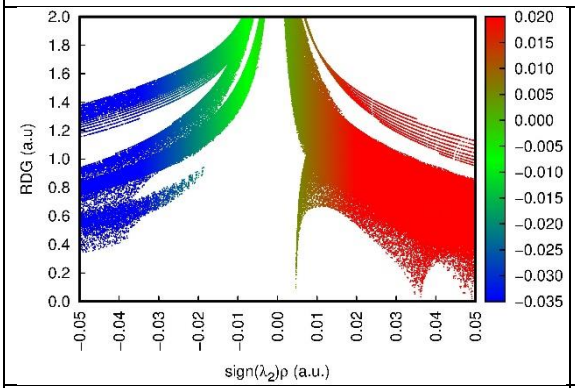
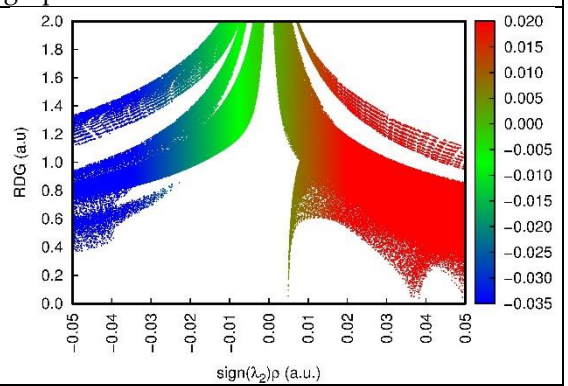


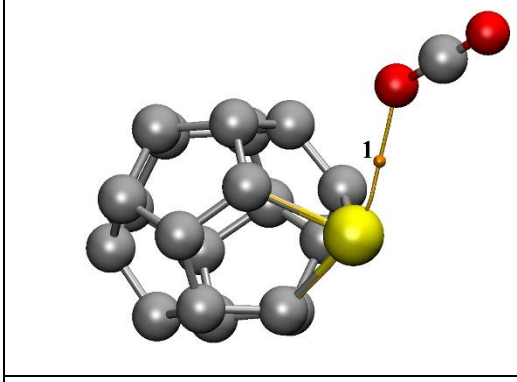
RDG

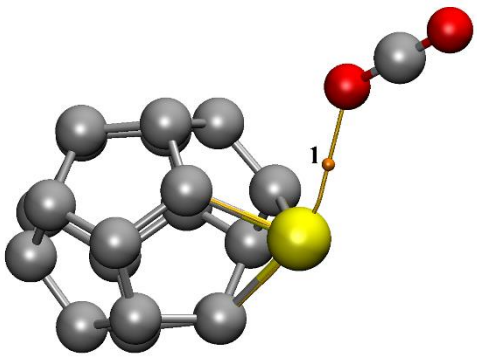




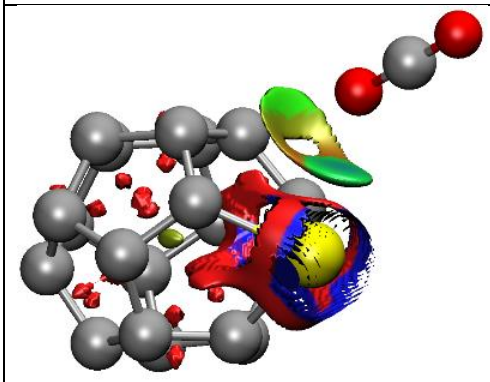
Scatter graph

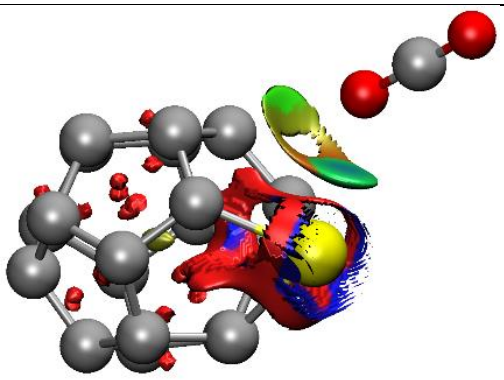
	
C_{19}Si-CO $F = 0.025\ a.u.$ $E_{ads}(BSSE) = -2.40028075eV$	**C_{19}Si-CO** $F = 0.025\ a.u.$ $E_{ads}(BSSE) = -2.57870530\ eV$
QTAIM	
	
RDG	
	
Scatter graph	
	
C_{19}Si-CO_2 $F = 0.025\ a.u.$ $E_{ads}(BSSE) = -0.33903162\ eV$	**C_{19}Si-CO_2** $F = 0.025\ a.u.$ $E_{ads}(BSSE) = -0.40174203eV$
QTAIM	



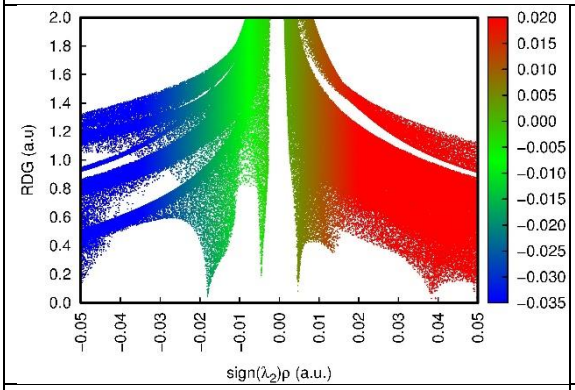


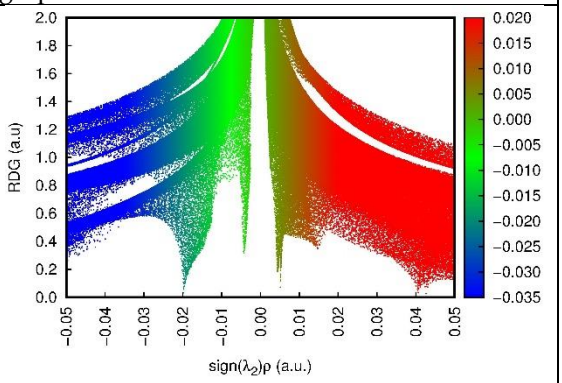
RDG





Scatter graph

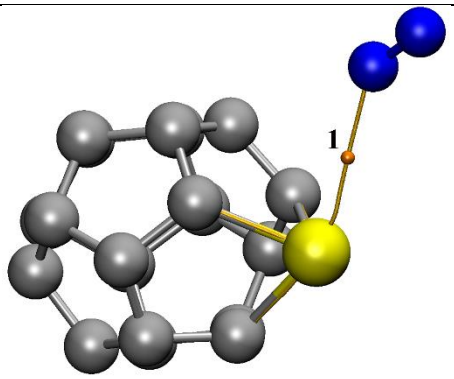


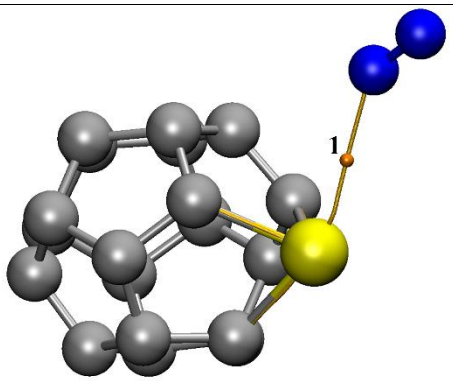


$C_{19}Si\text{-}N_2$
$F = 0.025\ a.u.$
$E_{ads}(BSSE) = -0.17736559\ eV$

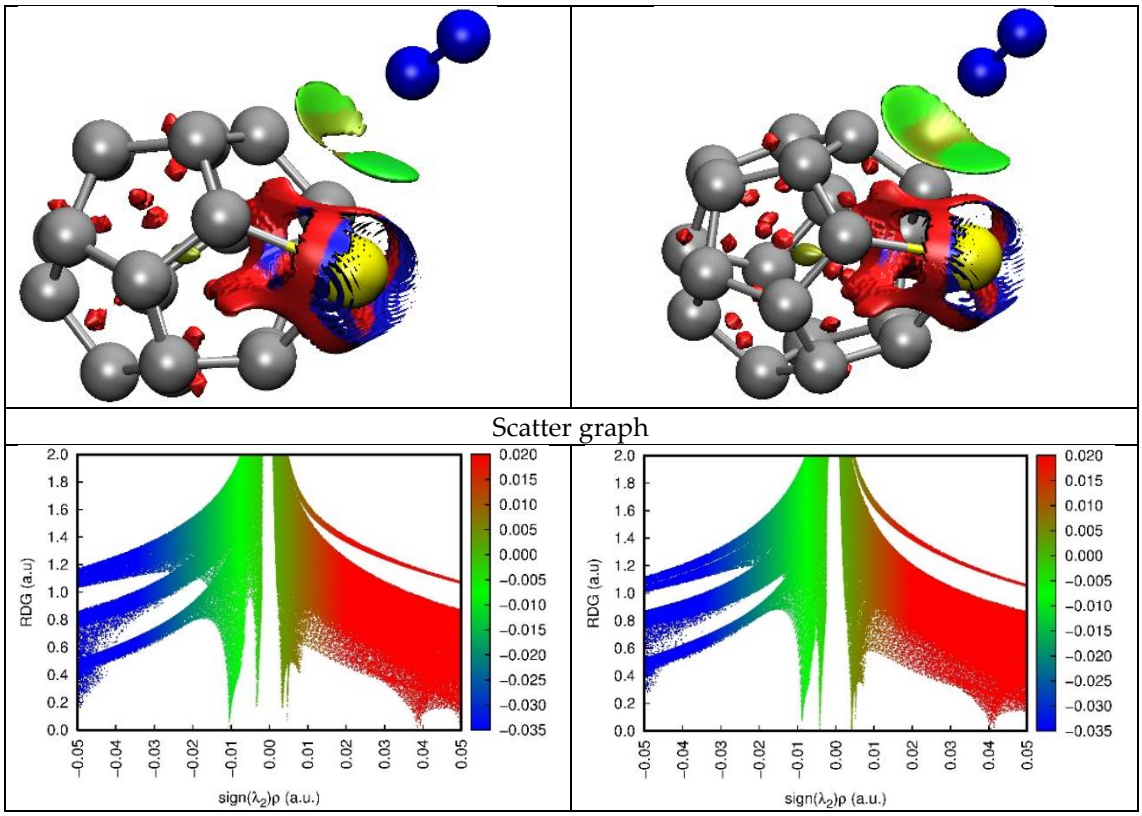
$C_{19}Si\text{-}N_2$
$F = 0.025\ a.u.$
$E_{ads}(BSSE) = -0.20140237 eV$

QTAIM





RDG


Scatter graph
RDG (a.u)
sign(λ2)ρ (a.u.)
RDG (a.u)
sign(λ2)ρ (a.u.)