

Supporting information

Comparative DFT analysis of CO₂ cycloaddition with ionic liquids in encapsulated and free states

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Cartesian Coordinates

TS-1

C	3.19732600	-1.12844400	0.82392700
C	1.81165500	-0.95793800	0.20472700
C	1.69997200	0.09491200	-0.83234700
O	1.47393400	-1.87774900	-0.76028400
H	3.94987400	-1.21189200	0.03288800
H	3.45267400	-0.28450100	1.47385000
H	3.22573900	-2.05146900	1.41244100
H	1.07805000	-0.83833900	1.03501100
H	0.76385400	0.17426100	-1.35556200
H	2.57393600	0.25736400	-1.45413400
N	-2.10962800	-0.14467000	0.07720100
C	-3.58274700	-0.35068600	0.28280800
C	-1.90217300	0.90865400	-0.98588200
C	-1.49904100	-1.47303900	-0.34401400
C	-1.49435200	0.34910900	1.36530400
H	-4.03659600	0.58823100	0.60208800
H	-4.02889600	-0.67898600	-0.65665700
H	-3.72945800	-1.11379400	1.04781600
H	-0.86167400	1.23983900	-0.96639500
H	-2.17479600	0.48673300	-1.95359500
H	-2.54414600	1.75954200	-0.75314300
H	-0.40734000	-1.44356100	-0.54687800
H	-1.68999400	-2.18483700	0.46092100
H	-2.02560200	-1.79574100	-1.24424700
H	-0.45527700	0.63109300	1.18256800
H	-2.05349500	1.22666200	1.69367700
H	-1.56514100	-0.44452000	2.10952500
Cl	1.41884500	2.18018700	0.01967900

Int-1

C	1.94526100	-1.86598100	-0.21036900
C	1.53094000	-0.52317400	0.41467200
C	2.28047900	0.65737600	-0.22810600
O	0.19266200	-0.25813900	0.24928100
H	1.70219700	-1.86711700	-1.28061600
H	3.01389000	-2.07597200	-0.09442300
H	1.37816100	-2.67557800	0.26193400
H	1.83933100	-0.54955300	1.48429000
H	1.94100600	1.59471200	0.21275100
H	2.11501100	0.67685000	-1.30760700
N	-2.76819200	0.15115400	-0.02790900
C	-4.23963400	0.35914900	-0.16776200

C	-2.47766900	-1.14631700	0.69358600
C	-2.14220600	1.28104300	0.75987300
C	-2.10566100	0.09506300	-1.38709500
H	-4.66591600	-0.46786600	-0.73800100
H	-4.69244900	0.39525900	0.82446000
H	-4.42046300	1.29988800	-0.69049600
H	-1.37264500	-1.20578000	0.74248500
H	-2.93979100	-1.09730100	1.68155100
H	-2.91626200	-1.96248400	0.11603800
H	-1.06284500	1.03843600	0.80938800
H	-2.33794100	2.21475600	0.22879200
H	-2.61057800	1.30794000	1.74576500
H	-1.02946500	-0.06404500	-1.18144100
H	-2.54990700	-0.73003100	-1.94743700
H	-2.29950700	1.03995000	-1.89872300
Cl	4.11736200	0.64658900	-0.00096400

TS-2

C	-1.13963200	-0.24941500	-0.55293600
C	0.33071400	-0.63871300	-0.57035200
C	1.03947200	-0.36903000	0.74827300
O	0.45050600	-2.06073800	-0.87680300
H	-1.66381400	-0.76424500	0.25996900
H	-1.21952700	0.82953400	-0.40591200
H	-1.61342700	-0.52372200	-1.49889700
H	0.85945800	-0.12574100	-1.37146700
H	2.11543600	-0.39519300	0.79463700
H	0.50818400	0.02624100	1.59601900
N	1.40608100	-4.58665900	3.79385500
C	0.18281300	-3.71490600	3.94936500
C	2.57675500	-3.71723800	3.40100300
C	1.15607900	-5.60509700	2.70425300
C	1.70103900	-5.28602100	5.08583100
H	0.35634000	-3.02367200	4.77570600
H	0.04480100	-3.16074200	3.01760800
H	-0.67161900	-4.35570500	4.17030400
H	3.44032200	-4.35956000	3.22492100
H	2.29349900	-3.16272200	2.50324300
H	2.78334800	-3.02707000	4.22054100
H	2.04724000	-6.22835600	2.61362100
H	0.30466200	-6.21846000	3.00376300
H	0.95006200	-5.07512400	1.76158400
H	2.58767000	-5.90820800	4.95817900
H	1.87817100	-4.54211700	5.86363100
H	0.84733800	-5.90912000	5.35514800
C	0.63660600	-2.82453700	0.22135000

O	0.83065800	-2.13544500	1.31551600
O	0.62613300	-4.05119200	0.13544600
Cl	1.37935200	1.97591900	0.27381600

TS-1_(E)

C	3.55941100	-3.78321500	-3.61197600
C	3.72453500	-3.93958600	-2.15816700
C	2.79522800	-4.72525900	-1.45837800
C	1.64454500	-5.13689900	-2.13442300
C	1.56668000	-4.92681800	-3.58837800
C	0.46805200	-5.43668400	-1.43339400
C	-0.74731100	-5.31510600	-2.11166700
C	-0.72958800	-5.09694500	-3.56588300
C	-1.93330700	-5.06957300	-1.40957700
C	-2.97821100	-4.43640200	-2.09189800
C	-2.86809600	-4.26236500	-3.54835500
C	4.83692800	-1.86486100	-3.62875600
C	5.06330800	-1.94431000	-2.17704300
C	4.57638800	-3.06116600	-1.48151300
C	5.15461600	0.41685400	-3.63537000
C	5.39738300	0.43571800	-2.18386800
C	5.45019000	-0.78398600	-1.49566300
C	4.45395200	2.61122800	-3.62873500
C	4.66291700	2.72306000	-2.17599300
C	5.24205700	1.64638800	-1.49458600
C	-3.94691300	-3.70284200	-1.39613500
C	-4.62279100	-2.68763800	-2.08426600
C	-4.44007700	-2.57970000	-3.53925400
C	2.87656900	4.28990400	-3.61187300
C	3.01230900	4.46714300	-2.15690200
C	3.99598200	3.74151800	-1.47889100
C	-5.18458700	-1.60521800	-1.39426900
C	-5.35582000	-0.40085000	-2.08677200
C	-5.14104900	-0.38341700	-3.54120500
C	-5.39718400	0.81960400	-1.39954800
C	-5.02754800	1.97561300	-2.09554400
C	-4.83039900	1.89684000	-3.55095600
C	-4.53199200	3.09073100	-1.40942500
C	-3.69060400	3.96404500	-2.10743300
C	-3.54932700	3.80306800	-3.56279400
C	-2.75440000	4.74410500	-1.42188600
C	-1.61420000	5.16223000	-2.12031200
C	-1.55817500	4.95857100	-3.57673300
C	-0.43272700	5.45662200	-1.43619000
C	0.77627900	5.33767900	-2.13653300
C	0.73324800	5.13187400	-3.59349500

C	1.97164600	5.09511400	-1.45611400
H	2.85414100	-4.81398200	-0.37475000
H	0.48155500	-5.53914000	-0.34935300
H	-1.96505700	-5.16270800	-0.32474000
H	4.67021900	-3.11636900	-0.39818400
H	5.56597700	-0.79773000	-0.41308700
H	5.35460800	1.68059800	-0.41195800
H	-4.01768000	-3.77006900	-0.31073300
H	4.07992400	3.81303200	-0.39551700
H	-5.28099400	-1.63360700	-0.30892000
H	-5.49868100	0.83699700	-0.31455400
H	-4.61470300	3.15018900	-0.32459400
H	-2.80119200	4.83038500	-0.33693700
H	-0.43618900	5.55180400	-0.35115300
H	2.01249700	5.18537800	-0.37156200
N	5.05086200	-0.73572000	-4.32635900
N	2.59303200	-4.42888900	-4.29632000
N	-1.83380200	-4.75937500	-4.25491600
N	-4.85080600	-1.50233700	-4.23512200
N	-4.26340900	2.89502600	-4.25464500
N	-0.42565000	5.13034900	-4.28143400
N	3.70760600	3.49784200	-4.31461300
N	1.82530100	4.78079200	-4.29720700
N	-2.59731200	4.44550600	-4.26590900
N	-5.06021700	0.76338300	-4.24218900
N	-3.70824300	-3.47009100	-4.23888600
N	0.41532500	-5.08316700	-4.27400400
N	4.24406900	-2.86379500	-4.31482600
N	4.85900000	1.53281600	-4.32653300
C	3.40145000	-3.76470600	2.71815500
C	3.58565500	-3.94152200	4.16722600
C	2.66784000	-4.75762100	4.84566100
C	1.48807100	-5.14297900	4.19003400
C	1.40209500	-4.91607700	2.73825300
C	0.30745000	-5.47876900	4.86874100
C	-0.92168600	-5.32455600	4.20914000
C	-0.89912100	-5.08971900	2.75616800
C	-2.13285200	-5.11845000	4.88527700
C	-3.17542300	-4.45495200	4.22090900
C	-3.05213100	-4.25823900	2.76709600
C	4.70360800	-1.85647600	2.70219700
C	4.95288500	-1.94613000	4.14952600
C	4.48391900	-3.08488200	4.82278100
C	5.04482200	0.42923300	2.69793200
C	5.30369700	0.44759500	4.14613100
C	5.38477500	-0.78585400	4.81137500

C	4.34031400	2.62571700	2.70368800
C	4.56343100	2.74939500	4.15315400
C	5.17993400	1.67548400	4.81459900
C	-4.18139300	-3.74698300	4.89386000
C	-4.83540600	-2.70149300	4.22530900
C	-4.63775100	-2.58191700	2.77116800
C	2.74452400	4.29524000	2.71670500
C	2.89531400	4.49970500	4.16636200
C	3.91586100	3.79662600	4.82562400
C	-5.43543000	-1.62612100	4.89580500
C	-5.56947400	-0.40195100	4.22471600
C	-5.33951200	-0.38364900	2.77045400
C	-5.63884600	0.82845600	4.89379600
C	-5.22331900	1.98649400	4.22102300
C	-5.01105900	1.89989300	2.76646100
C	-4.74529200	3.12372500	4.88821000
C	-3.86450500	3.98106000	4.21340700
C	-3.71384500	3.80693500	2.75904600
C	-2.93646600	4.79679500	4.87747200
C	-1.77069100	5.18304000	4.20066500
C	-1.71227400	4.95391200	2.74750100
C	-0.57974900	5.52052300	4.86118200
C	0.63812300	5.36417000	4.18369000
C	0.58917700	5.12284000	2.73234300
C	1.86101300	5.16361800	4.84226400
H	2.75965100	-4.89771500	5.92035500
H	0.32767500	-5.63744800	5.94461700
H	-2.18458900	-5.26642200	5.96164400
H	4.62989500	-3.17533900	5.89680400
H	5.55639600	-0.80966800	5.88515300
H	5.34568000	1.72563600	5.88836600
H	-4.29316100	-3.85519300	5.97041000
H	4.04305600	3.91013600	5.89986400
H	-5.58294900	-1.67283100	5.97248500
H	-5.79127100	0.85214400	5.97054700
H	-4.87130300	3.21351100	5.96488600
H	-3.00969800	4.93550100	5.95383700
H	-0.58453000	5.68329000	5.93664400
H	1.92796700	5.31722500	5.91698100
N	4.92345700	-0.72221200	2.00917200
N	2.43001200	-4.39719500	2.03771200
N	-2.00197300	-4.73703600	2.07228000
N	-5.05883700	-1.50591800	2.08127500
N	-4.42779000	2.89564800	2.07296400
N	-0.56910700	5.10335400	2.05009600
N	3.58106700	3.50015200	2.01974600

N	1.68478000	4.76281900	2.03456300
N	-2.75171200	4.44296400	2.06351700
N	-5.25098400	0.76771200	2.07877500
N	-3.89780700	-3.46968500	2.07970400
N	0.25309200	-5.06867700	2.05742400
N	4.09243000	-2.84189200	2.01955700
N	4.75238200	1.54720900	2.00929400
C	0.73614700	-1.11277000	-4.74864700
C	0.44166100	-1.19536500	-3.25877300
C	-0.92185400	-0.78424200	-2.83934700
O	-0.00263900	-2.41807900	-2.77534900
H	-0.07566000	-1.57510700	-5.31682600
H	0.84454600	-0.06780100	-5.05384000
H	1.66189400	-1.64697700	-4.97995300
H	1.25607700	-0.73597600	-2.67003200
H	-1.20665300	-0.84703500	-1.80300200
H	-1.71196800	-0.91714500	-3.56871900
N	0.77888700	-0.05733200	0.90227800
C	1.20396200	-0.02231600	2.33962100
C	-0.59198600	0.56047800	0.77217200
C	0.76847000	-1.50144500	0.44427900
C	1.76371900	0.74473100	0.08193800
H	1.22435900	1.01509000	2.67379200
H	0.48858500	-0.59575200	2.93085000
H	2.19833300	-0.45992600	2.41553900
H	-0.83771300	0.67725200	-0.28595300
H	-1.31554800	-0.07794800	1.28094400
H	-0.57028800	1.55126500	1.22899700
H	0.50739600	-1.57937000	-0.61284800
H	1.75960400	-1.92382800	0.61663700
H	0.03486900	-2.04933000	1.03757900
H	1.41182500	0.76435200	-0.94964700
H	1.80752400	1.75907800	0.48143200
H	2.74489100	0.27868900	0.17096000
Cl	-0.98163200	1.50526600	-2.64674600

Int-1_(E)

C	3.72340500	-3.64945100	-3.32829800
C	3.82709700	-3.85673100	-1.87319100
C	2.92311700	-4.72414200	-1.25122300
C	1.82835900	-5.18903500	-1.99801700
C	1.79954200	-4.91308600	-3.44442800
C	0.64468200	-5.59103200	-1.36800100
C	-0.55610200	-5.49495400	-2.08714600
C	-0.48828200	-5.19921300	-3.52849700
C	-1.77978500	-5.32243900	-1.42635400

C	-2.81451000	-4.67049100	-2.10919100
C	-2.65607400	-4.42489800	-3.55226400
C	4.93484700	-1.68925900	-3.21515900
C	5.08609300	-1.81186700	-1.75457500
C	4.60740500	-2.96254200	-1.12126500
C	5.22616900	0.59561400	-3.13007100
C	5.39396300	0.56953200	-1.66643900
C	5.42167700	-0.66676900	-1.01341700
C	4.52037000	2.78748600	-3.08431900
C	4.66541100	2.85713900	-1.61985700
C	5.21034900	1.75937400	-0.94396100
C	-3.81279100	-3.96977000	-1.41695100
C	-4.46274000	-2.91994100	-2.07585400
C	-4.23557900	-2.75300300	-3.52054700
C	2.92620800	4.44723900	-3.08026500
C	3.00577400	4.59121900	-1.61643600
C	3.97284400	3.85566400	-0.91879600
C	-5.05315600	-1.86529700	-1.36341000
C	-5.20389800	-0.63201500	-2.00636800
C	-4.94535900	-0.55311000	-3.45302200
C	-5.28394100	0.56474100	-1.27648800
C	-4.91432100	1.75324600	-1.91390100
C	-4.66989300	1.73263700	-3.36584400
C	-4.47555800	2.86347100	-1.17427100
C	-3.64960800	3.79368700	-1.81275900
C	-3.45662500	3.68910600	-3.26884400
C	-2.77412000	4.60559600	-1.07391700
C	-1.63697200	5.10068200	-1.72132700
C	-1.52473500	4.93960800	-3.18091800
C	-0.48851300	5.44322200	-0.99083400
C	0.74454600	5.39498200	-1.65259000
C	0.75878400	5.21835600	-3.11476500
C	1.93098000	5.17995200	-0.93627300
H	2.94676000	-4.84409800	-0.16988200
H	0.62877700	-5.73808300	-0.29011200
H	-1.84279800	-5.46598800	-0.34992800
H	4.66315400	-3.04788200	-0.03732700
H	5.49777200	-0.70800200	0.07257400
H	5.28922400	1.76884700	0.14321900
H	-3.91542800	-4.08028500	-0.33977600
H	4.02873300	3.91083800	0.16883000
H	-5.18508400	-1.93148900	-0.28551400
H	-5.41482700	0.54847500	-0.19605500
H	-4.59362700	2.89364100	-0.09204600
H	-2.85915400	4.67387300	0.01039200
H	-0.52647400	5.53226200	0.09515400

H	1.94449200	5.26434700	0.15090300
N	5.16950600	-0.53406000	-3.86094100
N	2.81910500	-4.31114500	-4.07689400
N	-1.58258200	-4.85231800	-4.23617000
N	-4.63508300	-1.64736000	-4.17969900
N	-4.10340400	2.76570900	-4.00958200
N	-0.37695300	5.17453800	-3.83898000
N	3.79730400	3.69084200	-3.77190700
N	1.88532200	4.92657100	-3.78797400
N	-2.51445800	4.39414400	-3.91672600
N	-4.85545700	0.61727700	-4.10205500
N	-3.49446700	-3.61743200	-4.23172400
N	0.68141600	-5.08859100	-4.17958000
N	4.40410700	-2.67850700	-3.96102700
N	4.96245300	1.73416300	-3.79604100
C	3.83705200	-3.39539400	2.94974000
C	3.94900500	-3.62022000	4.40004800
C	3.02928500	-4.49266600	5.00122500
C	1.89698800	-4.88622100	4.27357500
C	1.87293300	-4.59669400	2.83049400
C	0.69861200	-5.28937200	4.88145100
C	-0.50371800	-5.13165800	4.17671600
C	-0.42138400	-4.81606700	2.74179900
C	-1.74792900	-4.99000700	4.80893200
C	-2.77694300	-4.31171300	4.13930600
C	-2.59345500	-4.02704000	2.70735500
C	5.07263500	-1.45156700	3.06739900
C	5.24189400	-1.58469400	4.52347500
C	4.77928200	-2.76049000	5.13338700
C	5.33304700	0.83823500	3.15822900
C	5.52008300	0.81167200	4.61813900
C	5.60222400	-0.43935900	5.24763000
C	4.57160300	3.01541200	3.20863000
C	4.73157600	3.09277400	4.67004600
C	5.33720400	2.00949700	5.32354800
C	-3.82507100	-3.66140400	4.80759500
C	-4.47726700	-2.59438400	4.17211300
C	-4.22975800	-2.39638000	2.73543900
C	2.94509800	4.65253700	3.21516600
C	3.03468900	4.80966200	4.67621000
C	4.03904300	4.10270100	5.35294000
C	-5.12561700	-1.56568000	4.87126100
C	-5.26786300	-0.31344400	4.25449200
C	-4.99727400	-0.22316300	2.81059400
C	-5.38972500	0.88480200	4.97260400
C	-4.98788200	2.08250600	4.36201600

C	-4.73210700	2.06492900	2.91255900
C	-4.56358500	3.20497200	5.08722500
C	-3.69086000	4.11569300	4.47297600
C	-3.48892700	4.00404800	3.01911500
C	-2.81045600	4.93357200	5.19512800
C	-1.63683000	5.38001300	4.56976400
C	-1.52164600	5.20459400	3.11266000
C	-0.47987000	5.72644900	5.28175200
C	0.76338100	5.62616600	4.64045800
C	0.77350100	5.43338200	3.18098600
C	1.96410400	5.42891400	5.33702000
H	3.07482100	-4.67378600	6.07273300
H	0.67701200	-5.50259900	5.94775800
H	-1.84058200	-5.19791600	5.87249900
H	4.87440200	-2.88613400	6.20959700
H	5.72329800	-0.49585000	6.32709700
H	5.45439400	2.02570500	6.40481400
H	-3.97497100	-3.83083700	5.87144800
H	4.12267200	4.18173700	6.43456700
H	-5.30754600	-1.66756100	5.93871300
H	-5.57408900	0.85832300	6.04420100
H	-4.72262100	3.24800200	6.16236000
H	-2.92082800	5.03096800	6.27283100
H	-0.52425200	5.85116200	6.36139200
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N	-4.66292300	-1.30570400	2.08017200
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N	3.82585600	3.90317100	2.52620500
N	1.90018400	5.12708600	2.51203300
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C	0.62295600	-1.24935300	-4.91503800
C	-0.81379100	-0.63377200	-4.65411400
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O	-1.21409500	-0.98589300	-3.41269800
H	0.57410500	-2.33864300	-4.86267000
H	0.93804300	-0.93557200	-5.91366800
H	1.32878200	-0.86522600	-4.17593700

H	-0.69020300	0.46215900	-4.77393700
H	-2.79743600	-0.81382100	-5.52968600
H	-1.78381700	-2.25465200	-5.78169900
N	-0.33145000	-0.82881900	-0.13477900
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C	0.30272600	0.26884500	-0.94951200
C	-1.83161300	-0.66226100	-0.17354400
C	0.02573300	-2.16569900	-0.73797500
H	1.23583800	-0.92960000	1.29092900
H	-0.09716700	0.19093600	1.70807700
H	-0.33140000	-1.58203100	1.83810400
H	-0.07999500	0.16510500	-1.96952400
H	0.02440900	1.22997300	-0.51452000
H	1.38608200	0.14437100	-0.91863100
H	-2.12907800	-0.67939100	-1.22240000
H	-2.29520800	-1.47790900	0.38402200
H	-2.09187400	0.29310200	0.28476800
H	-0.34747200	-2.17118600	-1.76469100
H	1.11097700	-2.26924300	-0.71783600
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TS-2_(E)

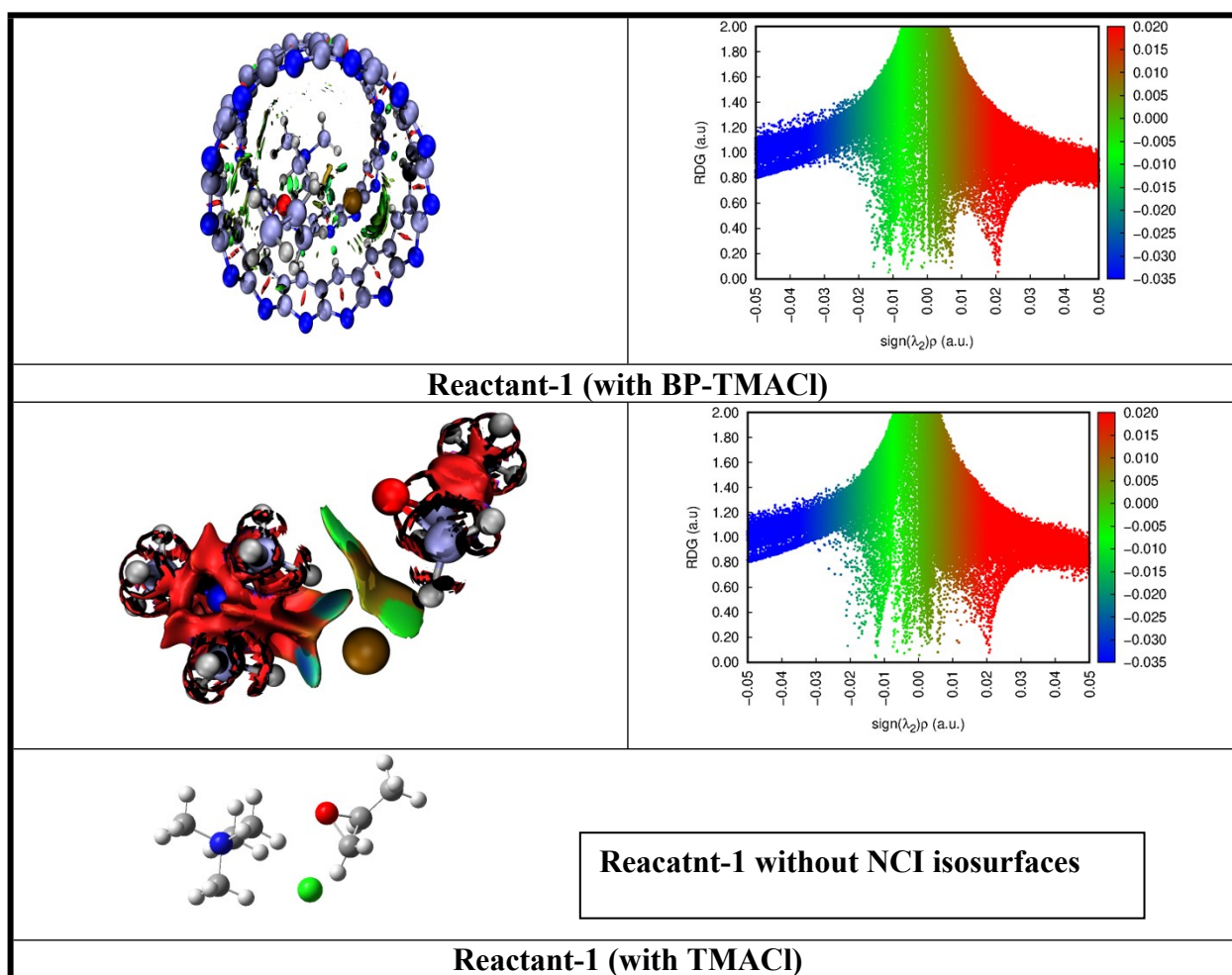
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C	2.73654700	-4.67072900	-1.85392500
C	1.56753600	-5.10013100	-2.49495300
C	1.45265300	-4.92027600	-3.95288800
C	0.41002100	-5.38968500	-1.75965800
C	-0.82592600	-5.28262200	-2.40903400
C	-0.84402500	-5.09554300	-3.87034500
C	-1.99814300	-5.02937400	-1.68378300
C	-3.06266500	-4.41020000	-2.34949500
C	-2.99035100	-4.25796500	-3.81306500
C	4.73843200	-1.85976700	-4.12369700
C	4.99545800	-1.91464700	-2.67391600
C	4.52190300	-3.01522700	-1.94801000
C	5.07155500	0.42009700	-4.17354000
C	5.34249400	0.46111500	-2.72600400
C	5.40541700	-0.74586000	-2.01877600
C	4.37944700	2.61838100	-4.18360000
C	4.61774500	2.75057200	-2.73578200
C	5.20662000	1.68115800	-2.05033700
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C	-4.70308300	-2.65635800	-2.32753800

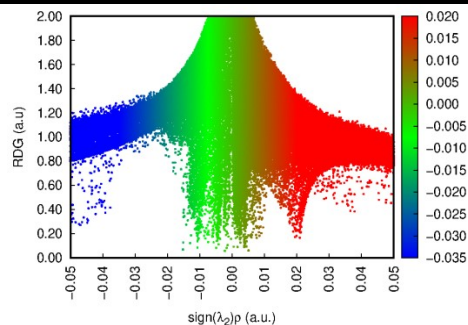
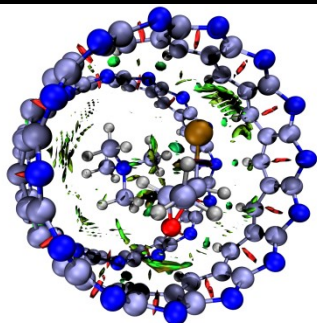
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C	3.97183600	3.78040400	-2.03849100
C	-5.24210500	-1.56094800	-1.63938400
C	-5.42392300	-0.36611800	-2.34601200
C	-5.25385800	-0.37526900	-3.80917500
C	-5.43858100	0.86480900	-1.67676300
C	-5.07897800	2.00915000	-2.39935600
C	-4.92213800	1.90440100	-3.86023200
C	-4.55968300	3.13334700	-1.74457500
C	-3.73338000	3.99578000	-2.47639100
C	-3.63163400	3.81166500	-3.93430700
C	-2.77857900	4.78987300	-1.82927000
C	-1.65582200	5.19562500	-2.56270700
C	-1.63894900	4.96530000	-4.01752800
C	-0.45325000	5.50474500	-1.91595600
C	0.73725400	5.37319000	-2.64345000
C	0.65763700	5.13812700	-4.09549000
C	1.95348500	5.14243900	-1.98985200
H	2.82606600	-4.73962800	-0.77046900
H	0.45470900	-5.47329100	-0.67454800
H	-1.99933900	-5.10293500	-0.59713600
H	4.64870500	-3.05554300	-0.86698800
H	5.54844500	-0.74172300	-0.93910800
H	5.34341600	1.73080600	-0.97098800
H	-4.05421800	-3.71186300	-0.55401100
H	4.08288400	3.86846700	-0.95850000
H	-5.30561000	-1.56987900	-0.55185200
H	-5.50733600	0.90079300	-0.58998500
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H	-0.42672600	5.62545900	-0.83355400
H	2.02547800	5.25478400	-0.90866200
N	4.95085200	-0.74161900	-4.84284800
N	2.46091500	-4.41796700	-4.69013500
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N	-4.99954300	-1.50851000	-4.48996500
N	-4.35892800	2.88683300	-4.58856600
N	-0.51872000	5.11314300	-4.74965900
N	3.62000300	3.49789600	-4.86355100
N	1.73375500	4.77590600	-4.81896300
N	-2.69390600	4.44003200	-4.66825400
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N	4.12669900	-2.86527400	-4.77694100
N	4.76902100	1.52984100	-4.87321900
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C	3.83893200	-3.73254400	3.71065100
C	2.93758700	-4.52171300	4.43312900
C	1.75195800	-4.92297100	3.80554900
C	1.63365600	-4.73210800	2.35241000
C	0.59301800	-5.21277500	4.53121600
C	-0.64772500	-5.07643300	3.89414800
C	-0.66454100	-4.88669500	2.43605600
C	-1.82503300	-4.82711700	4.60727800
C	-2.89102800	-4.19739000	3.95085800
C	-2.81516000	-4.04334400	2.48978300
C	4.92613000	-1.68659900	2.18455900
C	5.19347700	-1.74273400	3.63026300
C	4.73665900	-2.86096500	4.33977200
C	5.25372900	0.59733500	2.13445300
C	5.54050800	0.64317300	3.57716000
C	5.62842400	-0.57312900	4.26837600
C	4.55070000	2.79592600	2.12201400
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C	5.42995000	1.87754500	4.23242600
C	-3.86539100	-3.46799500	4.64416200
C	-4.56129100	-2.46056600	3.96382500
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C	2.96684900	4.47423000	2.15018300
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C	-5.33805300	1.05768600	4.60842300
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C	-4.79439000	2.10052600	2.43929500
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C	-3.58796400	4.18449100	3.83176800
C	-3.48713700	4.00088400	2.37496000
C	-2.63590400	4.99475600	4.46562900
C	-1.49859600	5.38355500	3.74586100
C	-1.48372100	5.14349800	2.29377900
C	-0.29104800	5.72201900	4.37321100
C	0.90436200	5.56606600	3.65954600
C	0.81701800	5.31087600	2.21244400
C	2.14025400	5.36693200	4.29189000
H	3.04915700	-4.63321600	5.50891400
H	0.63996300	-5.33129500	5.61075600

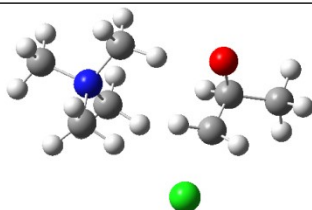
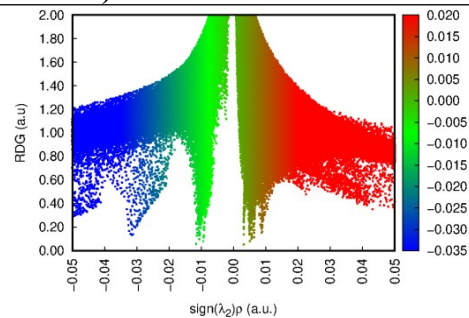
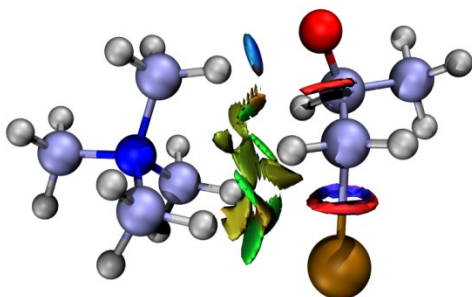
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H	4.33926800	4.12736500	5.30921900
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H	-5.41493400	1.08370600	5.69142900
H	-4.51641700	3.41470200	5.62907100
H	-2.67683600	5.13992400	5.54274700
H	-0.26620500	5.89530100	5.44671000
H	2.23663500	5.53565600	5.36206300
N	5.13856700	-0.56585800	1.46876000
N	2.64930500	-4.24589100	1.61601400
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N	0.46598500	-4.90249400	1.70618500
N	4.31955500	-2.69363400	1.53215300
N	4.94269800	1.70581500	1.43727700
C	0.35702800	-0.20052600	7.35992800
C	-0.59743300	-0.97851300	6.46239900
C	-1.53418600	-0.06794000	5.68345800
O	0.14075600	-1.81164800	5.54006800
H	0.95017800	0.49940700	6.76296500
H	-0.21136600	0.35841000	8.10764200
H	1.03565300	-0.88716200	7.87261800
H	-1.19190500	-1.67358000	7.05548400
H	-2.24931100	-0.49092200	4.99845800
H	-1.43732100	1.00253400	5.71924000
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C	-0.39497500	0.79337800	0.97474200
C	0.32640500	0.01208200	-1.24491000
C	-0.17374500	-1.62035700	0.53518400
C	1.83292700	-0.21423700	0.69496200
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H	-1.43252500	0.75475700	0.63865600
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H	-0.71469700	-0.03030900	-1.56641000

H	0.73883700	1.00105400	-1.44695800
H	0.37873400	-2.36778500	-0.03328400
H	-0.03355000	-1.80757200	1.59896400
H	-1.22980200	-1.63747800	0.26447100
H	2.40141200	-0.97446100	0.15988500
H	2.24631600	0.77521900	0.49593300
H	1.83828200	-0.44687100	1.76060800
C	0.40069400	-1.18141500	4.33852100
O	-0.19506700	-0.05521800	4.19814800
O	1.13974400	-1.75845000	3.53454800
Cl	-3.19256700	0.11069300	7.27136200



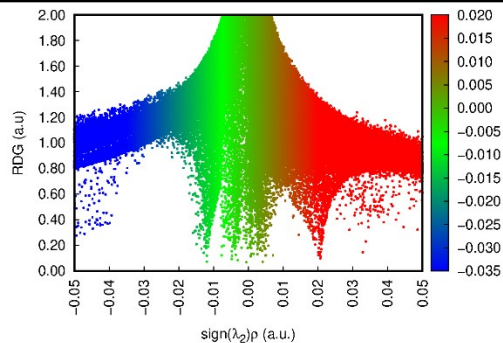
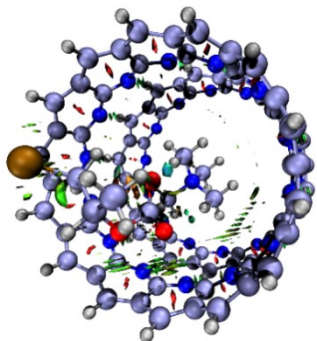


TS-1 (with BP-TMACI)

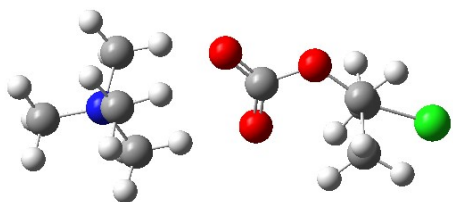
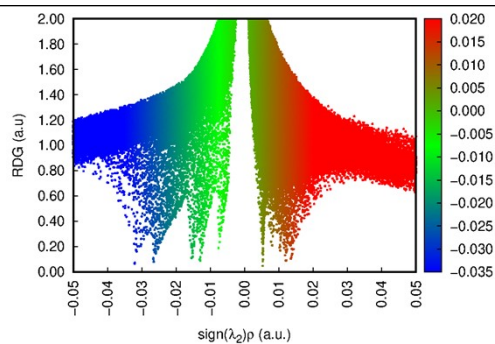
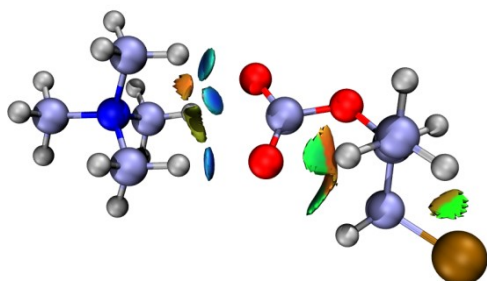


TS-1 without NCI isosurfaces

TS-1 (with TMACI)

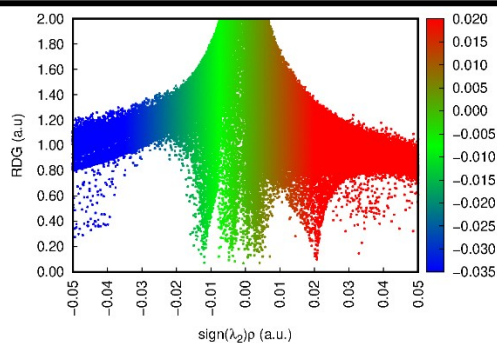
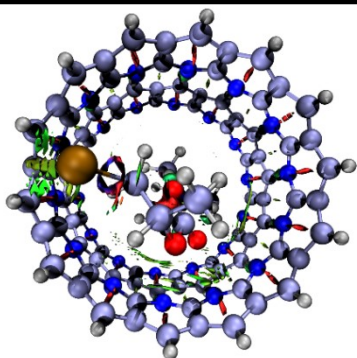


Reactant-2 (with BP-TMACI)

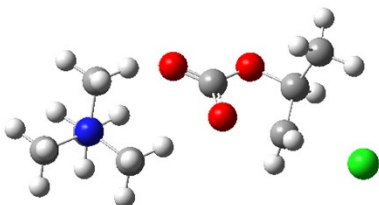
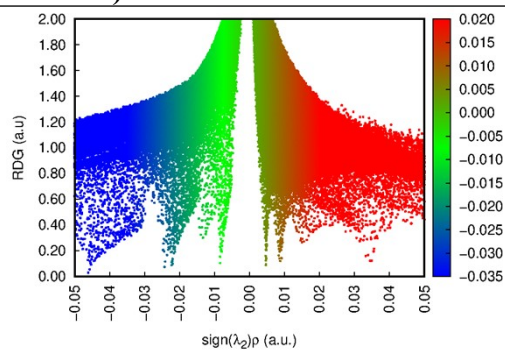
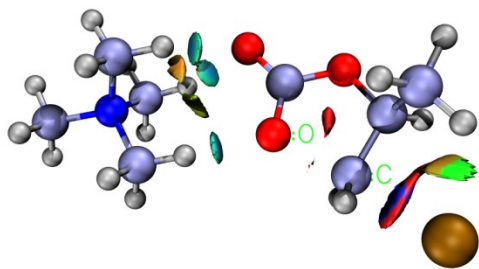


Reactant-2 without NCI isosurfaces

Reactant-2 (with TMACI)



TS-2 (with BP-TMACI)



TS-2 without NCI isosurfaces

TS-2 (with TMACI)

Figure S1. Results of NCI analysis computed at B3LYP/6-31G(d,p).