

Regioselective CF₂ functionalization of Sc₃N@D_{3h}(5)-C₇₈

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Supplementary information

Optimized PBE/Def2-TZVP coordinates of the isomers of Sc₃N@C₇₈(CF₂) (pp. 2-25), of the respective anionic intermediates (pp. 26-40) and transition states for ring closure (pp. 41-61), and the optimized coordinates of the starting Sc₃N@C₇₈ and the reference [6,6]-Sc₃N@C₈₀(CF₂) and Sc₃N@C₈₀ compounds (pp. 62-67).

Optimized isomers of Sc₃N@C₇₈

56-1

N	0.010133020	0.006937260	-0.029349260
Sc	2.018994720	0.037922270	-0.005960530
Sc	-1.020006900	-1.717977550	-0.001512150
Sc	-0.994241640	1.745562500	-0.043177210
C	3.622641650	1.419485770	-1.204241140
C	3.144941000	0.738358420	-2.395359240
C	2.190621680	1.425077470	-3.206162150
C	1.245578120	0.698152400	-4.007447170
C	1.246496490	-0.706046200	-4.001776290
C	4.158797310	0.743815840	-0.033468050
C	4.144029890	-0.697812760	-0.016320320
C	3.606466500	-1.391631540	-1.174325700
C	3.142151750	-0.730412230	-2.382903920
C	2.190059200	-1.425245590	-3.189130970
C	2.223332140	1.465676470	3.135666190
C	3.180195470	0.777456760	2.337721140
C	3.644656280	1.441087230	1.134211430
C	-1.217806180	0.716961850	-4.006320380
C	-1.216817260	-0.724482970	-4.003032100
C	-0.002649050	1.418986250	-4.008495880
C	-0.000730130	-1.426627820	-3.999504700
C	0.153281810	-2.601944420	-3.185340890
C	-0.921995390	-3.078493440	-2.375394180
C	-0.577803580	-3.809231230	-1.166642770
C	2.888870620	-2.555242930	-0.700394080
C	1.835805050	-3.157664610	-1.454977080
C	1.528079730	-2.629021920	-2.720646540
C	0.789998160	-3.767884610	-0.696540690
C	-3.015149720	2.428036850	-1.195186930
C	-2.195534780	2.349415360	-2.393534650
C	-2.316494310	1.175869240	-3.201649650
C	-3.035160430	0.000401700	-2.743302650
C	-3.689905580	-1.216530160	-0.739534950
C	-3.669388980	0.004593700	-1.491530850
C	-3.684741030	1.227876320	-0.741657470
C	-2.195815980	-2.347248850	-2.385468090
C	-2.316170670	-1.178689900	-3.197649480
C	-3.021339130	-2.419046510	-1.192039930
C	-0.924044400	3.083980230	-2.395799070
C	0.150816860	2.601303390	-3.206150570
C	-2.681336520	3.224400230	-0.020827110
C	-1.432904230	3.945739010	-0.023097850
C	-0.579493500	3.835346350	-1.199670720
C	-3.000959040	2.415044170	1.147571830
C	-2.166295740	2.321932280	2.337539230

C	-2.268972180	1.150453740	3.143696450
C	-3.699353440	-1.216753880	0.687133360
C	-3.668777440	0.008812720	1.433267420
C	-3.680956000	1.226097910	0.684269460
C	-3.022781840	0.007355520	2.677278160
C	0.795926620	3.816549210	-0.749879320
C	1.845966720	3.191044650	-1.501655560
C	1.529381520	2.637482420	-2.751664600
C	2.916140770	2.600072800	-0.751649130
C	0.799485570	3.814592150	0.676049830
C	1.532043890	2.638884850	2.668942770
C	1.850018670	3.197220420	1.423148560
C	2.925024370	2.610420470	0.674982200
C	-0.901864100	3.052443910	2.335223820
C	-0.568895320	3.820177550	1.143123950
C	0.166510700	2.557524430	3.139234920
C	-1.306050290	-0.786819370	4.033184230
C	-1.184828880	0.665084010	3.984347890
C	0.047808190	1.377202930	3.982065550
C	-0.266618270	-1.704679380	4.295509590
C	-3.044405920	-2.423443730	1.146485920
C	-2.234242340	-2.350702650	2.347674350
C	-2.350411660	-1.176768930	3.144073150
C	-0.594278780	-3.789470980	1.166672570
C	-1.444195380	-3.926402100	-0.005984730
C	-2.700507380	-3.219084100	-0.020808910
C	0.093345880	-2.610431690	3.235974220
C	-0.949517900	-3.051377680	2.352791960
C	2.875500910	-2.530741990	0.730181010
C	1.490417050	-2.546311050	2.781872630
C	1.801606660	-3.089034600	1.501869160
C	0.779388000	-3.741673970	0.734029120
C	1.366320540	0.757090380	4.028237230
C	1.643084880	-0.601416020	4.292019350
C	2.245140300	-1.367363240	3.232093600
C	3.145432840	-0.685475440	2.345166510
C	3.604282330	-1.363927220	1.158971410
C	0.805261490	-1.352609950	5.251020160
F	0.362210280	-0.582498580	6.296957120
F	1.442489180	-2.453950070	5.787022430

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N	-0.000173880	0.010996880	0.040959910
Sc	1.993308900	0.142143150	0.160709180
Sc	-0.968324240	-1.767369340	-0.007452610
Sc	-1.064569070	1.727059700	-0.002929590

C	3.574976990	1.414992040	-1.137372190
C	3.109008790	0.713892670	-2.308602260
C	2.183492370	1.410343080	-3.147710350
C	1.246751650	0.692937330	-3.958508530
C	1.245127590	-0.708211150	-3.942282010
C	4.127220190	0.760226190	0.025168850
C	4.171604300	-0.676000230	0.071250170
C	3.571679550	-1.434851150	-1.033764750
C	3.096446700	-0.752939760	-2.254368200
C	2.167805420	-1.427815390	-3.100989310
C	2.165342510	1.474889280	3.166115790
C	3.143738810	0.805371130	2.379272050
C	3.645802750	1.483383050	1.199110230
C	-1.217512310	0.722605520	-3.989105730
C	-1.221276010	-0.718785000	-3.986764180
C	-0.000254100	1.419511630	-3.981059630
C	-0.005332260	-1.423073140	-3.966380010
C	0.130370270	-2.598479920	-3.153961320
C	-0.957111770	-3.084021820	-2.369030430
C	-0.624857330	-3.848484340	-1.178647570
C	2.924707120	-2.695284450	-0.657808560
C	1.801158050	-3.178581270	-1.416981850
C	1.494595070	-2.624543010	-2.661793510
C	0.745169670	-3.842643780	-0.710876850
C	-3.031820590	2.440965700	-1.190955910
C	-2.202819210	2.358059970	-2.384184700
C	-2.320373110	1.184267870	-3.189815720
C	-3.045380720	0.010437800	-2.735572190
C	-3.709120280	-1.202046870	-0.728889680
C	-3.682046580	0.014806890	-1.483722140
C	-3.691686520	1.237263670	-0.732492280
C	-2.220381930	-2.338728190	-2.377612660
C	-2.329687550	-1.169132230	-3.190996570
C	-3.041051560	-2.402139770	-1.182541710
C	-0.928491670	3.087576990	-2.379605790
C	0.150193630	2.603560280	-3.183148710
C	-2.710499070	3.244956500	-0.019476420
C	-1.453977830	3.951455040	-0.016508530
C	-0.591759020	3.836148500	-1.181996530
C	-3.040288590	2.445569150	1.153320990
C	-2.218484520	2.369998990	2.352375910
C	-2.333403810	1.194794210	3.158397940
C	-3.709645160	-1.201074060	0.698471240
C	-3.685362650	0.018028470	1.449113200
C	-3.695562510	1.239379790	0.695102850
C	-3.051418220	0.017901840	2.701902300
C	0.779344800	3.834347850	-0.722245830
C	1.826005200	3.199226680	-1.464626930
C	1.523454450	2.632185040	-2.709942070

C	2.879281590	2.599451580	-0.699743250
C	0.776204810	3.842523560	0.704901370
C	1.502265350	2.686022320	2.719118240
C	1.825304440	3.233522960	1.468184030
C	2.901789260	2.633213020	0.726946660
C	-0.948615100	3.106352770	2.356139330
C	-0.600111700	3.845727800	1.155118140
C	0.125076510	2.635129890	3.172385990
C	-1.217779450	-0.703000810	3.941338940
C	-1.229778030	0.736852690	3.956833900
C	-0.018645080	1.442574750	3.962958620
C	0.004302990	-1.397427410	3.911346590
C	-3.038978600	-2.399989050	1.154984980
C	-2.215801470	-2.329267390	2.350190780
C	-2.328716110	-1.157596060	3.155060160
C	-0.633970660	-3.839724470	1.159171530
C	-1.489339960	-3.950685130	-0.012137540
C	-2.717634650	-3.202112790	-0.014040590
C	0.157132380	-2.570451160	3.105202420
C	-0.946743160	-3.066551810	2.342037080
C	3.045297720	-3.129719390	0.703541160
C	1.544850690	-2.634993250	2.651247000
C	1.842208490	-3.346402460	1.458812120
C	0.732479980	-3.852734170	0.712702730
C	1.233141590	0.726305060	3.949683490
C	1.249475150	-0.680845730	3.905683580
C	2.210506340	-1.402373530	3.109881950
C	3.233946120	-0.656562680	2.404172890
C	4.077212620	-1.268527310	1.397566160
C	4.284555430	-2.734669520	1.413491960
F	4.395840860	-3.268244800	2.671592940
F	5.423573370	-3.095677360	0.716992340

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N	-0.035535870	0.046343940	-0.002080420
Sc	1.934703330	0.206814170	-0.003310890
Sc	-0.957115580	-1.725062160	-0.003234070
Sc	-1.091011340	1.744916600	0.000351370
C	3.602420400	1.351880070	-1.177909420
C	3.092468320	0.703304710	-2.369205760
C	2.160411090	1.418504430	-3.186674770
C	1.213476700	0.718623330	-4.005823670
C	1.205213180	-0.684010450	-4.027535800
C	4.102636230	0.626691340	-0.006272230
C	4.028418220	-0.824467050	-0.007626130
C	3.588498370	-1.494095230	-1.236630530
C	3.069489070	-0.753550390	-2.377032270

C	2.148453550	-1.424927390	-3.236522580
C	2.167504810	1.412228890	3.179970740
C	3.097926820	0.698710300	2.359099570
C	3.605400580	1.349738410	1.168029590
C	-1.252408330	0.757708510	-3.996430930
C	-1.260212010	-0.684638910	-4.004371250
C	-0.030743050	1.449849810	-3.995547030
C	-0.049640890	-1.391008880	-4.019724430
C	0.104937420	-2.561802310	-3.203153450
C	-0.938216840	-3.045806990	-2.372728810
C	-0.547783850	-3.778687820	-1.171803890
C	3.184903490	-2.871563670	-1.105385190
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C	-3.056657740	0.033842810	-2.717192230
C	-3.692244480	-1.189836440	-0.711645590
C	-3.679562390	0.032694890	-1.461186640
C	-3.688802270	1.257956110	-0.710110710
C	-2.209988760	-2.313193840	-2.368326140
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C	-3.012342080	-2.384592430	-1.167157620
C	-0.933640370	3.105007310	-2.368068340
C	0.134931300	2.622628300	-3.183996750
C	-2.707978090	3.272035960	0.003927090
C	-1.435371150	3.963043240	0.003197300
C	-0.577471070	3.836382960	-1.165650090
C	-3.034788630	2.465848650	1.176106510
C	-2.208817950	2.380158160	2.372925410
C	-2.334031690	1.207219270	3.179501620
C	-3.690644750	-1.191239930	0.712830240
C	-3.676284150	0.029796630	1.464756380
C	-3.687197490	1.256527860	0.716124750
C	-3.050576630	0.028467020	2.719370170
C	0.798661720	3.798956050	-0.711996760
C	1.837381240	3.160376880	-1.465657260
C	1.514293780	2.633475160	-2.722930670
C	2.895628500	2.528719380	-0.716397600
C	0.800260510	3.797532300	0.713067980
C	1.520356240	2.628135740	2.720117160
C	1.840672730	3.157520150	1.463180690
C	2.897332010	2.527378360	0.710365430
C	-0.928355410	3.100290780	2.371610080
C	-0.574864860	3.834002380	1.169840760
C	0.142020750	2.616358330	3.184230100
C	-1.251280650	-0.692548320	4.001147750

C	-1.243496360	0.749808330	3.996043870
C	-0.021839620	1.441963720	3.993802800
C	-0.040675530	-1.398941170	4.012404620
C	-3.009687330	-2.386856080	1.164455130
C	-2.204684100	-2.317841260	2.363979560
C	-2.337940830	-1.149877000	3.182572040
C	-0.545159410	-3.780898230	1.160834250
C	-1.406439150	-3.903152470	-0.004626350
C	-2.663603100	-3.184541990	-0.002518870
C	0.112081980	-2.568095620	3.193151960
C	-0.932907240	-3.050435610	2.364093840
C	3.187441590	-2.873762140	1.087971950
C	1.485479910	-2.628110990	2.765787990
C	1.889119480	-3.256221260	1.581393500
C	0.845203940	-3.777970660	0.718996080
C	1.222403880	0.710722810	3.999831670
C	1.214192040	-0.691954910	4.018809780
C	2.155652370	-1.431276870	3.224202930
C	3.074851990	-0.758196570	2.364030660
C	3.591437930	-1.496565420	1.221102030
C	3.815444990	-3.633048590	-0.010183950
F	5.194791750	-3.551231710	-0.011725030
F	3.481174230	-4.965808960	-0.011144520

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N	0.109640940	-0.013443860	0.075540180
Sc	2.128088820	-0.255035280	0.167513010
Sc	-1.012608720	-1.701717630	0.017479570
Sc	-0.843614750	1.782352790	0.003982240
C	3.555919530	1.437084650	-1.217091180
C	3.116924510	0.771573010	-2.419803280
C	2.167418640	1.456933320	-3.226627570
C	1.218902170	0.725519630	-4.020343230
C	1.225433200	-0.679138890	-4.005236820
C	4.166105360	0.764970690	-0.107694270
C	4.506392930	-0.622323250	-0.302589970
C	3.683204980	-1.368853400	-1.235372050
C	3.115731980	-0.691778900	-2.397230070
C	2.169122600	-1.384818810	-3.186370030
C	2.171232560	1.388002810	3.144711860
C	3.161317920	0.687128610	2.360539190
C	3.626122850	1.367485240	1.129995290
C	-1.242785170	0.726387970	-4.001342400
C	-1.235606110	-0.716077860	-3.995633630
C	-0.032140130	1.438202880	-4.009377860
C	-0.015129620	-1.409653200	-3.988858350
C	0.151325560	-2.577113630	-3.166769350

C	-0.922549290	-3.057857140	-2.362744100
C	-0.568313220	-3.785968630	-1.161919360
C	2.960153820	-2.517688960	-0.678206600
C	1.859622640	-3.106388280	-1.431286550
C	1.528109850	-2.588745550	-2.695389760
C	0.803074930	-3.741279000	-0.696282840
C	-3.012020450	2.399501160	-1.171136000
C	-2.210270580	2.341108930	-2.373713730
C	-2.339605200	1.177130900	-3.191742650
C	-3.052881800	0.001649900	-2.726778080
C	-3.693860040	-1.218755300	-0.719309330
C	-3.686328690	0.001542540	-1.471784710
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C	-2.201804910	-2.338975960	-2.370624640
C	-2.330163640	-1.172592530	-3.182553120
C	-3.022510160	-2.415929120	-1.173843400
C	-0.948335750	3.088691000	-2.379689620
C	0.122617840	2.615786200	-3.196923010
C	-2.667575950	3.187717210	-0.005647840
C	-1.448574390	3.945578370	-0.004576070
C	-0.600945810	3.842880190	-1.182537010
C	-3.011549350	2.399096240	1.159617940
C	-2.204813180	2.338600400	2.358875310
C	-2.340167430	1.177188210	3.178796230
C	-3.699402370	-1.219125620	0.708233310
C	-3.691786850	0.002960140	1.459917130
C	-3.713716200	1.218482550	0.707622730
C	-3.062795940	0.004585280	2.717086900
C	0.769496640	3.805351900	-0.726984070
C	1.817813250	3.192920170	-1.484431000
C	1.503544420	2.655733770	-2.745708250
C	2.876409380	2.599877220	-0.733444100
C	0.781444510	3.788588510	0.700965000
C	1.516378770	2.596410930	2.691629410
C	1.834132990	3.144584150	1.442063970
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C	1.824729890	3.175802610	-1.474436420
C	1.512639470	2.632188030	-2.725771330
C	2.878964860	2.569736030	-0.717334310
C	0.781618610	3.829580700	0.698039650
C	1.520519520	2.673746570	2.703369420
C	1.837451220	3.223500050	1.451410570
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C	-1.183405340	-0.726681260	3.932448240
C	-1.179458300	0.704468810	3.935586230
C	0.042723070	1.389031650	3.925242340
C	0.034990260	-1.417964220	3.919156190
C	-3.034882740	-2.421496840	1.149238860
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C	-2.712661930	-3.219921290	-0.024014590
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C	-0.605435360	-3.852451170	-1.104877760
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C	1.807865230	-3.162495770	-1.412489610
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C	0.140169900	-2.621369280	-3.185293300
C	-0.934204610	-3.101070330	-2.374338950
C	-0.585454170	-3.846387240	-1.176617740
C	2.909458480	-2.610645030	-0.726401840
C	1.840712580	-3.201606930	-1.473394000
C	1.519554410	-2.654720950	-2.728175460
C	0.788711630	-3.823414410	-0.722232900
C	-3.004303090	2.395072890	-1.178001080
C	-2.201157590	2.324471810	-2.384275050
C	-2.327455410	1.154885970	-3.191257980
C	-3.041662020	-0.016559720	-2.725642160
C	-3.688359450	-1.233832570	-0.719726450
C	-3.674723790	-0.011474040	-1.470292540
C	-3.694877820	1.209216060	-0.722691740
C	-2.204697950	-2.366311660	-2.373642490
C	-2.325250180	-1.195387340	-3.183863750
C	-3.023812900	-2.436390310	-1.175316790
C	-0.933777560	3.059925140	-2.391960270
C	0.138051100	2.580411850	-3.204085460
C	-2.669931020	3.198144300	-0.014098160
C	-1.435372810	3.942762580	-0.016551040
C	-0.589442240	3.807522950	-1.192799130
C	-3.002002440	2.406104750	1.155318570
C	-2.175890790	2.339700910	2.348133460
C	-2.307297160	1.164516630	3.153182920
C	-3.686649670	-1.230128580	0.706452000

C	-3.669777710	-0.005917810	1.452429520
C	-3.690171740	1.212476210	0.705009500
C	-3.032984970	-0.005493780	2.705982900
C	0.781453010	3.763076990	-0.737207380
C	1.839708350	3.159633250	-1.501962710
C	1.520244560	2.608502590	-2.743593180
C	2.891016150	2.542820800	-0.738338380
C	0.790494350	3.804005780	0.679612190
C	1.605724220	2.750760140	2.910954900
C	1.981815830	3.402469280	1.446458220
C	2.923327460	2.570472460	0.678434600
C	-0.910559440	3.091914780	2.371442940
C	-0.563574640	3.847954370	1.157004920
C	0.141647790	2.617886070	3.202964600
C	-1.219258800	-0.732200500	3.970554780
C	-1.215391100	0.706136290	3.960477250
C	-0.004780990	1.413199420	3.944965190
C	-0.003672070	-1.435289480	3.969904600
C	-3.015473340	-2.428648290	1.163638120
C	-2.196684080	-2.357088550	2.361099520
C	-2.318430540	-1.184995380	3.169190020
C	-0.580983640	-3.836494830	1.162197240
C	-1.441019860	-3.954094600	-0.004300740
C	-2.689612120	-3.232267320	-0.003586160
C	0.151265090	-2.613472400	3.167845020
C	-0.926126750	-3.091752660	2.360309630
C	2.911186200	-2.605683790	0.701284320
C	1.529543050	-2.644478050	2.703445380
C	1.845593870	-3.196069540	1.449337000
C	0.792254050	-3.820781600	0.703934480
C	1.250307430	0.687273080	3.944248250
C	1.241130370	-0.714688430	3.959108780
C	2.182230100	-1.432192030	3.150643630
C	3.134731080	-0.731883830	2.345155830
C	3.603348650	-1.414352420	1.151650210
C	2.347254250	4.033163110	2.749314500
F	1.727247310	5.186071730	3.108345670
F	3.656056580	4.070600100	3.107294630

66-7

N	-0.022125230	0.000405520	-0.045355460
Sc	1.982603800	0.000663870	-0.057264710
Sc	-1.010385080	-1.748608170	-0.030113240
Sc	-1.011098130	1.749124300	-0.030249340
C	3.605319610	1.404853950	-1.170749880
C	3.136704720	0.733416370	-2.372702730
C	2.185770150	1.424060890	-3.190020070

C	1.244953830	0.702057760	-3.999832550
C	1.244918930	-0.701571700	-3.999626680
C	4.106922990	0.718643180	0.014590530
C	4.106857680	-0.717754160	0.014648720
C	3.605287830	-1.404075100	-1.170615820
C	3.136616610	-0.732775920	-2.372592630
C	2.185836260	-1.423563290	-3.189936020
C	2.216432750	1.530571320	3.238616790
C	3.106753380	0.745561230	2.421400750
C	3.553468710	1.392607940	1.180186780
C	-1.220470720	0.720600280	-4.005598020
C	-1.220449160	-0.720166580	-4.005548620
C	-0.004196910	1.422435240	-4.005847900
C	-0.004167250	-1.421981880	-4.005716500
C	0.147590420	-2.604008870	-3.204854340
C	-0.931502060	-3.085780200	-2.400207630
C	-0.590105150	-3.840644210	-1.209068300
C	2.896823950	-2.582769050	-0.727549460
C	1.838172750	-3.186444650	-1.489142890
C	1.525390560	-2.636203810	-2.741124000
C	0.785033570	-3.824208020	-0.753109800
C	-3.021441310	2.424929310	-1.192799710
C	-2.202538580	2.349927290	-2.394142820
C	-2.320450000	1.176773230	-3.200177110
C	-3.037151070	0.000199040	-2.740597980
C	-3.677406870	-1.219131890	-0.730685540
C	-3.662066970	0.000235220	-1.483223520
C	-3.676726540	1.219603720	-0.730772960
C	-2.202315250	-2.349296090	-2.393850430
C	-2.320412170	-1.176339640	-3.200140450
C	-3.021039750	-2.424104450	-1.192514790
C	-0.931720150	3.086404770	-2.400614230
C	0.147502180	2.604591960	-3.205146920
C	-2.695179450	3.230782040	-0.025423470
C	-1.449897280	3.959583340	-0.039692370
C	-0.590274620	3.841009870	-1.209332850
C	-3.008689310	2.424374910	1.150438150
C	-2.175751640	2.348829550	2.339762210
C	-2.245672030	1.171547530	3.149176730
C	-3.663925410	-1.218412840	0.697217220
C	-3.623483670	0.000249670	1.449795620
C	-3.663405110	1.218815190	0.697104000
C	-2.959456410	0.000376020	2.690458180
C	0.784843720	3.824641960	-0.753384680
C	1.838029020	3.187011080	-1.489391970
C	1.525295050	2.636744470	-2.741353570
C	2.896728060	2.583471470	-0.727769750
C	0.780443640	3.831496450	0.669997860
C	1.510341800	2.672729360	2.674478720

C	1.819077460	3.198285580	1.420905810
C	2.879086150	2.579227000	0.697145150
C	-0.925879260	3.101570440	2.320575970
C	-0.590837860	3.852409360	1.126419990
C	0.143433160	2.641895870	3.132674340
C	-1.145581300	-0.729743630	3.983348310
C	-1.145631380	0.730765680	3.983296130
C	0.020294570	1.529661640	4.039726350
C	0.020365070	-1.528584560	4.039830580
C	-3.008604140	-2.423631810	1.150607210
C	-2.175647010	-2.347946280	2.339894940
C	-2.245624460	-1.170672100	3.149306880
C	-0.590626230	-3.851619700	1.126737830
C	-1.449685230	-3.958919590	-0.039355120
C	-2.694787260	-3.229896960	-0.025180410
C	0.143541510	-2.640905870	3.132885520
C	-0.925733460	-3.100647330	2.320781440
C	2.879216260	-2.578429840	0.697361820
C	1.510450080	-2.671762280	2.674688980
C	1.819245490	-3.197484390	1.421189400
C	0.780683860	-3.830938090	0.670316270
C	1.356215400	1.054218850	4.286532520
C	1.356247740	-1.053009800	4.286500990
C	2.216510540	-1.529528420	3.238724060
C	3.106770630	-0.744544250	2.421439270
C	3.553445800	-1.391658840	1.180271330
C	1.706090110	0.000593550	5.243146880
F	3.031353300	0.000597380	5.614516160
F	0.939591160	0.000574230	6.382844360

Optimized anionic intermediates for the nucleophilic route

PHHJ-1

N	0.011578560	0.000021840	0.000288710
Sc	2.010126150	-0.151877010	0.000337560
Sc	-0.963384540	-1.759030000	0.000732620
Sc	-0.975411580	1.761840030	-0.000252830
C	3.573222240	1.409013610	-1.160604100
C	3.127657000	0.758421410	-2.369016120
C	2.169209760	1.449430050	-3.187054800
C	1.231790870	0.729778180	-4.000213050
C	1.236253120	-0.681222010	-3.979352130
C	4.117762850	0.740852140	0.000313270
C	4.425022950	-0.751785160	0.000772270
C	3.674500340	-1.400485760	-1.202764010
C	3.146469960	-0.710918080	-2.353503600
C	2.175638330	-1.393324150	-3.166618670
C	2.168715130	1.451299730	3.186967680
C	3.127297320	0.759817920	2.369491840
C	3.573029030	1.409685410	1.160751260
C	-1.237516930	0.725948860	-3.990294880
C	-1.231085820	-0.716674340	-3.987531960
C	-0.021878100	1.435619760	-3.993335150
C	-0.008861740	-1.408528120	-3.980363110
C	0.147108310	-2.594458060	-3.180700800
C	-0.930067510	-3.077809220	-2.370292630
C	-0.583055810	-3.825366230	-1.171670500
C	2.905766830	-2.529728620	-0.711803290
C	1.835149650	-3.127219270	-1.449252500
C	1.521117540	-2.607622290	-2.716100000
C	0.787762830	-3.772440360	-0.709381840
C	-3.032752750	2.411679960	-1.171055500
C	-2.218788230	2.345327100	-2.368627400
C	-2.335206990	1.174117540	-3.180580060
C	-3.049521630	-0.005615970	-2.720384760
C	-3.697821010	-1.228395250	-0.713696930
C	-3.685531230	-0.007614860	-1.467245080
C	-3.703307510	1.212884600	-0.714481850
C	-2.202114200	-2.348509190	-2.370003910
C	-2.331297310	-1.180676500	-3.185463640
C	-3.019559790	-2.422989170	-1.169159590
C	-0.950120280	3.090000460	-2.375456600
C	0.123148950	2.616369200	-3.183399960
C	-2.707013530	3.215364660	-0.000952370
C	-1.466020270	3.951829670	-0.001071220
C	-0.608086080	3.837908420	-1.172249800
C	-3.032973930	2.412384910	1.169576780

C	-2.219175060	2.346720140	2.367303040
C	-2.335726550	1.175982450	3.179924170
C	-3.697940810	-1.227977040	0.714223090
C	-3.685781270	-0.006754590	1.467063600
C	-3.703429880	1.213305320	0.713585800
C	-3.049960400	-0.004023830	2.720297820
C	0.764004070	3.809498110	-0.714396850
C	1.817865870	3.188943940	-1.465082100
C	1.507468100	2.650325280	-2.725436040
C	2.880138020	2.598465260	-0.711867440
C	0.763889140	3.809924020	0.712703370
C	1.507051140	2.651938650	2.724551420
C	1.817626560	3.189787820	1.463911370
C	2.880016250	2.598873120	0.711210170
C	-0.950505360	3.091405160	2.373904120
C	-0.608277080	3.838635440	1.170324550
C	0.122643140	2.618195320	3.182261600
C	-1.231750990	-0.714342130	3.988176040
C	-1.238167110	0.728284790	3.990072550
C	-0.022514320	1.437940860	3.992888450
C	-0.009507710	-1.406164790	3.981527430
C	-3.019767280	-2.422314310	1.170491680
C	-2.202517440	-2.347124230	2.371421280
C	-2.331813950	-1.178806050	3.186172320
C	-0.583249610	-3.824691570	1.174209280
C	-1.439918020	-3.950215260	0.001231420
C	-2.687929950	-3.222488290	0.000924760
C	0.146583720	-2.592544290	3.182575300
C	-0.930462490	-3.076409530	2.372315490
C	2.905641250	-2.529302460	0.714136610
C	1.520659530	-2.605987910	2.718222360
C	1.834923840	-3.126385150	1.451766890
C	0.787647250	-3.772038740	0.712111990
C	1.231163480	0.732117190	4.000389160
C	1.235626910	-0.678894870	3.980360740
C	2.175139210	-1.391472630	3.168184280
C	3.146067600	-0.709531710	2.354807180
C	3.674282930	-1.399766530	1.204557040
C	5.965476910	-0.999454730	0.000976120
F	6.541465540	-0.430353950	1.097517700
F	6.541632790	-0.431100840	-1.095863770
Cl	6.402466910	-2.764366260	0.001612430

PHHJ-2

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Sc	-1.059846240	1.720801580	0.042947790
C	3.618201610	1.399444240	-1.161040360
C	3.127055450	0.730770140	-2.349777400
C	2.185259270	1.426192600	-3.174045390
C	1.240725580	0.705821370	-3.984704220
C	1.233918490	-0.699881890	-3.985369680
C	4.144922880	0.704855920	0.017511280
C	4.142295370	-0.729656070	0.015597530
C	3.559143990	-1.392185160	-1.124714570
C	3.100784120	-0.733837060	-2.326643730
C	2.169020370	-1.427730840	-3.168619120
C	2.152343790	1.402724690	3.147932350
C	3.109193240	0.690881810	2.337346160
C	3.633084820	1.408915440	1.180870850
C	-1.227038200	0.732978330	-4.000407720
C	-1.231874960	-0.707080810	-4.000488540
C	-0.005328650	1.429814330	-3.990238190
C	-0.014923450	-1.415605310	-3.995774250
C	0.133977400	-2.593680460	-3.182216220
C	-0.946598930	-3.074531890	-2.379868020
C	-0.607370980	-3.835600690	-1.181725640
C	2.877194080	-2.587462050	-0.680920780
C	1.818435330	-3.157934390	-1.446842800
C	1.511067260	-2.625914910	-2.716991470
C	0.761689130	-3.784047210	-0.711707610
C	-3.025627500	2.441188750	-1.185213380
C	-2.203664150	2.362554530	-2.384571210
C	-2.327493450	1.194412830	-3.194155310
C	-3.047395110	0.016000980	-2.735629430
C	-3.709610500	-1.204214280	-0.729873820
C	-3.681078510	0.015581730	-1.481053380
C	-3.691160870	1.238910510	-0.729073810
C	-2.209616070	-2.331094780	-2.381591020
C	-2.332778230	-1.160810640	-3.197904350
C	-3.025169620	-2.397606560	-1.182352600
C	-0.927351830	3.089232550	-2.376841980
C	0.149022970	2.612175610	-3.186882010
C	-2.705881870	3.246534800	-0.015449510
C	-1.443294070	3.947710510	-0.010991170
C	-0.583251900	3.826914680	-1.176027690
C	-3.046272840	2.448428910	1.159891130
C	-2.219600270	2.363974400	2.357917670
C	-2.346295500	1.188952450	3.164995180
C	-3.713889640	-1.204508060	0.697834320
C	-3.695759600	0.015604270	1.450314180
C	-3.699262390	1.241147880	0.698599600
C	-3.067658400	0.012465320	2.705426610
C	0.792740830	3.816632500	-0.718458790

C	1.838671000	3.184068210	-1.464318420
C	1.525816770	2.639683800	-2.720424510
C	2.899792810	2.574387880	-0.706733610
C	0.789878720	3.812312230	0.709128740
C	1.510426350	2.621321770	2.709437830
C	1.836032730	3.185068480	1.460931030
C	2.902658490	2.578241440	0.719034330
C	-0.941786840	3.089294320	2.360147680
C	-0.587497970	3.835948360	1.161913100
C	0.129083430	2.602025690	3.170623650
C	-1.260793120	-0.716102500	3.979272780
C	-1.253879200	0.726615670	3.976143750
C	-0.033417150	1.422217600	3.972584490
C	-0.045578430	-1.424728570	3.975574230
C	-3.031876900	-2.396536180	1.154189690
C	-2.223634620	-2.335016570	2.359262490
C	-2.359198660	-1.166992910	3.175520260
C	-0.611013240	-3.832249910	1.167335330
C	-1.464842090	-3.949376460	-0.007106650
C	-2.695520740	-3.195841470	-0.013737540
C	0.116665470	-2.610149580	3.175764540
C	-0.962613620	-3.083068980	2.373597360
C	2.926494010	-2.655780800	0.740230600
C	1.511982620	-2.667473510	2.750324650
C	1.838639590	-3.191930590	1.468815810
C	0.763421090	-3.780355930	0.713535370
C	1.209487200	0.690772940	3.957424730
C	1.200388570	-0.709944620	3.954240030
C	2.144384140	-1.444424210	3.156064580
C	3.118611880	-0.755518670	2.351570930
C	3.887894230	-1.567591660	1.294688210
C	5.187943550	-2.229607470	1.850550850
F	5.809520680	-2.964350820	0.884070910
F	4.915853830	-3.077918710	2.880525960
Cl	6.387108260	-0.997322940	2.455149240

PHHJ-3

N	-0.018734950	0.017501860	-0.067647310
Sc	1.993951090	-0.102428090	-0.029007970
Sc	-0.846644400	-1.807203860	-0.117269500
Sc	-1.016418950	1.739810910	-0.012759940
C	3.597589370	1.420524390	-1.133998200
C	3.135934460	0.737917070	-2.323236380
C	2.198359120	1.425659130	-3.156856500
C	1.260420670	0.700074410	-3.970212370

C	1.256712860	-0.708683170	-3.946341220
C	4.097081890	0.724810150	0.040319490
C	4.132259610	-0.714412140	0.053303040
C	3.614329580	-1.412474690	-1.112498780
C	3.137306490	-0.732213330	-2.302818890
C	2.186347270	-1.421829140	-3.123034690
C	2.146330290	1.458875640	3.197903930
C	3.084843920	0.755985420	2.385690500
C	3.565273570	1.423520440	1.194953050
C	-1.205284770	0.712432610	-3.987128270
C	-1.208231890	-0.727278520	-3.971243370
C	0.016007420	1.417345130	-3.984875540
C	0.008027670	-1.429835750	-3.946165410
C	0.153836150	-2.604899990	-3.129328720
C	-0.944572860	-3.100911960	-2.338332430
C	-0.600150010	-3.868125900	-1.148037210
C	2.922101310	-2.602351690	-0.660714460
C	1.835768090	-3.153260190	-1.390913080
C	1.518840950	-2.627128980	-2.658558470
C	0.770304330	-3.812506510	-0.674719370
C	-3.023137310	2.432880150	-1.198245530
C	-2.190902860	2.350234410	-2.387686250
C	-2.306563930	1.172671230	-3.188798810
C	-3.032394180	-0.001706040	-2.725200440
C	-3.730461100	-1.204685570	-0.722799900
C	-3.690121520	0.010973660	-1.479804060
C	-3.703743540	1.239299340	-0.740135680
C	-2.203986190	-2.348923930	-2.350780480
C	-2.318510500	-1.178960220	-3.173180360
C	-3.034812490	-2.397466520	-1.161740190
C	-0.917911030	3.082672270	-2.381654010
C	0.164022190	2.599830990	-3.179068790
C	-2.700037270	3.241059540	-0.030658210
C	-1.448397840	3.957057460	-0.024189060
C	-0.579468540	3.835894710	-1.185428020
C	-3.043504310	2.450223680	1.142322190
C	-2.231644660	2.385575590	2.348464700
C	-2.361376970	1.220820450	3.165217160
C	-3.735956580	-1.191318810	0.706473160
C	-3.708284890	0.033178820	1.448102570
C	-3.713435550	1.251392690	0.689506510
C	-3.079706210	0.042731640	2.707500650
C	0.791595520	3.825399870	-0.718122510
C	1.853362310	3.202447520	-1.456587660
C	1.539299360	2.638513910	-2.707866560
C	2.921254320	2.626576720	-0.695177590
C	0.778306120	3.833020570	0.709124190
C	1.493704950	2.665983540	2.723322460
C	1.824818020	3.215027490	1.471820950

C	2.901834960	2.625850440	0.732703600
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C	-0.599490950	3.851683440	1.153053680
C	0.110679230	2.638091150	3.174428350
C	-1.274670510	-0.668113750	4.000568780
C	-1.274839130	0.771990190	3.993963870
C	-0.051747540	1.467342010	3.991407360
C	-0.056373150	-1.368062890	4.001786400
C	-3.031757020	-2.365700300	1.170540940
C	-2.238719200	-2.296706790	2.379446280
C	-2.369970250	-1.129187020	3.187291170
C	-0.611263430	-3.782109300	1.200420780
C	-1.466118250	-3.943056650	0.029371610
C	-2.686433890	-3.172781010	0.015683590
C	0.100175870	-2.541135020	3.190535180
C	-0.968301460	-3.029282340	2.388676110
C	3.148409860	-2.818253060	0.839198150
C	1.485481560	-2.582131260	2.740524260
C	1.823275080	-3.165781790	1.517692870
C	0.765649510	-3.743714920	0.753969850
C	1.196620910	0.746605590	4.012341210
C	1.198165970	-0.656475220	4.008095370
C	2.160012250	-1.398598660	3.235759820
C	3.095831580	-0.717474470	2.387516370
C	3.618329670	-1.397964040	1.233474860
C	4.266782300	-3.861780290	1.162595110
F	4.529865580	-3.897378600	2.500133520
F	5.435766820	-3.541678380	0.538773080
Cl	3.819618710	-5.551551080	0.642676160

PHHJ-4

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Sc	2.003042560	-0.256254540	0.243611910
Sc	-0.757666420	-1.847640310	0.234493090
Sc	-0.971302810	1.723613550	-0.000952030
C	3.575265710	1.435839600	-1.202904600
C	3.129346830	0.773747570	-2.405912100
C	2.173552410	1.462557450	-3.220745230
C	1.231133210	0.739619460	-4.023034790
C	1.232914850	-0.670322050	-4.021387270
C	4.091947810	0.737015020	-0.039597960
C	4.175412440	-0.692426530	-0.037918840
C	3.610991110	-1.355095120	-1.198009650
C	3.134393090	-0.687601390	-2.404850320
C	2.181333160	-1.384057510	-3.209361520
C	2.189344030	1.437828160	3.139496090
C	3.152047550	0.749237960	2.332650720

C	3.605914560	1.433929710	1.137554300
C	-1.237951680	0.746455520	-4.008759880
C	-1.236827050	-0.696595260	-4.017805710
C	-0.022955270	1.453722220	-4.011530580
C	-0.011774910	-1.394486630	-4.018434290
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C	-0.584297070	-3.796268070	-1.190067150
C	2.887562670	-2.513686740	-0.727017560
C	1.823518030	-3.107836720	-1.476839680
C	1.524715280	-2.599137360	-2.748621030
C	0.781716600	-3.735031500	-0.723114430
C	-3.021985070	2.422562360	-1.179144260
C	-2.209381640	2.361346630	-2.380421850
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C	-2.199596070	-2.327208330	-2.394900160
C	-2.328596100	-1.157064530	-3.210804370
C	-2.992295310	-2.386592570	-1.188758980
C	-0.942163750	3.099764910	-2.383458240
C	0.130395740	2.631206770	-3.202943500
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C	-2.311686900	1.174368860	3.160943610
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C	-3.671483200	-0.007643440	1.444621220
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C	-3.025266440	-0.004175730	2.698784480
C	0.784096010	3.828246350	-0.734615740
C	1.838936590	3.213663300	-1.489675250
C	1.510472860	2.660653540	-2.741725220
C	2.917007370	2.636170440	-0.744819330
C	0.792002160	3.828753430	0.692544640
C	1.533460340	2.648437470	2.689207370
C	1.852033550	3.205999470	1.433145310
C	2.926937950	2.637889860	0.685637930
C	-0.925119690	3.087700580	2.349841310
C	-0.581552460	3.838980520	1.155092190
C	0.157312300	2.611437610	3.155317980
C	-1.199387610	-0.713202790	3.952577270
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C	0.005936810	1.432771770	3.959258620
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C	-2.640082120	-3.181793170	-0.025316560
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C	-0.909678530	-3.108412970	2.368602140
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C	1.250630570	0.713626390	3.946767810
C	1.264998020	-0.693526540	3.938709090
C	2.231377040	-1.400860210	3.171323180
C	3.188090910	-0.725215920	2.358885050
C	3.721480690	-1.418031190	1.169941060
C	2.335462340	-3.857063230	3.846883020
F	2.188389500	-3.516453240	5.158246720
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Cl	1.657742340	-5.534488040	3.640293440

PHHJ-5

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Sc	1.983897420	-0.231879870	0.261668000
Sc	-1.073851090	-1.700349290	-0.059330610
Sc	-0.850665680	1.811257780	-0.006975060
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C	3.126287830	0.746120500	-2.401972240
C	2.181040250	1.442181380	-3.213324440
C	1.231177910	0.718225420	-4.015303650
C	1.233175690	-0.687581160	-4.017586300
C	4.074419480	0.713776050	-0.028389410
C	4.144666570	-0.721643830	-0.028398400
C	3.597414380	-1.390165580	-1.199999510
C	3.133664260	-0.716779880	-2.404774160
C	2.183209210	-1.409097130	-3.212622260
C	2.216021360	1.451036140	3.188052450
C	3.127143920	0.729144740	2.341210160
C	3.578154660	1.416691380	1.146407800
C	-1.234870150	0.729593050	-4.004657330
C	-1.233304490	-0.711392700	-4.003667460
C	-0.018183790	1.437015900	-4.007556920
C	-0.014382460	-1.409644340	-4.005334410
C	0.143132650	-2.593528140	-3.203874680
C	-0.933244670	-3.070120120	-2.387345890
C	-0.583445800	-3.811292300	-1.188886810

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C	1.844655890	-3.165067980	-1.492375980
C	1.522514330	-2.617790920	-2.744660920
C	0.790648050	-3.785691870	-0.736050600
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C	-2.203363690	2.346360110	-2.381195940
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C	-3.052658810	0.004233950	-2.738527800
C	-3.699616810	-1.221289890	-0.731969380
C	-3.686922960	0.003665190	-1.480320660
C	-3.713902180	1.221239670	-0.729259190
C	-2.211057920	-2.347106110	-2.386541220
C	-2.332501130	-1.168520230	-3.193628120
C	-3.044153230	-2.431217050	-1.191668210
C	-0.937327000	3.091014840	-2.384990130
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C	-2.670185760	3.199295500	-0.016339340
C	-1.450408010	3.967579000	-0.017193730
C	-0.592792620	3.852695900	-1.190051400
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C	-3.680860120	0.003929660	1.448362590
C	-3.711097580	1.221994290	0.699378530
C	-3.039817690	0.004670610	2.701795850
C	0.779531330	3.810208420	-0.729249610
C	1.837380800	3.191573090	-1.484829780
C	1.522408600	2.648640160	-2.742332390
C	2.904390580	2.608976190	-0.733422130
C	0.784254220	3.811756240	0.702133310
C	1.536910480	2.635716840	2.699802070
C	1.851897360	3.214924280	1.456316690
C	2.909619360	2.614623230	0.695400840
C	-0.928621490	3.088711310	2.349566560
C	-0.588628040	3.856607970	1.160517500
C	0.151086250	2.596438890	3.146789250
C	-1.212827190	-0.713933190	3.957009950
C	-1.217079120	0.720843380	3.957554740
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C	-1.442490930	-3.930404510	-0.018377140
C	-2.710875220	-3.227983770	-0.018355100
C	0.163046940	-2.581092140	3.141908380
C	-0.918742810	-3.059195050	2.346198440

C	2.944866940	-2.581483130	0.695688680
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C	1.254398440	0.698135770	3.958614480
C	1.259241180	-0.695956170	4.012324060
C	2.381539340	-1.537103990	3.388526000
C	3.172400210	-0.722724180	2.344740840
C	3.679264700	-1.431615790	1.162944850
C	3.326015690	-2.170918400	4.455294020
F	4.213599010	-3.029684840	3.872574660
F	2.625764260	-2.894188020	5.374516120
Cl	4.294691880	-0.923963500	5.359949320

PHHJ-6

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C	3.139150490	0.734651460	-2.375796040
C	2.193088630	1.424117870	-3.195196430
C	1.252551370	0.695606050	-4.005573020
C	1.252156770	-0.708916180	-3.999959370
C	4.159884920	0.745739740	-0.001922750
C	4.098326690	-0.700375190	0.004974870
C	3.574654970	-1.387096710	-1.156938570
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C	2.197684120	-1.431548670	-3.191507620
C	2.143460770	1.408462350	3.148244710
C	3.157277780	0.753551340	2.370220550
C	3.649950040	1.440175940	1.179815950
C	-1.213717920	0.715912440	-4.014234160
C	-1.214239700	-0.725172540	-4.010620090
C	0.004589630	1.416896070	-4.010592840
C	0.003113400	-1.429338440	-4.001563060
C	0.153679600	-2.605235970	-3.188979570
C	-0.927826190	-3.085755050	-2.386784270
C	-0.588569020	-3.844000200	-1.186358760
C	2.903447460	-2.588211010	-0.709498920
C	1.842294170	-3.177417630	-1.467567120
C	1.534552500	-2.641707080	-2.728318890
C	0.781525390	-3.793954960	-0.716920350
C	-3.029059640	2.428775620	-1.212914460
C	-2.196420140	2.348696820	-2.405677640
C	-2.315850970	1.174075510	-3.212006750
C	-3.038141080	-0.002068590	-2.755461330

C	-3.711615320	-1.215087300	-0.748852980
C	-3.677270190	0.002106460	-1.502458230
C	-3.692253080	1.228502210	-0.756543360
C	-2.192459840	-2.342590270	-2.390677990
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C	-3.007978540	-2.400139100	-1.193240560
C	-0.925595170	3.079059870	-2.404212860
C	0.155927750	2.602001510	-3.211364530
C	-2.710106650	3.236329640	-0.039549120
C	-1.445612440	3.936825480	-0.037918980
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C	-2.329302660	1.193511470	3.154839290
C	-3.710525890	-1.209155600	0.680274030
C	-3.682443190	0.012060120	1.428837460
C	-3.701722530	1.234616480	0.675376320
C	-3.041283330	0.015208200	2.680583550
C	0.790519090	3.815329760	-0.744028850
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C	1.531833930	2.638247170	-2.748777780
C	2.903187930	2.587660000	-0.733173450
C	0.785207930	3.814916550	0.682042130
C	1.493496060	2.627142910	2.678980300
C	1.826954470	3.181881820	1.437638820
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C	-0.944563800	3.087007560	2.331505830
C	-0.590858490	3.827789470	1.134338520
C	0.125214370	2.602320550	3.138214440
C	-1.230029510	-0.700784740	3.963539300
C	-1.254882210	0.747420610	3.992386890
C	-0.013653230	1.417266500	3.947641220
C	-0.035813990	-1.419767760	4.007958430
C	-3.018935650	-2.393818000	1.138112650
C	-2.203925940	-2.322922430	2.337808440
C	-2.321296560	-1.152785900	3.140154750
C	-0.593849150	-3.833751360	1.164242090
C	-1.449372820	-3.953395060	-0.014696330
C	-2.673290140	-3.190624860	-0.023601090
C	0.127278000	-2.548192380	3.160253970
C	-0.940435790	-3.054201900	2.350229680
C	2.896023930	-2.582429270	0.718369300
C	1.514091890	-2.590229490	2.711288350
C	1.831462100	-3.168925370	1.473961870
C	0.773243380	-3.782910190	0.711647860
C	1.231875300	0.727585020	3.992628680
C	1.333626140	-0.749337880	4.277578960
C	2.207617270	-1.426664480	3.210000780
C	3.122861510	-0.729004110	2.382447900

C	3.575810500	-1.393448100	1.175977040
C	1.798364080	-1.063003590	5.730426370
F	1.838440000	-2.406614850	5.968360920
F	0.937727600	-0.527927190	6.642513830
Cl	3.457494610	-0.401086930	6.090682740

THJ-1

N	-0.015412080	0.000569070	0.001192510
Sc	2.014823410	0.023716000	-0.053619980
Sc	-0.951295250	-1.771624880	0.015946200
Sc	-1.025013580	1.726967350	0.031818070
C	3.626253030	1.397816720	-1.167676480
C	3.137894310	0.727810390	-2.358997680
C	2.187307060	1.425768830	-3.183055690
C	1.245166730	0.703954240	-3.990415100
C	1.239383570	-0.703452060	-3.990281260
C	4.151464880	0.710170710	0.009012420
C	4.126604610	-0.735773820	0.021561540
C	3.596168400	-1.411475480	-1.156897080
C	3.128502340	-0.738131560	-2.357017310
C	2.176252400	-1.427696690	-3.174666830
C	2.155690960	1.388809890	3.162309580
C	3.134973910	0.717255890	2.380559350
C	3.584039920	1.371128620	1.180435360
C	-1.221968800	0.727596110	-4.005121270
C	-1.227874570	-0.713212860	-4.008072900
C	-0.002482960	1.427701620	-3.998735650
C	-0.010348270	-1.419639550	-3.998315100
C	0.134541760	-2.600478960	-3.190420980
C	-0.946325610	-3.076524600	-2.383541170
C	-0.611868790	-3.829597860	-1.183705810
C	2.864078090	-2.569006450	-0.698740730
C	1.808791670	-3.168521180	-1.458065330
C	1.511056190	-2.635780910	-2.722834510
C	0.759153920	-3.796855670	-0.714622020
C	-3.020607900	2.431884080	-1.193407400
C	-2.197685880	2.356211420	-2.388885150
C	-2.323082910	1.187423970	-3.202283430
C	-3.045524000	0.012485470	-2.745207980
C	-3.714712100	-1.205969670	-0.740798160
C	-3.683681710	0.013810690	-1.491958150
C	-3.695747830	1.235204260	-0.740521490
C	-2.211776900	-2.333120170	-2.388331170
C	-2.330396650	-1.165625460	-3.205467320
C	-3.030492510	-2.399059670	-1.192675290
C	-0.924304660	3.085075590	-2.385973760
C	0.151089920	2.609025810	-3.195490630

C	-2.699877740	3.234271880	-0.019809870
C	-1.442182840	3.943695240	-0.015597070
C	-0.581147460	3.821849190	-1.180629650
C	-3.040183820	2.436442570	1.150485850
C	-2.222958260	2.357899780	2.353397800
C	-2.343354260	1.183192390	3.160962510
C	-3.721437500	-1.207802560	0.687274250
C	-3.696336790	0.012471990	1.439864820
C	-3.704322090	1.236692540	0.688190370
C	-3.067593390	0.009700020	2.696118000
C	0.792124370	3.799104200	-0.720787810
C	1.843030800	3.171561980	-1.468206280
C	1.531820670	2.635111090	-2.730312600
C	2.904816990	2.570159360	-0.712656600
C	0.785178160	3.798594530	0.705528330
C	1.498483990	2.596285550	2.697645880
C	1.826506480	3.157498060	1.455874180
C	2.887506790	2.557272080	0.713278000
C	-0.942365710	3.077989720	2.356519390
C	-0.588103570	3.828108660	1.159952200
C	0.126320770	2.582784030	3.163180570
C	-1.259497100	-0.717645880	3.968190380
C	-1.257407240	0.723040900	3.980790340
C	-0.025054930	1.405742010	3.979816250
C	-0.047238340	-1.422751270	3.967111590
C	-3.047712420	-2.406296540	1.144339550
C	-2.236060160	-2.339568560	2.346667150
C	-2.357319190	-1.170026350	3.158255370
C	-0.621019550	-3.840709890	1.162610780
C	-1.475165230	-3.949794560	-0.018449230
C	-2.708911270	-3.203869100	-0.024488360
C	0.101513710	-2.596114980	3.165849710
C	-0.967256070	-3.079200740	2.355006790
C	2.854533350	-2.556187190	0.728058750
C	1.496119640	-2.617186900	2.721375220
C	1.812383900	-3.196649070	1.475867920
C	0.757552670	-3.798553850	0.716403400
C	1.223431950	0.692654430	4.011570390
C	1.222966580	-0.721890980	3.981053750
C	2.171982310	-1.465647470	3.230135900
C	3.416477720	-0.815883620	2.589685210
C	3.595536950	-1.413349160	1.185766860
C	4.689660380	-0.985579560	3.473344860
F	4.512204470	-0.436456130	4.706198260
F	5.764335730	-0.354646050	2.912103000
Cl	5.145485540	-2.731933120	3.703799150

THJ-2

N	-0.004882110	-0.023211040	0.136677680
Sc	1.995289330	0.143933250	0.217576270
Sc	-1.001494710	-1.752325470	0.023849000
Sc	-0.864692870	1.790827040	0.214245220
C	3.589873500	1.385079890	-1.149017000
C	3.128193310	0.724181950	-2.358339350
C	2.188119030	1.422432700	-3.172763510
C	1.244824360	0.700445180	-3.986600700
C	1.248590480	-0.703956740	-3.996829820
C	4.142993950	0.714352060	0.014133340
C	4.101969310	-0.727488540	0.006301380
C	3.578519410	-1.407469830	-1.161250520
C	3.129278330	-0.739832940	-2.365655380
C	2.193363540	-1.431498110	-3.189975410
C	2.149973960	1.398595720	3.153957370
C	3.157967210	0.707609770	2.389271750
C	3.646002400	1.415006230	1.200082400
C	-1.220374260	0.716430200	-3.997844430
C	-1.217740390	-0.724943820	-4.001691590
C	-0.004726450	1.419371850	-3.987256790
C	0.001355470	-1.426334170	-4.001271950
C	0.155902690	-2.606112130	-3.195680670
C	-0.921139550	-3.088810240	-2.390820650
C	-0.577394150	-3.839589060	-1.194865330
C	2.912421840	-2.610939190	-0.718729910
C	1.849041490	-3.195915180	-1.477355610
C	1.534044720	-2.640571700	-2.730894100
C	0.793748430	-3.823456460	-0.733461530
C	-3.001858100	2.377828890	-1.164358260
C	-2.197942650	2.324850160	-2.367924800
C	-2.325005680	1.167883960	-3.192270260
C	-3.038818360	-0.009751090	-2.733053640
C	-3.690355960	-1.243778640	-0.735740400
C	-3.678325990	-0.016255650	-1.480098030
C	-3.708036360	1.197350350	-0.722001330
C	-2.192411040	-2.357611010	-2.391479500
C	-2.315833380	-1.184045890	-3.196731770
C	-3.015286950	-2.437748350	-1.196197620
C	-0.931915920	3.060339440	-2.359817110
C	0.144489170	2.598574740	-3.174107080
C	-2.677689650	3.172467540	0.003168380
C	-1.452301700	3.933165280	0.011703330
C	-0.593652180	3.792930000	-1.150860500
C	-3.039868060	2.384824310	1.170693220
C	-2.219543980	2.322621710	2.369374090
C	-2.349875750	1.136237480	3.175248960
C	-3.699647250	-1.251792730	0.691641270

C	-3.699280280	-0.033023580	1.449867250
C	-3.722334320	1.193852680	0.707052810
C	-3.058461170	-0.036246170	2.700644800
C	0.774499490	3.765502550	-0.682074680
C	1.834966560	3.175012810	-1.449954580
C	1.520914810	2.627729540	-2.703356420
C	2.876137220	2.552738300	-0.682056980
C	0.768635070	3.798306830	0.737777480
C	1.507878290	2.608800510	2.741019010
C	1.986858430	3.444247740	1.583239220
C	2.901578530	2.560476580	0.737505520
C	-0.963754110	3.077591960	2.385586050
C	-0.597177630	3.856980500	1.197817240
C	0.138691690	2.553302530	3.151401670
C	-1.246104950	-0.767964380	3.968862900
C	-1.248215800	0.673310140	3.968804050
C	-0.029581410	1.369144420	3.965602220
C	-0.026970320	-1.469004940	3.969515190
C	-3.030932820	-2.455095890	1.142741590
C	-2.213888270	-2.387026140	2.344262670
C	-2.340723840	-1.219748070	3.156848580
C	-0.586169200	-3.860674830	1.143778080
C	-1.441247820	-3.965291330	-0.031872760
C	-2.690605750	-3.247219000	-0.032532850
C	0.133291040	-2.642627440	3.158130500
C	-0.938958390	-3.120129830	2.344859370
C	2.915486190	-2.624157260	0.710233840
C	1.517400250	-2.668451460	2.702816700
C	1.843159010	-3.221569640	1.452624620
C	0.790591460	-3.835336050	0.693895870
C	1.209630720	0.657153320	3.967407700
C	1.220234620	-0.746070200	3.969913540
C	2.174887450	-1.466524530	3.177747730
C	3.135765780	-0.757807980	2.372693090
C	3.602713990	-1.435987250	1.174220350
C	2.778846010	4.720201180	2.023912300
F	3.225344590	5.420581970	0.937939290
F	3.878844520	4.378497240	2.750739200
Cl	1.782145130	5.854787020	3.031356860

Optimized transition states for nucleophilic route

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N	0.052859950	0.016663950	0.000306350
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C	3.575319570	1.484008510	-1.176655510
C	3.138895840	0.800268450	-2.363075180
C	2.165591800	1.475805840	-3.180415790
C	1.237278490	0.748782300	-3.993802960
C	1.254583370	-0.662268550	-3.978552250
C	4.185899480	0.864493140	0.000336640
C	4.359070120	-0.759334040	0.000782580
C	3.683386700	-1.382398980	-1.205439010
C	3.171302240	-0.681497930	-2.354546600
C	2.199917200	-1.367132300	-3.166626450
C	2.164962240	1.477626980	3.180203630
C	3.138514520	0.801546590	2.363540450
C	3.575308010	1.484803000	1.176934920
C	-1.231908360	0.727660910	-3.990516870
C	-1.213388610	-0.714729220	-3.988557340
C	-0.022233900	1.445856540	-3.990625180
C	0.014480780	-1.397384040	-3.981123090
C	0.177516930	-2.580785240	-3.180097230
C	-0.894939100	-3.073194060	-2.370304330
C	-0.544985980	-3.820615290	-1.171841550
C	2.930222690	-2.513103940	-0.711853620
C	1.865461980	-3.112033300	-1.451902390
C	1.550509530	-2.583531330	-2.712619090
C	0.824344440	-3.761822060	-0.709910630
C	-3.046072540	2.400055980	-1.171501100
C	-2.228977850	2.339720580	-2.369485590
C	-2.334051830	1.167212140	-3.182144940
C	-3.036900930	-0.018422140	-2.721777760
C	-3.677032200	-1.245029790	-0.713797220
C	-3.671084780	-0.025939390	-1.467077430
C	-3.701250180	1.193753860	-0.714567650
C	-2.170931620	-2.353002430	-2.369410910
C	-2.308509450	-1.186338970	-3.185748740
C	-2.986429850	-2.432189510	-1.168698230
C	-0.968385750	3.092050840	-2.373635660
C	0.110256930	2.628474600	-3.182922250
C	-2.729067770	3.204538310	-0.000964770
C	-1.494003490	3.946570330	-0.001081180
C	-0.635503930	3.843425240	-1.171626770

C	-3.046285590	2.400747500	1.169993500
C	-2.229394860	2.341117120	2.368149830
C	-2.334600230	1.169078920	3.181479060
C	-3.677135420	-1.244613620	0.714328530
C	-3.671337060	-0.025078660	1.466883220
C	-3.701401940	1.194179710	0.713662290
C	-3.037357080	-0.016827780	2.721683830
C	0.735738570	3.837491030	-0.713990320
C	1.794664130	3.227029780	-1.464110290
C	1.488863600	2.670098280	-2.716543580
C	2.868051920	2.654082160	-0.715296590
C	0.735619350	3.837917260	0.712267410
C	1.488369540	2.671685100	2.715611860
C	1.794418370	3.227918000	1.462941780
C	2.867985370	2.654546880	0.714715270
C	-0.968805260	3.093456480	2.372068850
C	-0.635705060	3.844114060	1.169668580
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C	-1.232592340	0.729997580	3.990290570
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C	-2.171331510	-2.351629580	2.370856240
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C	-0.545185540	-3.819938690	1.174408920
C	-1.400249390	-3.948601270	0.001248250
C	-2.648532670	-3.226657770	0.000930070
C	0.176986670	-2.578949310	3.182059440
C	-0.895339540	-3.071825590	2.372381630
C	2.930136120	-2.512733230	0.714225630
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C	1.865234590	-3.111213190	1.454454950
C	0.824227450	-3.761419130	0.712675760
C	1.236567670	0.751111400	3.993910630
C	1.253909490	-0.659950860	3.979523560
C	2.199378980	-1.365302300	3.168182910
C	3.170957680	-0.680175790	2.355880100
C	3.683294240	-1.381790020	1.207301560
C	5.688497260	-0.203386030	0.000580960
F	6.342689750	0.089134110	1.114318270
F	6.342580540	0.088403550	-1.113425570
Cl	6.606091190	-2.691338770	0.001555680

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N	-0.002727570	0.011968340	0.042191530
Sc	2.026515920	0.006772970	0.057896360
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C	3.123304440	0.748652860	-2.348245240
C	2.176968730	1.435545430	-3.180166360
C	1.242307070	0.705632290	-3.989508530
C	1.246881080	-0.700101470	-3.981968750
C	4.146832680	0.754933930	0.030737950
C	4.153468680	-0.701996580	0.046612800
C	3.601070070	-1.371322440	-1.133616350
C	3.127654390	-0.712846670	-2.339453140
C	2.186468030	-1.412897600	-3.160163060
C	2.178053910	1.497819170	3.192419150
C	3.264254330	0.943958350	2.469957510
C	3.610407710	1.472894370	1.185152720
C	-1.224571880	0.713065560	-4.007132220
C	-1.219939400	-0.728210400	-4.002492960
C	-0.010231760	1.420860490	-4.003888850
C	0.001468800	-1.425606040	-3.990509520
C	0.152975180	-2.603250260	-3.179806330
C	-0.925093540	-3.082577800	-2.371000250
C	-0.585917610	-3.827814160	-1.168274360
C	2.875055050	-2.535539250	-0.687248190
C	1.829290870	-3.151364660	-1.445722090
C	1.527868550	-2.624990360	-2.709360840
C	0.784323610	-3.788103270	-0.700959350
C	-3.035740330	2.416527440	-1.203738270
C	-2.213243590	2.342033610	-2.399504300
C	-2.329097070	1.168529790	-3.206954760
C	-3.043959180	-0.009142330	-2.744930320
C	-3.700914580	-1.222213270	-0.733645970
C	-3.680416510	-0.006409010	-1.491087780
C	-3.702097630	1.217359600	-0.744582480
C	-2.195473160	-2.348419400	-2.377889090
C	-2.320296740	-1.184445710	-3.198554420
C	-3.014906920	-2.415666790	-1.181388220
C	-0.946228530	3.081390040	-2.400027470
C	0.133432950	2.606960160	-3.205717400
C	-2.719361550	3.225932470	-0.035840050
C	-1.471838180	3.950756090	-0.034897720
C	-0.609181810	3.830546080	-1.200398730
C	-3.051999280	2.430893360	1.138120850
C	-2.233981830	2.366263910	2.339361890
C	-2.338934210	1.194924750	3.151012130
C	-3.707368660	-1.217246210	0.694511440

C	-3.690028520	0.006127500	1.442213190
C	-3.709544620	1.225010880	0.683957190
C	-3.054713180	0.013998230	2.696086260
C	0.762705010	3.819556770	-0.739590550
C	1.817517560	3.192310290	-1.482563880
C	1.510627270	2.643793010	-2.737445520
C	2.879109160	2.601519840	-0.722720800
C	0.755964530	3.832160910	0.686867150
C	1.480305080	2.666554170	2.693953180
C	1.804465540	3.212553720	1.443584030
C	2.873021380	2.618983980	0.698605990
C	-0.964717280	3.101569580	2.340725050
C	-0.618025590	3.849707170	1.140672010
C	0.108977130	2.621472040	3.149146760
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C	-1.238988650	0.746378130	3.960990630
C	-0.017463890	1.438707040	3.957886560
C	-0.011990510	-1.383490730	3.957886680
C	-3.029320590	-2.410426960	1.156387160
C	-2.214672670	-2.331762060	2.355892390
C	-2.332963680	-1.157484330	3.159617020
C	-0.595173310	-3.828390460	1.176852520
C	-1.448521060	-3.947393950	-0.001437780
C	-2.688744410	-3.212234760	-0.009552060
C	0.125077590	-2.568658600	3.169346350
C	-0.943986920	-3.064010560	2.365990840
C	2.873799850	-2.539302880	0.734045060
C	1.507603300	-2.604590930	2.725080690
C	1.829870310	-3.173777640	1.484800970
C	0.781005950	-3.789623730	0.727769540
C	1.252844290	0.743197170	3.997340080
C	1.264396250	-0.680744360	3.977837450
C	2.205690290	-1.464907680	3.242414090
C	3.434830330	-0.959370740	2.593267460
C	3.650595190	-1.429849100	1.206204570
C	4.475895210	-0.309729720	3.327059290
F	4.354875890	0.014528710	4.601903610
F	5.629423960	0.055174340	2.785823130
Cl	5.393511480	-2.645968790	3.846891080

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N	0.016939610	-0.008234240	0.125825780
Sc	2.005992960	0.224421720	0.293833050
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Sc	-0.993145950	1.732304490	-0.026792610
C	3.605578170	1.361370920	-1.119974620
C	3.125355100	0.703764930	-2.315109690

C	2.204391570	1.406835770	-3.148602640
C	1.267756680	0.695380290	-3.975912000
C	1.261006690	-0.710606030	-3.980874890
C	4.217759330	0.699029590	0.005292120
C	4.082358070	-0.726064240	0.045160260
C	3.554137840	-1.418641560	-1.120786450
C	3.119726720	-0.757624890	-2.324877890
C	2.194577750	-1.443696430	-3.167184660
C	2.135262620	1.379630770	3.222486470
C	3.193084020	0.671220880	2.520544570
C	3.915591810	1.533213480	1.243411360
C	-1.198559720	0.728919080	-3.995897240
C	-1.205417130	-0.712443600	-4.003564330
C	0.024379300	1.423257520	-3.980845600
C	0.009473440	-1.421602390	-3.992428410
C	0.150391730	-2.604179390	-3.183651630
C	-0.934161290	-3.080849720	-2.388605050
C	-0.603375500	-3.837972720	-1.190990280
C	2.895315560	-2.626884430	-0.685599670
C	1.831256870	-3.200744050	-1.452710210
C	1.523750230	-2.642880070	-2.707808060
C	0.765056540	-3.820093880	-0.719630690
C	-3.007793070	2.432133090	-1.180966150
C	-2.175248390	2.355034220	-2.372248660
C	-2.298115980	1.187451880	-3.192469190
C	-3.026333000	0.012834210	-2.745009710
C	-3.700182260	-1.211419870	-0.750070100
C	-3.668960370	0.012006720	-1.495477810
C	-3.683369490	1.230780270	-0.736988560
C	-2.197927340	-2.336543530	-2.397720590
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C	-3.018312080	-2.404398250	-1.203880640
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C	-3.083341140	-0.015431460	2.696930810
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C	1.848103720	3.122396320	-1.415159100
C	1.551489470	2.612377050	-2.690049530
C	2.902887080	2.530471430	-0.653228880
C	0.806476850	3.741579280	0.752309430

C	1.519481170	2.590037050	2.775985560
C	1.872725400	3.140576370	1.511239150
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C	-0.572510410	3.784224510	1.193537460
C	0.117250580	2.569049940	3.211598450
C	-1.289147050	-0.753452360	3.983302750
C	-1.282273460	0.688424710	3.991143440
C	-0.063307570	1.385333910	4.002006360
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C	-3.050050880	-2.420464470	1.131758370
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C	-0.983837960	-3.110200080	2.349754300
C	2.894624840	-2.646648270	0.741062830
C	1.468980240	-2.672123140	2.719979950
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C	3.576353810	-1.444166930	1.211034870
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F	5.787965400	0.725842110	2.540392130
F	4.771142700	2.558986940	3.271836940
Cl	6.352569360	3.086709780	0.729134830

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N	0.021021390	0.011571020	0.056741980
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C	1.215761210	-0.714041610	-4.017826670
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C	4.137640390	-0.678009510	-0.035518660
C	3.580185440	-1.369953010	-1.191375440
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C	2.206230730	1.468335500	3.191286380
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C	0.136217180	-2.612597470	-3.190019250
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C	-2.351719410	1.153984670	-3.201862480
C	-3.061352220	-0.023290250	-2.730943550
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C	-3.703716650	1.206737490	-0.725748990
C	-2.203545600	-2.360515800	-2.368326650
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C	-3.009871840	-2.426535410	-1.164290260
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C	0.781407840	3.798061660	0.670826990
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C	-0.910403690	-3.066967100	2.370159100
C	2.924367580	-2.554748750	0.698338400
C	1.534983390	-2.585626470	2.689232050
C	1.862082350	-3.147243750	1.446989930
C	0.806786680	-3.783331950	0.706792180
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C	2.192620690	-1.381690630	3.145007860
C	3.195795670	-0.727684180	2.382114740
C	3.625018200	-1.362415060	1.158307750
C	4.699750730	1.369476950	2.662250420
F	4.894395390	2.594050720	3.127023440
F	5.815240930	0.741996520	2.315740250
Cl	4.915028770	0.289601040	5.103310340

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N	-0.017920810	0.004276260	-0.018063740
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C	2.188110810	1.433746630	-3.147735160
C	1.258721170	0.707954890	-3.965651660
C	1.266422710	-0.698858030	-3.967463340
C	4.126155870	0.743793170	0.051794740
C	4.149529010	-0.699657730	0.041515840
C	3.642109210	-1.390728340	-1.137131140
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C	2.205071430	-1.418848150	-3.155207030
C	2.178017850	1.526321060	3.332179610
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C	0.019783990	-1.424608630	-3.983180610
C	0.171114280	-2.605553400	-3.179720260

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C	-0.570776290	-3.826986020	-1.170951180
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C	0.799367420	-3.788880180	-0.702088330
C	-3.034572250	2.398849560	-1.198505710
C	-2.207108490	2.334099590	-2.390379720
C	-2.316986280	1.165030970	-3.202801500
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C	-3.681759010	-0.017481830	-1.499082420
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C	-2.304176580	-1.185743640	-3.198343830
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C	0.144913340	2.604687100	-3.177788370
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C	-3.709559770	-0.014792120	1.430295210
C	-3.732009470	1.205516760	0.677276630
C	-3.087014620	-0.009463360	2.691528540
C	0.753279870	3.800718340	-0.699949280
C	1.812057700	3.176304250	-1.437068480
C	1.519704890	2.641834090	-2.701363850
C	2.866607900	2.580820950	-0.672590130
C	0.741613390	3.802346170	0.728837360
C	1.468281150	2.663598450	2.753029390
C	1.793442420	3.203407510	1.501254690
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C	-0.637716630	3.841152050	1.167128070
C	0.084662590	2.599836540	3.167222240
C	-1.279736310	-0.714466930	3.982811080
C	-1.289131570	0.722366580	3.975257780
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C	1.185367690	0.729724680	4.024010100
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C	3.577134370	-1.361352100	1.204899560
C	3.975186380	1.371539830	3.743416890
F	4.058281770	0.753276200	4.909057430
F	4.525894430	2.575930770	3.738374220
Cl	6.324182740	0.185446150	2.995479870

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N	0.019054950	-0.007272170	-0.001881480
Sc	2.041071060	0.080875180	-0.008983860
Sc	-0.910718620	-1.784277970	-0.012900790
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C	1.206010350	-0.719603030	-4.024147600
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C	0.106897610	-2.613284030	-3.212239490
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C	-0.611409850	-3.844410920	-1.197777630
C	2.896586520	-2.625318330	-0.774170030
C	1.818550230	-3.203726950	-1.516643440
C	1.496123430	-2.659386950	-2.771260020
C	0.766995030	-3.816850310	-0.752785630
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C	-2.197759650	2.352928580	-2.361925950

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C	-3.704222770	-1.207012290	-0.701952400
C	-3.682756270	0.014525620	-1.448674040
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C	-2.225064860	-2.336416130	-2.372084580
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C	2.920803570	2.535006480	-0.755527610
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C	1.596775840	2.665526990	2.735675610
C	1.889510710	3.142197170	1.461762010
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C	2.909175550	-2.628237120	0.653441950
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F	4.555831530	2.593011740	3.612297940
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Cl	2.562296300	3.294428750	5.769088080

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N	-0.023937800	-0.014058340	-0.018263920
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C	1.228014690	0.722940780	-3.972627810
C	1.247478820	-0.684663520	-3.977987550
C	4.078510280	0.762719480	0.026562780
C	4.132291440	-0.671352680	0.016581020
C	3.625908460	-1.371861650	-1.158417010
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C	-1.216759720	-0.726715360	-3.987861900
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C	1.238937690	-0.717264380	-3.999571760
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C	1.560303320	2.607753590	2.738514220
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Cl	3.411794420	5.889588540	0.681800380

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N	0.013764380	0.004436260	0.011512500
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C	4.128592460	-0.716779150	-0.053327340
C	3.590156780	-1.419787570	-1.205537650
C	3.122854350	-0.770211660	-2.414645260

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C	-1.248409220	-0.775569320	-4.002375820
C	-0.032914870	1.368113910	-4.034963390
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C	-3.053574780	-0.035128190	-2.729128700
C	-3.689080110	-1.230916680	-0.705671420
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C	-3.022619410	-2.436486650	-1.151451760
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C	1.539350140	-2.649019780	-2.701829790
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