

Charge controlled changes in the cluster and spin dynamics of $\text{Sc}_3\text{N@C}_{80}(\text{CF}_3)_2$: the flexible spin density distribution and its impact on ESR spectra

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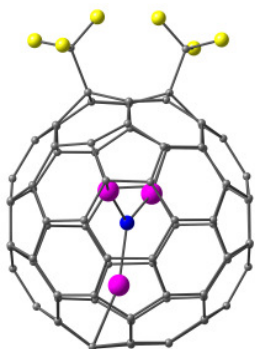
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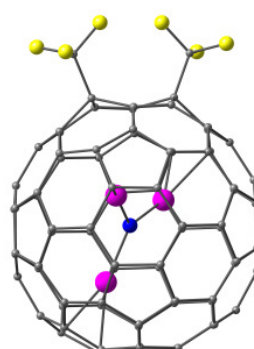
To study as much configurations of the Sc_3N cluster inside $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2$ as possible, we have degenerated multiple conformations by (a) considering C_s and C_3 conformers of parent $\text{Sc}_3\text{N}@C_{80}$ (see ref. 16) and then (b) by adding a pair of CF_3 groups in all possible symmetry-non-equivalent positions of these two conformers. This way, more than 50 initial structures were generated, which were then fully optimized in different charged states without symmetry restrictions. The procedure resulted in 30-40 different conformers for each charged state listed below.

Table S1. PEB/TZ2P relative energies of conformers of non-charged $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2$

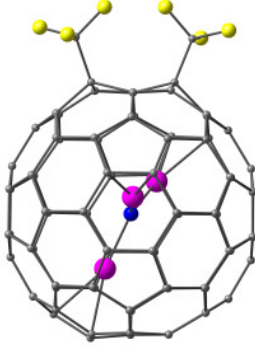
conformer	ΔE , kJ/mol
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Cnf2	1.7
Cnf3	13.0
Cnf4	15.5
Cnf5	16.4
Cnf6	21.1
Cnf7	21.4
Cnf8	25.4
Cnf9	25.9
Cnf10	27.4
Cnf11	35.2
Cnf12	38.4
Cnf13	40.9
Cnf14	43.6
Cnf15	45.6
Cnf16	46.4
Cnf17	46.6
Cnf18	46.8
Cnf19	47.6
Cnf20	47.7
Cnf21	48.7
Cnf22	48.8
Cnf23	49.2
Cnf24	51.1
Cnf25	51.8
Cnf26	53.0
Cnf27	55.8
Cnf28	56.5
Cnf29	58.7
Cnf30	61.2
Cnf31	62.0
Cnf32	62.4
Cnf33	64.9



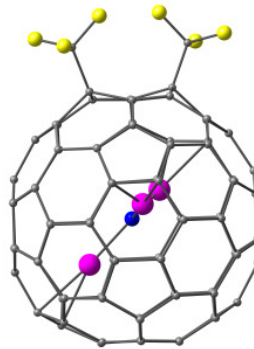
Cnf1



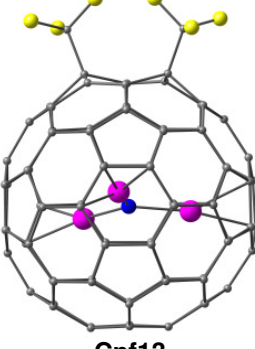
Cnf2



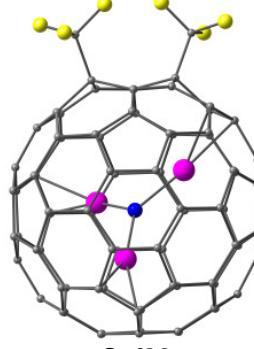
Cnf3



Cnf4



Cnf13



Cnf33

PBE/TZ2P Cartesian coordinates of Sc₃N@C₈₀(CF₃)₂, Cnf1, ΔE=0.0 kJ/mol

C	-3.715026510	-1.597919280	0.710893390
C	-3.683751480	-1.587792280	-0.723330870
C	-3.909015650	-0.236902710	-1.180884220
C	-4.051608560	0.594081870	-0.008136200
C	-3.932888320	-0.249652370	1.158929420
C	-3.335305560	0.253573490	2.348452290
C	-2.555634590	-0.661675400	3.144989600
C	-2.310457210	-1.993177560	2.663525060
C	-2.870248440	-2.489584610	1.437924680
C	-2.113822960	-3.457788280	0.725063810
C	-2.101852560	-3.456760660	-0.717434940
C	-2.838989100	-2.480444730	-1.445574220
C	-2.281237770	-1.974597210	-2.662101370
C	-2.530593880	-0.645809540	-3.115120080
C	-3.365906560	0.263168950	-2.419066850
C	-3.035151270	1.688716010	-2.474642230
C	-3.143800670	2.509152950	-1.256672780
C	-3.622340580	1.961382610	-0.004896690
C	-3.079360060	2.467880340	1.221747480
C	-2.949039170	1.621407090	2.377441290
C	-1.778844820	2.040449060	3.114513000
C	-0.997814500	1.124810680	3.895141710
C	-1.448895470	-0.256700650	3.992571980
C	-0.483841040	-1.369829510	3.999953910
C	-1.032652670	-2.418363300	3.154314100
C	-0.235794870	-3.335070990	2.372870510
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C	0.008366300	-4.114895670	0.022293060
C	-0.790972900	-3.851830530	-1.149711860
C	-0.217291180	-3.285091430	-2.321321340
C	-0.994062940	-2.402474970	-3.128817470
C	-0.396725960	-1.342594180	-3.884135990
C	-1.465662340	-0.263173390	-4.156369550
C	-0.917206360	1.119000410	-3.826513700
C	-1.761556750	2.027718570	-3.090060690
C	-1.156136670	3.086892370	-2.325841210
C	-1.984292540	3.370762580	-1.190744660
C	-1.397854590	3.860423800	0.035261880
C	-1.996792260	3.422605750	1.251504690
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C	1.188194280	-3.049907100	-2.310861090
C	1.801262330	-1.986896730	-3.059567220
C	0.971465620	-1.082906670	-3.814560530
C	1.525959090	0.299482620	-4.130180450
C	0.453139080	1.378016470	-3.870791920
C	1.040360880	2.436612380	-3.107465500
C	0.251325380	3.317135220	-2.308723380

C	0.810198500	3.881265050	-1.129478550
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C	0.219255670	3.356650010	2.387424540
C	1.013077540	2.456390980	3.167714650
C	0.418467550	1.359935130	3.897142530
C	1.371550970	0.262304730	3.902310980
C	0.943315380	-1.111550960	3.906003530
C	1.739234960	-2.021572370	3.134777080
C	1.174520990	-3.151553680	2.422042810
C	1.990945900	-3.405405010	1.273095830
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C	2.107488810	3.484563650	0.764946850
C	2.862815080	2.523584680	1.499759500
C	2.317472350	2.048806390	2.734139000
C	2.540112940	0.697977660	3.177444660
C	3.312450710	-0.219209390	2.402668490
C	2.913159460	-1.589922440	2.418447810
C	3.062753170	-2.434094900	1.263525120
C	3.626556360	-1.929688150	0.046638780
C	4.063040130	-0.563772200	0.051492740
C	3.933621240	0.269740300	-1.122652900
C	3.694763220	1.617853510	-0.664681020
C	3.704055900	1.624558320	0.769765490
C	3.925645490	0.277202400	1.216181360
Sc	-1.592023520	0.816836160	-0.977363400
Sc	1.619709340	-0.763579790	-0.924757550
Sc	-0.296579480	-0.237655090	2.025758710
N	-0.048893080	-0.068338250	0.030845220
C	-2.112029010	-0.335369530	-5.571583240
F	-1.258240250	0.016339160	-6.556944880
F	-2.567912970	-1.586472370	-5.841775210
F	-3.177548120	0.512829320	-5.635319070
C	2.190907790	0.376053370	-5.536757100
F	2.645153930	1.629017560	-5.799634200
F	3.259996490	-0.468178200	-5.587899100
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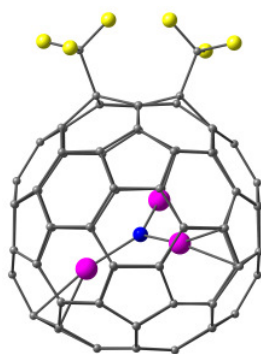
PBE/TZ2P Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2$, Cnf2, $\Delta E=1.7$ kJ/mol

C	1.144155680	-0.833089760	3.834684890
C	0.958512440	-2.149950160	3.290574810
C	2.084068590	-2.489874790	2.489339160
C	3.200207620	-1.455456080	2.718821390
C	2.400586170	-0.315001910	3.383983900
C	2.544938590	1.029986950	3.049403550
C	1.440192750	1.914756930	3.284566240
C	0.195893920	1.388879440	3.770632680
C	0.011557080	0.004433500	4.041058120
C	-1.297345930	-0.531174110	3.856178130
C	-1.473472320	-1.865579900	3.359377130
C	-0.347308050	-2.675242800	3.032164390
C	-0.462568430	-3.565143340	1.929105910
C	0.677986450	-3.876900900	1.103950460
C	1.995821350	-3.369376830	1.382133030
C	2.884223060	-3.150763140	0.243682710
C	3.644404370	-1.910533980	0.251701620
C	3.750143940	-1.002684790	1.371591000
C	3.989310060	0.346849330	1.109224150
C	3.620784050	1.491702790	2.076793840
C	3.024520450	2.522230200	1.098146950
C	1.982006770	3.439998980	1.386874560
C	1.174767490	3.157942750	2.578389330
C	-0.281545720	3.315065300	2.549610120
C	-0.866848620	2.225443330	3.304135470
C	-2.158659960	1.660565550	3.026982600
C	-2.362642100	0.286595720	3.340277480
C	-3.200523580	-0.543527270	2.505972880
C	-2.643116150	-1.876860130	2.520813420
C	-2.724861880	-2.705373120	1.366366380
C	-1.643382190	-3.601692950	1.107664530
C	-1.233665740	-3.912227670	-0.237044400
C	0.196224440	-4.082916540	-0.240870240
C	0.999596050	-3.744314430	-1.381162750
C	2.355537530	-3.311652910	-1.126174260
C	2.853699030	-2.219333130	-1.929655590
C	3.654994520	-1.377541420	-1.086967570
C	3.825278510	0.013096830	-1.360528700
C	4.009730440	0.863366330	-0.226834370
C	3.414245370	2.167574400	-0.229583850
C	2.725134320	2.670279020	-1.375238190
C	1.644632070	3.565814930	-1.113468590
C	1.266406260	3.946734410	0.232120520
C	-0.175901140	4.118424350	0.221713630
C	-0.975253020	3.756719310	1.359022560
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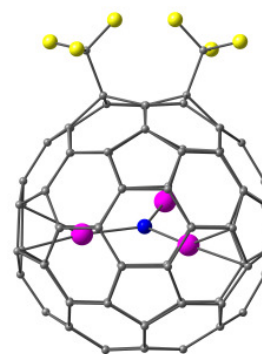
C	-3.710059800	1.369150570	1.097640290
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C	-3.026553580	-2.495083580	-1.097872300
C	-1.888676860	-3.339563780	-1.363476380
C	-1.118615140	-3.053507230	-2.523482770
C	0.311886440	-3.241040800	-2.528953770
C	0.887141100	-2.227986250	-3.381992440
C	2.156868210	-1.666509420	-3.068854510
C	2.379762070	-0.295726720	-3.375664600
C	3.206216980	0.530561020	-2.530033290
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C	1.489732110	1.856576840	-3.381025330
C	0.366681940	2.678829500	-3.070778860
C	0.480857330	3.569560190	-1.951421890
C	-0.647242400	3.884655500	-1.125829020
C	-1.931313220	3.317664200	-1.386155810
C	-2.751624370	3.019582770	-0.255445750
C	-3.626416020	1.877797350	-0.256294340
C	-3.736073440	1.008905220	-1.390305430
C	-4.046930730	-0.386984600	-1.140151480
C	-3.349118520	-1.377290570	-1.939980540
C	-2.501393640	-1.045788240	-3.065409540
C	-1.418575620	-1.921677210	-3.362065960
C	-0.179669490	-1.412275480	-3.894248780
C	0.010051520	-0.013374210	-4.114610600
C	1.316899950	0.525741580	-3.899756120
C	-0.933482010	2.177929750	-3.376331200
C	-2.060527600	2.485294370	-2.535789070
C	-2.937252150	1.343436440	-2.530913850
C	-2.346744760	0.332883210	-3.380060270
C	-1.111683510	0.849731450	-3.900777320
N	-0.044442090	-0.061661600	0.220453240
Sc	0.438302490	1.785670200	0.925599070
Sc	1.273779070	-1.597863070	-0.007535240
Sc	-2.000947660	-0.348100930	-0.099888250
C	4.837252520	2.145550150	2.796003270
F	4.431900990	3.258440310	3.470011340
F	5.786958830	2.531346790	1.903496950
F	5.421786560	1.320997940	3.691451980
C	4.286343680	-2.101202820	3.628756070
F	3.767871970	-2.469022690	4.829480630
F	5.332049300	-1.279088890	3.863645400
F	4.781178230	-3.224083300	3.033456370

Table S2. Relative energies of the conformers of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$

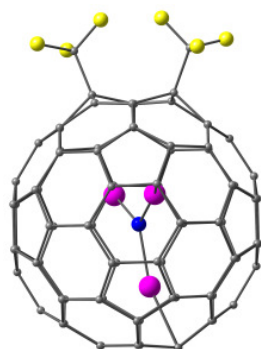
conformer	ΔE , kJ/mol
Cnf1	0.0
Cnf2	3.8
Cnf3	4.4
Cnf4	7.4
Cnf5	8.1
Cnf6	8.5
Cnf7	9.0
Cnf8	9.6
Cnf9	9.8
Cnf10	10.0
Cnf11	11.7
Cnf12	13.7
Cnf13	13.9
Cnf14	14.8
Cnf15	15.2
Cnf16	15.5
Cnf17	16.0
Cnf18	16.0
Cnf19	17.1
Cnf20	17.7
Cnf21	18.1
Cnf22	18.2
Cnf23	18.4
Cnf24	19.8
Cnf25	20.8
Cnf26	21.2
Cnf27	21.7
Cnf28	24.1
Cnf29	24.2
Cnf30	26.6
Cnf31	31.2
Cnf32	37.3
Cnf33	38.5
Cnf34	39.6
Cnf35	43.1
Cnf36	48.9



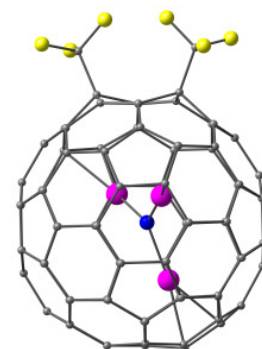
Cnf1



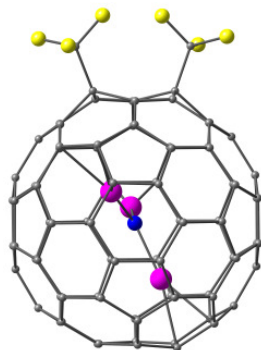
Cnf2



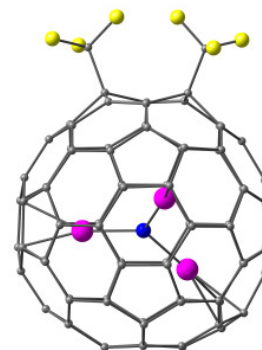
Cnf3



Cnf4



Cnf5



Cnf6

PBE/TZ2P Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$, Cnf1, $\Delta E = 0.0$ kJ/mol

C	-3.706014240	-1.589446020	0.761754940
C	-3.707039900	-1.575061070	-0.680570250
C	-3.917030420	-0.221781380	-1.106764770
C	-4.049304270	0.606288700	0.055104440
C	-3.935837580	-0.233349960	1.227759960
C	-3.398176200	0.249269660	2.472284180
C	-2.664755220	-0.708079690	3.296526010
C	-2.410667070	-2.069772310	2.788359670
C	-2.908417590	-2.514328550	1.503125350
C	-2.128994610	-3.455618650	0.746907080
C	-2.139482030	-3.445865000	-0.692126480
C	-2.881894830	-2.478385430	-1.415377210
C	-2.324950140	-2.009307420	-2.661285420
C	-2.509640600	-0.639581270	-3.053238400
C	-3.291276510	0.277790880	-2.291889120
C	-2.889804940	1.633619310	-2.333220490
C	-3.022668420	2.471411020	-1.160139460
C	-3.572956330	1.949292370	0.057759760
C	-3.057009680	2.460268030	1.275866200
C	-2.928336090	1.606431270	2.442419600
C	-1.748772130	2.044412430	3.153442980
C	-0.942594960	1.101441540	3.850254560
C	-1.415289540	-0.261393550	3.902549640
C	-0.454140830	-1.331375400	3.830123650
C	-1.050441430	-2.429080270	3.128468870
C	-0.237577890	-3.335155680	2.354600000
C	-0.817961760	-3.873522670	1.170994230
C	-0.018526530	-4.115999300	0.000093910
C	-0.831152750	-3.846963060	-1.156948040
C	-0.271625630	-3.351486260	-2.381938600
C	-1.080747780	-2.482910790	-3.225823700
C	-0.489225010	-1.370266390	-3.986409660
C	-1.375501440	-0.222703130	-3.823560490
C	-0.974472710	1.160136130	-3.802090390
C	-1.764283290	2.067656820	-3.100538950
C	-1.263567260	3.404238840	-2.519830090
C	-1.988471000	3.420536200	-1.158739020
C	-1.400153350	3.860845300	0.054595650
C	-1.983034990	3.403849220	1.280364580
C	-1.173823980	3.153369690	2.442849430
C	1.142990860	-3.124207510	-2.380586230
C	1.727526730	-2.014027970	-3.106930700
C	0.938015230	-1.091516490	-3.880794770
C	1.355794210	0.268198630	-3.839877510
C	0.470833280	1.489248540	-4.145422340
C	1.032728700	2.521211520	-3.143867790
C	0.253264970	3.373144170	-2.355399340

C	0.800415630	3.866221970	-1.142752700
C	0.000934350	4.129663670	0.043883970
C	0.804827860	3.861547150	1.195322750
C	0.238120590	3.330182240	2.396746740
C	1.045085130	2.430466100	3.157799690
C	0.467128580	1.330828390	3.883202170
C	1.405497760	0.243352590	3.872807400
C	0.965505270	-1.107700570	3.814918760
C	1.762649470	-2.045556040	3.106621050
C	1.173246790	-3.145164710	2.389879370
C	1.980219490	-3.408251360	1.224997930
C	1.383087660	-3.843348140	0.000684320
C	1.962079970	-3.383100840	-1.219265230
C	3.050148770	-2.448279390	-1.223595700
C	2.896023100	-1.594538300	-2.372952680
C	3.267367930	-0.228287680	-2.334697910
C	2.485842830	0.689596840	-3.092866560
C	2.296762450	2.058767110	-2.668660680
C	2.845861910	2.513851540	-1.437674680
C	2.095236770	3.459076880	-0.703157200
C	2.112198130	3.445211300	0.747358810
C	2.921404480	2.533363430	1.487400340
C	2.354317810	2.031361080	2.709668920
C	2.585493290	0.669556790	3.154503240
C	3.393933580	-0.253695660	2.404223980
C	2.933550350	-1.611541800	2.382429950
C	3.059311980	-2.465615390	1.216335090
C	3.576521340	-1.940770400	0.002413700
C	4.052328190	-0.576442440	0.028066040
C	3.857083290	0.258795280	-1.122891640
C	3.679747250	1.608988840	-0.679984210
C	3.818431860	1.646680780	0.759751100
C	4.061424780	0.264462540	1.214437480
Sc	-0.171785320	-0.977210420	-1.771409270
Sc	-1.399515030	-0.476360720	1.460624130
Sc	1.867868580	0.439270320	0.718079670
N	0.067776970	-0.239843720	0.099365010
C	-1.735601050	4.664466170	-3.324252520
F	-1.455513710	5.788278270	-2.615747360
F	-1.121870010	4.766333300	-4.519215710
F	-3.073484620	4.623773020	-3.537387320
C	0.661514780	1.863652280	-5.652049940
F	1.953091970	2.184942310	-5.905186780
F	0.335829220	0.791762180	-6.425838090
F	-0.115721380	2.894657580	-6.029996520

PBE/TZ2P Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$, Cnf2, $\Delta E = 3.8$ kJ/mol

C	-3.740484410	-1.539333060	0.712885980
C	-3.738171600	-1.541662180	-0.727919010
C	-3.956133740	-0.180776470	-1.179690100
C	-4.072251060	0.652755430	-0.004112710
C	-3.955057760	-0.186745050	1.155454160
C	-3.347875180	0.309490480	2.348239060
C	-2.587057180	-0.612805860	3.156738320
C	-2.348830200	-1.945114610	2.661965860
C	-2.910951130	-2.436515420	1.439745480
C	-2.149282550	-3.401457290	0.716136770
C	-2.153518480	-3.399721960	-0.723242490
C	-2.933654030	-2.467366340	-1.471732880
C	-2.434034880	-2.014616910	-2.757927230
C	-2.678643670	-0.646374450	-3.246437380
C	-3.408020720	0.309545770	-2.417363940
C	-2.933541700	1.661196910	-2.376633760
C	-3.063859970	2.508054890	-1.213559430
C	-3.603467710	2.001844940	0.002866150
C	-3.080707500	2.522830530	1.225887860
C	-2.948151270	1.673568560	2.373333630
C	-1.763003200	2.075144850	3.103732350
C	-0.998350750	1.164223370	3.902591280
C	-1.467408780	-0.215126950	3.994653570
C	-0.499398340	-1.323915370	3.933968110
C	-1.060629480	-2.369395630	3.114875670
C	-0.270292420	-3.299338090	2.344672470
C	-0.853673340	-3.832323070	1.159897690
C	-0.031465720	-4.084868330	-0.011707950
C	-0.837664770	-3.825197640	-1.160030620
C	-0.265372970	-3.287242220	-2.335543270
C	-1.077740650	-2.374818170	-3.103145950
C	-0.479035140	-1.275191970	-3.793564410
C	-1.433101160	-0.199757420	-3.850191200
C	-0.956885600	1.164125440	-3.802443160
C	-1.754864850	2.104312850	-3.098895150
C	-1.173283420	3.201691050	-2.385373060
C	-1.977216660	3.447363430	-1.216041630
C	-1.387829990	3.898852450	0.005603290
C	-1.979342920	3.450424410	1.227930930
C	-1.170583690	3.182231180	2.382186040
C	1.144976380	-3.106220810	-2.352186300
C	1.733708580	-1.984269060	-3.053324660
C	0.936003570	-1.054640900	-3.780416570
C	1.379166840	0.290242940	-3.839160990
C	0.451659200	1.389834540	-3.854294330
C	1.042568340	2.479331770	-3.127935680
C	0.246461960	3.374292620	-2.352961900

C	0.822118580	3.892311920	-1.157051310
C	0.017004400	4.161209920	0.005894360
C	0.820311670	3.914562310	1.170839110
C	0.240233800	3.369632130	2.359789800
C	1.027969270	2.466125820	3.135647990
C	0.423603050	1.377227400	3.867012920
C	1.362112830	0.269132660	3.841727380
C	0.916805560	-1.086759230	3.816171150
C	1.700048370	-2.025774710	3.054594220
C	1.129254360	-3.132648950	2.390324090
C	2.089454410	-3.642842050	1.299430570
C	1.370446970	-3.860632100	-0.033056110
C	1.958417510	-3.432538890	-1.227220670
C	3.278136820	-2.639658110	-1.323527400
C	2.914813910	-1.586537240	-2.383934280
C	3.358188980	-0.235266750	-2.384188940
C	2.560402870	0.699978640	-3.124235730
C	2.352776990	2.065897660	-2.683461760
C	2.937266430	2.558210050	-1.470374230
C	2.127490160	3.467597830	-0.714157000
C	2.120341910	3.485654870	0.733015100
C	2.864023090	2.519009920	1.454041760
C	2.329729040	2.043828650	2.693990110
C	2.533304300	0.690931830	3.122568290
C	3.264853230	-0.242661180	2.328285210
C	2.883196190	-1.605858160	2.334951950
C	3.064739770	-2.453750770	1.195377120
C	3.573807880	-1.953704350	0.002106530
C	4.006284830	-0.582529520	-0.030323740
C	4.041806450	0.273818400	-1.205198560
C	3.829527470	1.656198840	-0.750769300
C	3.692552460	1.615414300	0.690906930
C	3.838995890	0.250978000	1.120316040
Sc	-1.435941630	-0.448483760	-1.378797060
Sc	-0.482577740	-0.069954990	1.967123330
Sc	1.842750060	0.567110320	-0.650239420
N	-0.012218000	0.013233190	-0.002845350
C	2.741622200	-4.963376510	1.836825440
F	3.444808870	-4.720447250	2.970657390
F	1.767196480	-5.862968520	2.131104230
F	3.569399910	-5.529204660	0.939616540
C	4.499078770	-3.461182980	-1.854323580
F	5.533645260	-2.614071260	-2.110270690
F	4.928399060	-4.377196240	-0.966423690
F	4.183817350	-4.097627120	-3.007391900

PBE/TZ2P Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$, Cnf3, $\Delta E=4.4$ kJ/mol

C	-3.774980610	-1.555827040	0.738458440
C	-3.788502640	-1.553329470	-0.691498940
C	-3.961911050	-0.188546200	-1.134360940
C	-4.069699530	0.647924490	0.028563550
C	-3.944661340	-0.193775410	1.194933450
C	-3.396755820	0.289296760	2.430609960
C	-2.674650840	-0.655111650	3.268685090
C	-2.397992980	-1.970328990	2.710910940
C	-2.940326510	-2.457100020	1.465344710
C	-2.192057390	-3.424493320	0.738924700
C	-2.190345840	-3.411836320	-0.703474780
C	-2.944491820	-2.438689810	-1.422436500
C	-2.393811220	-1.946495870	-2.657964070
C	-2.655026610	-0.628914640	-3.198874030
C	-3.377768880	0.301382100	-2.349817100
C	-2.941291800	1.662225750	-2.348934800
C	-3.067554010	2.507974700	-1.187950710
C	-3.600833990	1.994032540	0.030109870
C	-3.056304730	2.494371900	1.250428530
C	-2.943523800	1.653362030	2.421809930
C	-1.753672940	2.065976360	3.144241620
C	-0.972518310	1.129947420	3.901743770
C	-1.467073830	-0.234640900	3.998887720
C	-0.496012440	-1.308064940	3.870054550
C	-1.081177570	-2.374631260	3.110093530
C	-0.296424690	-3.309028000	2.350264110
C	-0.886962090	-3.850056270	1.176306710
C	-0.085431320	-4.111951830	0.008580660
C	-0.888800130	-3.827610790	-1.148865220
C	-0.301087590	-3.276425770	-2.325931970
C	-1.082295550	-2.346204590	-3.071598020
C	-0.491539950	-1.282204240	-3.832735220
C	-1.481700130	-0.218199970	-3.971208100
C	-0.986275840	1.147531410	-3.870364380
C	-1.756811310	2.071410190	-3.082868170
C	-1.155286160	3.151613950	-2.348101820
C	-1.963382360	3.424625280	-1.188006450
C	-1.361988660	3.868276660	0.029149370
C	-1.955308140	3.413357870	1.250704580
C	-1.147322710	3.151704960	2.408834190
C	1.105083200	-3.094163840	-2.382164360
C	1.711594250	-2.051318060	-3.149441670
C	0.934397590	-1.108927750	-3.823706340
C	1.484013520	0.272540250	-4.148267700
C	0.423309740	1.340311810	-3.825600520
C	1.022635680	2.386752290	-3.081294990
C	0.257038040	3.322683380	-2.314444170

C	0.841480870	3.868519870	-1.138975250
C	0.039517390	4.133972040	0.028186640
C	0.845800590	3.875389300	1.189880140
C	0.267197780	3.337980060	2.377096810
C	1.055107970	2.436881320	3.162112680
C	0.447325370	1.337614320	3.870637980
C	1.387542160	0.240273650	3.865431040
C	0.931252690	-1.103721200	3.828077000
C	1.716390780	-2.054929080	3.117943460
C	1.117474870	-3.142632240	2.394513990
C	1.910994250	-3.392709240	1.221642050
C	1.306964960	-3.826050260	0.008230350
C	1.899180710	-3.333996640	-1.200781970
C	3.008786350	-2.455805940	-1.202929880
C	3.113809520	-1.767369630	-2.575034800
C	3.308271620	-0.270197830	-2.380934270
C	2.592298850	0.651872930	-3.145692440
C	2.341986740	1.974628320	-2.665898970
C	2.861553440	2.447242890	-1.432055180
C	2.135740450	3.429846260	-0.698465930
C	2.143296770	3.436729400	0.741108970
C	2.881545490	2.467502370	1.478453000
C	2.354341180	2.021184110	2.725857240
C	2.563700550	0.658551490	3.151134520
C	3.339366810	-0.275713860	2.386709130
C	2.888247040	-1.631992110	2.388746910
C	3.014972170	-2.470163120	1.212172690
C	3.619487370	-1.994977670	-0.001240670
C	4.188788310	-0.653841340	0.012136070
C	3.901134670	0.180516310	-1.150338870
C	3.652509320	1.518399220	-0.690239510
C	3.699505230	1.533549140	0.742362520
C	4.026761270	0.197339290	1.196246870
Sc	-0.949707570	0.025025550	-1.775479470
Sc	-1.104801750	0.002164680	1.764397170
Sc	1.970438060	-0.292025080	0.293981370
N	-0.038494470	-0.082309780	0.041362660
C	1.887908030	0.422221640	-5.652317430
F	2.405340560	1.651011690	-5.888724860
F	2.790910580	-0.500477430	-6.033331490
F	0.783604580	0.272096020	-6.430943150
C	4.288645940	-2.430667470	-3.367035950
F	4.479687400	-1.860782540	-4.571243730
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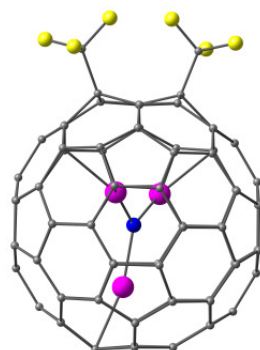
Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$, Cnf4 , $\Delta E = 7.4$ kJ/mol

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C	-0.964238210	2.155058380	-3.292041440
C	-2.085508090	2.491767730	-2.499892850
C	-3.199576900	1.453755420	-2.718561140
C	-2.404325220	0.310651080	-3.378907490
C	-2.557205700	-1.038406880	-3.056344240
C	-1.456626140	-1.928249470	-3.303041510
C	-0.207134140	-1.391605830	-3.767063300
C	-0.020886920	-0.004610500	-4.040217180
C	1.288550710	0.533004450	-3.847731740
C	1.469312140	1.871070510	-3.360666310
C	0.345047480	2.678430000	-3.031466640
C	0.460301450	3.574317650	-1.934910040
C	-0.677859580	3.886312650	-1.112941340
C	-1.988787610	3.367954680	-1.383696960
C	-2.865209150	3.138028530	-0.244654320
C	-3.620111670	1.891577880	-0.256703440
C	-3.754162780	0.999159020	-1.376277680
C	-3.997939340	-0.349009610	-1.118301850
C	-3.635255030	-1.496783440	-2.083351450
C	-3.038153900	-2.525482140	-1.102744010
C	-1.972259810	-3.429236460	-1.387424090
C	-1.184254830	-3.174500220	-2.588758620
C	0.274151770	-3.317573080	-2.546438100
C	0.856292680	-2.221848600	-3.291641930
C	2.148427990	-1.653236420	-3.014482830
C	2.354778430	-0.281500220	-3.335105040
C	3.197469340	0.551057940	-2.510069590
C	2.643251710	1.883323830	-2.528200330
C	2.720009210	2.707880770	-1.373181800
C	1.639557890	3.600001280	-1.108763600
C	1.234831670	3.913211790	0.233958570
C	-0.197278890	4.096403340	0.237830710
C	-1.003455660	3.771708650	1.376567690
C	-2.367870150	3.328614340	1.121774950
C	-2.859052540	2.225445160	1.924609130
C	-3.645781240	1.373433710	1.080972380
C	-3.821771420	-0.016814940	1.352080270
C	-3.994123880	-0.855487450	0.219431380
C	-3.406491740	-2.172650400	0.221705240
C	-2.724103960	-2.681241970	1.373893600
C	-1.648859090	-3.577065690	1.116358620
C	-1.263853970	-3.915883620	-0.229418440
C	0.179350910	-4.095562310	-0.216839460
C	0.971541710	-3.747690390	-1.350712180
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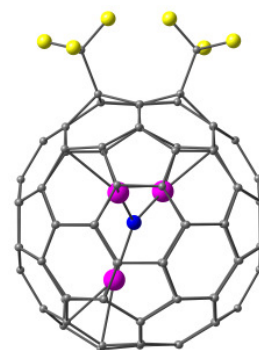
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C	3.453821170	2.192454930	-0.238774200
C	3.019385600	2.490398380	1.096567960
C	1.889920530	3.344582760	1.361229290
C	1.118062910	3.058723620	2.517914520
C	-0.313070130	3.242343630	2.514397210
C	-0.884589630	2.223875660	3.364915830
C	-2.154493820	1.659999000	3.050179830
C	-2.378491280	0.288182380	3.363288980
C	-3.203532790	-0.539544890	2.524838390
C	-2.661256800	-1.869258390	2.537927000
C	-1.487437610	-1.863041020	3.372893280
C	-0.364148240	-2.687168050	3.064394660
C	-0.477259470	-3.582422740	1.954252240
C	0.652665690	-3.902425230	1.133488730
C	1.930493000	-3.321370810	1.387473720
C	2.746474850	-3.011178370	0.259053630
C	3.633257900	-1.869652470	0.261057510
C	3.775483030	-1.008352290	1.402153270
C	4.086910880	0.393343930	1.154338220
C	3.370799920	1.384108760	1.948138250
C	2.503136160	1.052531070	3.057289360
C	1.419933730	1.929067950	3.358473020
C	0.179469220	1.412988280	3.875942860
C	-0.011361800	0.008502290	4.100534410
C	-1.314554070	-0.530870750	3.886606690
C	0.938454910	-2.180551150	3.367690520
C	2.063975330	-2.488170220	2.534648040
C	2.939494160	-1.336819710	2.520828970
C	2.341222120	-0.327757750	3.366177520
C	1.109709590	-0.848203540	3.887989530
N	0.055306070	0.063146280	-0.163814250
Sc	-0.451854950	-1.684306340	-1.058272580
Sc	-1.168608820	1.660290740	0.112151490
Sc	2.020873040	0.203039820	0.278744780
C	-4.857771340	-2.156226670	-2.801819330
F	-4.445207380	-3.275638190	-3.454101660
F	-5.802312500	-2.518433850	-1.901444310
F	-5.423646270	-1.335805330	-3.706326930
C	-4.293253180	2.098618710	-3.633180900
F	-3.769325880	2.449842370	-4.831621980
F	-5.332583420	1.271436250	-3.849963670
F	-4.771923670	3.222762080	-3.036199640

Table S3. PBE/TZ2P relative energies of the conformers of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^-$

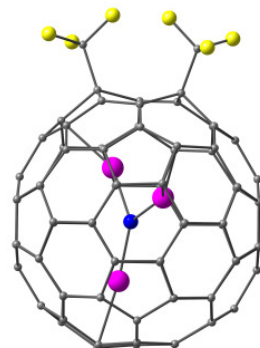
conformer	ΔE , kJ/mol
Cnf1	0.0
Cnf2	5.5
Cnf3	23.0
Cnf4	26.3
Cnf5	26.6
Cnf6	27.0
Cnf7	31.6
Cnf8	32.4
Cnf9	34.8
Cnf10	35.3
Cnf11	35.4
Cnf12	35.5
Cnf13	35.6
Cnf14	36.7
Cnf15	37.2
Cnf16	38.9
Cnf17	39.2
Cnf18	40.5
Cnf19	42.7
Cnf20	43.6
Cnf21	45.9
Cnf22	48.7
Cnf23	49.2
Cnf24	49.6
Cnf25	51.0
Cnf26	51.6
Cnf27	52.6
Cnf28	55.2
Cnf29	55.9
Cnf30	56.6
Cnf31	57.1
Cnf32	57.6
Cnf33	58.4
Cnf34	59.3
Cnf35	60.4
Cnf36	60.9
Cnf37	61.5
Cnf38	64.2



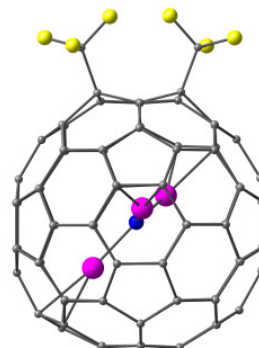
Cnf1



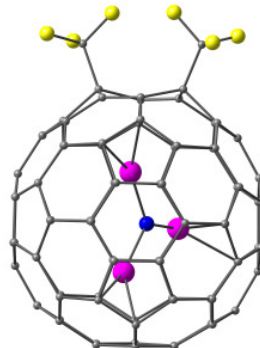
Cnf2



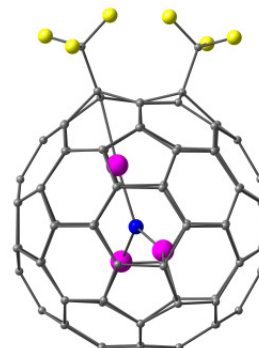
Cnf3



Cnf4



Cnf18



Cnf38

Cartesian coordinates of Sc₃N@C₈₀(CF₃)₂⁻, Cnf1, ΔE = 0.0 kJ/mol

C	-3.653495070	-1.564809780	0.702776470
C	-3.685412820	-1.556434830	-0.727057430
C	-3.948168050	-0.220768170	-1.191662280
C	-4.365759200	0.649270080	0.014271610
C	-3.878464750	-0.227361770	1.180731970
C	-3.370521120	0.243649100	2.417852890
C	-2.543505210	-0.693420010	3.138377540
C	-2.314327240	-2.043012830	2.671678350
C	-2.847213740	-2.493837350	1.424596900
C	-2.103538870	-3.464230990	0.690428520
C	-2.099049560	-3.437625300	-0.745069490
C	-2.841904730	-2.449319500	-1.450634140
C	-2.280977710	-1.948463090	-2.664227540
C	-2.529314660	-0.610644240	-3.142491630
C	-3.323886590	0.283580150	-2.339432620
C	-3.139359860	1.783065170	-2.541662570
C	-3.078675960	2.500979080	-1.174637280
C	-3.580614130	1.954997680	0.014371970
C	-3.033019580	2.411199220	1.263699710
C	-3.004771550	1.657761310	2.513301860
C	-1.769159020	2.048651180	3.210196490
C	-0.918239070	1.079818690	3.862949890
C	-1.359773050	-0.285449850	3.862465120
C	-0.426162000	-1.385775070	3.855774330
C	-1.021364750	-2.470270600	3.121388040
C	-0.225629600	-3.360737950	2.329085490
C	-0.799834530	-3.890481030	1.134772980
C	0.005984530	-4.145112650	-0.032578570
C	-0.794915820	-3.859969290	-1.197709120
C	-0.208413440	-3.316555610	-2.375363420
C	-1.000132870	-2.382243780	-3.139379620
C	-0.442132140	-1.323069240	-3.947146840
C	-1.419121230	-0.223095850	-4.004437880
C	-0.957443050	1.161290130	-3.872410910
C	-1.717338070	2.045921340	-3.066898210
C	-1.131814030	3.124322580	-2.319584530
C	-1.945758360	3.380508260	-1.169568840
C	-1.332782670	3.807035290	0.046455740
C	-1.904430050	3.306713150	1.252038500
C	-1.117656890	3.076485270	2.428446800
C	1.209696350	-3.155245760	-2.418835720
C	1.796049600	-2.048233220	-3.135852710
C	0.978284180	-1.089929130	-3.832320280
C	1.413435310	0.277143410	-3.833405060
C	0.469763080	1.369952860	-3.829230330
C	1.076028140	2.459702030	-3.091589310

C	0.282429710	3.332237020	-2.288090180
C	0.864570710	3.879230210	-1.106796210
C	0.058319770	4.108688600	0.061017270
C	0.867788140	3.851982030	1.226922250
C	0.306569630	3.300476290	2.413811740
C	1.105990890	2.427043320	3.210477540
C	0.498386650	1.310992820	3.896679740
C	1.425975990	0.210100940	3.871082050
C	0.979156570	-1.146979290	3.817961900
C	1.782692050	-2.081337470	3.093985340
C	1.191761920	-3.170767800	2.360038170
C	1.993540420	-3.417555330	1.194700200
C	1.405509400	-3.866776490	-0.031778510
C	2.001182400	-3.405797560	-1.245829860
C	3.085966640	-2.452022600	-1.231121180
C	2.960352100	-1.621821650	-2.414602210
C	3.340332240	-0.247939600	-2.355965040
C	2.595808660	0.697423840	-3.120525830
C	2.382331690	2.047381330	-2.665758350
C	2.909480900	2.498450830	-1.417300420
C	2.171218730	3.457642480	-0.667619320
C	2.177763680	3.445910130	0.774912180
C	2.924429700	2.479049440	1.509670510
C	2.404568840	2.013602720	2.753363460
C	2.605650330	0.639907300	3.159933180
C	3.398037590	-0.280757870	2.394807550
C	2.959732540	-1.648924900	2.382467270
C	3.095179820	-2.484041450	1.200419970
C	3.679600130	-1.983532270	-0.013494400
C	4.219152670	-0.630181930	0.013631030
C	3.953802180	0.218652380	-1.138024110
C	3.698054400	1.558806230	-0.675851100
C	3.740601070	1.554043610	0.758807120
C	4.076648430	0.214304000	1.210202010
Sc	-0.481812860	-0.089447240	-1.957232070
Sc	-1.317739680	0.674490250	1.384299580
Sc	1.993010780	-0.297507990	0.381575670
N	0.063927130	0.102680570	0.006572200
C	-5.898588710	0.863410260	0.154061570
F	-6.424740190	1.650600540	-0.816076270
F	-6.576851660	-0.319027210	0.128059680
F	-6.186497380	1.463559240	1.348858910
C	-4.162702470	2.389978610	-3.540917320
F	-3.991288000	3.735041790	-3.682919600
F	-4.003279520	1.833341690	-4.779754460
F	-5.453521910	2.184386250	-3.182470830

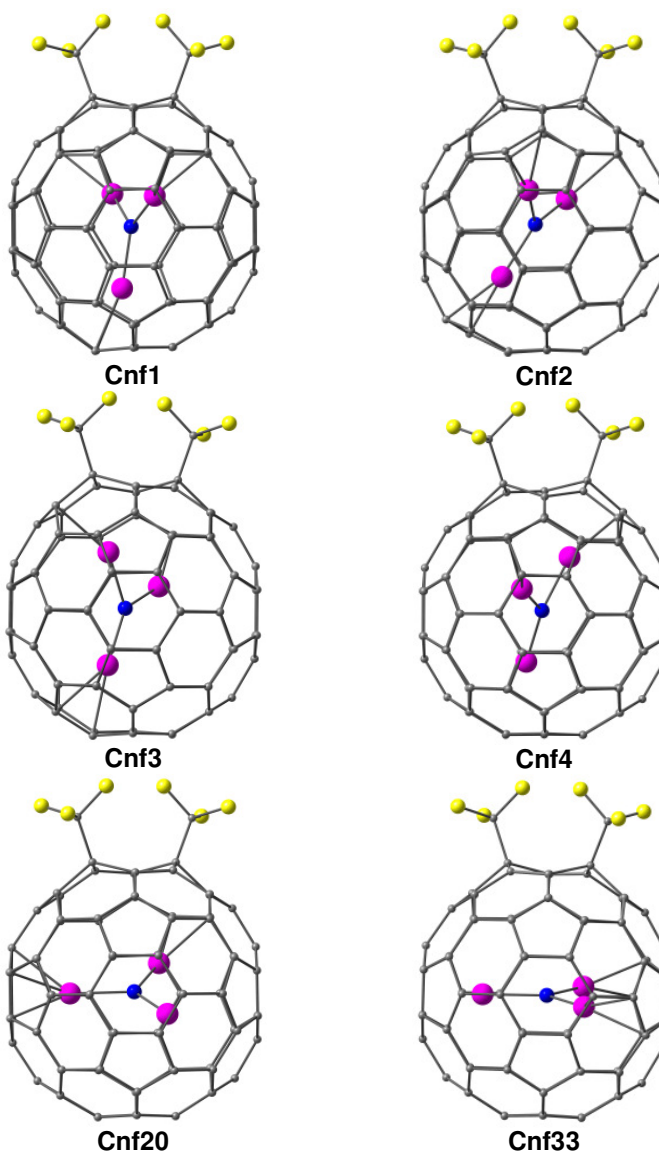
Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^-$, Cnf2, $\Delta E = 5.5$ kJ/mol

C	-1.150708900	0.834467730	-3.802491300
C	-0.999792900	2.172328630	-3.311111850
C	-2.141241370	2.525746180	-2.516925250
C	-3.221583230	1.435861150	-2.694907250
C	-2.382914170	0.296626060	-3.298794980
C	-2.583542410	-1.088008710	-3.070047030
C	-1.432476060	-1.923079610	-3.311684870
C	-0.187662720	-1.398798780	-3.828450420
C	-0.017489280	-0.000453460	-4.046986730
C	1.285614370	0.552849720	-3.866375290
C	1.442974050	1.879694970	-3.337431930
C	0.301718100	2.670324800	-3.011761700
C	0.406016840	3.535531700	-1.883508680
C	-0.728451020	3.892918230	-1.067325340
C	-2.010088080	3.312424230	-1.362154180
C	-3.037872740	3.245395350	-0.238319830
C	-3.719332450	1.858581500	-0.230906820
C	-3.748652770	0.995272400	-1.335470700
C	-3.925252240	-0.415103860	-1.103583980
C	-3.476375490	-1.489668820	-1.980670070
C	-3.101277290	-2.617724960	-1.106794150
C	-1.900397030	-3.391107870	-1.323077930
C	-1.110692070	-3.059945160	-2.478532840
C	0.318750900	-3.236518280	-2.490266400
C	0.888183420	-2.214084450	-3.331124470
C	2.159021200	-1.633409620	-3.040438650
C	2.358764740	-0.258334520	-3.356809230
C	3.191249850	0.571829300	-2.517076700
C	2.623303010	1.900654530	-2.512631980
C	2.708912950	2.729700730	-1.357906060
C	1.590252020	3.592512570	-1.079081820
C	1.208417380	4.008962690	0.252088760
C	-0.240561600	4.266278920	0.260001650
C	-1.051235860	3.823769340	1.398538560
C	-2.299220190	3.209274640	1.113126360
C	-2.867620450	2.166172940	1.929483320
C	-3.708488910	1.347812660	1.111770330
C	-3.806131320	-0.049522450	1.383309600
C	-3.923612770	-0.910331950	0.250474570
C	-3.403474930	-2.246693410	0.257013250
C	-2.691918290	-2.750600380	1.408777880
C	-1.609416130	-3.643578710	1.161035190
C	-1.209903910	-3.946404720	-0.192307080
C	0.218541410	-4.118377460	-0.203117900
C	0.994522910	-3.713117630	-1.328437590
C	2.298564580	-3.167936170	-1.071623460
C	2.894143380	-2.164810570	-1.917324980

C	3.832018230	-1.386887450	-1.126547790
C	3.889005300	0.046356180	-1.379519220
C	4.002372180	0.915842640	-0.244582220
C	3.453758790	2.254525800	-0.241584410
C	3.037111460	2.560236920	1.101157510
C	1.885371110	3.382588050	1.360921020
C	1.098663200	3.066466090	2.515943870
C	-0.336342000	3.254185920	2.519707160
C	-0.894383970	2.206038670	3.347640420
C	-2.162819030	1.621752230	3.043814790
C	-2.364593210	0.251323380	3.380559410
C	-3.184585290	-0.582707820	2.546545730
C	-2.627966380	-1.913729990	2.558469790
C	-1.454152710	-1.894672940	3.396119750
C	-0.321921490	-2.709406930	3.085417380
C	-0.429848790	-3.616217230	1.985891390
C	0.702089790	-3.910287740	1.142966660
C	1.968545120	-3.308390110	1.394373510
C	2.813851890	-2.993790460	0.261741720
C	3.789734530	-1.914950640	0.251948220
C	3.783739460	-0.998611200	1.386804510
C	3.935512780	0.405986950	1.109381220
C	3.332456600	1.424380390	1.934771070
C	2.508022360	1.075048310	3.050784210
C	1.411453700	1.935291450	3.357402220
C	0.177868520	1.407223660	3.869424060
C	0.009622690	0.002830660	4.108571140
C	-1.289173220	-0.555089460	3.900175820
C	0.977226650	-2.185187300	3.391176090
C	2.098562760	-2.482618880	2.548521730
C	2.966973800	-1.321292350	2.518102850
C	2.368031000	-0.310582320	3.356898540
C	1.139506440	-0.842276010	3.887540470
N	0.060873700	0.069248880	-0.176465300
Sc	-1.547721230	-0.889161160	-0.982443470
Sc	-0.051588390	2.027861120	0.337286740
Sc	1.897527910	-0.713942190	-0.121691320
C	-4.351669810	1.809173120	-3.694420800
F	-5.138689200	0.720241040	-3.948965550
F	-5.172163490	2.788084720	-3.241363670
F	-3.848097840	2.225674890	-4.891584220
C	-4.021226840	4.448526410	-0.242605410
F	-4.701461340	4.585989020	-1.407132100
F	-4.943483190	4.348791570	0.756134220
F	-3.340140510	5.618051770	-0.043287910

Table S4. PBE/TZ2P relative energies of the conformers of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^{3-}$

conformer	ΔE , kJ/mol
Cnf1	0.0
Cnf2*	7.8
Cnf3*	6.6
Cnf4	18.8
Cnf5	26.7
Cnf6	28.3
Cnf7	32.1
Cnf8	32.8
Cnf9	34.2
Cnf10	34.4
Cnf11	35.4
Cnf12	36.1
Cnf13	37.0
Cnf14	37.6
Cnf15	38.1
Cnf16	38.4
Cnf17	39.2
Cnf18	39.6
Cnf19	39.7
Cnf20	40.4
Cnf21	40.7
Cnf22	41.1
Cnf23	41.2
Cnf24	41.7
Cnf25	42.1
Cnf26	42.4
Cnf27	42.6
Cnf28	43.1
Cnf29	44.3
Cnf30	46.5
Cnf31	46.9
Cnf32	54.1
Cnf33	69.3



* for the sake of comparison to $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2$ and $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^-$, **Cnf2** is the structure with the relative energy 7.8 kJ/mol, while the lower energy structure (6.6 kJ/mol) is titled **Cnf3**.

Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^{3-}$, Cnf1, $\Delta E = 0.0$ kJ/mol

C	-3.821888370	-1.582088470	0.733241510
C	-3.819674040	-1.569690780	-0.708426400
C	-3.999467460	-0.205605670	-1.143439860
C	-4.119633550	0.626871780	0.026433810
C	-3.993069760	-0.222534560	1.189091120
C	-3.394159760	0.260166790	2.408886430
C	-2.657836260	-0.675504810	3.251972590
C	-2.384397890	-1.989526370	2.693146530
C	-2.945020580	-2.467203200	1.451944420
C	-2.183368980	-3.430456440	0.718594200
C	-2.185743990	-3.417278170	-0.725935900
C	-2.952207150	-2.445120620	-1.441725170
C	-2.381141460	-1.938934060	-2.668720150
C	-2.650844540	-0.621889610	-3.200354240
C	-3.374251360	0.291955390	-2.343392080
C	-2.938075870	1.665381860	-2.345979660
C	-3.071093230	2.500563800	-1.177159140
C	-3.613571070	1.974913990	0.036492920
C	-3.072758710	2.481174360	1.259099820
C	-2.944215610	1.631486110	2.420801000
C	-1.764252950	2.051263880	3.150093660
C	-0.963436720	1.118006870	3.910201790
C	-1.459315820	-0.250741610	3.989070020
C	-0.476019540	-1.317622650	3.860470900
C	-1.063751420	-2.394429230	3.098232460
C	-0.282357620	-3.326677950	2.345501920
C	-0.873194520	-3.853502380	1.155802620
C	-0.069137010	-4.108413740	-0.012796890
C	-0.874831440	-3.823257450	-1.169622360
C	-0.275489870	-3.256506290	-2.337728090
C	-1.061518570	-2.324894450	-3.081853520
C	-0.474685040	-1.247912120	-3.844847810
C	-1.480962610	-0.194651090	-3.991870790
C	-0.976593340	1.174673830	-3.872042030
C	-1.763850740	2.089126090	-3.073037870
C	-1.166180530	3.186680350	-2.333374310
C	-1.973830810	3.437074250	-1.173736360
C	-1.384284320	3.886609740	0.055385790
C	-1.974699340	3.418512070	1.270159900
C	-1.167120440	3.154529290	2.432025620
C	1.139303080	-3.079450240	-2.386747120
C	1.745121630	-2.031021660	-3.169927090
C	0.948292630	-1.062196100	-3.818227030
C	1.495163710	0.321519680	-4.160559270
C	0.427707870	1.380654280	-3.829903980
C	1.038688040	2.470092380	-3.096327530
C	0.254087240	3.365878820	-2.302439390

C	0.826554090	3.907196190	-1.108004030
C	0.018954680	4.160257270	0.061089170
C	0.826960860	3.897669520	1.229184020
C	0.252009290	3.351028120	2.417991160
C	1.052083660	2.459294130	3.216552960
C	0.457462620	1.348527660	3.916095720
C	1.420865870	0.261450700	3.934806650
C	0.944023510	-1.090345110	3.820635510
C	1.734476500	-2.044683380	3.104518970
C	1.137921360	-3.138865960	2.372737230
C	1.935396730	-3.390230580	1.209166330
C	1.333888210	-3.819271680	-0.021866950
C	1.933821110	-3.359260940	-1.231604980
C	3.038879770	-2.415411010	-1.214218740
C	3.145511270	-1.727152830	-2.585815850
C	3.309823230	-0.223461170	-2.372117890
C	2.607395600	0.711950350	-3.160113970
C	2.329414560	2.039993330	-2.662293990
C	2.848273400	2.493288650	-1.413893580
C	2.122875590	3.473343340	-0.663714230
C	2.130750740	3.469953340	0.778356340
C	2.877205200	2.500451660	1.517947400
C	2.362465980	2.048844520	2.773632500
C	2.582691410	0.689500980	3.207746120
C	3.325304260	-0.237584010	2.387955700
C	2.906048040	-1.617795110	2.381881770
C	3.042896460	-2.447632670	1.208192380
C	3.655866820	-1.968556490	-0.013341350
C	4.216334850	-0.614813910	0.019170630
C	3.912284520	0.220875120	-1.144968050
C	3.644225980	1.563514110	-0.676780740
C	3.683556350	1.572148110	0.756996640
C	4.000690920	0.237285980	1.205043050
Sc	-0.887539820	0.038426260	-1.827210450
Sc	-1.053377050	0.000794450	1.742201770
Sc	1.977989170	-0.382525390	0.169563870
N	-0.032641070	-0.080312620	0.012276180
C	4.320447910	-2.354182740	-3.384274840
F	4.535404790	-1.797484630	-4.612914970
F	5.510399470	-2.227150470	-2.704981250
F	4.150374070	-3.698968490	-3.600157410
C	1.899542480	0.457364290	-5.653731930
F	2.428911450	1.689392630	-5.946367930
F	2.817186220	-0.460162730	-6.079306760
F	0.810878060	0.306348680	-6.482255270

Cartesian coordinates of Sc₃N@C₈₀(CF₃)₂³⁻, Cnf2, ΔE = 7.8 kJ/mol

C	-1.154051120	0.858166650	-3.885718840
C	-0.989400530	2.191767600	-3.358161910
C	-2.124076060	2.477136940	-2.513301010
C	-2.989336450	1.326205620	-2.523766890
C	-2.387179830	0.322625640	-3.364580100
C	-2.519502270	-1.072316910	-3.062460580
C	-1.417386670	-1.928469830	-3.368262440
C	-0.183182410	-1.396204310	-3.893007990
C	-0.017681010	0.012209970	-4.103348030
C	1.283626170	0.575054870	-3.895233880
C	1.444788870	1.917543670	-3.382635070
C	0.304879530	2.712546810	-3.057841840
C	0.414488040	3.597646050	-1.915370300
C	-0.716355880	3.879759240	-1.069826070
C	-1.991876870	3.272938300	-1.332828790
C	-2.815193630	2.978091740	-0.204391520
C	-3.687297970	1.843522000	-0.220310910
C	-3.732462710	0.972158570	-1.354465590
C	-3.943618860	-0.420501690	-1.104141580
C	-3.338980580	-1.426338130	-1.938101320
C	-3.018900190	-2.557554340	-1.111820980
C	-1.867053540	-3.371147460	-1.374621580
C	-1.098151610	-3.066982630	-2.538003230
C	0.337415940	-3.238800570	-2.546505200
C	0.898621170	-2.197785470	-3.377465750
C	2.160995410	-1.606250840	-3.066036850
C	2.358839700	-0.224333570	-3.373552730
C	3.192135310	0.620053850	-2.544330170
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C	-1.056620680	3.748583200	1.389083830
C	-2.364267330	3.252891310	1.136524280
C	-3.153067560	2.343335430	2.105907950
C	-3.745448990	1.310512400	1.125219260
C	-3.945324070	-0.067079500	1.407648970
C	-4.015995180	-0.936866450	0.250410530
C	-3.433621320	-2.262708930	0.239584180
C	-2.712825880	-2.786840830	1.376608910
C	-1.596480890	-3.661857920	1.105355500
C	-1.194057720	-3.955207130	-0.247511100
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C	3.752432750	-1.322050580	-1.124479170
C	3.836673380	0.098008020	-1.375855610
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C	3.428980900	2.283779790	-0.249275250
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C	-2.390680600	0.244479580	3.309639240
C	-3.339271830	-0.635799400	2.619077400
C	-2.706907920	-1.975479170	2.575254110
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C	2.010996880	-3.339075380	1.335679810
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C	3.772577990	-0.961771470	1.340550300
C	3.947108940	0.451832040	1.091840740
C	3.332319670	1.445609660	1.925967420
C	2.483095390	1.081397610	3.031375260
C	1.385141930	1.928084600	3.318620090
C	0.149078220	1.405044690	3.825505400
C	0.005300170	0.002268230	4.029703030
C	-1.284475410	-0.557381550	3.769820810
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C	2.971631870	-1.312211760	2.489840120
C	2.367677640	-0.315745470	3.334605440
C	1.133007200	-0.851191520	3.831896950
N	0.093388390	0.033291030	0.361612580
Sc	-1.674373760	-0.515759010	1.119171060
Sc	0.479852770	1.999338010	0.125634120
Sc	1.637395560	-1.195461620	0.105632650
C	-4.317280560	3.056764390	2.847434760
F	-5.115325340	2.153047230	3.511466800
F	-3.916059870	3.957817590	3.791648150
F	-5.147661110	3.740878070	1.995926640
C	-0.407821790	4.769495610	3.659498270
F	-1.652651830	5.275790990	3.905303020
F	0.157647160	4.532443920	4.887842590
F	0.310945860	5.802634640	3.104316940

Cartesian coordinates of $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^{3-}$, Cnf3, $\Delta E = 6.6$ kJ/mol

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C	-3.769167930	-1.610473790	-0.687326690
C	-3.939704940	-0.241596720	-1.137730220
C	-4.076203230	0.590209210	0.027544410
C	-3.951769710	-0.252385820	1.190775670
C	-3.357855230	0.238647910	2.406264000
C	-2.628999700	-0.685963490	3.264668180
C	-2.347786820	-2.004567290	2.720972450
C	-2.901113460	-2.493868020	1.483218850
C	-2.124178400	-3.449388560	0.758447130
C	-2.120701320	-3.442044930	-0.683443370
C	-2.879961260	-2.464856560	-1.417256660
C	-2.354164590	-1.968764030	-2.661565560
C	-2.709267090	-0.678281730	-3.261848020
C	-3.371490910	0.248080810	-2.371047450
C	-2.938251310	1.621404640	-2.356277270
C	-3.070664800	2.460605580	-1.180771820
C	-3.615028650	1.954431810	0.034209690
C	-3.069046390	2.460617230	1.257115890
C	-2.931530200	1.615375490	2.416561480
C	-1.755120780	2.042744950	3.147558140
C	-0.954925450	1.122854070	3.919642840
C	-1.437590410	-0.251209600	4.011372590
C	-0.452188000	-1.312290440	3.902740200
C	-1.026639450	-2.392917900	3.140405560
C	-0.223091430	-3.316868200	2.389245130
C	-0.811136030	-3.858539490	1.205856400
C	0.004271920	-4.104405650	0.043627170
C	-0.812375470	-3.832052850	-1.120217250
C	-0.242073980	-3.233235620	-2.279812390
C	-1.033204950	-2.326277200	-3.061972600
C	-0.467054790	-1.288738080	-3.904161770
C	-1.553512300	-0.236022320	-4.251729800
C	-0.962324120	1.166545860	-3.898355960
C	-1.749270260	2.038432930	-3.074697220
C	-1.159651810	3.130901760	-2.323164500
C	-1.980117300	3.400414860	-1.175922160
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C	-1.981254410	3.405299590	1.269076520
C	-1.169530150	3.148806440	2.433684720
C	1.168152920	-3.019743280	-2.277666560
C	1.753156440	-1.915613280	-2.990121540
C	0.925261770	-0.997377020	-3.717933840
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C	0.448920130	1.397225870	-3.852912810
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C	0.248069910	3.344718170	-2.292092780

C	0.820864460	3.904216690	-1.103539820
C	0.008856580	4.152195740	0.059299200
C	0.818838240	3.906324850	1.231705730
C	0.247463490	3.358283680	2.421800950
C	1.053081660	2.473334910	3.217848410
C	0.466540580	1.365171170	3.931680210
C	1.426446040	0.284599200	3.949486770
C	0.972405580	-1.074616650	3.864959790
C	1.781851940	-2.027056730	3.166367090
C	1.194808130	-3.135359170	2.448194550
C	2.008545900	-3.392170970	1.290661100
C	1.404858390	-3.821751700	0.066424050
C	2.003845040	-3.330391310	-1.156112660
C	3.181966430	-2.478668640	-1.201247750
C	3.044721160	-1.615466520	-2.397356810
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C	2.128563890	3.502620250	-0.655318270
C	2.128784880	3.499532220	0.785522800
C	2.889374490	2.535862440	1.528184450
C	2.362809420	2.066155520	2.767901530
C	2.593757020	0.711004790	3.219997680
C	3.343644750	-0.215404250	2.429858190
C	2.958805270	-1.601460690	2.450049910
C	3.104506080	-2.442885230	1.287071780
C	3.676858730	-1.9444446720	0.056123050
C	4.108722100	-0.560639780	0.056269070
C	3.964822090	0.288857040	-1.114708300
C	3.715164520	1.637764910	-0.657304970
C	3.719606180	1.631422230	0.780378290
C	3.939478150	0.280561400	1.222448390
Sc	-1.022836780	-0.061369630	-1.801120900
Sc	-0.969657470	-0.105706200	1.772866400
Sc	1.738718160	-0.781284880	-0.742960620
N	-0.103095980	-0.282455870	-0.032252320
C	-2.115360480	-0.278839230	-5.704045810
F	-1.261188940	0.186121470	-6.663827690
F	-2.466003420	-1.549416960	-6.083227740
F	-3.251057940	0.486307860	-5.815806550
C	2.157447800	0.337421870	-5.531968260
F	2.562149300	1.588180360	-5.925210600
F	3.278802220	-0.459495320	-5.582462700
F	1.334069340	-0.125988610	-6.515999050

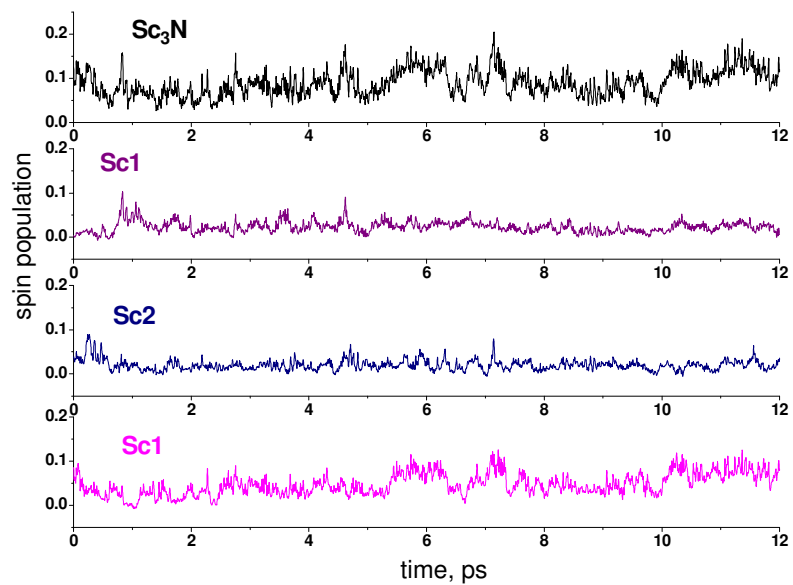


Figure S1. Spin populations in $\text{Sc}_3\text{N}@C_{80}(\text{CF}_3)_2^+$ as a functions of time.

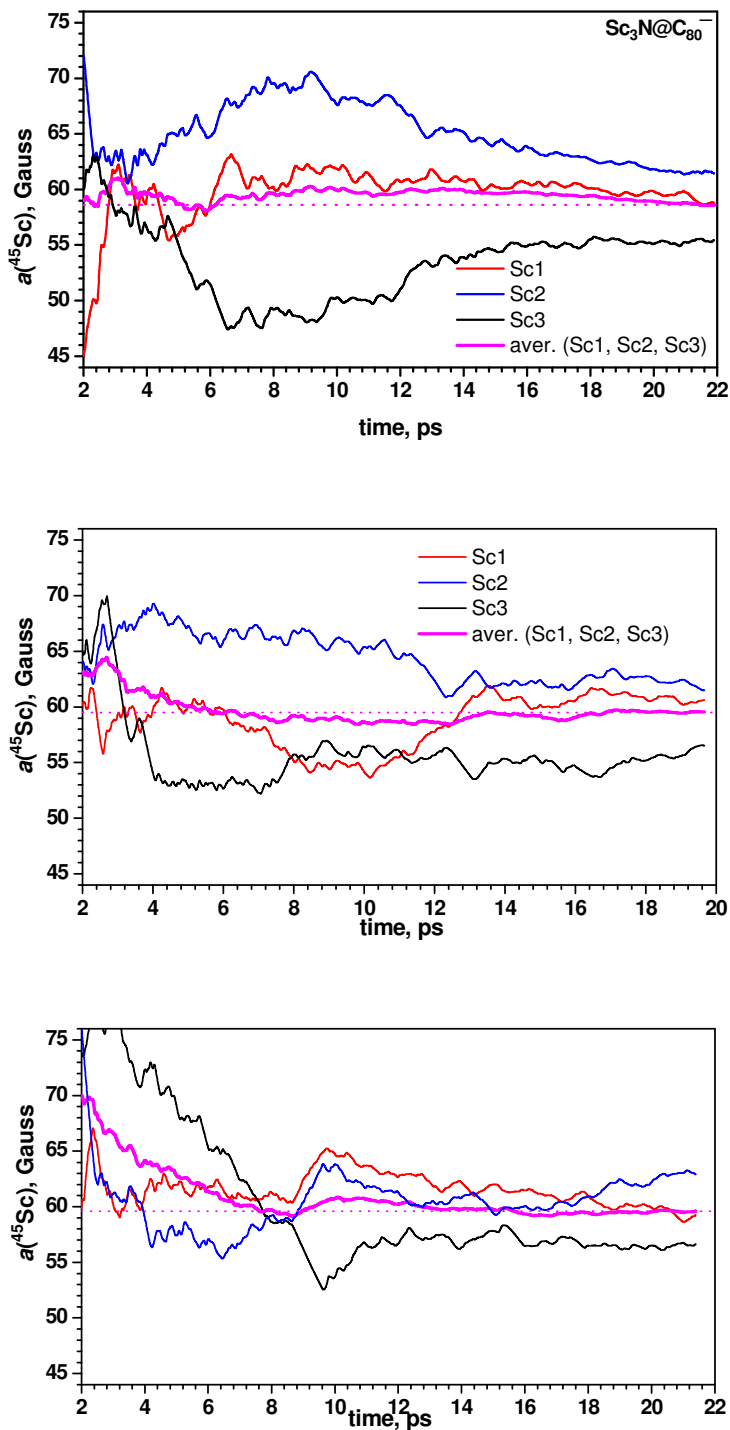


Figure S2. Time-averaged $a(^{45}\text{Sc})$ values in $\text{Sc}_3\text{N}@C_{80}^-$ as a function of propagation time in three independent trajectories (BOMD simulations, 300 K, PBE/DZ(P) level). Large oscillations of $a(^{45}\text{Sc})$ values during the first two picoseconds are not shown. In all figures the mean value is shown in magenta, note that the mean values converge to the same value in all three runs.

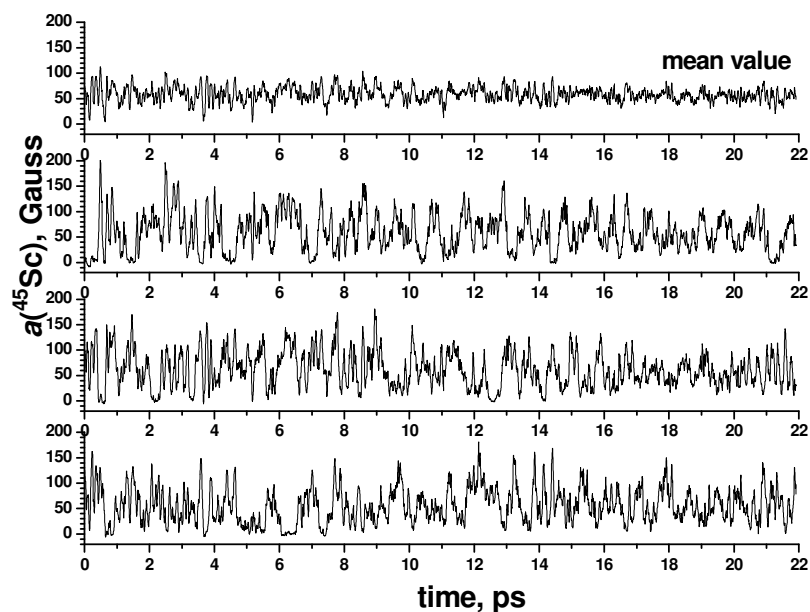


Figure S3. Instant $a(^{45}\text{Sc})$ values in $\text{Sc}_3\text{N@C}_{80}^-$ as a function of time in BOMD trajectory (300 K, PBE/DZ(P) level). Note that the values for individual atoms oscillate in the range of 0-200 Gauss, while the mean value for three Sc atoms oscillates in much smaller range.

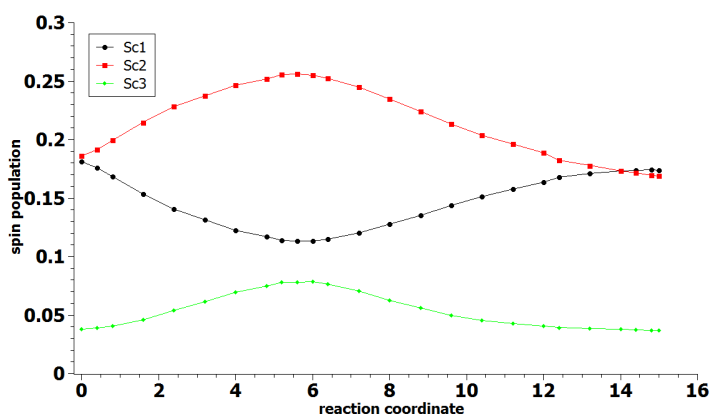


Figure S4. Mulliken spin population for Sc1-Sc3 atoms in $\text{Sc}_3\text{N@C}_{80}(\text{CF}_3)_2^-$ along the reaction coordinate (PBE0/6-311G* calculations with CP3P basis for Sc atoms)