

Supporting Information

Endohedral Metallofullerene Sc₃NC@C₈₄: A Theoretical Prediction

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A. Cartesian coordinates (in Å) and energies for isomers (a-e) of Sc₃NC@C₈₄ computed at the B3LYP/6-31G* level of theory

Sc₃NC@C₈₄ (a) Energy=-5575.9266397 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.727605	4.385241
2	6	0	0.000000	-0.727605	4.385241
3	6	0	1.164170	1.409105	3.845604
4	6	0	-1.164170	1.409105	3.845604
5	6	0	1.164170	-1.409105	3.845604
6	6	0	-1.164170	-1.409105	3.845604
7	6	0	2.365651	0.734591	3.405194
8	6	0	2.365651	-0.734591	3.405194
9	6	0	-2.365651	0.734591	3.405194
10	6	0	-2.365651	-0.734591	3.405194
11	6	0	0.708223	2.574338	3.103959
12	6	0	-0.708223	2.574338	3.103959
13	6	0	0.708223	-2.574338	3.103959
14	6	0	-0.708223	-2.574338	3.103959
15	6	0	3.178713	1.424000	2.468975
16	6	0	3.178713	-1.424000	2.468975
17	6	0	-3.178713	1.424000	2.468975
18	6	0	-3.178713	-1.424000	2.468975
19	6	0	1.460754	3.188762	2.049695
20	6	0	-1.460754	3.188762	2.049695
21	6	0	1.460754	-3.188762	2.049695
22	6	0	-1.460754	-3.188762	2.049695
23	6	0	2.749937	2.644609	1.822449
24	6	0	2.749937	-2.644609	1.822449
25	6	0	-2.749937	2.644609	1.822449
26	6	0	-2.749937	-2.644609	1.822449
27	6	0	3.950215	0.690281	1.493203
28	6	0	3.950215	-0.690281	1.493203
29	6	0	-3.950215	0.690281	1.493203
30	6	0	-3.950215	-0.690281	1.493203
31	6	0	0.726362	3.870449	0.975743
32	6	0	-0.726362	3.870449	0.975743
33	6	0	0.726362	-3.870449	0.975743

34	6	0	-0.726362	-3.870449	0.975743
35	6	0	3.302623	2.637691	0.492583
36	6	0	3.302623	-2.637691	0.492583
37	6	0	-3.302623	2.637691	0.492583
38	6	0	-3.302623	-2.637691	0.492583
39	6	0	3.966583	1.403952	0.244025
40	6	0	3.966583	-1.403952	0.244025
41	6	0	-3.966583	1.403952	0.244025
42	6	0	-3.966583	-1.403952	0.244025
43	6	0	1.410596	4.035269	-0.309512
44	6	0	-1.410596	4.035269	-0.309512
45	6	0	1.410596	-4.035269	-0.309512
46	6	0	-1.410596	-4.035269	-0.309512
47	6	0	2.614694	3.284754	-0.532942
48	6	0	-2.614694	3.284754	-0.532942
49	6	0	2.614694	-3.284754	-0.532942
50	6	0	-2.614694	-3.284754	-0.532942
51	6	0	3.853588	0.723999	-1.019684
52	6	0	3.853588	-0.723999	-1.019684
53	6	0	-3.853588	0.723999	-1.019684
54	6	0	-3.853588	-0.723999	-1.019684
55	6	0	0.711482	4.075293	-1.593292
56	6	0	-0.711482	4.075293	-1.593292
57	6	0	0.711482	-4.075293	-1.593292
58	6	0	-0.711482	-4.075293	-1.593292
59	6	0	2.595632	2.710367	-1.844111
60	6	0	-2.595632	2.710367	-1.844111
61	6	0	2.595632	-2.710367	-1.844111
62	6	0	-2.595632	-2.710367	-1.844111
63	6	0	3.183961	1.432355	-2.106745
64	6	0	3.183961	-1.432355	-2.106745
65	6	0	-3.183961	1.432355	-2.106745
66	6	0	-3.183961	-1.432355	-2.106745
67	6	0	1.399849	3.180992	-2.503438
68	6	0	-1.399849	3.180992	-2.503438
69	6	0	1.399849	-3.180992	-2.503438
70	6	0	-1.399849	-3.180992	-2.503438
71	6	0	2.621106	0.710919	-3.192526
72	6	0	2.621106	-0.710919	-3.192526
73	6	0	-2.621106	0.710919	-3.192526
74	6	0	-2.621106	-0.710919	-3.192526
75	6	0	0.730782	2.340200	-3.480495
76	6	0	-0.730782	2.340200	-3.480495
77	6	0	0.730782	-2.340200	-3.480495

78	6	0	-0.730782	-2.340200	-3.480495
79	6	0	1.420665	1.169835	-3.878187
80	6	0	1.420665	-1.169835	-3.878187
81	6	0	-1.420665	1.169835	-3.878187
82	6	0	-1.420665	-1.169835	-3.878187
83	6	0	0.699659	0.000000	-4.294431
84	6	0	-0.699659	0.000000	-4.294431
85	21	0	0.000000	-2.118554	-0.729831
86	21	0	0.000000	2.118554	-0.729831
87	21	0	0.000000	0.000000	2.292420
88	7	0	0.000000	0.000000	0.194454
89	6	0	0.000000	0.000000	-1.085131

Sc₃NC@C₈₄ (b) Energy=-5575.907154 a.u.

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.569402	0.458849	4.391403
2	6	0	0.569402	-0.458849	4.391403
3	6	0	-0.371447	1.790424	3.835590
4	6	0	-1.828288	-0.031521	3.837957
5	6	0	1.828288	0.031521	3.837957
6	6	0	0.371447	-1.790424	3.835590
7	6	0	0.908130	2.313738	3.386620
8	6	0	2.047962	1.389650	3.386069
9	6	0	-2.047962	-1.389650	3.386069
10	6	0	-0.908130	-2.313738	3.386620
11	6	0	-1.554246	2.153014	3.072243
12	6	0	-2.438488	1.046610	3.076045
13	6	0	2.438488	-1.046610	3.076045
14	6	0	1.554246	-2.153014	3.072243
15	6	0	0.873399	3.370832	2.442659
16	6	0	3.091830	1.595742	2.438112
17	6	0	-3.091830	-1.595742	2.438112
18	6	0	-0.873399	-3.370832	2.442659
19	6	0	-1.566902	3.118070	2.013443
20	6	0	-3.381381	0.848696	2.009472
21	6	0	3.381381	-0.848696	2.009472
22	6	0	1.566902	-3.118070	2.013443
23	6	0	-0.348449	3.798492	1.786698

24	6	0	3.768963	0.499540	1.781069
25	6	0	-3.768963	-0.499540	1.781069
26	6	0	0.348449	-3.798492	1.786698
27	6	0	1.921466	3.517243	1.462776
28	6	0	2.997260	2.651369	1.466028
29	6	0	-2.997260	-2.651369	1.466028
30	6	0	-1.921466	-3.517243	1.462776
31	6	0	-2.539435	2.961182	0.924008
32	6	0	-3.471554	1.839113	0.936259
33	6	0	3.471554	-1.839113	0.936259
34	6	0	2.539435	-2.961182	0.924008
35	6	0	0.000000	4.242897	0.462367
36	6	0	4.148498	0.939528	0.450540
37	6	0	-4.148498	-0.939528	0.450540
38	6	0	0.000000	-4.242897	0.462367
39	6	0	1.380783	3.991167	0.218506
40	6	0	3.554583	2.216220	0.212261
41	6	0	-3.554583	-2.216220	0.212261
42	6	0	-1.380783	-3.991167	0.218506
43	6	0	-2.229763	3.601448	-0.323849
44	6	0	-4.065357	1.396243	-0.338487
45	6	0	4.065357	-1.396243	-0.338487
46	6	0	2.229763	-3.601448	-0.323849
47	6	0	-0.932813	4.142166	-0.566347
48	6	0	-4.352933	-0.005363	-0.594578
49	6	0	4.352933	0.005363	-0.594578
50	6	0	0.932813	-4.142166	-0.566347
51	6	0	1.834463	3.480512	-1.050996
52	6	0	2.959717	2.573801	-1.059186
53	6	0	-2.959717	-2.573801	-1.059186
54	6	0	-1.834463	-3.480512	-1.050996
55	6	0	-2.642154	3.006016	-1.572323
56	6	0	-3.518562	1.916172	-1.571994
57	6	0	3.518562	-1.916172	-1.571994
58	6	0	2.642154	-3.006016	-1.572323
59	6	0	-0.495985	3.776973	-1.889932
60	6	0	-3.836134	-0.364720	-1.913069
61	6	0	3.836134	0.364720	-1.913069
62	6	0	0.495985	-3.776973	-1.889932
63	6	0	0.860335	3.413701	-2.140899
64	6	0	3.133447	1.614737	-2.158041
65	6	0	-3.133447	-1.614737	-2.158041
66	6	0	-0.860335	-3.413701	-2.140899
67	6	0	-1.582810	3.080189	-2.526477

68	6	0	-3.346955	0.853721	-2.528549
69	6	0	3.346955	-0.853721	-2.528549
70	6	0	1.582810	-3.080189	-2.526477
71	6	0	1.075337	2.497079	-3.206430
72	6	0	2.193488	1.611640	-3.219058
73	6	0	-2.193488	-1.611640	-3.219058
74	6	0	-1.075337	-2.497079	-3.206430
75	6	0	-1.365740	2.032894	-3.480775
76	6	0	-2.271162	0.880842	-3.486029
77	6	0	2.271162	-0.880842	-3.486029
78	6	0	1.365740	-2.032894	-3.480775
79	6	0	-0.023174	1.836513	-3.884710
80	6	0	1.793773	0.384413	-3.911615
81	6	0	-1.793773	-0.384413	-3.911615
82	6	0	0.023174	-1.836513	-3.884710
83	6	0	0.440438	0.549643	-4.319320
84	6	0	-0.440438	-0.549643	-4.319320
85	21	0	2.117441	-0.200272	-0.439413
86	21	0	-2.117441	0.200272	-0.439413
87	21	0	0.000000	0.000000	2.319871
88	7	0	0.000000	0.000000	0.250744
89	6	0	0.000000	0.000000	-1.031122

Sc₃NC@C₈₄ (c) Energy=-5575.9017482 a.u.

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.601069	2.297733	-0.548187
2	6	0	-4.040654	1.406750	0.446113
3	6	0	-2.652017	3.311369	-0.229527
4	6	0	-3.355489	1.830537	-1.883568
5	6	0	-3.528144	1.500890	1.774234
6	6	0	-4.223564	0.025345	0.115674
7	6	0	-2.129439	3.427975	1.083687
8	6	0	-2.574016	2.488578	2.108118
9	6	0	-3.552026	0.468997	-2.237455
10	6	0	-4.002789	-0.457931	-1.193159
11	6	0	-1.818427	3.510113	-1.411731
12	6	0	-2.245207	2.584681	-2.416236
13	6	0	-3.409526	0.149424	2.309673

14	6	0	-3.828878	-0.755339	1.283262
15	6	0	-0.813637	3.987845	1.192326
16	6	0	-1.662355	2.140138	3.167078
17	6	0	-2.753764	-0.023015	-3.310480
18	6	0	-3.614928	-1.842951	-1.291445
19	6	0	-0.460863	3.866166	-1.303493
20	6	0	-1.339272	2.028741	-3.360954
21	6	0	-2.435938	-0.223403	3.270631
22	6	0	-3.307149	-2.067774	1.181985
23	6	0	0.000000	4.195106	0.019295
24	6	0	-1.621911	0.856473	3.829733
25	6	0	-1.684483	0.739648	-3.869560
26	6	0	-3.350054	-2.681013	-0.141477
27	6	0	0.064296	3.620384	2.250858
28	6	0	-0.350441	2.692263	3.217000
29	6	0	-2.338579	-1.410994	-3.350568
30	6	0	-2.777640	-2.301713	-2.371625
31	6	0	0.510008	3.364486	-2.297408
32	6	0	0.067386	2.437776	-3.325213
33	6	0	-1.875474	-1.567651	3.222444
34	6	0	-2.293493	-2.482854	2.164781
35	6	0	1.374903	4.025149	0.405022
36	6	0	-0.270120	0.669316	4.370174
37	6	0	-0.660018	-0.200334	-4.285867
38	6	0	-2.357565	-3.669535	-0.553126
39	6	0	1.410732	3.552894	1.763223
40	6	0	0.548472	1.757039	3.837985
41	6	0	-1.029484	-1.531351	-3.906406
42	6	0	-1.921329	-3.369455	-1.904592
43	6	0	1.921329	3.369455	-1.904592
44	6	0	1.029484	1.531351	-3.906406
45	6	0	-0.548472	-1.757039	3.837985
46	6	0	-1.410732	-3.552894	1.763223
47	6	0	2.357565	3.669535	-0.553126
48	6	0	0.660018	0.200334	-4.285867
49	6	0	0.270120	-0.669316	4.370174
50	6	0	-1.374903	-4.025149	0.405022
51	6	0	2.293493	2.482854	2.164781
52	6	0	1.875474	1.567651	3.222444
53	6	0	-0.067386	-2.437776	-3.325213
54	6	0	-0.510008	-3.364486	-2.297408
55	6	0	2.777640	2.301713	-2.371625
56	6	0	2.338579	1.410994	-3.350568
57	6	0	0.350441	-2.692263	3.217000

58	6	0	-0.064296	-3.620384	2.250858
59	6	0	3.350054	2.681013	-0.141477
60	6	0	1.684483	-0.739648	-3.869560
61	6	0	1.621911	-0.856473	3.829733
62	6	0	0.000000	-4.195106	0.019295
63	6	0	3.307149	2.067774	1.181985
64	6	0	2.435938	0.223403	3.270631
65	6	0	1.339272	-2.028741	-3.360954
66	6	0	0.460863	-3.866166	-1.303493
67	6	0	3.614928	1.842951	-1.291445
68	6	0	2.753764	0.023015	-3.310480
69	6	0	1.662355	-2.140138	3.167078
70	6	0	0.813637	-3.987845	1.192326
71	6	0	3.828878	0.755339	1.283262
72	6	0	3.409526	-0.149424	2.309673
73	6	0	2.245207	-2.584681	-2.416236
74	6	0	1.818427	-3.510113	-1.411731
75	6	0	4.002789	0.457931	-1.193159
76	6	0	3.552026	-0.468997	-2.237455
77	6	0	2.574016	-2.488578	2.108118
78	6	0	2.129439	-3.427975	1.083687
79	6	0	4.223564	-0.025345	0.115674
80	6	0	3.528144	-1.500890	1.774234
81	6	0	3.355489	-1.830537	-1.883568
82	6	0	2.652017	-3.311369	-0.229527
83	6	0	4.040654	-1.406750	0.446113
84	6	0	3.601069	-2.297733	-0.548187
85	21	0	-1.284269	-1.691449	-0.429806
86	21	0	1.284269	1.691449	-0.429806
87	21	0	0.000000	0.000000	2.317194
88	7	0	0.000000	0.000000	0.247101
89	6	0	0.000000	0.000000	-1.032265

Sc₃NC@C₈₄ (d) Energy=-5575.8528633 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	0.000000	0.709849	-4.281338
2	6	0	0.000000	-0.709849	-4.281338
3	6	0	-1.158115	1.417246	-3.851481

4	6	0	1.158115	1.417246	-3.851481
5	6	0	-1.158115	-1.417246	-3.851481
6	6	0	1.158115	-1.417246	-3.851481
7	6	0	-2.334976	0.735636	-3.443876
8	6	0	-2.334976	-0.735636	-3.443876
9	6	0	2.334976	0.735636	-3.443876
10	6	0	2.334976	-0.735636	-3.443876
11	6	0	-0.714614	2.628523	-3.165947
12	6	0	0.714614	2.628523	-3.165947
13	6	0	-0.714614	-2.628523	-3.165947
14	6	0	0.714614	-2.628523	-3.165947
15	6	0	-3.155213	1.422569	-2.508387
16	6	0	-3.155213	-1.422569	-2.508387
17	6	0	3.155213	1.422569	-2.508387
18	6	0	3.155213	-1.422569	-2.508387
19	6	0	-1.473596	3.282627	-2.141981
20	6	0	1.473596	3.282627	-2.141981
21	6	0	-1.473596	-3.282627	-2.141981
22	6	0	1.473596	-3.282627	-2.141981
23	6	0	-2.737493	2.653788	-1.870294
24	6	0	-2.737493	-2.653788	-1.870294
25	6	0	2.737493	2.653788	-1.870294
26	6	0	2.737493	-2.653788	-1.870294
27	6	0	-3.943055	0.694057	-1.557069
28	6	0	-3.943055	-0.694057	-1.557069
29	6	0	3.943055	0.694057	-1.557069
30	6	0	3.943055	-0.694057	-1.557069
31	6	0	-0.746836	4.068210	-1.089333
32	6	0	0.746836	4.068210	-1.089333
33	6	0	-0.746836	-4.068210	-1.089333
34	6	0	0.746836	-4.068210	-1.089333
35	6	0	-3.317460	2.651175	-0.549215
36	6	0	-3.317460	-2.651175	-0.549215
37	6	0	3.317460	2.651175	-0.549215
38	6	0	3.317460	-2.651175	-0.549215
39	6	0	-3.983244	1.413318	-0.309712
40	6	0	-3.983244	-1.413318	-0.309712
41	6	0	3.983244	1.413318	-0.309712
42	6	0	3.983244	-1.413318	-0.309712
43	6	0	-1.407462	4.017868	0.219681
44	6	0	1.407462	4.017868	0.219681
45	6	0	-1.407462	-4.017868	0.219681
46	6	0	1.407462	-4.017868	0.219681
47	6	0	-2.633730	3.310206	0.469059

48	6	0	2.633730	3.310206	0.469059
49	6	0	-2.633730	-3.310206	0.469059
50	6	0	2.633730	-3.310206	0.469059
51	6	0	-3.843347	0.729406	0.945613
52	6	0	-3.843347	-0.729406	0.945613
53	6	0	3.843347	0.729406	0.945613
54	6	0	3.843347	-0.729406	0.945613
55	6	0	-0.690125	3.959767	1.486259
56	6	0	0.690125	3.959767	1.486259
57	6	0	-0.690125	-3.959767	1.486259
58	6	0	0.690125	-3.959767	1.486259
59	6	0	-2.633401	2.748867	1.792838
60	6	0	2.633401	2.748867	1.792838
61	6	0	-2.633401	-2.748867	1.792838
62	6	0	2.633401	-2.748867	1.792838
63	6	0	-3.178891	1.457724	2.019342
64	6	0	-3.178891	-1.457724	2.019342
65	6	0	3.178891	1.457724	2.019342
66	6	0	3.178891	-1.457724	2.019342
67	6	0	-1.423049	3.185901	2.455178
68	6	0	1.423049	3.185901	2.455178
69	6	0	-1.423049	-3.185901	2.455178
70	6	0	1.423049	-3.185901	2.455178
71	6	0	-2.559709	0.709820	3.075064
72	6	0	-2.559709	-0.709820	3.075064
73	6	0	2.559709	0.709820	3.075064
74	6	0	2.559709	-0.709820	3.075064
75	6	0	-0.734287	2.367250	3.395298
76	6	0	0.734287	2.367250	3.395298
77	6	0	-0.734287	-2.367250	3.395298
78	6	0	0.734287	-2.367250	3.395298
79	6	0	-1.410720	1.166418	3.833386
80	6	0	-1.410720	-1.166418	3.833386
81	6	0	1.410720	1.166418	3.833386
82	6	0	1.410720	-1.166418	3.833386
83	6	0	-0.729380	0.000000	4.383652
84	6	0	0.729380	0.000000	4.383652
85	21	0	0.000000	-2.030208	-0.615767
86	21	0	0.000000	2.030208	-0.615767
87	21	0	0.000000	0.000000	2.317315
88	7	0	0.000000	0.000000	0.216091
89	6	0	0.000000	0.000000	-1.074642

Sc₃NC@C₈₄ (e) Energy=-5575.9422684 a.u.

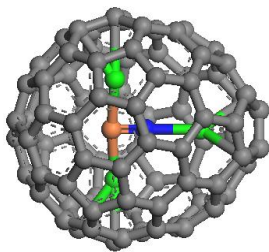
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.248050	1.266705	0.138348
2	6	0	4.272543	-0.880017	-0.764556
3	6	0	4.266620	-0.996737	0.676732
4	6	0	4.252371	0.516023	-1.092856
5	6	0	4.234699	0.332186	1.226735
6	6	0	3.574628	2.516027	0.251537
7	6	0	3.596437	-1.824902	-1.582188
8	6	0	3.596747	-2.062985	1.330580
9	6	0	3.519159	0.973241	-2.222593
10	6	0	3.508498	0.620401	2.421692
11	6	0	3.011549	-2.956757	-0.915501
12	6	0	3.031922	-3.109793	0.512999
13	6	0	2.949026	3.052078	-0.932152
14	6	0	2.974650	2.858620	1.491580
15	6	0	2.888526	2.257920	-2.122814
16	6	0	2.912733	1.906008	2.556776
17	6	0	2.947461	-1.367948	-2.770795
18	6	0	2.928271	-1.785304	2.564573
19	6	0	2.892689	0.027686	-3.072589
20	6	0	2.862632	-0.461475	3.089044
21	6	0	1.801991	3.948489	-0.909167
22	6	0	1.754370	3.653779	1.525268
23	6	0	1.842522	-3.617968	-1.412447
24	6	0	1.900280	-3.928349	0.914020
25	6	0	1.668508	2.582869	-2.819448
26	6	0	1.650734	2.078256	3.246375
27	6	0	1.718744	-1.968799	-3.220658
28	6	0	1.692473	-2.459038	2.884897
29	6	0	1.592633	0.301433	-3.659135
30	6	0	1.563769	-0.289755	3.699419
31	6	0	1.109512	4.167541	0.361703
32	6	0	1.155931	-4.258679	-0.309680
33	6	0	1.053713	3.690733	-2.132860
34	6	0	0.999648	3.197585	2.661456
35	6	0	1.158242	-3.090795	-2.569751
36	6	0	1.175001	-3.544658	2.120681
37	6	0	0.913041	1.522876	-3.479655

38	6	0	0.890505	0.957516	3.708451
39	6	0	0.867835	-0.922836	-3.741610
40	6	0	0.839514	-1.501258	3.572251
41	6	0	-0.368888	4.251817	0.368161
42	6	0	-0.295205	-4.313729	-0.331204
43	6	0	-0.368250	3.701840	-2.088966
44	6	0	-0.387043	3.279089	2.659511
45	6	0	-0.250140	-3.235885	-2.600948
46	6	0	-0.254884	-3.632855	2.085543
47	6	0	-0.545335	1.517070	-3.366877
48	6	0	-0.570731	0.970443	3.596987
49	6	0	-0.546249	-0.963823	-3.602277
50	6	0	-0.574317	-1.521269	3.423829
51	6	0	-1.069503	4.077214	-0.886901
52	6	0	-1.077563	3.874670	1.557003
53	6	0	-0.965961	-3.880329	-1.526098
54	6	0	-0.977845	-4.090937	0.915691
55	6	0	-1.137570	2.668171	-2.740036
56	6	0	-1.170686	2.192777	3.175881
57	6	0	-1.088368	-2.205905	-3.144985
58	6	0	-1.101874	-2.674521	2.767692
59	6	0	-1.291987	0.267527	-3.387736
60	6	0	-1.317471	-0.269885	3.409606
61	6	0	-2.372309	3.468112	-0.938973
62	6	0	-2.385388	3.272721	1.500039
63	6	0	-2.282666	-3.318043	-1.484885
64	6	0	-2.292362	-3.516751	0.958487
65	6	0	-2.409740	2.598397	-2.094553
66	6	0	-2.428893	2.222440	2.508325
67	6	0	-2.345603	-2.271202	-2.493517
68	6	0	-2.360209	-2.644895	2.115665
69	6	0	-2.623430	0.201187	-2.761192
70	6	0	-2.640536	-0.245348	2.774740
71	6	0	-3.032909	3.090164	0.262296
72	6	0	-2.954222	-3.160453	-0.247114
73	6	0	-3.179412	1.406240	-2.135554
74	6	0	-3.199764	1.048824	2.349737
75	6	0	-3.150006	-1.113030	-2.341062
76	6	0	-3.165557	-1.474196	2.149184
77	6	0	-3.954519	2.003700	0.166559
78	6	0	-3.905885	-2.101391	-0.163646
79	6	0	-4.162067	1.280552	-1.076100
80	6	0	-4.169183	1.090836	1.271174
81	6	0	-4.129614	-1.190218	-1.276008

82	6	0	-4.139765	-1.379327	1.078618
83	6	0	-4.690281	0.001356	-0.724670
84	6	0	-4.697395	-0.115499	0.719154
85	21	0	-2.531287	-0.041359	0.005327
86	21	0	0.703431	-2.096085	0.328063
87	21	0	0.620232	2.003696	-0.718412
88	7	0	-0.386113	-0.041064	-0.066407
89	6	0	0.890561	-0.049549	-0.200195

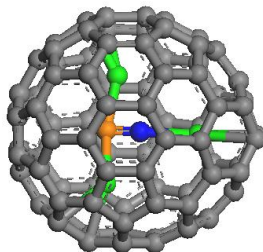
B B3LYP/6-31G* optimized geometries of Sc₃NC@C₈₄ (50322) and Sc₃NC@C₈₄ (51425). The total energies (E_t , in hartree) and HOMO-LUMO gaps (ΔE , in eV) are given.



$E_t=-5575.90502$

$\Delta E=1.67$

Sc₃NC@C₈₄ (50322)



$E_t=-5575.91582$

$\Delta E=1.77$

Sc₃NC@C₈₄ (51425)

C. Harmonic frequencies, IR intensities, and Raman scattering activities of IPR D_{2d} (23) C₈₄⁶⁻ calculated at the B3LYP/6-31G* level

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	B1	E	E
Frequencies --	208.1357	214.0216	214.0216
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.3063	0.3239	0.3239
IR Inten --	0.0000	0.3874	0.3874
Raman Activ --	24.2172	14.1270	14.1270
	4	5	6
	B2	A1	E
Frequencies --	214.0541	215.3511	276.5447

Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.3240	0.3279	0.5407
IR Inten --	0.0000	0.0000	0.0017
Raman Activ --	69.2747	58.9352	0.4052
	7	8	9
	E	A2	E
Frequencies --	276.5447	276.6104	278.8455
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.5407	0.5410	0.5497
IR Inten --	0.0017	0.0000	0.1526
Raman Activ --	0.4052	0.0000	0.0261
	10	11	12
	E	B2	A1
Frequencies --	278.8455	282.5026	284.5839
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.5497	0.5643	0.5726
IR Inten --	0.1526	0.0387	0.0000
Raman Activ --	0.0261	1.3337	0.0479
	13	14	15
	A1	A2	B1
Frequencies --	328.4754	329.0214	329.8362
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.7628	0.7654	0.7692
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.4626	0.0000	46.8051
	16	17	18
	E	E	B2
Frequencies --	330.4232	330.4232	346.2813
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.7719	0.7719	0.8478
IR Inten --	0.2140	0.2140	0.4999
Raman Activ --	22.0212	22.0212	6.8279
	19	20	21
	B1	A1	E
Frequencies --	349.2648	353.3434	357.1913
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.8625	0.8827	0.9021
IR Inten --	0.0000	0.0000	0.0105
Raman Activ --	0.5562	3.9422	1.4052
	22	23	24
	E	A2	A1
Frequencies --	357.1913	359.0964	359.7980
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.9021	0.9117	0.9153

IR Inten	--	0.0105	0.0000	0.0000
Raman Activ	--	1.4052	0.0000	2.8860
		25	26	27
		E	E	E
Frequencies	--	365.5745	365.5745	406.5521
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	0.9449	0.9449	1.1686
IR Inten	--	0.2044	0.2044	2.7296
Raman Activ	--	1.8178	1.8178	11.7186
		28	29	30
		E	A1	B2
Frequencies	--	406.5521	407.3869	414.2929
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	1.1686	1.1734	1.2135
IR Inten	--	2.7296	0.0000	0.3323
Raman Activ	--	11.7186	162.3761	4.7305
		31	32	33
		E	E	B1
Frequencies	--	425.6718	425.6718	426.6367
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	1.2811	1.2811	1.2869
IR Inten	--	0.0027	0.0027	0.0000
Raman Activ	--	20.1976	20.1976	16.2047
		34	35	36
		A2	A1	B2
Frequencies	--	432.0695	444.6273	452.1257
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	1.3199	1.3977	1.4453
IR Inten	--	0.0000	0.0000	3.0928
Raman Activ	--	0.0000	25.8220	22.8277
		37	38	39
		E	E	E
Frequencies	--	454.0585	454.0585	469.0846
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	1.4577	1.4577	1.5557
IR Inten	--	2.1223	2.1223	16.2205
Raman Activ	--	0.8481	0.8481	1.1488
		40	41	42
		E	B1	A2
Frequencies	--	469.0846	472.9887	474.2360
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	1.5557	1.5817	1.5901
IR Inten	--	16.2205	0.0000	0.0000
Raman Activ	--	1.1488	2.9488	0.0000

	43	44	45
	B2	E	E
Frequencies --	484.4714	486.2843	486.2843
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.6595	1.6719	1.6719
IR Inten --	59.9113	47.1762	47.1762
Raman Activ --	2.5504	0.6775	0.6775
	46	47	48
	B1	E	E
Frequencies --	488.7970	489.4890	489.4890
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.6892	1.6940	1.6940
IR Inten --	0.0000	55.9618	55.9618
Raman Activ --	15.1092	4.7995	4.7995
	49	50	51
	A1	A2	E
Frequencies --	491.3484	500.7251	502.2691
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.7069	1.7727	1.7836
IR Inten --	0.0000	0.0000	0.5200
Raman Activ --	5.1868	0.0000	0.0066
	52	53	54
	E	B2	E
Frequencies --	502.2691	504.3856	505.4517
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.7836	1.7987	1.8063
IR Inten --	0.5200	8.7172	19.0811
Raman Activ --	0.0066	0.9072	0.3899
	55	56	57
	E	B2	B1
Frequencies --	505.4517	509.1166	525.2887
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.8063	1.8326	1.9509
IR Inten --	19.0811	51.0577	0.0000
Raman Activ --	0.3899	16.8398	0.4079
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571
	58	59	60
	A2	E	E
Frequencies --	535.4763	543.6524	543.6524
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.0273	2.0897	2.0897
IR Inten --	0.0000	0.4877	0.4877
Raman Activ --	0.0000	18.9786	18.9786

	61	62	63
	E	E	B2
Frequencies --	600.6189	600.6189	601.7628
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.5505	2.5505	2.5602
IR Inten --	0.2191	0.2191	1.4062
Raman Activ --	3.5848	3.5848	2.8997
	64	65	66
	A1	B1	E
Frequencies --	603.0995	608.3961	611.8874
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.5716	2.6170	2.6471
IR Inten --	0.0000	0.0000	0.2573
Raman Activ --	0.5393	171.3712	0.0216
	67	68	69
	E	B2	B1
Frequencies --	611.8874	617.4323	620.1459
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.6471	2.6953	2.7191
IR Inten --	0.2573	0.7810	0.0000
Raman Activ --	0.0216	21.3195	71.9418
	70	71	72
	B1	A2	A1
Frequencies --	621.1838	622.6543	624.6233
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.7282	2.7411	2.7585
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0412	0.0000	38.6942
	73	74	75
	E	E	A2
Frequencies --	630.8066	630.8066	635.0206
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.8134	2.8134	2.8511
IR Inten --	30.8777	30.8777	0.0000
Raman Activ --	10.2136	10.2136	0.0000
	76	77	78
	E	E	A1
Frequencies --	643.0710	643.0710	643.5896
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.9238	2.9238	2.9285
IR Inten --	2.4453	2.4453	0.0000
Raman Activ --	3.1059	3.1059	94.0358
	79	80	81
	B2	B1	E

Frequencies --	645.0559	648.0196	648.9941
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.9419	2.9690	2.9779
IR Inten --	6.3944	0.0000	10.5818
Raman Activ --	0.3604	3.1169	3.4848
	82	83	84
	E	E	E
Frequencies --	648.9941	654.6481	654.6481
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.9779	3.0300	3.0300
IR Inten --	10.5818	48.5337	48.5337
Raman Activ --	3.4848	57.5706	57.5706
	85	86	87
	A1	B2	E
Frequencies --	659.5340	659.9724	660.4902
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.0754	3.0795	3.0844
IR Inten --	0.0000	9.1988	0.4616
Raman Activ --	13.4810	2.6111	2.0606
	88	89	90
	E	E	E
Frequencies --	660.4902	663.1473	663.1473
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.0844	3.1092	3.1092
IR Inten --	0.4616	0.5233	0.5233
Raman Activ --	2.0606	15.4539	15.4539
	91	92	93
	A2	B2	B1
Frequencies --	664.1675	666.0184	666.4566
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.1188	3.1362	3.1403
IR Inten --	0.0000	5.1381	0.0000
Raman Activ --	0.0000	37.4560	3.5945
	94	95	96
	E	E	B2
Frequencies --	668.6535	668.6535	670.6149
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.1611	3.1611	3.1796
IR Inten --	0.5931	0.5931	0.9508
Raman Activ --	7.9075	7.9075	1.7805
	97	98	99
	A2	E	E
Frequencies --	670.8842	671.6662	671.6662
Red. masses --	12.0000	12.0000	12.0000

Frc consts	--	3.1822	3.1896	3.1896
IR Inten	--	0.0000	0.2435	0.2435
Raman Activ	--	0.0000	3.0850	3.0850
		100	101	102
		E	E	A1
Frequencies	--	675.3358	675.3358	676.0326
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.2246	3.2246	3.2312
IR Inten	--	0.0759	0.0759	0.0000
Raman Activ	--	2.7828	2.7828	26.2002
		103	104	105
		B1	A2	A1
Frequencies	--	677.9054	678.1833	686.1610
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.2491	3.2518	3.3288
IR Inten	--	0.0000	0.0000	0.0000
Raman Activ	--	24.5655	0.0000	16.2242
		106	107	108
		E	E	B1
Frequencies	--	686.1862	686.1862	686.4019
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3290	3.3290	3.3311
IR Inten	--	21.7726	21.7726	0.0000
Raman Activ	--	5.8841	5.8841	14.5926
		109	110	111
		E	E	A2
Frequencies	--	687.3907	687.3907	688.0734
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3407	3.3407	3.3473
IR Inten	--	4.6556	4.6556	0.0000
Raman Activ	--	0.0025	0.0025	0.0000
		112	113	114
		B1	B1	B2
Frequencies	--	693.1239	705.5408	721.3572
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3967	3.5195	3.6790
IR Inten	--	0.0000	0.0000	2.1321
Raman Activ	--	0.5801	38.5586	4.5394
		115	116	117
		A1	A2	E
Frequencies	--	729.3365	733.9768	751.0530
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.7609	3.8089	3.9882
IR Inten	--	0.0000	0.0000	7.3023

Raman Activ --	1.5538	0.0000	0.2331
	118	119	120
	E	A2	E
Frequencies --	751.0530	764.0322	777.4663
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.9882	4.1272	4.2736
IR Inten --	7.3023	0.0000	0.1319
Raman Activ --	0.2331	0.0000	1.8505
	121	122	123
	E	E	E
Frequencies --	777.4663	803.1249	803.1249
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	4.2736	4.5603	4.5603
IR Inten --	0.1319	1.8088	1.8088
Raman Activ --	1.8505	0.3949	0.3949
	124	125	126
	A2	A2	E
Frequencies --	809.7079	849.0560	854.7228
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	4.6354	5.0969	5.1651
IR Inten --	0.0000	0.0000	0.4483
Raman Activ --	0.0000	0.0000	14.4871
	127	128	129
	E	A1	B2
Frequencies --	854.7228	859.7088	863.6164
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.1651	5.2256	5.2732
IR Inten --	0.4483	0.0000	3.8658
Raman Activ --	14.4871	0.2916	0.4773
	130	131	132
	E	E	B1
Frequencies --	865.2001	865.2001	877.3667
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.2925	5.2925	5.4424
IR Inten --	3.1540	3.1540	0.0000
Raman Activ --	3.4819	3.4819	0.6505
	133	134	135
	E	E	A2
Frequencies --	881.4961	881.4961	894.5018
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.4938	5.4938	5.6571
IR Inten --	1.0753	1.0753	0.0000
Raman Activ --	3.0082	3.0082	0.0000
	136	137	138

	B1	A1	A1
Frequencies --	940.4628	996.4937	1012.6913
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	6.2534	7.0207	7.2508
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0036	10.3536	8.9709
	139	140	141
	B1	B2	E
Frequencies --	1013.5047	1015.4614	1018.5326
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.2624	7.2905	7.3347
IR Inten --	0.0000	2.7067	7.1894
Raman Activ --	6.6609	1.7492	20.4664
	142	143	144
	E	E	E
Frequencies --	1018.5326	1038.5396	1038.5396
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.3347	7.6257	7.6257
IR Inten --	7.1894	11.5010	11.5010
Raman Activ --	20.4664	7.0391	7.0391
	145	146	147
	A2	B2	E
Frequencies --	1045.5882	1104.5436	1111.7702
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.7295	8.6258	8.7390
IR Inten --	0.0000	0.7155	10.4562
Raman Activ --	0.0000	6.8715	4.4911
	148	149	150
	E	A1	B2
Frequencies --	1111.7702	1133.6843	1136.5099
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	8.7390	9.0869	9.1323
IR Inten --	10.4562	0.0000	17.8444
Raman Activ --	4.4911	0.0455	4.0242
	151	152	153
	B1	E	E
Frequencies --	1139.2397	1142.8761	1142.8761
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	9.1762	9.2348	9.2348
IR Inten --	0.0000	16.0455	16.0455
Raman Activ --	37.2941	5.4356	5.4356
	154	155	156
	E	E	A1
Frequencies --	1163.0329	1163.0329	1176.2933

Red. masses --	12.0000	12.0000	12.0000
Frc consts --	9.5635	9.5635	9.7828
IR Inten --	3.3613	3.3613	0.0000
Raman Activ --	48.8211	48.8211	31.4609
	157	158	159
	B1	A2	E
Frequencies --	1176.4281	1176.9559	1188.3802
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	9.7850	9.7938	9.9849
IR Inten --	0.0000	0.0000	48.0965
Raman Activ --	166.2939	0.0000	60.8024
	160	161	162
	E	A2	B2
Frequencies --	1188.3802	1210.7973	1217.0919
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	9.9849	10.3651	10.4732
IR Inten --	48.0965	0.0000	1.7778
Raman Activ --	60.8024	0.0000	2.0658
	163	164	165
	E	E	B2
Frequencies --	1223.5274	1223.5274	1229.1400
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	10.5842	10.5842	10.6815
IR Inten --	12.5290	12.5290	0.2416
Raman Activ --	128.2352	128.2352	0.6076
	166	167	168
	A1	E	E
Frequencies --	1232.3231	1247.2471	1247.2471
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	10.7369	10.9986	10.9986
IR Inten --	0.0000	63.7005	63.7005
Raman Activ --	79.9503	11.4118	11.4118
	169	170	171
	B2	E	E
Frequencies --	1252.7738	1253.3247	1253.3247
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.0963	11.1060	11.1060
IR Inten --	71.3666	20.9181	20.9181
Raman Activ --	49.5742	10.7812	10.7812
	172	173	174
	B1	A1	A2
Frequencies --	1262.5172	1265.2593	1272.1868
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.2695	11.3185	11.4428

IR Inten	--	0.0000	0.0000	0.0000
Raman Activ	--	8.1469	15.7375	0.0000
		175	176	177
		E	E	B1
Frequencies	--	1280.4031	1280.4031	1284.3812
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	11.5911	11.5911	11.6632
IR Inten	--	27.8668	27.8668	0.0000
Raman Activ	--	3.5029	3.5029	84.6059
		178	179	180
		E	E	A1
Frequencies	--	1290.8081	1290.8081	1298.4741
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	11.7803	11.7803	11.9206
IR Inten	--	0.1946	0.1946	0.0000
Raman Activ	--	124.3108	124.3108	300.0870
		181	182	183
		A2	E	E
Frequencies	--	1305.2064	1309.0180	1309.0180
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	12.0445	12.1150	12.1150
IR Inten	--	0.0000	29.4444	29.4444
Raman Activ	--	0.0000	0.0008	0.0008
		184	185	186
		B1	A1	A2
Frequencies	--	1309.4018	1320.7373	1322.7642
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	12.1221	12.3329	12.3708
IR Inten	--	0.0000	0.0000	0.0000
Raman Activ	--	0.3227	7.2349	0.0000
		187	188	189
		B2	E	E
Frequencies	--	1323.5721	1329.0372	1329.0372
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	12.3859	12.4884	12.4884
IR Inten	--	25.6646	0.4371	0.4371
Raman Activ	--	10.3158	135.6668	135.6668
		190	191	192
		B2	E	E
Frequencies	--	1332.2239	1337.7598	1337.7598
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	12.5483	12.6528	12.6528
IR Inten	--	76.4013	2.7019	2.7019
Raman Activ	--	0.3111	21.4184	21.4184

	193	194	195
	A1	B2	E
Frequencies --	1339.2454	1347.2651	1348.4914
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.6809	12.8333	12.8566
IR Inten --	0.0000	82.3936	199.3785
Raman Activ --	19.4110	0.0363	310.8908
	196	197	198
	E	E	E
Frequencies --	1348.4914	1355.3434	1355.3434
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.8566	12.9876	12.9876
IR Inten --	199.3785	3.7282	3.7282
Raman Activ --	310.8908	47.7364	47.7364
	199	200	201
	B1	B1	B2
Frequencies --	1359.6649	1368.0287	1369.7730
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.0706	13.2319	13.2657
IR Inten --	0.0000	0.0000	62.9522
Raman Activ --	93.2841	133.9715	0.6810
	202	203	204
	A2	E	E
Frequencies --	1370.2974	1371.3038	1371.3038
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.2758	13.2953	13.2953
IR Inten --	0.0000	0.6353	0.6353
Raman Activ --	0.0000	234.6362	234.6362
	205	206	207
	E	E	A1
Frequencies --	1377.0037	1377.0037	1377.0659
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.4061	13.4061	13.4073
IR Inten --	39.1016	39.1016	0.0000
Raman Activ --	7.2506	7.2506	33.8957
	208	209	210
	A2	E	E
Frequencies --	1384.4894	1387.2828	1387.2828
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.5522	13.6070	13.6070
IR Inten --	0.0000	1.6011	1.6011
Raman Activ --	0.0000	16.9498	16.9498
	211	212	213
	B2	B1	A1

Frequencies --	1405.6045	1407.5715	1413.5078
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.9688	14.0079	14.1263
IR Inten --	23.2261	0.0000	0.0000
Raman Activ --	74.1064	63.0331	50.9437
	214	215	216
	E	E	B2
Frequencies --	1419.3131	1419.3131	1420.7945
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.2426	14.2426	14.2723
IR Inten --	0.0081	0.0081	25.7460
Raman Activ --	23.6223	23.6223	9.8503
	217	218	219
	A1	A2	E
Frequencies --	1433.6950	1441.8222	1463.3136
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.5327	14.6979	15.1393
IR Inten --	0.0000	0.0000	6.3044
Raman Activ --	221.3520	0.0000	37.4372
	220	221	222
	E	E	E
Frequencies --	1463.3136	1464.2936	1464.2936
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.1393	15.1596	15.1596
IR Inten --	6.3044	0.3029	0.3029
Raman Activ --	37.4372	2.9685	2.9685
	223	224	225
	A2	A1	B1
Frequencies --	1464.3198	1470.5567	1480.8361
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.1601	15.2896	15.5041
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	29.1276	129.4107
	226	227	228
	E	E	E
Frequencies --	1485.7032	1485.7032	1503.4725
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.6061	15.6061	15.9817
IR Inten --	0.1527	0.1527	1.1190
Raman Activ --	28.0222	28.0222	75.3596
	229	230	231
	E	B1	A2
Frequencies --	1503.4725	1504.5159	1504.6802
Red. masses --	12.0000	12.0000	12.0000

Frc consts	--	15.9817	16.0039	16.0074
IR Inten	--	1.1190	0.0000	0.0000
Raman Activ	--	75.3596	106.2268	0.0000
		232	233	234
		B2	A2	B1
Frequencies	--	1504.8889	1516.4400	1518.1011
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.0118	16.2586	16.2942
IR Inten	--	3.3384	0.0000	0.0000
Raman Activ	--	43.8882	0.0000	0.8452
		235	236	237
		B2	E	E
Frequencies	--	1520.2339	1521.7423	1521.7423
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.3400	16.3724	16.3724
IR Inten	--	0.8032	0.0718	0.0718
Raman Activ	--	32.0091	1.1392	1.1392
		238	239	240
		A1	B1	A1
Frequencies	--	1525.3196	1566.4893	1567.3672
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.4495	17.3495	17.3689
IR Inten	--	0.0000	0.0000	0.0000
Raman Activ	--	263.8931	48.2238	211.8218
		241	242	243
		E	E	E
Frequencies	--	1570.4967	1570.4967	1575.6101
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	17.4384	17.4384	17.5521
IR Inten	--	1.2111	1.2111	32.3973
Raman Activ	--	23.8333	23.8333	157.4427
		244	245	246
		E	B2	A1
Frequencies	--	1575.6101	1582.3508	1600.5461
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	17.5521	17.7026	18.1121
IR Inten	--	32.3973	1.0305	0.0000
Raman Activ	--	157.4427	71.4384	36.9633

D. Harmonic frequencies, IR intensities, and Raman scattering activities of Sc₃NC@C₈₄ (a) calculated at the B3LYP/6-31G* level

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering

activities (A^{**4}/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	B2	B1	B1
Frequencies --	55.8358	76.0662	89.6779
Red. masses --	35.1135	31.3788	23.5766
Frc consts --	0.0645	0.1070	0.1117
IR Inten --	1.8278	0.0111	0.0508
Raman Activ --	3.4821	5.7269	0.7264
	4	5	6
	A2	B2	B1
Frequencies --	101.2329	145.4966	173.3303
Red. masses --	37.0166	32.7168	14.5602
Frc consts --	0.2235	0.4081	0.2577
IR Inten --	0.0000	0.8109	0.5278
Raman Activ --	1.2198	0.7421	4.3260
	7	8	9
	A1	B1	B2
Frequencies --	183.8790	196.0104	204.1180
Red. masses --	25.6721	14.0194	17.4031
Frc consts --	0.5114	0.3174	0.4272
IR Inten --	0.3620	0.3372	1.4189
Raman Activ --	1.2468	0.5773	1.4500
	10	11	12
	A1	A2	A1
Frequencies --	214.6206	219.3337	221.8783
Red. masses --	13.6236	12.0770	15.2658
Frc consts --	0.3697	0.3423	0.4428
IR Inten --	0.1300	0.0000	0.5957
Raman Activ --	44.5419	34.3808	40.4126
	13	14	15
	B1	B2	A1
Frequencies --	231.6350	241.0821	262.2664
Red. masses --	12.1103	13.0450	14.0050
Frc consts --	0.3828	0.4467	0.5676
IR Inten --	0.0297	0.2414	1.0550
Raman Activ --	19.4419	16.3285	18.4115
	16	17	18
	A2	A1	B2
Frequencies --	285.4166	293.8700	294.5922
Red. masses --	12.0010	12.6019	12.4025
Frc consts --	0.5760	0.6412	0.6342
IR Inten --	0.0000	1.6416	0.1005
Raman Activ --	0.0946	2.1824	4.7425
	19	20	21
	B1	B1	A1
Frequencies --	295.3975	298.8486	324.0445
Red. masses --	12.0297	12.0983	16.3352
Frc consts --	0.6185	0.6366	1.0106
IR Inten --	0.0019	0.3773	0.4406
Raman Activ --	0.4701	2.4123	1.6154
	22	23	24
	B1	B2	A2
Frequencies --	330.4046	332.7403	335.9843
Red. masses --	12.0243	12.0024	12.0005

Frc consts --	0.7734	0.7829	0.7982
IR Inten --	2.1980	0.5836	0.0000
Raman Activ --	8.6264	7.8382	7.9429
	25	26	27
	A2	B2	A1
Frequencies --	338.0149	342.1240	349.6952
Red. masses --	12.0021	12.9253	13.3710
Frc consts --	0.8079	0.8914	0.9634
IR Inten --	0.0000	7.7842	1.3082
Raman Activ --	0.9333	1.4827	3.3383
	28	29	30
	A1	B2	A1
Frequencies --	351.0588	359.7071	371.2338
Red. masses --	12.0155	12.2320	12.1494
Frc consts --	0.8725	0.9325	0.9865
IR Inten --	0.0080	0.2280	0.3475
Raman Activ --	7.4570	0.0003	2.7960
	31	32	33
	B1	A2	B1
Frequencies --	371.5487	373.9874	389.7413
Red. masses --	12.0088	12.0119	12.1043
Frc consts --	0.9767	0.9899	1.0833
IR Inten --	0.4175	0.0000	0.0742
Raman Activ --	0.3567	0.0151	0.5692
	34	35	36
	A2	A1	A1
Frequencies --	389.8249	391.3510	402.2821
Red. masses --	12.0513	12.3388	13.8603
Frc consts --	1.0790	1.1134	1.3216
IR Inten --	0.0000	2.1923	0.0246
Raman Activ --	1.2903	36.5480	24.3385
	37	38	39
	B2	B2	A1
Frequencies --	409.8632	419.1703	424.7653
Red. masses --	12.5017	14.8907	12.7488
Frc consts --	1.2374	1.5415	1.3552
IR Inten --	2.2667	0.4265	1.3963
Raman Activ --	0.3989	8.8111	92.9479
	40	41	42
	B2	A1	B2
Frequencies --	442.8059	446.5409	449.1008
Red. masses --	12.1033	12.2766	12.0163
Frc consts --	1.3982	1.4423	1.4279
IR Inten --	4.1854	1.0309	0.0848
Raman Activ --	6.1136	13.2742	1.5701
	43	44	45
	A2	B1	B1
Frequencies --	451.9759	452.9672	463.4426
Red. masses --	12.0167	12.1297	12.0094
Frc consts --	1.4463	1.4663	1.5197
IR Inten --	0.0000	0.9499	0.7559
Raman Activ --	1.3598	2.6675	0.3132
	46	47	48
	A2	A1	B2
Frequencies --	463.6472	465.9249	481.3151
Red. masses --	12.0211	12.7206	12.0105
Frc consts --	1.5225	1.6270	1.6393

IR Inten --	0.0000	2.5642	4.9650
Raman Activ --	0.1639	3.5250	0.0125
	49	50	51
	B1	A1	A2
Frequencies --	485.4672	488.5308	490.9455
Red. masses --	12.0784	12.5447	12.0070
Frc consts --	1.6772	1.7640	1.7051
IR Inten --	0.4478	10.8716	0.0000
Raman Activ --	2.1789	1.9235	0.0010
	52	53	54
	B1	B1	B2
Frequencies --	491.0365	497.5550	497.5945
Red. masses --	12.0083	12.0108	12.0476
Frc consts --	1.7059	1.7519	1.7575
IR Inten --	13.6664	0.2510	4.2125
Raman Activ --	0.0244	0.4254	3.8647
	55	56	57
	A2	A1	A1
Frequencies --	498.0061	499.4665	504.1954
Red. masses --	12.0016	13.8128	12.4824
Frc consts --	1.7537	2.0302	1.8696
IR Inten --	0.0000	1.3284	0.1120
Raman Activ --	0.3670	13.5959	4.2906
	58	59	60
	B2	B1	B2
Frequencies --	505.7722	509.2534	512.4311
Red. masses --	12.0167	12.0048	12.0439
Frc consts --	1.8111	1.8343	1.8633
IR Inten --	0.4522	0.8094	0.1568
Raman Activ --	0.2631	0.0131	0.0349
	61	62	63
	A1	A2	A2
Frequencies --	518.1241	519.9872	520.9062
Red. masses --	12.2218	12.0582	12.0009
Frc consts --	1.9331	1.9210	1.9186
IR Inten --	2.2643	0.0000	0.0000
Raman Activ --	2.0364	3.0217	0.0001
	64	65	66
	B1	B1	B2
Frequencies --	523.2326	533.0892	545.7545
Red. masses --	12.0113	12.1733	12.2465
Frc consts --	1.9374	2.0383	2.1491
IR Inten --	1.1724	1.3007	0.8414
Raman Activ --	2.5774	0.1335	0.0047
	67	68	69
	A2	A1	B2
Frequencies --	548.2915	571.8047	575.9793
Red. masses --	12.0232	12.7386	12.4577
Frc consts --	2.1296	2.4540	2.4350
IR Inten --	0.0000	3.2411	14.8315
Raman Activ --	0.0634	15.2286	0.0925
	70	71	72
	B1	A2	B2
Frequencies --	585.7658	585.8398	587.2442
Red. masses --	12.0282	12.0835	12.1113
Frc consts --	2.4316	2.4434	2.4608
IR Inten --	10.8997	0.0000	0.3496

Raman Activ --	1.0811	3.3669	0.8430
	73	74	75
	A1	A1	A1
Frequencies --	588.1240	606.9281	612.0381
Red. masses --	13.2625	12.0031	12.1323
Frc consts --	2.7028	2.6051	2.6776
IR Inten --	4.2724	0.9674	0.9613
Raman Activ --	21.4606	5.6806	1.1626
	76	77	78
	B2	B1	A2
Frequencies --	613.9454	618.3118	619.9268
Red. masses --	12.0015	12.0003	12.0035
Frc consts --	2.6653	2.7031	2.7179
IR Inten --	0.0195	0.0137	0.0000
Raman Activ --	0.1530	0.2058	1.8513
	79	80	81
	A2	A2	B1
Frequencies --	625.3760	631.5285	641.7967
Red. masses --	12.0015	12.0014	12.0124
Frc consts --	2.7655	2.8201	2.9153
IR Inten --	0.0000	0.0000	0.2251
Raman Activ --	0.2008	1.1595	0.2712
	82	83	84
	B2	A1	B1
Frequencies --	646.0122	651.7290	655.2131
Red. masses --	12.0244	12.0159	12.0029
Frc consts --	2.9566	3.0070	3.0360
IR Inten --	0.0258	2.1265	1.0675
Raman Activ --	0.0126	0.0134	7.1654
	85	86	87
	B2	A1	B1
Frequencies --	655.7592	660.3640	660.8744
Red. masses --	12.0020	12.0019	12.0224
Frc consts --	3.0408	3.0837	3.0937
IR Inten --	5.9097	3.6062	2.4380
Raman Activ --	6.7307	8.7176	0.3385
	88	89	90
	B2	A2	B1
Frequencies --	661.8309	666.7398	671.2982
Red. masses --	12.0415	12.0000	12.0072
Frc consts --	3.1076	3.1430	3.1880
IR Inten --	2.0357	0.0000	0.0023
Raman Activ --	2.4734	3.2022	25.2501
	91	92	93
	A2	B2	A2
Frequencies --	671.3940	674.7656	680.5923
Red. masses --	12.0058	12.0465	12.0061
Frc consts --	3.1886	3.2316	3.2766
IR Inten --	0.0000	0.0107	0.0000
Raman Activ --	12.6866	10.6574	38.7716
	94	95	96
	A1	B1	B2
Frequencies --	683.0299	690.4455	690.5867
Red. masses --	12.0849	12.0029	12.0121
Frc consts --	3.3218	3.3713	3.3753
IR Inten --	0.0366	5.3332	4.6793
Raman Activ --	10.5091	0.2405	1.8720

	97	98	99
	A2	A1	B2
Frequencies --	692.2188	692.7714	704.3866
Red. masses --	12.0026	12.1050	12.0229
Frc consts --	3.3885	3.4229	3.5147
IR Inten --	0.0000	4.7896	0.0521
Raman Activ --	0.0113	31.1067	11.0640
	100	101	102
	A1	B1	A2
Frequencies --	706.3335	707.1958	710.6751
Red. masses --	12.0181	12.0082	12.0015
Frc consts --	3.5327	3.5384	3.5713
IR Inten --	0.3393	20.7806	0.0000
Raman Activ --	5.5315	13.3842	26.5969
	103	104	105
	B1	A1	B1
Frequencies --	715.8841	717.7335	719.4469
Red. masses --	12.0171	12.0532	12.0019
Frc consts --	3.6286	3.6583	3.6601
IR Inten --	1.8447	0.3400	4.1920
Raman Activ --	12.5170	14.0000	0.6813
	106	107	108
	A2	A1	A1
Frequencies --	721.8289	727.1114	729.2651
Red. masses --	12.0012	12.0888	12.0582
Frc consts --	3.6842	3.7656	3.7784
IR Inten --	0.0000	2.9815	0.0007
Raman Activ --	16.0518	16.2577	0.4284
	109	110	111
	B2	B2	A2
Frequencies --	729.5433	730.3051	732.0125
Red. masses --	12.0070	12.0363	12.0018
Frc consts --	3.7652	3.7823	3.7891
IR Inten --	8.4079	0.0353	0.0000
Raman Activ --	0.4078	1.1798	0.0042
	112	113	114
	A1	A2	A2
Frequencies --	741.6789	742.7681	745.6736
Red. masses --	12.0032	12.0000	12.0001
Frc consts --	3.8903	3.9007	3.9313
IR Inten --	0.0875	0.0000	0.0000
Raman Activ --	1.1175	1.0229	0.5085
	115	116	117
	A2	B1	B2
Frequencies --	748.1088	749.0942	749.8131
Red. masses --	12.0001	12.0086	12.0137
Frc consts --	3.9570	3.9702	3.9795
IR Inten --	0.0000	0.4797	1.3794
Raman Activ --	3.2866	5.3510	0.0522
	118	119	120
	B1	B2	A1
Frequencies --	750.3902	752.3092	752.5685
Red. masses --	12.0013	12.0162	12.0569
Frc consts --	3.9816	4.0069	4.0232
IR Inten --	0.1469	0.0041	0.0784
Raman Activ --	0.0455	1.4578	9.9469
	121	122	123

	A1	B2	A2
Frequencies --	755.4318	755.5551	756.8417
Red. masses --	12.0387	12.0034	12.0001
Frc consts --	4.0478	4.0373	4.0499
IR Inten --	0.3586	1.3438	0.0000
Raman Activ --	6.3704	0.0519	0.0498
	124	125	126
	B1	A1	B1
Frequencies --	758.8660	761.4983	762.8126
Red. masses --	12.0023	12.0102	12.0011
Frc consts --	4.0723	4.1033	4.1144
IR Inten --	1.0483	0.2527	1.8422
Raman Activ --	0.3021	12.4309	0.1493
	127	128	129
	B2	A2	A2
Frequencies --	762.9923	764.0685	768.6306
Red. masses --	12.1425	12.0006	12.0003
Frc consts --	4.1648	4.1278	4.1771
IR Inten --	16.9483	0.0000	0.0000
Raman Activ --	7.4436	3.0623	4.9356
	130	131	132
	B2	B1	B2
Frequencies --	769.1331	769.5550	774.3934
Red. masses --	12.6329	12.0020	12.0635
Frc consts --	4.4031	4.1878	4.2623
IR Inten --	13.2260	5.1763	0.0416
Raman Activ --	8.3080	0.0770	1.1302
	133	134	135
	A2	B2	B1
Frequencies --	778.1334	787.9848	789.6437
Red. masses --	12.0122	12.0044	12.0036
Frc consts --	4.2853	4.3916	4.4099
IR Inten --	0.0000	0.2473	0.6602
Raman Activ --	1.4717	0.2218	0.3704
	136	137	138
	B2	B1	A2
Frequencies --	813.5154	813.8503	817.9976
Red. masses --	12.0139	12.0009	12.0006
Frc consts --	4.6845	4.6833	4.7310
IR Inten --	1.5359	1.3222	0.0000
Raman Activ --	0.1227	0.5967	0.0002
	139	140	141
	A2	B1	B2
Frequencies --	858.3334	863.2552	864.6023
Red. masses --	12.0005	12.0009	12.0170
Frc consts --	5.2091	5.2692	5.2927
IR Inten --	0.0000	3.0446	0.5848
Raman Activ --	1.7722	5.5987	8.5589
	142	143	144
	A1	B2	B1
Frequencies --	866.1607	874.3869	875.0173
Red. masses --	12.0363	12.0031	12.0038
Frc consts --	5.3203	5.4070	5.4151
IR Inten --	0.2144	0.6519	2.7481
Raman Activ --	4.4105	0.0868	0.7975
	145	146	147
	A1	A2	B2

Frequencies --	878.2645	884.9292	887.7522
Red. masses --	12.0208	12.0000	12.0093
Frc consts --	5.4630	5.5367	5.5764
IR Inten --	4.0044	0.0000	1.5139
Raman Activ --	0.8385	0.0019	1.1729
	148	149	150
	B1	A2	A2
Frequencies --	891.1469	907.3302	947.6690
Red. masses --	12.0003	12.0003	12.0000
Frc consts --	5.6149	5.8207	6.3496
IR Inten --	0.0640	0.0000	0.0000
Raman Activ --	0.0431	0.1968	0.0324
	151	152	153
	A1	B1	A2
Frequencies --	991.1459	1019.6715	1024.6496
Red. masses --	12.0081	12.0009	12.0002
Frc consts --	6.9503	7.3517	7.4232
IR Inten --	1.1931	8.2287	0.0000
Raman Activ --	18.7379	26.8703	2.3188
	154	155	156
	A1	B2	A1
Frequencies --	1025.5959	1029.4945	1032.8303
Red. masses --	12.0026	12.0046	12.0012
Frc consts --	7.4384	7.4963	7.5428
IR Inten --	2.5886	13.5373	0.3942
Raman Activ --	8.2059	0.0980	4.0569
	157	158	159
	B1	B2	A2
Frequencies --	1043.8278	1050.3561	1056.4667
Red. masses --	12.0009	12.0012	12.0005
Frc consts --	7.7041	7.8010	7.8915
IR Inten --	2.5005	4.2511	0.0000
Raman Activ --	0.0228	1.6061	4.0350
	160	161	162
	B1	B2	A1
Frequencies --	1114.2136	1118.7337	1121.3134
Red. masses --	12.0000	12.0003	12.0018
Frc consts --	8.7775	8.8490	8.8910
IR Inten --	1.5729	4.3482	0.2746
Raman Activ --	2.4299	0.0013	10.0807
	163	164	165
	A1	A2	B2
Frequencies --	1134.3241	1142.8610	1153.3826
Red. masses --	12.0008	12.0004	12.0003
Frc consts --	9.0978	9.2349	9.4056
IR Inten --	7.8153	0.0000	2.0866
Raman Activ --	95.2497	10.8379	10.8107
	166	167	168
	A1	B1	A2
Frequencies --	1155.5890	1158.5249	1160.4712
Red. masses --	12.0003	12.0000	12.0001
Frc consts --	9.4417	9.4895	9.5215
IR Inten --	7.7647	0.1321	0.0000
Raman Activ --	23.5038	0.0582	42.0295
	169	170	171
	B2	B1	A2
Frequencies --	1169.9426	1177.8400	1192.5298

Red. masses --	12.0004	12.0000	12.0001
Frc consts --	9.6777	9.8085	10.0548
IR Inten --	4.9901	0.2242	0.0000
Raman Activ --	8.9791	8.7773	16.4185
	172	173	174
	A1	B1	B2
Frequencies --	1194.4992	1202.1519	1206.9032
Red. masses --	12.0011	12.0000	12.0002
Frc consts --	10.0889	10.2177	10.2987
IR Inten --	4.0863	0.7112	16.3454
Raman Activ --	10.3554	8.8123	7.4254
	175	176	177
	B1	A2	A1
Frequencies --	1220.8976	1223.0239	1223.4207
Red. masses --	12.0006	12.0000	12.0003
Frc consts --	10.5393	10.5755	10.5826
IR Inten --	19.2523	0.0000	0.7129
Raman Activ --	68.7717	14.9656	18.1328
	178	179	180
	B1	B2	A1
Frequencies --	1236.0293	1239.6528	1240.1552
Red. masses --	12.0000	12.0003	12.0005
Frc consts --	10.8017	10.8653	10.8743
IR Inten --	2.9941	14.7370	23.3419
Raman Activ --	25.9203	6.4786	161.7864
	181	182	183
	A2	A1	B2
Frequencies --	1249.5265	1255.2464	1259.2457
Red. masses --	12.0000	12.0004	12.0004
Frc consts --	11.0388	11.1405	11.2116
IR Inten --	0.0000	0.5163	4.9572
Raman Activ --	17.9837	112.4791	1.4779
	184	185	186
	A1	B2	B1
Frequencies --	1268.8004	1268.8340	1270.1953
Red. masses --	12.0001	12.0004	12.0001
Frc consts --	11.3821	11.3830	11.4071
IR Inten --	4.0817	21.4493	0.3499
Raman Activ --	55.7398	6.1652	2.1872
	187	188	189
	A2	A1	B2
Frequencies --	1276.4383	1281.6217	1287.4511
Red. masses --	12.0000	12.0008	12.0008
Frc consts --	11.5194	11.6140	11.7199
IR Inten --	0.0000	37.9542	23.9628
Raman Activ --	0.0828	41.4472	35.4769
	190	191	192
	A2	B1	B2
Frequencies --	1295.0193	1297.1158	1307.1631
Red. masses --	12.0000	12.0000	12.0003
Frc consts --	11.8573	11.8957	12.0809
IR Inten --	0.0000	9.2224	3.1847
Raman Activ --	26.0978	5.1507	19.3459
	193	194	195
	A1	B1	A2
Frequencies --	1310.2018	1318.4009	1319.4372
Red. masses --	12.0003	12.0000	12.0000

Frc consts	--	12.1372	12.2893	12.3086
IR Inten	--	2.5075	5.5041	0.0000
Raman Activ	--	201.2581	2.9518	0.7312
		196	197	198
		B2	A2	B1
Frequencies	--	1320.0885	1326.5583	1332.6647
Red. masses	--	12.0004	12.0001	12.0004
Frc consts	--	12.3212	12.4419	12.5570
IR Inten	--	25.7916	0.0000	25.5506
Raman Activ	--	4.5866	4.8504	72.0554
		199	200	201
		A1	B2	A1
Frequencies	--	1332.8817	1334.9855	1337.5072
Red. masses	--	12.0004	12.0001	12.0001
Frc consts	--	12.5612	12.6005	12.6482
IR Inten	--	0.7452	4.1434	6.3158
Raman Activ	--	30.8095	39.4320	65.0808
		202	203	204
		B1	A1	A2
Frequencies	--	1340.2869	1344.4460	1345.9103
Red. masses	--	12.0001	12.0004	12.0000
Frc consts	--	12.7007	12.7801	12.8075
IR Inten	--	15.7316	11.2402	0.0000
Raman Activ	--	28.3149	17.1787	25.3599
		205	206	207
		B1	B2	B1
Frequencies	--	1348.6273	1351.0121	1352.7463
Red. masses	--	12.0009	12.0003	12.0017
Frc consts	--	12.8602	12.9051	12.9397
IR Inten	--	48.2818	10.7045	121.4812
Raman Activ	--	37.2504	0.0093	112.5787
		208	209	210
		A2	A1	B1
Frequencies	--	1357.4080	1363.8271	1365.4399
Red. masses	--	12.0006	12.0004	12.0000
Frc consts	--	13.0279	13.1512	13.1819
IR Inten	--	0.0000	7.1874	7.2156
Raman Activ	--	61.9234	15.1875	48.9764
		211	212	213
		B2	B1	A1
Frequencies	--	1366.7927	1369.0524	1371.8388
Red. masses	--	12.0002	12.0001	12.0002
Frc consts	--	13.2082	13.2518	13.3059
IR Inten	--	6.6649	0.3949	24.6479
Raman Activ	--	81.4524	33.8245	70.7469
		214	215	216
		A2	B2	B2
Frequencies	--	1374.1462	1374.8580	1391.7531
Red. masses	--	12.0000	12.0010	12.0010
Frc consts	--	13.3505	13.3654	13.6960
IR Inten	--	0.0000	61.8836	26.1959
Raman Activ	--	0.1804	7.1666	54.2840
		217	218	219
		A1	B1	B1
Frequencies	--	1395.7913	1402.8642	1404.0695
Red. masses	--	12.0011	12.0006	12.0001
Frc consts	--	13.7757	13.9151	13.9383

IR Inten	--	12.4978	58.0885	0.0217
Raman Activ	--	19.2010	1.3859	21.9013
		220	221	222
		A2	A1	A2
Frequencies	--	1404.6776	1405.1920	1408.3506
Red. masses	--	12.0000	12.0005	12.0000
Frc consts	--	13.9504	13.9612	14.0234
IR Inten	--	0.0000	0.1944	0.0000
Raman Activ	--	0.1441	8.8854	0.1569
		223	224	225
		B2	A2	B2
Frequencies	--	1411.0061	1414.6881	1418.3262
Red. masses	--	12.0004	12.0000	12.0001
Frc consts	--	14.0768	14.1499	14.2229
IR Inten	--	21.2503	0.0000	9.5874
Raman Activ	--	58.8578	41.3289	7.5635
		226	227	228
		A1	A1	B2
Frequencies	--	1418.7721	1439.7374	1440.3898
Red. masses	--	12.0005	12.0011	12.0003
Frc consts	--	14.2322	14.6567	14.6690
IR Inten	--	0.5530	3.0323	13.5671
Raman Activ	--	147.8885	34.5119	0.1129
		229	230	231
		A1	A2	B1
Frequencies	--	1445.9886	1450.3538	1450.3747
Red. masses	--	12.0007	12.0000	12.0000
Frc consts	--	14.7838	14.8724	14.8728
IR Inten	--	44.0065	0.0000	2.1368
Raman Activ	--	38.5949	0.0540	73.0087
		232	233	234
		A1	A2	B1
Frequencies	--	1463.4331	1463.7363	1468.8421
Red. masses	--	12.0001	12.0000	12.0001
Frc consts	--	15.1419	15.1481	15.2540
IR Inten	--	2.4438	0.0000	1.6534
Raman Activ	--	37.9679	9.5386	7.8780
		235	236	237
		B2	A1	B2
Frequencies	--	1470.5160	1471.2777	1478.0925
Red. masses	--	12.0001	12.0002	12.0001
Frc consts	--	15.2888	15.3048	15.4468
IR Inten	--	3.6712	10.7009	0.0002
Raman Activ	--	30.8136	120.6894	0.8920
		238	239	240
		B1	A1	B1
Frequencies	--	1492.8928	1493.1770	1497.6737
Red. masses	--	12.0000	12.0001	12.0002
Frc consts	--	15.7576	15.7637	15.8589
IR Inten	--	4.7290	4.2798	3.0737
Raman Activ	--	2.9553	112.8502	32.8779
		241	242	243
		B2	A2	A1
Frequencies	--	1497.8520	1501.6212	1513.6041
Red. masses	--	12.0005	12.0000	12.9169
Frc consts	--	15.8631	15.9424	17.4355
IR Inten	--	31.5680	0.0000	0.0040

Raman Activ --	36.5300	15.3964	6.4941
	244	245	246
	A2	B2	A1
Frequencies --	1513.6614	1516.5257	1520.4833
Red. masses --	12.0000	12.0001	12.0008
Frc consts --	16.1991	16.2605	16.3464
IR Inten --	0.0000	2.1514	9.6066
Raman Activ --	0.0257	35.2128	77.6130
	247	248	249
	B1	B2	A2
Frequencies --	1526.8996	1528.7922	1530.0020
Red. masses --	12.0000	12.0002	12.0000
Frc consts --	16.4837	16.5247	16.5507
IR Inten --	0.8928	5.1245	0.0000
Raman Activ --	0.1164	95.3550	12.3198
	250	251	252
	B1	A1	A2
Frequencies --	1531.9673	1536.4568	1541.5188
Red. masses --	12.0001	12.0016	12.0001
Frc consts --	16.5933	16.6928	16.8010
IR Inten --	3.7087	0.8879	0.0000
Raman Activ --	0.3959	50.9529	0.1673
	253	254	255
	B2	A2	A1
Frequencies --	1548.8726	1555.8475	1584.1706
Red. masses --	12.0000	12.0000	12.0014
Frc consts --	16.9615	17.1145	17.7454
IR Inten --	1.0027	0.0000	3.8390
Raman Activ --	9.3659	5.2906	66.9245
	256	257	258
	A1	B1	A2
Frequencies --	1596.0255	1596.7352	1601.6041
Red. masses --	12.0010	12.0000	12.0000
Frc consts --	18.0113	18.0260	18.1360
IR Inten --	6.2717	1.2509	0.0000
Raman Activ --	186.3559	0.1996	15.7114
	259	260	261
	B2	B1	A1
Frequencies --	1609.8772	1625.8958	1634.0625
Red. masses --	12.0001	12.0000	12.0000
Frc consts --	18.3241	18.6904	18.8786
IR Inten --	23.1805	8.1201	2.8849
Raman Activ --	33.3166	30.5326	28.6313

E. Harmonic frequencies, IR intensities, and Raman scattering activities of non-IPR C_s (51365) C₈₄⁶⁻ calculated at the B3LYP/6-31G* level

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1	2	3
A'	A''	A''

Frequencies --	199.6730	203.5717	209.5645
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.2819	0.2930	0.3105
IR Inten --	0.0145	0.0719	0.0044
Raman Activ --	27.6882	35.0987	25.2114
	4	5	6
	A'	A'	A'
Frequencies --	227.7966	228.4590	266.6833
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.3669	0.3690	0.5028
IR Inten --	0.0379	0.0005	0.6534
Raman Activ --	31.8168	27.8498	0.2151
	7	8	9
	A''	A''	A'
Frequencies --	270.5617	272.2053	275.3205
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.5176	0.5239	0.5359
IR Inten --	0.0059	0.2061	0.0287
Raman Activ --	0.6241	0.1527	0.5065
	10	11	12
	A''	A'	A'
Frequencies --	280.0787	296.6602	297.2795
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.5546	0.6222	0.6248
IR Inten --	0.0575	0.0009	0.0045
Raman Activ --	0.0572	0.1829	0.3833
	13	14	15
	A''	A''	A'
Frequencies --	312.0291	319.3252	339.7517
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.6884	0.7209	0.8161
IR Inten --	0.0161	0.0212	0.2731
Raman Activ --	0.4565	0.2272	0.5090
	16	17	18
	A''	A'	A''
Frequencies --	345.3299	347.0716	347.2563
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.8431	0.8517	0.8526
IR Inten --	0.1179	0.3392	0.0069
Raman Activ --	0.0587	0.6822	0.1544
	19	20	21
	A'	A''	A''
Frequencies --	349.7085	350.6282	357.0500
Red. masses --	12.0000	12.0000	12.0000

Frc consts --	0.8647	0.8692	0.9013
IR Inten --	0.2114	0.0001	0.0642
Raman Activ --	1.0031	0.8273	0.5784
	22	23	24
	A'	A''	A'
Frequencies --	357.8705	359.1598	359.6335
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.9055	0.9120	0.9144
IR Inten --	0.0156	0.0236	0.0618
Raman Activ --	0.1627	0.4299	1.9931
	25	26	27
	A'	A'	A''
Frequencies --	365.3715	377.5238	405.5853
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	0.9438	1.0077	1.1630
IR Inten --	0.0278	0.3535	0.0002
Raman Activ --	1.2341	1.4103	1.4112
	28	29	30
	A'	A''	A'
Frequencies --	406.9900	407.8058	414.4201
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.1711	1.1758	1.2143
IR Inten --	0.0079	0.0057	0.0464
Raman Activ --	137.6537	0.0845	12.7271
	31	32	33
	A'	A''	A''
Frequencies --	415.2969	416.3219	430.8472
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.2194	1.2254	1.3124
IR Inten --	0.4901	0.1552	0.0017
Raman Activ --	12.6105	0.6703	1.9964
	34	35	36
	A'	A''	A'
Frequencies --	439.0890	442.7290	450.5083
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.3631	1.3858	1.4350
IR Inten --	0.0866	0.0033	0.8728
Raman Activ --	6.8131	2.9518	0.8577
	37	38	39
	A'	A''	A''
Frequencies --	458.1696	459.1659	465.1076
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.4842	1.4906	1.5295
IR Inten --	0.1263	51.0460	1.6888

Raman Activ --	1.8958	0.2578	3.5142
	40	41	42
	A''	A'	A''
Frequencies --	466.8955	472.2848	476.2840
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.5412	1.5770	1.6038
IR Inten --	25.4760	4.9292	4.3457
Raman Activ --	0.2601	0.8947	1.0105
	43	44	45
	A'	A'	A''
Frequencies --	476.3636	480.3104	481.0079
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.6044	1.6311	1.6358
IR Inten --	1.4631	0.2664	6.6061
Raman Activ --	0.7491	1.4515	0.1229
	46	47	48
	A''	A'	A'
Frequencies --	485.9404	489.2670	494.5518
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.6695	1.6925	1.7292
IR Inten --	0.0419	2.8723	1.4747
Raman Activ --	1.3427	0.8437	0.5031
	49	50	51
	A''	A''	A'
Frequencies --	498.6883	503.4907	505.2018
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.7583	1.7923	1.8045
IR Inten --	3.8711	1.6218	96.1504
Raman Activ --	3.4621	1.8567	0.4256
	52	53	54
	A'	A'	A'
Frequencies --	506.7884	520.4950	520.7925
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.8159	1.9154	1.9176
IR Inten --	91.8256	17.1415	9.3010
Raman Activ --	0.5838	0.5972	0.8245
	55	56	57
	A''	A''	A'
Frequencies --	525.4378	536.0026	547.7588
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	1.9520	2.0313	2.1213
IR Inten --	0.0052	0.0155	8.4088
Raman Activ --	3.6500	0.2679	0.2703
	58	59	60

	A'	A''	A'
Frequencies --	563.4888	581.3117	582.3497
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.2449	2.3892	2.3977
IR Inten --	1.0353	0.0057	1.2485
Raman Activ --	3.3636	0.2283	7.4239
	61	62	63
	A''	A''	A'
Frequencies --	583.9290	594.5702	595.1733
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.4107	2.4994	2.5045
IR Inten --	0.6337	0.8734	0.4549
Raman Activ --	5.3891	3.2290	1.2130
	64	65	66
	A'	A''	A''
Frequencies --	603.2985	603.9734	608.0215
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.5733	2.5791	2.6138
IR Inten --	0.5083	0.1003	1.6246
Raman Activ --	11.2746	0.2764	0.2268
	67	68	69
	A''	A'	A''
Frequencies --	616.3767	616.5663	620.5766
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.6861	2.6878	2.7228
IR Inten --	0.2601	0.1139	0.0672
Raman Activ --	0.1179	0.3677	0.1947
	70	71	72
	A'	A''	A'
Frequencies --	623.9157	624.5198	626.2333
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.7522	2.7576	2.7727
IR Inten --	0.0310	2.7551	2.7695
Raman Activ --	1.3873	1.7348	0.8011
	73	74	75
	A''	A'	A'
Frequencies --	635.4043	637.0353	642.2712
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.8545	2.8692	2.9165
IR Inten --	0.0384	13.1448	1.2519
Raman Activ --	0.7382	1.6165	0.7696
	76	77	78
	A''	A'	A''
Frequencies --	642.6061	648.4793	648.9094

Red. masses --	12.0000	12.0000	12.0000
Frc consts --	2.9196	2.9732	2.9771
IR Inten --	0.2027	1.8317	0.7293
Raman Activ --	2.0921	1.6779	5.8066
	79	80	81
	A'	A"	A'
Frequencies --	651.7848	652.3896	653.9654
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.0036	3.0092	3.0237
IR Inten --	4.7339	8.4391	1.8786
Raman Activ --	4.6204	3.7320	11.4248
	82	83	84
	A"	A'	A"
Frequencies --	655.9075	656.3269	660.5060
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.0417	3.0456	3.0845
IR Inten --	6.9594	4.9442	8.7422
Raman Activ --	2.3537	3.5638	4.2446
	85	86	87
	A'	A"	A'
Frequencies --	663.2549	663.5927	664.1979
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.1102	3.1134	3.1191
IR Inten --	4.2544	5.5279	4.8047
Raman Activ --	2.1267	1.4938	2.7119
	88	89	90
	A"	A'	A"
Frequencies --	666.3645	669.4915	669.6208
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.1395	3.1690	3.1702
IR Inten --	0.0004	1.7402	0.0253
Raman Activ --	0.0980	1.7335	0.0504
	91	92	93
	A'	A"	A"
Frequencies --	670.2508	670.2878	671.6468
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.1762	3.1765	3.1894
IR Inten --	1.0360	0.7890	0.6244
Raman Activ --	3.0023	1.6793	3.5710
	94	95	96
	A'	A'	A'
Frequencies --	672.8715	676.1870	676.2967
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.2011	3.2327	3.2337

IR Inten	--	0.5213	0.8455	0.3228
Raman Activ	--	6.4470	3.3338	0.7560
		97	98	99
		A'	A'	A''
Frequencies	--	677.8978	679.4100	680.4402
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.2491	3.2636	3.2735
IR Inten	--	5.6963	1.9447	0.5527
Raman Activ	--	6.2031	7.0716	1.2191
		100	101	102
		A''	A'	A'
Frequencies	--	681.2106	682.1016	682.7687
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.2809	3.2895	3.2959
IR Inten	--	0.3735	2.3396	0.9867
Raman Activ	--	0.4106	3.4872	2.4054
		103	104	105
		A''	A'	A'
Frequencies	--	685.7350	686.1301	687.2313
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3246	3.3285	3.3392
IR Inten	--	1.2845	4.6373	1.4554
Raman Activ	--	3.1152	5.3213	8.7626
		106	107	108
		A''	A'	A''
Frequencies	--	687.8024	689.3872	691.2459
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3447	3.3601	3.3783
IR Inten	--	0.8249	0.0890	0.0003
Raman Activ	--	1.4141	1.0022	2.6673
		109	110	111
		A''	A'	A''
Frequencies	--	692.6141	695.4196	697.0449
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.3917	3.4192	3.4352
IR Inten	--	1.0368	1.2011	0.2786
Raman Activ	--	2.1330	0.4866	1.1301
		112	113	114
		A'	A''	A'
Frequencies	--	698.6620	705.8800	706.0546
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	3.4512	3.5228	3.5246
IR Inten	--	2.6358	0.1846	1.1477
Raman Activ	--	0.4680	1.0822	0.3910

	115	116	117
	A'	A''	A'
Frequencies --	732.4181	732.5501	739.0968
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.7927	3.7941	3.8622
IR Inten --	1.2194	0.6228	1.8162
Raman Activ --	3.3698	7.6684	3.8013
	118	119	120
	A''	A'	A''
Frequencies --	746.4480	752.7555	763.8865
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	3.9394	4.0063	4.1256
IR Inten --	0.0556	1.7048	0.0945
Raman Activ --	1.8150	5.2883	0.1673
	121	122	123
	A''	A'	A'
Frequencies --	794.8597	802.9551	826.8400
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	4.4670	4.5584	4.8336
IR Inten --	0.0073	1.6318	0.5483
Raman Activ --	1.9610	3.1387	0.3522
	124	125	126
	A''	A'	A''
Frequencies --	837.4389	838.1610	838.3622
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	4.9584	4.9669	4.9693
IR Inten --	0.3642	0.1124	0.0732
Raman Activ --	0.3773	0.8847	0.3556
	127	128	129
	A'	A'	A''
Frequencies --	843.4016	854.7442	864.5970
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.0292	5.1654	5.2852
IR Inten --	0.4137	0.3893	0.4894
Raman Activ --	0.8465	2.4101	0.5461
	130	131	132
	A''	A'	A''
Frequencies --	875.0458	875.2833	881.0004
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.4137	5.4166	5.4876
IR Inten --	1.0266	0.2211	0.0175
Raman Activ --	0.0960	0.0764	0.2170
	133	134	135
	A'	A''	A''

Frequencies --	891.4559	892.4813	896.9570
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.6186	5.6316	5.6882
IR Inten --	7.1967	9.0154	0.0033
Raman Activ --	4.6613	0.1163	0.8075
	136	137	138
	A'	A''	A'
Frequencies --	919.1677	1004.1269	1004.1544
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	5.9734	7.1287	7.1291
IR Inten --	0.4124	0.3897	1.4789
Raman Activ --	0.0213	0.0263	1.9364
	139	140	141
	A'	A''	A'
Frequencies --	1005.7434	1017.4670	1024.9245
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.1516	7.3193	7.4270
IR Inten --	1.2458	0.0235	1.6630
Raman Activ --	2.3267	0.1675	5.4586
	142	143	144
	A'	A''	A'
Frequencies --	1035.9497	1037.3047	1039.0319
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.5877	7.6075	7.6329
IR Inten --	0.3155	3.6936	2.3711
Raman Activ --	1.0303	1.4842	3.4681
	145	146	147
	A''	A'	A''
Frequencies --	1041.8687	1115.4110	1118.4795
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	7.6746	8.7963	8.8448
IR Inten --	4.2116	7.8216	0.5493
Raman Activ --	0.9040	4.4620	0.9438
	148	149	150
	A''	A'	A''
Frequencies --	1125.5200	1130.0925	1136.4480
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	8.9565	9.0294	9.1313
IR Inten --	11.3305	6.9279	0.7326
Raman Activ --	1.8177	2.4161	0.2074
	151	152	153
	A'	A''	A'
Frequencies --	1138.7727	1150.4346	1160.2652
Red. masses --	12.0000	12.0000	12.0000

Frc consts	--	9.1687	9.3574	9.5180
IR Inten	--	9.0431	1.9263	2.2397
Raman Activ	--	5.1660	2.1163	2.4181
		154	155	156
		A'	A''	A''
Frequencies	--	1164.8863	1165.0604	1175.7965
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	9.5940	9.5968	9.7745
IR Inten	--	6.0668	8.5475	2.0444
Raman Activ	--	3.6843	3.1431	0.9176
		157	158	159
		A'	A'	A'
Frequencies	--	1179.8408	1196.2668	1200.4323
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	9.8419	10.1178	10.1884
IR Inten	--	0.1351	3.3878	7.5347
Raman Activ	--	5.2823	11.6956	2.9210
		160	161	162
		A''	A''	A''
Frequencies	--	1201.2453	1209.1490	1214.5766
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	10.2022	10.3369	10.4299
IR Inten	--	7.5978	0.1452	5.2555
Raman Activ	--	2.5789	2.8087	1.5711
		163	164	165
		A'	A''	A'
Frequencies	--	1224.8429	1229.4722	1229.8681
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	10.6070	10.6873	10.6942
IR Inten	--	2.1912	0.0122	0.3012
Raman Activ	--	5.7501	2.1973	8.6669
		166	167	168
		A'	A''	A'
Frequencies	--	1235.0063	1245.0155	1245.4751
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	10.7837	10.9593	10.9673
IR Inten	--	6.3965	16.4310	9.6984
Raman Activ	--	11.3864	0.8290	1.9543
		169	170	171
		A''	A'	A''
Frequencies	--	1250.1667	1253.0036	1254.6100
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	11.0501	11.1003	11.1288
IR Inten	--	6.2873	8.8371	7.2811

Raman Activ --	0.0643	4.9477	12.6736
	172	173	174
	A'	A''	A'
Frequencies --	1259.1518	1263.8224	1270.5702
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.2095	11.2928	11.4138
IR Inten --	14.9070	0.4069	0.5745
Raman Activ --	1.5455	5.9201	10.2257
	175	176	177
	A''	A'	A''
Frequencies --	1275.7430	1285.1069	1286.1659
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.5069	11.6764	11.6957
IR Inten --	2.8932	0.5276	0.9034
Raman Activ --	10.7819	1.2036	5.3668
	178	179	180
	A'	A''	A''
Frequencies --	1293.7650	1294.5641	1296.2787
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.8343	11.8489	11.8803
IR Inten --	4.0044	2.2410	0.5012
Raman Activ --	11.6369	1.4739	15.4334
	181	182	183
	A'	A''	A''
Frequencies --	1298.7255	1299.8460	1304.8698
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	11.9252	11.9458	12.0383
IR Inten --	10.6674	3.8160	4.0601
Raman Activ --	29.7516	19.2692	8.3875
	184	185	186
	A'	A''	A'
Frequencies --	1305.7962	1310.1606	1313.7968
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.0554	12.1361	12.2036
IR Inten --	0.6787	2.9826	1.8009
Raman Activ --	25.6482	32.2293	32.1270
	187	188	189
	A''	A'	A''
Frequencies --	1315.9860	1318.8977	1331.6744
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.2443	12.2985	12.5380
IR Inten --	0.0618	9.8486	6.8717
Raman Activ --	14.0785	6.7585	1.5127
	190	191	192

	A''	A'	A''
Frequencies --	1342.6936	1343.6585	1346.5164
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.7463	12.7647	12.8190
IR Inten --	102.3300	10.0558	4.4017
Raman Activ --	10.6602	10.7397	3.2707
	193	194	195
	A'	A'	A''
Frequencies --	1349.8600	1356.1338	1357.9217
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	12.8828	13.0028	13.0371
IR Inten --	12.6975	1.5601	8.7820
Raman Activ --	33.6792	7.3664	15.2454
	196	197	198
	A'	A'	A''
Frequencies --	1359.3904	1361.4372	1371.1381
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.0653	13.1047	13.2921
IR Inten --	21.5686	0.3463	1.6645
Raman Activ --	7.5034	9.2736	11.1279
	199	200	201
	A'	A''	A'
Frequencies --	1373.7267	1377.2490	1379.5908
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.3423	13.4109	13.4565
IR Inten --	69.7651	50.3563	22.3131
Raman Activ --	2.3556	0.6102	19.6807
	202	203	204
	A''	A'	A'
Frequencies --	1379.9727	1382.6537	1388.5808
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.4639	13.5163	13.6324
IR Inten --	26.2379	20.0013	24.5260
Raman Activ --	10.8747	4.4323	1.9113
	205	206	207
	A''	A'	A''
Frequencies --	1395.2505	1400.6678	1405.6812
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	13.7637	13.8708	13.9703
IR Inten --	2.1766	12.4924	5.2195
Raman Activ --	11.4367	14.3152	12.9557
	208	209	210
	A'	A''	A''
Frequencies --	1407.1998	1408.2728	1419.0536

Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.0005	14.0218	14.2373
IR Inten --	31.9420	0.1888	34.3132
Raman Activ --	17.5517	8.5436	25.1155
	211	212	213
	A'	A''	A'
Frequencies --	1420.1170	1432.8907	1433.3141
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.2587	14.5164	14.5249
IR Inten --	4.5969	0.5097	13.7762
Raman Activ --	36.5427	39.5375	22.4513
	214	215	216
	A'	A''	A'
Frequencies --	1438.9661	1450.3034	1450.6491
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.6397	14.8713	14.8784
IR Inten --	20.4183	5.3565	4.8101
Raman Activ --	5.8619	21.6090	54.5549
	217	218	219
	A'	A'	A''
Frequencies --	1455.8231	1456.2087	1457.4299
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	14.9847	14.9927	15.0178
IR Inten --	1.1506	0.3441	0.9727
Raman Activ --	38.5212	16.8574	5.8067
	220	221	222
	A''	A'	A'
Frequencies --	1460.8080	1461.3890	1468.6303
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.0875	15.0995	15.2495
IR Inten --	0.0147	2.6048	7.8573
Raman Activ --	11.6096	47.3189	5.5909
	223	224	225
	A''	A'	A'
Frequencies --	1473.3614	1478.8363	1481.9281
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.3479	15.4622	15.5269
IR Inten --	2.6768	12.5998	26.4639
Raman Activ --	6.5317	8.4468	12.8567
	226	227	228
	A''	A'	A''
Frequencies --	1485.9906	1486.4121	1490.5796
Red. masses --	12.0000	12.0000	12.0000
Frc consts --	15.6122	15.6210	15.7088

IR Inten	--	1.0556	10.0476	0.5536
Raman Activ	--	2.9744	10.9586	74.6504
		229	230	231
		A'	A''	A''
Frequencies	--	1491.3983	1500.5385	1506.4192
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	15.7260	15.9194	16.0444
IR Inten	--	0.9713	1.0758	3.4043
Raman Activ	--	3.0497	6.6902	6.4526
		232	233	234
		A''	A'	A''
Frequencies	--	1507.5370	1511.5703	1516.2520
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.0682	16.1543	16.2545
IR Inten	--	0.3809	2.2469	2.5907
Raman Activ	--	11.3693	13.4420	15.9096
		235	236	237
		A'	A''	A'
Frequencies	--	1520.6269	1522.2508	1527.7998
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.3485	16.3834	16.5031
IR Inten	--	2.6054	1.4088	0.7013
Raman Activ	--	115.8885	8.7263	5.8759
		238	239	240
		A''	A'	A''
Frequencies	--	1528.9385	1532.4133	1532.6566
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.5277	16.6029	16.6081
IR Inten	--	0.4214	0.0556	0.0001
Raman Activ	--	36.4574	48.9137	11.8575
		241	242	243
		A''	A'	A'
Frequencies	--	1539.6925	1542.8437	1550.6399
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	16.7610	16.8297	17.0002
IR Inten	--	0.2524	0.5368	1.7618
Raman Activ	--	9.4523	44.5119	135.2034
		244	245	246
		A'	A''	A'
Frequencies	--	1559.8216	1560.1509	1590.5749
Red. masses	--	12.0000	12.0000	12.0000
Frc consts	--	17.2021	17.2094	17.8871
IR Inten	--	1.7868	7.0105	0.2466
Raman Activ	--	69.5076	7.4224	47.5366

F. Harmonic frequencies, IR intensities, and Raman scattering activities of Sc₃NC@C₈₄ (e) calculated at the B3LYP/6-31G* level

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	85.1411	101.1081	133.9577
Red. masses --	28.8827	26.8040	30.8107
Frc consts --	0.1234	0.1614	0.3258
IR Inten --	0.6212	1.0164	0.3090
Raman Activ --	1.1886	0.6842	0.6837
	4	5	6
	A	A	A
Frequencies --	146.8929	157.7889	174.5958
Red. masses --	25.7455	21.2533	29.2820
Frc consts --	0.3273	0.3118	0.5259
IR Inten --	0.6589	2.4350	0.0480
Raman Activ --	2.3903	2.1818	7.7183
	7	8	9
	A	A	A
Frequencies --	178.3082	202.1502	207.8632
Red. masses --	17.7946	15.4049	13.1101
Frc consts --	0.3333	0.3709	0.3337
IR Inten --	2.0454	0.4097	0.1142
Raman Activ --	0.9438	13.0300	25.9941
	10	11	12
	A	A	A
Frequencies --	220.8511	228.0030	229.1248
Red. masses --	13.1338	13.6269	14.5766
Frc consts --	0.3774	0.4174	0.4509
IR Inten --	0.4746	0.2941	0.4717
Raman Activ --	19.9380	17.4703	20.5557
	13	14	15
	A	A	A
Frequencies --	256.3248	269.8051	272.2169
Red. masses --	13.3103	13.7879	14.2169
Frc consts --	0.5153	0.5914	0.6207
IR Inten --	0.4502	0.8749	0.4495
Raman Activ --	12.3796	1.9909	3.5324

	16	17	18
	A	A	A
Frequencies --	281.0864	281.4967	286.5182
Red. masses --	13.2448	12.5165	12.3716
Frc consts --	0.6166	0.5844	0.5984
IR Inten --	1.2000	0.2379	0.6753
Raman Activ --	1.5725	0.5889	1.2030
	19	20	21
	A	A	A
Frequencies --	291.8759	309.2374	314.7345
Red. masses --	12.7375	12.4647	12.0909
Frc consts --	0.6393	0.7023	0.7057
IR Inten --	0.7538	0.4363	0.2662
Raman Activ --	1.1164	0.4584	0.2595
	22	23	24
	A	A	A
Frequencies --	321.9038	336.7512	339.7741
Red. masses --	12.0978	12.4012	13.0985
Frc consts --	0.7386	0.8286	0.8909
IR Inten --	0.5072	0.5523	2.6904
Raman Activ --	0.2187	0.8383	3.1657
	25	26	27
	A	A	A
Frequencies --	344.1217	345.9457	350.4561
Red. masses --	13.3445	13.2414	12.0991
Frc consts --	0.9311	0.9337	0.8755
IR Inten --	1.3030	2.3343	0.0306
Raman Activ --	1.2910	1.7333	0.5877
	28	29	30
	A	A	A
Frequencies --	358.7493	361.9357	365.1547
Red. masses --	12.7592	13.3018	12.4609
Frc consts --	0.9675	1.0267	0.9789
IR Inten --	6.7103	7.5705	3.8530
Raman Activ --	0.6078	2.2243	0.6401
	31	32	33
	A	A	A
Frequencies --	367.9665	369.3413	372.9696
Red. masses --	12.3179	13.1786	12.5481
Frc consts --	0.9827	1.0592	1.0284
IR Inten --	0.9652	5.7079	0.8333
Raman Activ --	0.5390	3.3557	1.2623
	34	35	36
	A	A	A

Frequencies --	382.8800	389.2820	394.3928
Red. masses --	12.6455	12.7397	12.2760
Frc consts --	1.0922	1.1375	1.1250
IR Inten --	2.3445	0.6655	0.4343
Raman Activ --	3.2676	7.9199	1.7828
	37	38	39
	A	A	A
Frequencies --	400.0146	407.7463	411.9125
Red. masses --	12.4029	12.3790	13.3426
Frc consts --	1.1693	1.2126	1.3338
IR Inten --	1.1841	1.1081	3.7384
Raman Activ --	1.5980	1.7438	114.9910
	40	41	42
	A	A	A
Frequencies --	429.8186	430.5609	439.4648
Red. masses --	12.1343	12.1473	12.1237
Frc consts --	1.3208	1.3268	1.3795
IR Inten --	0.4938	0.0904	0.2510
Raman Activ --	0.6333	0.2259	1.1766
	43	44	45
	A	A	A
Frequencies --	445.6073	450.6980	458.3164
Red. masses --	12.2290	12.3369	12.1645
Frc consts --	1.4307	1.4765	1.5055
IR Inten --	0.7465	1.1008	0.4425
Raman Activ --	2.1570	2.1623	1.1422
	46	47	48
	A	A	A
Frequencies --	462.9375	469.1845	477.2535
Red. masses --	12.1145	12.0364	12.5068
Frc consts --	1.5297	1.5611	1.6784
IR Inten --	5.3943	1.0689	1.5553
Raman Activ --	2.6831	0.9469	7.2195
	49	50	51
	A	A	A
Frequencies --	479.6657	483.1417	483.8447
Red. masses --	12.6475	12.0797	12.0509
Frc consts --	1.7145	1.6613	1.6622
IR Inten --	1.4971	5.8124	0.0215
Raman Activ --	8.7864	0.2899	0.7986
	52	53	54
	A	A	A
Frequencies --	485.7696	490.2836	492.0356
Red. masses --	12.0956	12.1463	12.1922

Frc consts --	1.6817	1.7202	1.7391
IR Inten --	0.4010	1.7919	0.7763
Raman Activ --	1.7090	1.4168	2.8855
	55	56	57
	A	A	A
Frequencies --	502.1140	504.8316	508.0166
Red. masses --	12.5598	12.1614	12.0254
Frc consts --	1.8657	1.8261	1.8285
IR Inten --	2.6988	2.3216	0.4304
Raman Activ --	3.7504	2.1190	1.2970
	58	59	60
	A	A	A
Frequencies --	512.1285	515.3940	524.1296
Red. masses --	12.0742	12.1089	12.0554
Frc consts --	1.8658	1.8951	1.9512
IR Inten --	0.2313	5.5315	4.6715
Raman Activ --	0.4990	0.5352	0.3479
	61	62	63
	A	A	A
Frequencies --	528.9786	532.2971	536.1806
Red. masses --	12.3056	12.2001	12.0449
Frc consts --	2.0288	2.0367	2.0402
IR Inten --	2.3696	0.9590	1.8858
Raman Activ --	2.7550	1.6981	0.7573
	64	65	66
	A	A	A
Frequencies --	541.4708	548.0466	551.0079
Red. masses --	12.0480	12.3381	12.4605
Frc consts --	2.0812	2.1834	2.2290
IR Inten --	1.6937	4.2869	5.4550
Raman Activ --	0.4567	3.2271	2.9850
	67	68	69
	A	A	A
Frequencies --	558.1526	563.0555	575.6236
Red. masses --	12.2243	12.0677	12.2641
Frc consts --	2.2438	2.2541	2.3942
IR Inten --	2.4213	2.5482	1.3379
Raman Activ --	1.2979	0.2045	2.7108
	70	71	72
	A	A	A
Frequencies --	582.6502	588.1425	602.0073
Red. masses --	12.3544	12.0305	12.0186
Frc consts --	2.4711	2.4519	2.5663
IR Inten --	3.8107	0.1827	0.6421

Raman Activ --	5.1713	0.7478	1.3125
	73	74	75
	A	A	A
Frequencies --	607.5789	609.7600	616.9399
Red. masses --	12.0557	12.0094	12.0213
Frc consts --	2.6221	2.6308	2.6958
IR Inten --	1.9100	0.4790	0.6823
Raman Activ --	1.1690	0.2913	0.8546
	76	77	78
	A	A	A
Frequencies --	620.3150	621.7932	628.7663
Red. masses --	12.0327	12.0326	12.0156
Frc consts --	2.7280	2.7409	2.7988
IR Inten --	0.3015	0.2435	0.2489
Raman Activ --	0.9414	1.0445	0.4513
	79	80	81
	A	A	A
Frequencies --	632.6871	632.9867	637.8452
Red. masses --	12.0216	12.0094	12.0051
Frc consts --	2.8352	2.8350	2.8777
IR Inten --	0.7957	0.5851	0.0361
Raman Activ --	0.2974	1.4774	1.2676
	82	83	84
	A	A	A
Frequencies --	638.9756	647.5171	655.2088
Red. masses --	12.0228	12.0039	12.0129
Frc consts --	2.8922	2.9653	3.0385
IR Inten --	0.7921	0.1212	1.1402
Raman Activ --	1.2209	0.8086	0.8046
	85	86	87
	A	A	A
Frequencies --	656.8834	661.3301	663.8296
Red. masses --	12.0020	12.0106	12.0098
Frc consts --	3.0513	3.0949	3.1182
IR Inten --	0.4436	0.2694	3.6063
Raman Activ --	2.0801	5.4918	1.3231
	88	89	90
	A	A	A
Frequencies --	668.6247	669.0639	672.2265
Red. masses --	12.0394	12.0398	12.0163
Frc consts --	3.1712	3.1754	3.1993
IR Inten --	2.0942	1.0810	0.2863
Raman Activ --	11.2625	8.9986	3.3479
	91	92	93

	A	A	A
Frequencies --	672.5001	676.6083	681.2252
Red. masses --	12.0519	12.0155	12.0103
Frc consts --	3.2114	3.2409	3.2839
IR Inten --	1.0140	6.3182	1.9092
Raman Activ --	5.3239	2.9158	3.8446
	94	95	96
	A	A	A
Frequencies --	688.0057	693.1584	695.3187
Red. masses --	12.0120	12.0402	12.0156
Frc consts --	3.3500	3.4084	3.4227
IR Inten --	1.7619	0.5965	1.6735
Raman Activ --	1.4753	6.2317	2.4522
	97	98	99
	A	A	A
Frequencies --	698.2954	699.0494	702.7336
Red. masses --	12.0191	12.0361	12.0292
Frc consts --	3.4530	3.4654	3.5000
IR Inten --	0.6990	2.7698	0.4372
Raman Activ --	8.0382	11.3815	8.3396
	100	101	102
	A	A	A
Frequencies --	706.5048	707.0918	709.6045
Red. masses --	12.0106	12.0277	12.0101
Frc consts --	3.5322	3.5431	3.5631
IR Inten --	0.2184	0.5480	0.4256
Raman Activ --	1.7954	9.0869	3.1223
	103	104	105
	A	A	A
Frequencies --	711.8019	716.6167	720.6325
Red. masses --	12.0095	12.0127	12.0086
Frc consts --	3.5850	3.6347	3.6743
IR Inten --	1.1473	2.7132	0.3054
Raman Activ --	1.7374	0.8121	2.0729
	106	107	108
	A	A	A
Frequencies --	723.8342	725.2588	731.8956
Red. masses --	12.0126	12.0068	12.0060
Frc consts --	3.7082	3.7210	3.7892
IR Inten --	1.0559	0.7287	0.9936
Raman Activ --	2.1619	0.7888	0.6454
	109	110	111
	A	A	A
Frequencies --	735.6065	738.1000	741.5109

Red. masses --	12.0055	12.0027	12.0041
Frc consts --	3.8276	3.8527	3.8888
IR Inten --	0.8017	0.7789	0.2784
Raman Activ --	2.3367	1.4774	0.8856
	112	113	114
	A	A	A
Frequencies --	741.6607	742.6633	745.8044
Red. masses --	12.0106	12.0138	12.0162
Frc consts --	3.8925	3.9040	3.9379
IR Inten --	1.2434	0.2277	0.6306
Raman Activ --	3.5886	3.8557	6.1123
	115	116	117
	A	A	A
Frequencies --	747.5222	749.7424	752.1908
Red. masses --	12.0048	12.0043	12.0053
Frc consts --	3.9523	3.9757	4.0020
IR Inten --	0.1605	0.1348	1.2539
Raman Activ --	0.9527	2.5614	2.2278
	118	119	120
	A	A	A
Frequencies --	753.9546	755.2187	758.3951
Red. masses --	12.0060	12.0051	12.0048
Frc consts --	4.0210	4.0342	4.0681
IR Inten --	1.1285	0.3653	0.6389
Raman Activ --	1.6868	1.7383	2.2129
	121	122	123
	A	A	A
Frequencies --	760.8352	762.8354	763.5431
Red. masses --	12.0016	12.0022	12.0084
Frc consts --	4.0933	4.1150	4.1248
IR Inten --	0.9796	0.4449	0.5743
Raman Activ --	1.0799	0.6117	1.2891
	124	125	126
	A	A	A
Frequencies --	764.9701	767.5480	769.7858
Red. masses --	12.0030	12.0057	12.0034
Frc consts --	4.1384	4.1673	4.1908
IR Inten --	1.0051	0.1762	1.2935
Raman Activ --	1.3685	1.2132	1.2874
	127	128	129
	A	A	A
Frequencies --	770.6420	772.1786	774.9183
Red. masses --	12.0047	12.0082	12.0013
Frc consts --	4.2006	4.2185	4.2461

IR Inten	--	1.9434	1.9213	0.2535
Raman Activ	--	2.9980	0.7687	0.3911
		130	131	132
		A	A	A
Frequencies	--	775.3231	779.9851	781.8015
Red. masses	--	12.0041	12.0116	12.0031
Frc consts	--	4.2515	4.3055	4.3225
IR Inten	--	0.9401	0.2235	0.7709
Raman Activ	--	1.4848	1.1578	0.7691
		133	134	135
		A	A	A
Frequencies	--	798.4174	801.8622	806.8037
Red. masses	--	12.7879	12.0761	12.0025
Frc consts	--	4.8030	4.5748	4.6032
IR Inten	--	15.9953	1.2636	0.1940
Raman Activ	--	0.4645	1.1837	0.4045
		136	137	138
		A	A	A
Frequencies	--	816.4440	833.3911	847.0103
Red. masses	--	12.0015	12.0292	12.0037
Frc consts	--	4.7134	4.9225	5.0739
IR Inten	--	1.0320	1.1922	0.2478
Raman Activ	--	1.1427	0.3321	0.9664
		139	140	141
		A	A	A
Frequencies	--	848.0648	852.1142	853.3571
Red. masses	--	12.0008	12.0045	12.0053
Frc consts	--	5.0853	5.1356	5.1509
IR Inten	--	0.0201	0.2613	0.4907
Raman Activ	--	0.3010	0.8210	0.6305
		142	143	144
		A	A	A
Frequencies	--	864.2130	873.6684	884.9563
Red. masses	--	12.0021	12.0047	12.0073
Frc consts	--	5.2814	5.3988	5.5404
IR Inten	--	0.1164	1.2494	0.3107
Raman Activ	--	1.1858	0.3145	0.5904
		145	146	147
		A	A	A
Frequencies	--	885.3518	891.6813	900.8062
Red. masses	--	12.0034	12.0009	12.0113
Frc consts	--	5.5435	5.6219	5.7425
IR Inten	--	1.5033	0.2806	4.7707
Raman Activ	--	0.4987	0.2239	0.6983

	148	149	150
	A	A	A
Frequencies --	902.8461	908.6136	929.8480
Red. masses --	12.0184	12.0007	12.0003
Frc consts --	5.7720	5.8373	6.1132
IR Inten --	5.3986	0.1177	0.0983
Raman Activ --	1.5545	0.4245	0.1322
	151	152	153
	A	A	A
Frequencies --	1005.9427	1013.7122	1020.0307
Red. masses --	12.0036	12.0037	12.0013
Frc consts --	7.1566	7.2677	7.3571
IR Inten --	1.1089	0.5692	1.6397
Raman Activ --	0.9986	0.8905	1.4123
	154	155	156
	A	A	A
Frequencies --	1030.3051	1037.9419	1040.0500
Red. masses --	12.0011	12.0014	12.0033
Frc consts --	7.5059	7.6178	7.6500
IR Inten --	1.0775	1.5622	1.2914
Raman Activ --	1.0477	4.2681	6.1871
	157	158	159
	A	A	A
Frequencies --	1046.3806	1049.5299	1055.8444
Red. masses --	12.0009	12.0010	12.0011
Frc consts --	7.7418	7.7885	7.8826
IR Inten --	1.3289	1.2002	1.4001
Raman Activ --	1.6815	1.4848	1.9301
	160	161	162
	A	A	A
Frequencies --	1124.0082	1128.7965	1133.0325
Red. masses --	12.0006	12.0004	12.0009
Frc consts --	8.9329	9.0090	9.0771
IR Inten --	1.2565	2.4119	4.7766
Raman Activ --	1.8674	2.6730	0.8542
	163	164	165
	A	A	A
Frequencies --	1138.4867	1146.7773	1150.0691
Red. masses --	12.0002	12.0004	12.0002
Frc consts --	9.1642	9.2983	9.3516
IR Inten --	2.1848	8.4681	1.0161
Raman Activ --	4.2436	8.6712	2.6083
	166	167	168
	A	A	A

Frequencies --	1154.2209	1170.2514	1174.4699
Red. masses --	12.0004	12.0006	12.0001
Frc consts --	9.4194	9.6831	9.7525
IR Inten --	5.5460	3.6767	1.1275
Raman Activ --	0.3397	5.0837	8.9061
	169	170	171
	A	A	A
Frequencies --	1178.0803	1190.9862	1193.2042
Red. masses --	12.0003	12.0001	12.0002
Frc consts --	9.8128	10.0288	10.0662
IR Inten --	1.5640	1.0749	3.0721
Raman Activ --	1.8027	1.2944	2.6862
	172	173	174
	A	A	A
Frequencies --	1202.3737	1206.5982	1210.3032
Red. masses --	12.0002	12.0001	12.0003
Frc consts --	10.2215	10.2935	10.3569
IR Inten --	5.2015	1.6836	7.4829
Raman Activ --	3.3316	8.3188	3.2636
	175	176	177
	A	A	A
Frequencies --	1216.4423	1232.9235	1236.0418
Red. masses --	12.0001	12.0001	12.0002
Frc consts --	10.4621	10.7475	10.8020
IR Inten --	2.6946	1.3115	2.4247
Raman Activ --	1.4364	1.4451	2.9944
	178	179	180
	A	A	A
Frequencies --	1237.3515	1245.3486	1249.9747
Red. masses --	12.0001	12.0001	12.0001
Frc consts --	10.8248	10.9652	11.0468
IR Inten --	0.5231	2.0956	1.5484
Raman Activ --	5.3451	2.5192	0.9104
	181	182	183
	A	A	A
Frequencies --	1256.6291	1258.7619	1262.6954
Red. masses --	12.0001	12.0001	12.0001
Frc consts --	11.1647	11.2027	11.2728
IR Inten --	5.1651	3.3870	0.3714
Raman Activ --	2.2039	2.8293	5.6897
	184	185	186
	A	A	A
Frequencies --	1268.6904	1273.7756	1277.6430
Red. masses --	12.0001	12.0002	12.0001

Frc consts	--	11.3801	11.4716	11.5412
IR Inten	--	0.9323	0.7365	5.0824
Raman Activ	--	4.6613	8.3928	9.9284
		187	188	189
		A	A	A
Frequencies	--	1281.5836	1282.8378	1290.5362
Red. masses	--	12.0003	12.0002	12.0002
Frc consts	--	11.6128	11.6354	11.7755
IR Inten	--	11.0653	9.7992	9.0836
Raman Activ	--	12.2434	6.7283	3.1036
		190	191	192
		A	A	A
Frequencies	--	1293.9376	1298.0478	1301.9627
Red. masses	--	12.0001	12.0001	12.0001
Frc consts	--	11.8375	11.9128	11.9848
IR Inten	--	2.2149	0.8015	1.2673
Raman Activ	--	6.3303	1.7853	15.1657
		193	194	195
		A	A	A
Frequencies	--	1307.0874	1310.3951	1313.8582
Red. masses	--	12.0001	12.0004	12.0001
Frc consts	--	12.0793	12.1409	12.2048
IR Inten	--	1.9022	15.3934	3.5466
Raman Activ	--	6.9691	8.3240	6.6681
		196	197	198
		A	A	A
Frequencies	--	1317.5454	1320.0044	1322.4544
Red. masses	--	12.0000	12.0001	12.0000
Frc consts	--	12.2734	12.3193	12.3650
IR Inten	--	0.7314	2.1924	3.6357
Raman Activ	--	6.3264	6.4802	14.5788
		199	200	201
		A	A	A
Frequencies	--	1323.3420	1327.5970	1334.2530
Red. masses	--	12.0001	12.0002	12.0002
Frc consts	--	12.3816	12.4615	12.5868
IR Inten	--	0.9870	5.0781	6.3361
Raman Activ	--	13.3642	8.3981	17.9653
		202	203	204
		A	A	A
Frequencies	--	1335.9025	1347.2843	1350.6569
Red. masses	--	12.0002	12.0004	12.0002
Frc consts	--	12.6179	12.8340	12.8981
IR Inten	--	4.9382	20.2543	3.1191

Raman Activ --	5.9328	13.2500	5.4607
	205	206	207
	A	A	A
Frequencies --	1358.2841	1359.9347	1363.6756
Red. masses --	12.0002	12.0003	12.0004
Frc consts --	13.0443	13.0761	13.1482
IR Inten --	2.5862	17.5444	7.4696
Raman Activ --	7.7507	18.2726	3.7151
	208	209	210
	A	A	A
Frequencies --	1371.2079	1375.4306	1377.8493
Red. masses --	12.0002	12.0002	12.0003
Frc consts --	13.2936	13.3756	13.4229
IR Inten --	15.5192	9.0337	23.4925
Raman Activ --	5.2666	12.7677	15.0914
	211	212	213
	A	A	A
Frequencies --	1382.1764	1386.0727	1392.4380
Red. masses --	12.0004	12.0002	12.0001
Frc consts --	13.5074	13.5835	13.7084
IR Inten --	14.3816	29.0289	8.9585
Raman Activ --	8.2050	5.0202	0.4483
	214	215	216
	A	A	A
Frequencies --	1393.9324	1398.4613	1401.5614
Red. masses --	12.0002	12.0001	12.0005
Frc consts --	13.7380	13.8272	13.8891
IR Inten --	34.1953	3.3712	24.5842
Raman Activ --	7.6989	7.9495	5.6913
	217	218	219
	A	A	A
Frequencies --	1406.7296	1409.7330	1412.7678
Red. masses --	12.0005	12.0002	12.0003
Frc consts --	13.9917	14.0512	14.1119
IR Inten --	30.8874	19.0272	10.2144
Raman Activ --	5.6467	15.4017	10.3877
	220	221	222
	A	A	A
Frequencies --	1418.3001	1422.3680	1423.3282
Red. masses --	12.0003	12.0002	12.0002
Frc consts --	14.2225	14.3042	14.3235
IR Inten --	16.8350	23.6512	11.3879
Raman Activ --	16.5940	16.6608	6.2617
	223	224	225

	A	A	A
Frequencies --	1427.6272	1431.6932	1437.6411
Red. masses --	12.0001	12.0000	12.0002
Frc consts --	14.4100	14.4922	14.6130
IR Inten --	1.3696	3.1208	4.2753
Raman Activ --	7.5310	2.9332	5.7751
	226	227	228
	A	A	A
Frequencies --	1441.7857	1443.3724	1449.7743
Red. masses --	12.0002	12.0001	12.0002
Frc consts --	14.6973	14.7296	14.8607
IR Inten --	5.2932	4.2382	9.9304
Raman Activ --	11.4839	21.4141	17.8333
	229	230	231
	A	A	A
Frequencies --	1460.3431	1465.5403	1468.2422
Red. masses --	12.0001	12.0004	12.0002
Frc consts --	15.0780	15.1859	15.2417
IR Inten --	10.0610	7.2236	1.7363
Raman Activ --	17.0493	12.8458	5.5448
	232	233	234
	A	A	A
Frequencies --	1471.7294	1473.9460	1480.6163
Red. masses --	12.0004	12.0002	12.0002
Frc consts --	15.3144	15.3604	15.4997
IR Inten --	3.2905	1.6741	12.5744
Raman Activ --	9.2004	8.4296	21.9417
	235	236	237
	A	A	A
Frequencies --	1486.3238	1489.2629	1490.9252
Red. masses --	12.0015	12.0031	12.0229
Frc consts --	15.6211	15.6851	15.7461
IR Inten --	1.1669	0.7273	13.1941
Raman Activ --	2.5778	13.0933	8.1297
	238	239	240
	A	A	A
Frequencies --	1493.7715	1498.8485	1499.6317
Red. masses --	12.0030	12.7234	12.1153
Frc consts --	15.7801	16.8410	16.0528
IR Inten --	5.4451	1.6761	11.7306
Raman Activ --	3.2230	10.5521	11.7603
	241	242	243
	A	A	A
Frequencies --	1502.1105	1504.4505	1506.4211

Red. masses --	12.0000	12.0287	12.0020
Frc consts --	15.9528	16.0408	16.0471
IR Inten --	1.4870	5.2204	1.7683
Raman Activ --	7.4373	13.4253	3.0044
	244	245	246
	A	A	A
Frequencies --	1513.7896	1517.1535	1521.2098
Red. masses --	12.0011	12.0001	12.0002
Frc consts --	16.2033	16.2740	16.3612
IR Inten --	1.9682	0.5001	1.3249
Raman Activ --	8.1504	23.3451	12.1737
	247	248	249
	A	A	A
Frequencies --	1523.9413	1529.7200	1532.5009
Red. masses --	12.0000	12.0003	12.0001
Frc consts --	16.4199	16.5449	16.6048
IR Inten --	0.1022	1.8245	6.7009
Raman Activ --	19.8920	8.0750	11.3742
	250	251	252
	A	A	A
Frequencies --	1536.2592	1539.6709	1544.7765
Red. masses --	12.0000	12.0001	12.0004
Frc consts --	16.6864	16.7606	16.8723
IR Inten --	6.2346	4.7951	6.9211
Raman Activ --	16.0748	6.0325	40.0207
	253	254	255
	A	A	A
Frequencies --	1547.3715	1550.3952	1555.1221
Red. masses --	12.0001	12.0000	12.0000
Frc consts --	16.9287	16.9949	17.0987
IR Inten --	6.0384	3.7796	4.8550
Raman Activ --	11.0536	12.2834	27.2125
	256	257	258
	A	A	A
Frequencies --	1556.3508	1563.2148	1566.3765
Red. masses --	12.0001	12.0002	12.0002
Frc consts --	17.1257	17.2773	17.3472
IR Inten --	2.8380	2.0770	0.8979
Raman Activ --	30.4624	15.7632	26.9119
	259	260	261
	A	A	A
Frequencies --	1566.8140	1575.3150	1617.7740
Red. masses --	12.0001	12.0001	12.0000
Frc consts --	17.3568	17.5457	18.5041

IR Inten	--	1.1240	10.2989	9.0223
Raman Activ	--	64.7223	46.3059	23.3197

G. The calculated ¹³C chemical shifts (δ, ppm) of Sc₃NC@C₈₄ (a) and Sc₃NC@C₈₄ (e)

The calculated ¹³C chemical shifts (δ, ppm) of Sc₃NC@C₈₄ (a).

no.	δ/ppm	intensity
1	125.6	4
2	128	4
3	131.1	4
4	132	4
5	132.4	4
6	133.5	2
7	134.2	4
8	135.9	4
9	137	4
10	137.2	4
11	137.4	4
12	139.3	2
13	141.4	4
14	142	4
15	142.2	4
16	143	4
17	144.4	4
18	149.5	4
19	150.7	4
20	153.1	4
21	156.2	4
22	158.9	4
23	405.7	1

The calculated ¹³C chemical shifts (δ, ppm) of Sc₃NC@C₈₄ (e).

no.	δ/ppm	intensity	no.	δ/ppm	intensity	no.	δ/ppm	intensity
1	125.7	1	31	137.6	1	61	144.8	1
2	126.6	1	32	137.7	1	62	144.8	1
3	127.7	1	33	137.8	1	63	145.8	1
4	127.8	1	34	137.8	1	64	145.9	1
5	130.7	1	35	137.9	1	65	146.0	1
6	131.3	1	36	138.4	1	66	146.1	1
7	131.4	1	37	138.8	1	67	148.8	1

8	131.9	1	38	138.9	1	68	149.2	1
9	132.1	1	39	139.6	1	69	150.3	1
10	132.2	1	40	139.6	1	70	150.3	1
11	132.2	1	41	139.7	1	71	150.9	1
12	132.3	1	42	139.7	1	72	150.9	1
13	132.6	1	43	139.7	1	73	151.1	1
14	132.6	1	44	139.9	1	74	151.1	1
15	132.8	1	45	140.0	1	75	151.2	1
16	133.5	1	46	140.1	1	76	151.8	1
17	134.1	1	47	140.2	1	77	151.9	1
18	134.7	1	48	140.7	1	78	152.7	1
19	134.7	1	49	141.2	1	79	153.0	1
20	134.8	1	50	141.5	1	80	153.2	1
21	135.9	1	51	141.8	1	81	153.3	1
22	136.3	1	52	142.4	1	82	154.9	1
23	136.4	1	53	142.5	1	83	158.4	1
24	136.5	1	54	142.9	1	84	162.1	1
25	136.6	1	55	143.6	1	85	362.0	1
26	137.0	1	56	143.7				
27	137.0	1	57	144.0				
28	137.1	1	58	144.3				
29	137.2	1	59	144.4				
30	137.5	1	60	144.7				
