Electronic Supporting Information

$Sc_3N@C_s(39715)$-C_{82}: a missing isomer linked to $Sc_3N@C_{2v}(39718)$-C_{82} by a single step Stone-Wales transformation†

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Table S1. The singlet-triplet splitting energies Δ*E*(S-T).

Isomer	Spin	ΔE(kcal/mol)
$Sc_3N@C_{2v}(39718)$-C_{82}	singlet	0.0
	triplet	17.1
$Sc_3N@C_{2v}(39705)$-C_{82}	singlet	6.7
	triplet	34.6
$Sc_3N@C_s(39663)$-C_{82}	singlet	7.4
	triplet	34.7
$Sc_3N@C_s(39715)$-C_{82}	singlet	13.9
	triplet	23.4
$Sc_3N@C_{3v}(39717)$-C_{82}	singlet	14.0
	triplet	19.0
$Sc_3N@C_2(39714)$-C_{82}	singlet	19.1
	triplet	36.6
$Sc_3N@C_s(39704)$-C_{82}	singlet	23.4
	triplet	39.5
$Sc_3N@C_1(39656)$-C_{82}	singlet	36.0
	triplet	46.5
$Sc_3N@C_2(36652)$-C_{82}	singlet	38.8
	triplet	54.9

Table S2. Relative Energies(in kcal/mol) of Sc_3N in several molecules.

Sc_3N	Δ*E*
Sc_3Nneutraloptimized	0.0
Sc_3N From 39718 Cage	14.9
Sc_3N^{6+}From 39718 Cage	2435.1
Sc_3N From 39715 Cage	19.3
Sc_3N^{6+}From 39715 Cage	2422.8

Table S3. Relative Energies (in kcal/mol)and HOMO-LUMO gaps of $Sc_3N@C_{82}$.

			B3LYP/6-31G*~Lanl2dz		M06-2X/6-31G*~Lanl2dz		wB97XD/6-31G*~Lanl2dz		
	PA	ground state	ΔE	gap	ΔE	gap	ΔE	gap	$\Delta(\Delta E)_{max}$[a]
$Sc_3N@C_{2v}$(39718)-C_{82}	0	singlet	0.0	1.66	0.0	3.09	0.0	4.50	0.0
$Sc_3N@C_{2v}$(39705)-C_{82}	1	singlet	6.7	2.10	4.0	3.55	6.2	4.91	3.7
$Sc_3N@C_s$(39663)-C_{82}	1	singlet	7.4	2.34	5.4	3.82	8.0	5.14	2.6
$Sc_3N@C_s$(39715)-C_{82}	0	singlet	13.9	1.33	14.7	2.64	17.7	3.98	3.8
$Sc_3N@C_{3v}$(39717)-C_{82}	0	singlet	14.0	1.21	16.0	2.52	17.0	3.92	3.0
$Sc_3N@C_2$(39714)-C_{82}	0	singlet	19.1	1.59	20.4	2.90	21.2	4.26	2.1
$Sc_3N@C_s$(39704)-C_{82}	1	singlet	23.4	1.74	21.4	3.15	24.7	4.53	3.3
$Sc_3N@C_1$(39656)-C_{82}	1	singlet	36.0	1.35	37.9	2.64	40.2	4.04	4.2
$Sc_3N@C_2$(36652)-C_{82}	2	singlet	38.8	1.84	37.3	3.22	39.2	4.68	1.9

Table S4. Natural electron configuration populations of Sc atoms and N atoms in $Sc_3N@C_{2v}$(39718)-C_{82} and $Sc_3N@C_s$(39715)-C_{82}.

	Atoms	Charge	Populations
$Sc3N@C_{2v}$(39718)-C_{82}	Sc1	1.414	4s(0.07)3d(1.17)4p(0.24)4d(0.14)
	Sc2	1.344	4s(0.08)3d(1.20)4p(0.26)4d(0.16)
	Sc3	1.322	4s(0.08)3d(1.21)4p(0.27)4d(0.17)
	N	-1.316	2s(1.53)2p(4.78)
Sc3N_from 39718_+6 charged	Sc1	2.627	4s(0.01)3d(0.37)
	Sc2	2.586	4s(0.01)3d(0.40)4p(0.01)
	Sc3	2.593	4s(0.01)3d(0.39)4p(0.01)
	N	-1.806	2s(1.91)2p(4.89)
$Sc3N@C_s$(39715)-C_{82}	Sc1	1.299	4s(0.08)3d(1.19)4p(0.28)4d(0.19)
	Sc2	1.384	4s(0.08)3d(1.18)4p(0.25)4d(0.15)
	Sc3	1.386	4s(0.08)3d(1.18)4p(0.25)4d(0.15)
	N	-1.309	2s(1.53)2p(4.77)
Sc3N_from 39715_+6 charged	Sc1	2.593	4s(0.01)3d(0.39)4p(0.01)
	Sc2	2.606	4s(0.01)3d(0.39)4p(0.01)
	Sc3	2.606	4s(0.01)3d(0.38)4p(0.01)
	N	-1.805	2s(1.92)2p(4.89)
Sc3N_optimized	Sc1	0.519	4s(1.06)3d(1.18)4p(0.25)4d(0.01)
	Sc2	0.519	4*s*(1.06)3*d*(1.18)4*p*(0.25)4*d*(0.01)
	Sc3	0.518	4*s*(1.06)3*d*(1.18)4*p*(0.25)4*d*(0.01)
	N	-1.556	2*s*(1.78)2*p*(4.78)

Table S5. Values of Mayer Bond Order.

$Sc_3N@C_{2v}(39718)-C_{82}$				$Sc_3N@C_s(39715)-C_{82}$			
		d(Å)	MBO			d(Å)	MBO
Sc84	C1	2.654	0.134	Sc84	C34	2.494	0.182
	C2	2.380	0.197		C35	2.695	0.109
	C3	2.631	0.155		C36	2.495	0.182
	C4	2.706	0.128		C50	2.821	0.107
	C20	2.762	0.136		C51	2.434	0.205
	C63	2.297	0.191		C52	2.300	0.213
	C64	2.492	0.193		C53	2.300	0.213
	C65	2.941	0.074		C54	2.434	0.205
	C76	2.614	0.166		C55	2.822	0.106
	C77	2.395	0.176		C61	2.605	0.128
	C78	2.765	0.131		C62	2.605	0.128
	C79	3.060	0.074				
	N83	2.014	0.892		N83	2.091	0.808
Sc85	C9	2.662	0.130	Sc85	C1	2.295	0.183
	C10	2.355	0.210		C2	2.450	0.202
	C11	2.254	0.206		C3	2.741	0.108
	C12	2.344	0.228		C19	2.690	0.133
	C13	2.655	0.100		C20	2.432	0.204
	C29	2.813	0.104		C21	2.358	0.194
	C30	2.748	0.111		C22	2.588	0.169
	C31	2.396	0.224		C23	2.756	0.112
	C32	2.725	0.145		C39	2.835	0.107
	C33	2.867	0.093		C40	2.656	0.153
	C69	2.580	0.182		C75	2.757	0.141
	C70	2.589	0.146		C76	2.775	0.118
	N83	2.043	0.839		N83	2.056	0.864
Sc86	C24	2.827	0.107	Sc86	C11	2.748	0.106
	C25	2.823	0.087		C12	2.450	0.202
	C26	2.417	0.205		C13	2.295	0.183
	C27	2.664	0.103		C14	2.427	0.204
	C28	2.663	0.130		C15	2.682	0.134
	C43	2.704	0.127		C27	2.753	0.113
	C44	2.435	0.214		C28	2.593	0.167
	C45	2.253	0.206		C29	2.363	0.194
	C46	2.280	0.229		C30	2.668	0.150
	C47	2.503	0.175		C31	2.847	0.104
	C58	2.754	0.111		C69	2.769	0.119
	C59	2.514	0.197		C70	2.747	0.144
	N83	2.059	0.785		N83	2.055	0.864

Figure S1. Concentration-temperature curves.

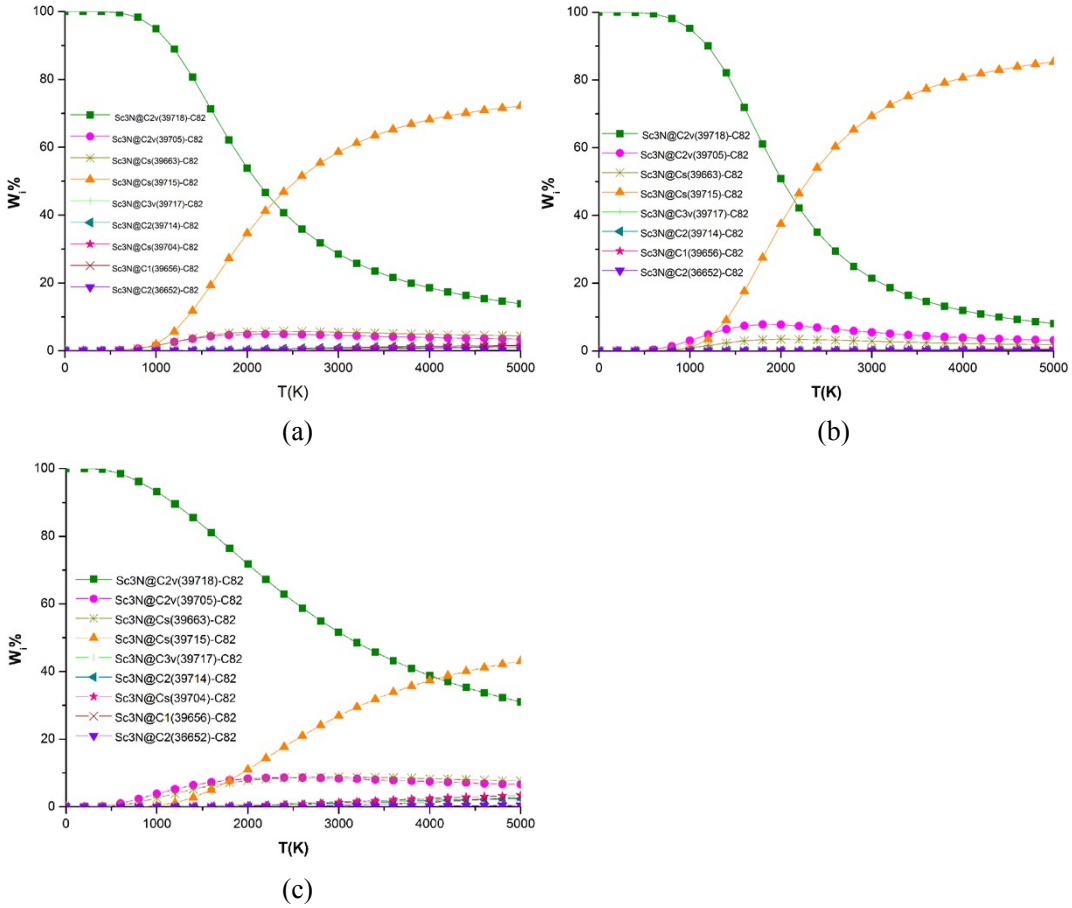
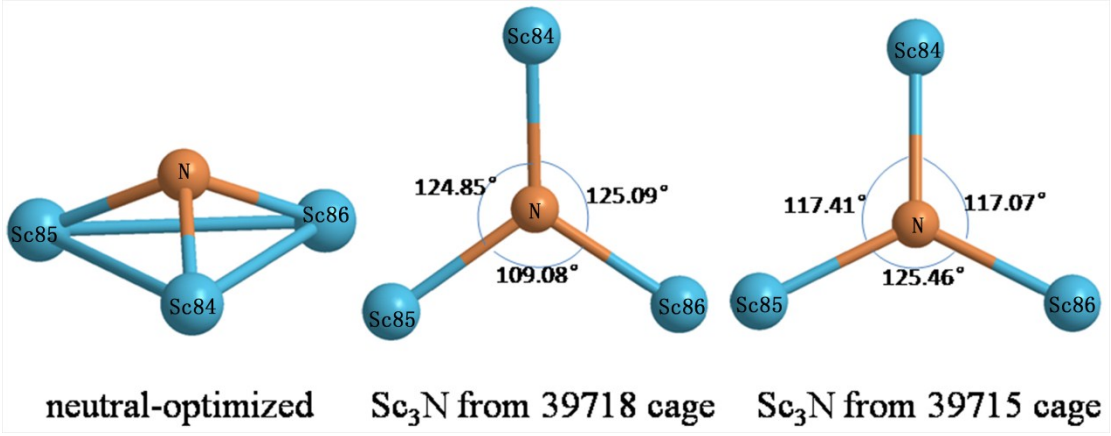


Figure S1.Concentration-temperature curves of $Sc_3N@C_{82}$ series calculated with (a) B3LYP, (b) wB97XD, (C) M06-2X methods.

Figure S2. Comparisons of shape of Sc3N unites from free optimization, $Sc_3N@C_{2v}(39718)$-C_{82} and $Sc_3N@C_s(39715)$-C_{82}.



Ⅰ.Cartesian coordinates of the nine lowest energy isomers of $Sc_3N@C_{82}$

(B3LYP/6-31G*~Lanl2dz).

$Sc_3N@C_{2v}$ (39718)-C_{82}

C	0.093176	1.352317	-7.786270	C	3.518624	-0.993640	-5.563600
C	-0.222590	2.735192	-7.541280	C	2.587413	-2.031010	-5.142910
C	0.825899	3.599117	-7.044380	C	2.462609	-2.476280	-3.769930
C	0.243682	4.542999	-6.151490	C	3.286194	-1.852810	-2.779840
C	0.996082	5.177346	-5.111760	C	2.683496	-1.426840	-1.523110
C	0.236025	5.610571	-3.988890	C	3.427882	-0.293280	-1.067440
C	0.823738	5.621551	-2.688940	C	2.874979	0.637041	-0.171940
C	-0.144730	5.157966	-1.731650	C	3.194310	2.020014	-0.303750
C	0.247494	4.346325	-0.637930	C	4.043145	2.494324	-1.357560
C	-0.740590	3.397736	-0.133060	C	3.793209	3.802045	-1.830430
C	-0.360440	2.131098	0.4676270	C	4.028314	4.124444	-3.207780
C	-1.246250	1.099766	-0.036270	C	4.603421	3.194835	-4.067910
C	-0.770800	-0.223380	-0.448000	C	4.137991	3.094883	-5.421820
C	-1.547990	-0.909340	-1.416560	C	4.367110	1.735953	-5.837640
C	-0.962200	-1.870970	-2.299370	C	4.820891	0.965073	-4.714900
C	-1.699600	-1.838740	-3.545750	C	4.376685	-0.369120	-4.539770
C	-1.042300	-2.06738	-4.780400	C	4.222249	-0.824560	-3.173820
C	-1.454620	-1.32447	-5.925700	C	4.332742	0.122738	-2.082260
C	-0.497700	-0.91318	-6.920760	C	4.646534	1.509742	-2.276980
C	-0.883620	0.380983	-7.393470	C	4.972613	1.892873	-3.593480
C	1.461607	0.966804	-7.767610	C	-1.482110	3.149889	-6.932620
C	1.850725	-0.342450	-7.327130	C	-1.167760	4.267413	-6.063000
C	0.884837	-1.258840	-6.840250	C	-1.862830	4.536480	-4.832220
C	1.272650	-2.091050	-5.741330	C	-1.163700	5.253438	-3.829490
C	0.332754	-2.464270	-4.727930	C	-1.399910	4.962092	-2.443320
C	1.050581	-2.630440	-3.486860	C	-2.299870	3.937586	-2.060770
C	0.422278	-2.180050	-2.245110	C	-1.934570	3.153403	-0.911770
C	1.252915	-1.506310	-1.261780	C	-2.252320	1.753407	-0.839570
C	0.655326	-0.513810	-0.362850	C	-2.976400	1.081819	-1.881970
C	1.514671	0.490500	0.229706	C	-2.657890	-0.280760	-2.109670
C	1.025361	1.822062	0.531681	C	-2.723990	-0.840940	-3.427460
C	2.024367	2.764592	0.107362	C	-3.074020	-0.020540	-4.545860
C	1.681017	4.028909	-0.490740	C	-2.44508	-0.29805	-5.79763
C	2.621918	4.562684	-1.405220	C	-2.10055	0.768487	-6.71130
C	2.175264	5.321638	-2.537360	C	-2.42088	2.140988	-6.45405
C	2.982738	4.987515	-3.681390	C	-3.08809	2.391185	-5.21427
C	2.402277	4.819422	-4.974570	C	-2.85806	3.591105	-4.43679
C	3.005502	3.834015	-5.883580	C	-3.08133	3.282842	-3.06168
C	2.203355	3.211113	-6.928620	C	-3.428990	1.882879	-2.97150
C	2.510334	1.904764	-7.402580	C	-3.444640	1.335274	-4.29322
C	3.565562	1.148515	-6.812130	N	0.581715	1.332847	-3.62759
C	3.155335	-0.226280	-6.698240	Sc	-0.344210	2.054785	-5.26406

Sc	0.181177	1.910543	-1.70895	Sc	1.792265	-0.33267	-3.59023

$Sc_3N@C_{2v}$ (39705)-C_{82}

C	-0.254984	0.159606	0.027850	C	-2.763762	3.033136	-2.633536
C	1.157210	0.333413	0.105024	C	-3.199654	1.909995	-3.391673
C	1.741290	1.645573	0.000738	C	-3.083297	1.853074	-4.813174
C	2.987401	1.529344	-0.687951	C	-2.404196	2.887041	-5.551547
C	3.452070	2.545244	-1.561107	C	-1.791763	2.477474	-6.762869
C	4.282342	2.101305	-2.651545	C	-0.625744	3.127035	-7.271537
C	4.324314	2.806995	-3.891905	C	-0.080164	4.252440	-6.611758
C	4.592399	1.870111	-4.949421	C	1.341960	4.443185	-6.746719
C	4.007207	2.091224	-6.250743	C	2.088280	5.077490	-5.708877
C	3.528919	0.943215	-6.942645	C	1.411071	5.662924	-4.641417
C	2.352066	1.000884	-7.755599	C	1.910115	5.565050	-3.283388
C	1.687706	-0.26809	-7.656400	C	0.799525	5.797468	-2.415657
C	0.262872	-0.348034	-7.662032	C	0.545698	4.948514	-1.289753
C	-0.335736	-1.387414	-6.885170	C	-0.866579	4.638495	-1.316881
C	-1.596362	-1.179819	-6.233770	C	-1.399770	5.062198	-2.597313
C	-1.606086	-1.948810	-5.004506	C	-2.186686	4.148701	-3.376681
C	-2.362687	-1.544854	-3.860181	C	-1.917197	4.050320	-4.837295
C	-1.762124	-1.809295	-2.585474	C	-0.781861	4.783080	-5.437280
C	-1.922437	-0.924099	-1.452712	C	-0.034261	5.673990	-4.593000
C	-0.74269	-1.006369	-0.646707	C	-0.396172	5.866727	-3.219696
C	-1.056054	1.334505	0.006103	C	2.050766	-0.601409	-0.515137
C	-2.254423	1.402511	-0.794301	C	3.198828	0.126986	-0.97653
C	-2.643212	0.295568	-1.584118	C	3.925206	-0.293293	-2.125594
C	-3.228975	0.569070	-2.874981	C	4.583992	0.713121	-2.918471
C	-3.178375	-0.350575	-3.989444	C	4.768256	0.558941	-4.363285
C	-3.101065	0.461295	-5.206760	C	4.192699	-0.585827	-5.046178
C	-2.295006	0.060987	-6.332276	C	3.595998	-0.366145	-6.331292
C	-1.713844	1.081263	-7.137337	C	2.459873	-1.11933	-6.788753
C	-0.468736	0.872322	-7.821523	C	1.852306	-2.106629	-5.955926
C	0.196571	2.138827	-7.920505	C	0.440785	-2.271496	-6.056791
C	1.617620	2.226018	-7.863314	C	-0.334371	-2.612609	-4.895790
C	2.176717	3.398724	-7.284814	C	0.267288	-2.826262	-3.615701
C	3.374836	3.335034	-6.483794	C	-0.481034	-2.449959	-2.460014
C	3.278580	4.341362	-5.445483	C	0.150788	-1.941978	-1.269941
C	3.643731	4.041790	-4.090592	C	1.562624	-1.739097	-1.234692
C	2.894277	4.572574	-2.956284	C	2.315400	-2.187318	-2.364103
C	2.716711	3.785044	-1.706212	C	3.479535	-1.471358	-2.796214
C	1.490072	3.939541	-0.895662	C	3.581828	-1.594380	-4.237343
C	0.959190	2.817924	-0.112996	C	2.459141	-2.372871	-4.688522
C	-0.465009	2.648856	0.026953	C	1.687288	-2.742156	-3.534147
C	-1.366849	3.520030	-0.654003	N	0.636024	1.609053	-3.819530
C	-2.402358	2.762537	-1.271920	Sc	0.422384	3.655665	-3.336894

Sc	-1.057044	0.520344	-4.097570	Sc	2.526562	0.881951	-4.006664

$Sc_3N@C_{3v}$ (39717)-C_{82}

C	-0.06191	-0.056686	0.109544	C	-2.424974	3.305279	-2.249294
C	1.387332	-0.083727	0.195123	C	-3.106709	2.313967	-3.003710
C	2.157925	1.164953	0.160977	C	-3.110036	2.333312	-4.435276
C	3.326319	0.933013	-0.6434	C	-2.415185	3.334653	-5.154256
C	3.986847	1.963752	-1.396291	C	-1.90971	2.963863	-6.446603
C	4.736089	1.518447	-2.517228	C	-0.736145	3.571445	-7.000644
C	4.864668	2.357027	-3.677699	C	-0.109815	4.600417	-6.284716
C	4.756942	1.567346	-4.855578	C	1.328501	4.772524	-6.262444
C	3.983046	2.045907	-5.957601	C	1.648797	5.593215	-5.107256
C	3.307398	1.042287	-6.718357	C	2.850100	5.278142	-4.363657
C	2.113227	1.297152	-7.465002	C	2.813393	5.189829	-2.918622
C	1.400183	0.044519	-7.645397	C	1.646556	5.429211	-2.192186
C	-0.054789	0.076712	-7.593298	C	1.336022	4.668280	-1.042064
C	-0.707302	-0.964237	-6.855839	C	-0.108542	4.541435	-1.041859
C	-1.929839	-0.729472	-6.129098	C	-0.677748	5.081006	-2.259251
C	-1.942541	-1.586972	-4.983986	C	-1.771678	4.401728	-2.947866
C	-2.552329	-1.165499	-3.760396	C	-1.755747	4.407271	-4.393161
C	-1.958741	-1.63214	-2.545997	C	-0.660318	5.080729	-5.056597
C	-1.943511	-0.801631	-1.382416	C	0.417532	5.747937	-4.353505
C	-0.713814	-1.055195	-0.671766	C	0.392898	5.690849	-2.946136
C	-0.681370	1.231942	0.133158	C	2.100680	-1.043809	-0.619867
C	-1.915351	1.507222	-0.587191	C	3.309177	-0.429438	-1.095790
C	-2.524253	0.504611	-1.393300	C	3.963772	-0.845290	-2.298879
C	-3.178395	0.939447	-2.578527	C	4.696779	0.151683	-2.989737
C	-3.203460	0.105944	-3.749849	C	4.696451	0.184245	-4.428501
C	-3.184507	0.965462	-4.898814	C	3.972955	-0.789353	-5.158229
C	-2.523939	0.572072	-6.090859	C	3.327602	-0.349242	-6.371323
C	-1.909228	1.592507	-6.870455	C	2.156512	-0.986594	-6.93587
C	-0.684634	1.350252	-7.593398	C	1.478256	-1.994078	-6.13742
C	0.061949	2.600225	-7.646584	C	0.042948	-1.979283	-6.142954
C	1.482179	2.587094	-7.427760	C	-0.726988	-2.358789	-4.987822
C	2.147234	3.653616	-6.691119	C	-0.090103	-2.757405	-3.775067
C	3.410845	3.379132	-5.949758	C	-0.750982	-2.424607	-2.555120
C	3.705509	4.213861	-4.811626	C	0.020913	-2.065155	-1.405260
C	4.358341	3.647766	-3.639393	C	1.444219	-2.053745	-1.424334
C	3.740827	4.169647	-2.461344	C	2.106077	-2.495818	-2.603792
C	3.415344	3.311596	-1.361592	C	3.352869	-1.906191	-3.031334
C	2.176458	3.556542	-0.624095	C	3.354970	-1.865048	-4.459378
C	1.522919	2.462374	0.081575	C	2.103292	-2.425019	-4.926738
C	0.089485	2.445961	0.178019	C	1.337379	-2.823201	-3.773549
C	-0.717211	3.465613	-0.438856	N	1.102151	1.520797	-3.767117
C	-1.911710	2.880514	-0.977014	Sc	1.037485	0.320963	-5.411759

Sc	1.297835	3.503097	-4.285291	Sc	1.062089	0.885077	-1.853095

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C	-0.04329	0.019473	0.208716	C	-2.009460	2.746950	-1.111050
C	1.405758	0.077982	0.131289	C	-2.517680	3.117472	-2.393680
C	2.150389	1.321234	0.035559	C	-3.123080	2.067745	-3.138530
C	3.421886	1.246634	-0.591950	C	-3.079960	2.068727	-4.556520
C	3.973491	2.379105	-1.272990	C	-2.429980	3.119566	-5.261990
C	4.763239	1.881034	-2.381600	C	-1.843940	2.750522	-6.511330
C	4.824099	2.600375	-3.602440	C	-0.688190	3.431855	-7.014260
C	4.837442	1.882210	-4.825230	C	-0.204750	4.547208	-6.357170
C	4.118124	2.381760	-5.980300	C	1.235362	4.747414	-6.268050
C	3.610012	1.250008	-6.69549	C	1.467787	5.579098	-5.135740
C	2.379597	1.325321	-7.399920	C	2.692243	5.482197	-4.387990
C	1.642023	0.082454	-7.541130	C	2.647736	5.480963	-2.947380
C	0.200962	0.023790	-7.708400	C	1.379511	5.576805	-2.276730
C	-0.301440	-1.071770	-6.912770	C	1.077514	4.744291	-1.161680
C	-1.516150	-0.972890	-6.121240	C	-0.365240	4.544222	-1.161720
C	-1.595930	-1.794690	-4.964560	C	-0.935390	5.034003	-2.369230
C	-2.353940	-1.373580	-3.825710	C	-1.937760	4.266283	-3.089930
C	-1.667750	-1.796550	-2.642440	C	-1.893910	4.267615	-4.530180
C	-1.659550	-0.975910	-1.482700	C	-0.848610	5.036285	-5.186880
C	-0.494990	-1.074120	-0.618870	C	0.183205	5.709410	-4.441460
C	-0.750860	1.245955	0.164459	C	0.140308	5.708487	-3.048810
C	-1.923820	1.372787	-0.676920	C	3.885742	0.054595	-1.263410
C	-2.388340	0.297920	-1.511600	C	4.692608	0.452417	-2.381600
C	-3.084690	0.682425	-2.68842	C	4.658550	-0.287090	-3.609030
C	-3.051030	-0.152880	-3.84672	C	4.767320	0.453827	-4.831170
C	-3.012940	0.683904	-5.004110	C	4.031444	0.057173	-5.997590
C	-2.245340	0.300879	-6.136260	C	3.224836	-1.111000	-5.981230
C	-1.730880	1.376627	-6.939690	C	2.028990	-1.065590	-6.765250
C	-0.507520	1.250212	-7.705610	C	0.841346	-1.766260	-6.370740
C	0.203953	2.497886	-7.632120	C	0.798268	-2.521780	-5.155810
C	1.644062	2.583482	-7.422140	C	-0.455640	-2.563710	-4.479270
C	2.166040	3.736670	-6.722890	C	-0.499560	-2.564820	-3.057000
C	3.419242	3.611094	-5.966720	C	0.710366	-2.523170	-2.304660
C	3.617229	4.448651	-4.804180	C	0.678912	-1.769260	-1.088680
C	4.220117	3.890318	-3.620900	C	1.839902	-1.069130	-0.620960
C	3.545548	4.447248	-2.476290	C	3.081688	-1.113670	-1.330160
C	3.276230	3.608078	-1.329380	C	3.136514	-1.922890	-2.496410
C	1.978574	3.732693	-0.652360	C	3.909568	-1.503070	-3.632600
C	1.414875	2.579429	0.013578	C	3.207769	-1.921330	-4.814600
C	-0.035640	2.493504	0.134671	C	2.006865	-2.610960	-4.408230
C	-0.887840	3.427968	-0.536600	C	1.962853	-2.612050	-2.976630

N	0.741235	1.679883	-3.729570	Sc	0.285056	0.832030	-1.912410
Sc	1.541339	3.611849	-3.704280	Sc	0.396673	0.822562	-5.565300

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C	0.092046	-0.155474	0.151631	C	-1.803239	2.721739	-0.967020
C	1.537952	-0.174824	0.088136	C	-2.450239	3.170380	-2.157683
C	2.340470	1.036878	0.039473	C	-3.064355	2.184072	-2.982097
C	3.623380	0.909623	-0.555331	C	-3.015014	2.300203	-4.407557
C	4.273877	2.039301	-1.125054	C	-2.350756	3.40285	-5.016642
C	5.080103	1.568511	-2.237799	C	-1.618989	3.147924	-6.215611
C	5.236783	2.369198	-3.397956	C	-0.384748	3.826139	-6.493787
C	5.163929	1.767713	-4.680301	C	0.137063	4.821269	-5.636763
C	4.433346	2.41671	-5.754758	C	1.594654	4.951423	-5.545958
C	3.830409	1.397223	-6.543063	C	2.093787	5.695191	-4.419429
C	2.589955	1.625986	-7.193707	C	3.42617	5.484896	-3.92959
C	1.798648	0.443595	-7.488778	C	3.376931	5.367894	-2.49465
C	0.361962	0.480899	-7.652746	C	2.012838	5.503541	-2.06991
C	-0.196047	-0.662494	-6.97076	C	1.441627	4.589047	-1.116435
C	-1.419054	-0.598111	-6.190868	C	-0.018199	4.453737	-1.147879
C	-1.538400	-1.522927	-5.118688	C	-0.78238	5.028262	-2.217393
C	-2.288276	-1.177124	-3.947304	C	-1.93204	4.34458	-2.765177
C	-1.618883	-1.711716	-2.798222	C	-1.883035	4.461297	-4.193895
C	-1.578419	-0.972638	-1.585461	C	-0.702463	5.218434	-4.543659
C	-0.412272	-1.170981	-0.742462	C	-0.116328	5.646414	-3.315867
C	-0.552178	1.111802	0.153045	C	1.254514	5.872187	-3.250095
C	-1.74234	1.326506	-0.629812	C	4.039940	-0.269695	-1.285899
C	-2.277966	0.315079	-1.513208	C	4.890833	0.152898	-2.356723
C	-3.00592	0.776658	-2.643595	C	4.814071	-0.476819	-3.644674
C	-2.973216	0.038438	-3.872378	C	4.974516	0.352626	-4.805183
C	-2.925534	0.965583	-4.965388	C	4.201502	0.113148	-5.985929
C	-2.118906	0.688470	-6.102661	C	3.319209	-0.993502	-6.066008
C	-1.529776	1.826302	-6.774008	C	2.127631	-0.801764	-6.835055
C	-0.289954	1.736525	-7.503474	C	0.905664	-1.470452	-6.505946
C	0.475835	2.927463	-7.217643	C	0.817969	-2.337187	-5.367695
C	1.901042	2.903470	-7.000255	C	-0.435949	-2.376339	-4.697772
C	2.488146	3.950895	-6.174855	C	-0.485351	-2.492438	-3.275122
C	3.824157	3.693237	-5.606250	C	0.719559	-2.568417	-2.523377
C	4.231819	4.427960	-4.438589	C	0.723938	-1.896805	-1.256507
C	4.789087	3.718659	-3.303610	C	1.916698	-1.296647	-0.739911
C	4.152081	4.238186	-2.109474	C	3.159391	-1.369036	-1.44708
C	3.669298	3.326458	-1.106862	C	3.176364	-2.092709	-2.668874
C	2.296194	3.496443	-0.597483	C	3.979513	-1.629845	-3.767345
C	1.658901	2.333090	0.005855	C	3.256879	-1.905631	-4.978913
C	0.222741	2.329393	0.121140	C	2.017449	-2.55656	-4.629897
C	-0.593584	3.338814	-0.499859	C	1.967857	-2.671835	-3.20311

N	1.132451	1.733843	-3.589393	Sc	0.570163	0.762011	-1.886101
Sc	2.243545	3.497221	-3.407669	Sc	0.659951	1.088211	-5.468157

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C	-0.062482	-0.050384	0.187150	C	1.855915	3.596608	-0.460486
C	1.415217	-0.053392	0.207768	C	1.418595	2.396005	0.189800
C	2.167646	1.178940	0.126538	C	-0.044255	2.389405	0.196862
C	3.361574	1.196623	-0.676851	C	-0.467121	3.622380	-0.393637
C	3.770182	2.376294	-1.381823	C	-1.673842	3.666211	-1.086944
C	4.406991	1.968133	-2.611844	C	-1.763702	4.435404	-2.306698
C	4.310197	2.740584	-3.801769	C	-0.635510	5.116051	-2.806430
C	4.244547	2.061203	-5.092469	C	-0.543977	5.232444	-4.245088
C	3.611591	2.788744	-6.185729	C	0.674451	5.505192	-4.962762
C	2.804198	2.105118	-7.152835	C	1.919190	5.479818	-4.212301
C	1.587277	2.824153	-7.400375	C	1.861154	5.217802	-2.792004
C	0.306721	2.144196	-7.497093	C	0.632322	5.089885	-2.050774
C	-0.855761	2.769028	-6.898587	C	0.683224	4.359261	-0.836107
C	-1.990610	1.977563	-6.458105	C	4.309728	-0.154527	-3.878745
C	-2.797714	2.394967	-5.300848	C	4.240438	0.605692	-5.126842
C	-3.510054	1.404968	-4.572907	C	3.605998	-0.072624	-6.270407
C	-3.596311	1.479516	-3.134435	C	2.780709	0.707155	-7.151602
C	-3.364784	0.170433	-2.570695	C	1.590669	-0.006581	-7.473662
C	-2.507679	0.009156	-1.440563	C	0.329270	0.697679	-7.627157
C	-1.696675	-1.201098	-1.392790	C	-0.825306	-0.038762	-7.330149
C	-0.478501	-1.161563	-0.623340	C	-1.992577	0.591965	-6.802866
C	0.687146	-1.867153	-1.070170	C	-2.692093	-0.389566	-6.011765
C	1.846969	-1.163004	-0.611631	C	-3.419778	0.009400	-4.900498
C	3.037381	-1.135791	-1.436561	C	-3.341531	-0.752207	-3.668653
C	3.798666	0.053007	-1.442432	C	-2.553784	-1.902336	-3.620370
C	4.433314	0.539858	-2.646309	C	-1.730117	-2.137694	-2.465452
C	-0.810215	1.183854	0.075899	C	-0.543879	-2.834754	-2.913295
C	-2.043511	1.212992	-0.723989	C	0.685980	-2.676550	-2.251376
C	-2.477642	2.488813	-1.204621	C	1.899431	-2.714835	-3.003874
C	-3.182922	2.604922	-2.458027	C	3.038196	-1.934707	-2.616043
C	-2.692273	3.735529	-3.181157	C	3.686976	-1.457764	-3.816879
C	-2.448035	3.612688	-4.572001	C	3.003096	-2.047473	-4.937237
C	-1.393508	4.409657	-5.084225	C	2.986003	-1.387445	-6.200668
C	-0.660806	4.051404	-6.254091	C	1.707581	-1.335657	-6.906960
C	0.596417	4.752712	-6.206331	C	0.504996	-1.983997	-6.405112
C	1.733345	4.079061	-6.726741	C	-0.739989	-1.399314	-6.763094
C	2.979271	4.059904	-5.980718	C	-1.908318	-1.603757	-5.975057
C	3.042696	4.726496	-4.725609	C	-1.847000	-2.356636	-4.788564
C	3.695202	4.039506	-3.641573	C	-0.595219	-2.909879	-4.365156
C	3.015250	4.414878	-2.433184	C	0.580544	-2.740782	-5.145595
C	3.014169	3.577623	-1.288488	C	1.844130	-2.739374	-4.441184

N	1.005591	1.380525	-3.682308	Sc	1.670598	-0.065096	-4.956692
Sc	1.114411	3.332380	-4.400211	Sc	0.732590	0.795120	-1.816047

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C	-0.032215	0.006350	0.084470	C	-1.994701	2.788853	-0.942485
C	1.400951	-0.023922	0.145929	C	-2.388128	3.214422	-2.262219
C	2.110467	1.234374	0.043957	C	-2.952375	2.225528	-3.095804
C	3.351276	1.203949	-0.649148	C	-2.820326	2.298453	-4.515296
C	3.883418	2.336540	-1.340738	C	-2.050801	3.314070	-5.127295
C	4.662602	1.863268	-2.441811	C	-1.425716	2.961515	-6.367433
C	4.759019	2.594738	-3.659716	C	-0.220906	3.579158	-6.811228
C	4.942996	1.832134	-4.851445	C	0.393031	4.641621	-6.099437
C	4.394763	2.288974	-6.089125	C	1.807514	4.778572	-6.275094
C	3.856140	1.169105	-6.806468	C	2.599206	5.245704	-5.194081
C	2.627686	1.301405	-7.504001	C	1.967379	5.765393	-4.071331
C	1.796722	0.126656	-7.591130	C	2.478728	5.495568	-2.749916
C	0.360610	0.186677	-7.723794	C	1.393634	5.710090	-1.838269
C	-0.194648	-0.888970	-6.950770	C	1.088401	4.776944	-0.799890
C	-1.412952	-0.754015	-6.186732	C	-0.342022	4.565386	-0.830871
C	-1.565320	-1.615470	-5.067384	C	-0.864804	5.148380	-2.045347
C	-2.330564	-1.203052	-3.929853	C	-1.721521	4.364359	-2.889542
C	-1.694294	-1.697065	-2.746803	C	-1.467938	4.383729	-4.340821
C	-1.667115	-0.913038	-1.567129	C	-0.285533	5.101403	-4.888063
C	-0.494203	-1.058006	-0.746343	C	0.521654	5.865642	-3.988543
C	-0.756724	1.197626	0.193939	C	0.189594	5.943959	-2.602870
C	-1.927095	1.380285	-0.612050	C	3.827859	0.006431	-1.319036
C	-2.371480	0.374552	-1.521583	C	4.631224	0.426368	-2.432610
C	-3.008785	0.828870	-2.711369	C	4.665628	-0.330147	-3.643578
C	-2.957099	0.054424	-3.910099	C	4.849137	0.386885	-4.851472
C	-2.829083	0.935623	-5.030942	C	4.175396	-0.025263	-6.052358
C	-2.070379	0.556894	-6.168271	C	3.303097	-1.146176	-6.051041
C	-1.478118	1.631251	-6.933820	C	2.125233	-1.068378	-6.858641
C	-0.294819	1.454643	-7.752865	C	0.896785	-1.702837	-6.472417
C	0.516656	2.634352	-7.619177	C	0.788755	-2.457506	-5.267966
C	1.966859	2.613154	-7.546525	C	-0.466808	-2.442514	-4.597169
C	2.582392	3.719505	-6.926125	C	-0.540079	-2.481055	-3.167736
C	3.792225	3.541957	-6.167935	C	0.653458	-2.514943	-2.395509
C	3.749005	4.397143	-5.016746	C	0.653084	-1.842697	-1.127833
C	4.125170	3.905638	-3.721398	C	1.844340	-1.231918	-0.556878
C	3.410548	4.421859	-2.542452	C	3.060707	-1.205099	-1.334997
C	3.195353	3.574796	-1.359605	C	3.084793	-1.936575	-2.559444
C	1.975393	3.675662	-0.538602	C	3.891823	-1.535718	-3.682929
C	1.380049	2.494530	0.104781	C	3.218487	-1.948479	-4.872034
C	-0.047783	2.441867	0.309729	C	1.986248	-2.604492	-4.497124
C	-0.911523	3.426195	-0.270224	C	1.907463	-2.606774	-3.076488

N	0.905271	1.688368	-3.622339	Sc	1.354135	0.276754	-2.223224
Sc	0.837224	3.684383	-2.947112	Sc	0.460245	1.263782	-5.603405

$Sc_3N@C_2(36652)$-C_{82}

C	0.089318	-0.071840	0.061482	C	-1.822699	2.880623	-0.691253
C	1.521245	-0.094259	0.035037	C	-2.660422	3.371601	-1.754038
C	2.342099	1.110956	0.059940	C	-3.580605	2.450333	-2.303580
C	3.529969	0.844067	-0.677209	C	-3.956753	2.512628	-3.684645
C	3.906873	1.721987	-1.744965	C	-3.328081	3.458822	-4.557121
C	4.020294	0.938357	-2.953577	C	-3.060325	3.038706	-5.899372
C	3.622288	1.442100	-4.218989	C	-1.858581	3.456113	-6.580269
C	3.117758	0.510853	-5.228181	C	-0.918408	4.345446	-5.972679
C	2.415652	1.045957	-6.384240	C	0.484853	4.137624	-6.290201
C	1.564720	0.222968	-7.165109	C	1.445493	4.317204	-5.238923
C	0.330755	0.734161	-7.754571	C	1.133061	4.880621	-3.958196
C	-0.636413	-0.326248	-7.735250	C	1.987665	4.535253	-2.888813
C	-2.018768	-0.057563	-7.458970	C	1.461245	4.350047	-1.561982
C	-2.752520	-1.023954	-6.709478	C	0.057627	4.413432	-1.353764
C	-3.675852	-0.602881	-5.680895	C	-0.788782	4.894807	-2.400206
C	-3.569722	-1.514483	-4.576691	C	-2.137028	4.409008	-2.577940
C	-3.574234	-1.047033	-3.207153	C	-2.435277	4.407663	-3.982295
C	-2.625676	-1.612191	-2.253028	C	-1.250437	4.850408	-4.681103
C	-2.039497	-0.794150	-1.196889	C	-0.242807	5.154219	-3.694569
C	-0.648162	-1.062071	-0.715169	C	2.247927	-1.061632	-0.749847
C	-0.525394	1.216573	0.310369	C	3.468011	-0.480995	-1.186922
C	-1.845043	1.514377	-0.217623	C	3.731588	-0.430420	-2.593823
C	-2.606995	0.535543	-0.969607	C	3.074726	-1.298868	-3.477549
C	-3.555052	1.051936	-1.908591	C	2.870608	-0.889636	-4.868373
C	-4.000506	0.285477	-3.021019	C	2.011157	-1.702109	-5.706396
C	-4.240992	1.181894	-4.129524	C	1.368954	-1.142014	-6.848629
C	-3.973828	0.770565	-5.463429	C	0.014865	-1.499638	-7.233799
C	-3.388933	1.722638	-6.355322	C	-0.720275	-2.495831	-6.529620
C	-2.398673	1.311252	-7.315243	C	-2.120159	-2.237467	-6.275126
C	-1.435624	2.375529	-7.449000	C	-2.698001	-2.568058	-4.986465
C	-0.039595	2.110895	-7.693212	C	-1.975993	-3.305282	-4.030280
C	0.924951	3.011492	-7.108876	C	-1.892741	-2.780592	-2.681408
C	2.109892	2.455945	-6.451516	C	-0.537449	-3.010864	-2.225185
C	2.446080	3.293556	-5.354900	C	0.136958	-2.111392	-1.375663
C	3.241234	2.852962	-4.261206	C	1.582904	-1.991519	-1.546764
C	3.086729	3.600872	-3.057928	C	2.168763	-2.268758	-2.867419
C	3.345744	2.998903	-1.792226	C	1.431087	-3.097361	-3.724629
C	2.292924	3.383943	-0.874992	C	1.338358	-2.846766	-5.138828
C	1.719411	2.393523	-0.025935	C	0.014226	-3.292553	-5.580279
C	0.288798	2.408995	0.147885	C	-0.675380	-3.812643	-4.412895
C	-0.508187	3.414228	-0.482052	C	0.185411	-3.657428	-3.286704

N	-0.291120	0.595382	-3.904862	Sc	-0.082976	2.006795	-5.338276
Sc	-0.456832	-1.492545	-4.144944	Sc	-0.439807	1.158003	-1.994439

$Sc_3N@C_2(39656)$-C_{82}

C	0.011020	-0.007830	0.136724	C	1.467249	2.405160	0.270051
C	1.452683	-0.020979	0.156390	C	0.031382	2.410233	0.312547
C	2.183656	1.193348	0.108239	C	-0.416714	3.675795	-0.210716
C	3.373287	1.209262	-0.679015	C	-1.623519	3.732857	-0.923264
C	3.770838	2.400990	-1.368188	C	-1.702197	4.552417	-2.123185
C	4.425177	1.987249	-2.571305	C	-0.580091	5.272746	-2.544672
C	4.323898	2.782601	-3.721098	C	-0.269270	5.317193	-3.954139
C	4.309584	2.221680	-5.038235	C	1.164860	5.377082	-4.072156
C	3.594973	3.175957	-5.910958	C	1.727444	5.238184	-2.729507
C	2.730471	2.669856	-6.958176	C	0.643151	5.225336	-1.799276
C	1.448038	3.300017	-7.133668	C	0.725673	4.422866	-0.638624
C	0.282160	2.576779	-7.571273	C	4.135400	-0.061922	-3.965969
C	-0.867869	3.169708	-6.936458	C	4.161121	0.786397	-5.164667
C	-1.973455	2.370757	-6.528543	C	3.483157	0.340298	-6.335370
C	-2.695542	2.742112	-5.295106	C	2.749859	1.261947	-7.194022
C	-3.427044	1.668210	-4.600452	C	1.623107	0.543836	-7.730183
C	-3.527162	1.632472	-3.136130	C	0.347880	1.189876	-7.874732
C	-3.146334	0.308585	-2.670611	C	-0.829690	0.426282	-7.641518
C	-2.322641	0.088541	-1.488357	C	-1.967103	1.016743	-6.987475
C	-1.536026	-1.135663	-1.462403	C	-2.583303	-0.027801	-6.212909
C	-0.436233	-1.178552	-0.554492	C	-3.205764	0.310698	-5.002117
C	0.743471	-1.947129	-0.852678	C	-2.999866	-0.513723	-3.833168
C	1.904898	-1.194627	-0.536279	C	-2.187480	-1.689427	-3.874677
C	2.987366	-1.117794	-1.492313	C	-1.522263	-2.061320	-2.618705
C	3.731016	0.077312	-1.494565	C	-0.441333	-3.010665	-2.718015
C	4.345776	0.563387	-2.700885	C	0.755289	-2.824669	-1.927858
C	-0.710641	1.211617	0.090961	C	1.922604	-2.933283	-2.787032
C	-1.929391	1.251465	-0.715098	C	2.937672	-1.908862	-2.722495
C	-2.411570	2.560750	-1.122791	C	3.447955	-1.352693	-3.999658
C	-3.068034	2.726540	-2.402134	C	2.878577	-1.809607	-5.276916
C	-2.552160	3.901754	-3.072882	C	2.858443	-0.930388	-6.403931
C	-2.227580	3.858760	-4.490773	C	1.711826	-0.810635	-7.290478
C	-1.067510	4.648160	-4.925883	C	0.527818	-1.561976	-7.052415
C	-0.425834	4.274698	-6.144045	C	-0.738461	-0.951093	-7.233033
C	0.997912	4.366969	-6.272977	C	-1.839041	-1.224473	-6.322599
C	1.813326	4.853900	-5.209685	C	-1.668217	-2.088866	-5.185868
C	3.104498	4.231331	-5.041338	C	-0.504230	-2.926054	-5.210556
C	3.568712	3.993662	-3.700486	C	0.002728	-3.489486	-4.003802
C	2.879688	4.438879	-2.515704	C	1.446623	-3.433986	-4.045711
C	2.982081	3.605014	-1.310437	C	1.833054	-2.805983	-5.272290
C	1.892077	3.622118	-0.396126	C	0.625557	-2.583369	-6.050840

N	0.513425	0.816530	-4.095225	Sc	1.958216	2.026002	-4.822642
Sc	0.682542	-1.245207	-3.918526	Sc	-1.318004	1.477450	-3.680622