Structure, stability and cluster-cage interactions in nitride clusterfullerenes $M_3N@C_{2n}$ (M = Sc, Y; $2n$ = 68 – 98): a density functional theory study

Alexey A. Popov,[*,†] and Lothar Dunsch*[‡]

Supporting information:

Table S1. Relative energies (ΔE, kJ/mol), binding energies (BE-1, eV) and averaged M–N and M-–C distances ($d_{M–N}$, $d_{M–C}$, Å) in selected $M_3N@C_{2n}$ isomers (M = Sc, Y; $2n$ = 68–98) as computed at the DFT level

	Cage	$Sc_3N@C_{2n}$				$Y_3N@C_{2n}$			
C_{2n}	isomer	ΔE	BE-1	$d_{Sc–N}$	$d_{Sc–C}$	ΔE	BE-1	$d_{Y–N}$	$d_{Y–C}$
C_{68}	D_3: 6140	0.0	-12.50	1.993	2.326		-9.01	2.039	2.415
C_{68}	C_{2v}: 6073	246.0	-9.07	2.025	2.287				
C_{70}	C_{2v}: 7854	0.0	-12.43	2.036	2.331		-9.30	2.058	2.410
C_{70}	D_{5h}: 8149	163.7	-6.91	1.969	2.266				
C_{72}	C_s: 10528	0.0	-10.56	2.043	2.322	33.4	-7.84	2.062	2.414
C_{72}	C_1: 10482	26.7	-11.75	2.057	2.342	0.0	-9.65	2.085	2.443
C_{72}	C_1: 10468	48.9	-11.45	2.073	2.347	25.5	-9.32	2.070	2.438
C_{72}	D_2: 10611	54.6	-10.51	1.985	2.265				
C_{74}	C_{2v}: 14239	0.0	-10.59	2.034	2.311	86.8	-7.77	2.090	2.409
C_{74}	C_3: 13492	9.9	-11.74	2.051	2.352	0.0	-9.93	2.100	2.455
C_{74}	C_2: 13295	18.7	-11.31	2.007	2.309				
C_{76}	T_d: 19151	0.0	-10.10	2.017	2.307	37.7	-7.61	2.092	2.403
C_{76}	C_s: 17490	20.0	-11.71	2.070	2.323	0.0	-9.81	2.105	2.431
C_{78}	D_{3h}: 24109	0.0	-10.51	2.012	2.307	83.6	-7.53	2.076	2.393
C_{78}	C_2: 22010	80.4	-12.10	2.077	2.352	0.0	-10.82	2.100	2.466
C_{80}	I_h: 31924	0.0	-12.48	2.034	2.315	0.0	-10.38	2.060	2.406
C_{80}	D_{5h}: 31923	67.0	-12.38	2.041	2.308	70.2	-10.25	2.065	2.401
C_{80}	C_1: 28325	262.8	-11.25	2.085	2.352	90.0	-10.58	2.135	2.492
C_{82}	C_{2v}: 39718	0.0	-10.78	2.062	2.332	29.6	-9.29	2.099	2.426
C_{82}	C_{2v}: 39705	17.7	-11.99	2.082	2.355	0.0	-10.98	2.119	2.470
C_{82}	C_s: 39663	49.8	-11.36	2.059	2.337	32.6	-10.35	2.131	2.457
C_{84}	C_s: 51365	0.0	-11.90	2.089	2.335	0.0	-11.32	2.156	2.482
C_{84}	D_2: 51589	13.8	-9.64	2.107	2.360	33.2	-8.85	2.136	2.454
C_{86}	C_s: 63757	0.0	-10.12	2.079	2.329	26.1	-9.52	2.157	2.476
C_{86}	D_3: 63761	12.2	-10.04	2.083	2.351	3.7	-9.79	2.173	2.480
C_{86}	C_{2v}: 63751	28.6	-10.44	2.084	2.345	0.0	-10.40	2.196	2.515
C_{88}	D_2: 81738	0.0	-10.56	2.083	2.351	0.0	-10.37	2.195	2.507
C_{90}	C_2: 44	52.8	-9.52	2.103	2.378	0.0	-9.53	2.230	2.541
C_{90}	C_2: 43	0.0	-10.51	2.043	2.323	8.0	-9.89	2.224	2.530
C_{92}	D_3: 85		-10.90	2.173	2.404		-10.90	2.171	2.492
C_{94}	C_2: 121		-10.14	2.030	2.323		-10.02	2.257	2.541
C_{96}	D_2: 186		-10.40	2.061	2.327		-10.06	2.255	2.525
C_{98}	C_2: 166		-9.36	2.056	2.324		-9.24	2.260	2.537

Table S2. Relative energies (ΔE, kJ/mol), and binding energies (BE-2, eV) of the most stable $M_3N@C_{2n}$ ($2n$ = 68-88; M = Sc, Y) isomers as computed at the DFT level

Cage	$Sc_3N@C_{2n}$			Cage	$Sc_3N@C_{2n}$				$Sc_3N@C_{2n}$		$Y_3N@C_{2n}$		Cage	$Sc_3N@C_{2n}$		$Y_3N@C_{2n}$	
C_{2n} isomer	APPs	ΔE	BE-2	C_{2n} isomer	APPs	ΔE	BE-2	C_{2n} isomer	APPs	ΔE	BE-2	ΔE	BE-2	C_{2n} isomer	APPs	ΔE	BE-2	ΔE	BE-2
C_{68} D_3: 6140	3	0.0	-137.7	C_{70} C_{2v}: 7854	3	0.0	-136.7	C_{76} C_s: 17490	2	20.0	-134.7	0.0	-125.5	C_{80} I_h: 31924	0	0.0	-133.2	0.0	-123.9
C_{68} C_{2v}: 6073	2	246.0	-135.3	C_{70} C_2: 7957	2	140.0	135.4	C_{76} C_{2v}: 19138	1	41.7	-134.6	103.2	-124.6	C_{80} D_{5h}: 31923	0	67.0	-133.4	70.2	-124.1
C_{68} C_1: 6102	3	95.6	-137.2	C_{70} C_1: 7852	3	21.6	-136.9	C_{76} T_d: 19151	0	0.0	-135.1	37.7	-125.3	C_{80} C_{2v}: 31922	0	166.5	-133.5	93.9	-124.9
C_{68} C_2: 6118	3	71.4	-137.6	C_{70} D_{5h}: 8149	0	163.7	-135.5	C_{76} C_1: 17465	2	83.1	-134.6	55.4	-125.5	C_{80} C_1: 31891	1	185.1	-133.9	149.8	-124.9
C_{68} C_2: 6146	2	191.7	-136.4	C_{70} C_s: 7960	2	179.0	-135.4	C_{76} C_2: 17765	2	116.4	-134.2	80.2	-125.3	C_{80} C_1: 28325	2	227.4	-133.6	90.0	-125.7
C_{68} C_s: 6072	3	205.9	-136.4	C_{70} C_1: 7886	3	39.2	-136.9	C_{76} C_2: 17512	2	176.6	-133.7	71.1	-125.4	C_{80} C_1: 28319	1	239.7	-133.7	145.2	-125.3
C_{68} C_s: 6089	3	256.9	-135.8	C_{70} C_s: 7922	3	68.0	-136.6	C_{76} C_2: 18161	2	70.0	-134.8	26.1	-125.9	C_{80} C_2: 29591	2	255.4	-133.6	110.6	-125.7
C_{68} C_1: 6138	3	87.9	-137.6	C_{70} C_1: 7887	3	43.6	-136.9	C_{76} C_1: 17588	2	81.1	-134.8	85.7	-125.4	C_{80} C_1: 28324	1	261.4	-133.6	168.5	-125.2
C_{68} C_1: 6116	3	123.9	-137.4	C_{70} C_1: 7851	3	28.6	-137.1	C_{76} C_1: 17760	2	95.7	-134.7	83.7	-125.5	C_{80} C_{2v}: 31920	0	290.5	-133.3	124.5	-125.7
C_{68} C_1: 6039	3	200.9	-136.6	C_{70} C_1: 7849	3	35.6	-137.1	C_{76} C_1: 17459	1	106.2	-134.6	149.7	-124.8	C_{80} C_1:31876	1	232.1	-133.9	144.2	-125.5
C_{72} D_2: 10611	2	54.6	-134.9	C_{74} C_2: 13295	2	18.7	-134.7	C_{82} C_{2v}: 39718	0	0.0	-133.1	29.6	-124.3	C_{84} D_2: 51589	0	13.8	-132.4	33.2	-124.4
C_{72} C_1: 10610	2	34.6	-135.9	C_{74} C_2: 13333	2	51.3	-134.6	C_{82} C_{2v}: 39705	1	17.7	-133.2	0.0	-124.9	C_{84} C_s:51365	1	0.0	-132.6	0.0	-124.8
C_{72} C_s: 10616	2	49.9	-135.7	C_{74} D_{3h}: 14246	0	21.3	-135.0	C_{82} C_{3v}: 39717	0	58.1	-133.0	119.1	-123.9	C_{84} D_{2d}: 51591	0	18.0	-132.7	48.8	-124.5
C_{72} C_1: 10482	3	26.7	-136.0	C_{74} C_1: 13408	2	58.5	-134.7	C_{82} C_s: 39715	0	41.2	-133.2	51.0	-124.7	C_{84} C_s: 51578	0	43.4	-132.5	49.3	-124.6
C_{72} C_s: 10528	2	0.0	-136.3	C_{74} C_2: 13290	2	51.9	-134.8	C_{82} C_s: 39663	1	49.8	-133.2	32.6	-124.9	C_{84} C_s: 51583	0	43.5	-132.5	60.7	-124.5
C_{72} C_{2v}: 11188	1	21.2	-136.1	C_{74} C_2: 13291	2	63.1	-134.8	C_{82} C_2: 39714	0	89.5	-133.1	54.4	-125.0	C_{84} D_2: 51590	0	39.0	-132.6	77.3	-124.3
C_{72} C_1: 10518	3	40.5	-136.1	C_{74} C_2: 13292	2	70.7	-134.9	C_{82} C_s: 39704	1	94.2	-133.2	103.2	-124.7	C_{84} C_{2v}: 51575	0	31.8	-132.8	73.4	-124.5
C_{72} C_1: 10468	3	48.9	-136.0	C_{74} C_1: 13391	2	98.5	-134.6	C_{82} C_s: 36652	2	146.7	-132.8	65.1	-125.2	C_{84} C_2: 50322	1	83.1	-132.3	68.1	-124.6
C_{72} C_1: 10557	2	107.7	-135.4	C_{74} C_3: 13492	3	9.9	-135.6	C_{82} C_1: 39656	1	147.8	-133.0	104.2	-125.0	C_{84} C_1: 51350	1	70.8	-132.5	63.0	-124.7
C_{72} C_2: 10612	1	36.9	-136.2	C_{74} C_{2v}: 14239	2	0.0	-135.8	C_{82} C_s: 39713	0	118.8	-133.2	104.0	-124.9	C_{84} C_s: 51425	1	57.0	-132.6	58.9	-124.8
C_{72} C_2: 10626	2	116.6	-135.4	C_{74} C_1: 13384	2	104.4	-134.8												
C_{72} C_1: 10526	3	55.6	-136.1	C_{74} C_s: 13336	2	50.4	-135.4	C_{86} D_3: 63761	0	12.2	-131.4	3.7	-123.9	C_{88} D_2: 81738	0	0.0	-131.2	0.0	-123.8
C_{72} C_2: 10693	2	53.5	-136.2	C_{74} C_1: 13479	3	38.4	-135.6	C_{86} C_{2v}: 63751	0	28.6	-131.6	0.0	-124.3	C_{88} C_s: 81735	0	64.5	-131.3	55.5	-123.9
C_{72} C_1: 10688	3	56.6	-136.2	C_{74} C_2: 13961	2	132.1	-134.6	C_{86} C_s: 63757	0	0.0	-132.1	26.1	-124.3	C_{88} C_s: 81734	0	60.9	-131.4	77.4	-123.8
C_{72} C_1: 10469	3	70.9	-136.0	C_{74} C_1: 13771	2	57.1	-135.4	C_{86} C_1: 58832	1	45.8	-131.8	40.8	-124.3	C_{88} C_1: 81733	0	58.0	-131.5	91.3	-123.7
C_{72} C_1: 10774	3	40.9	-136.4	C_{74} C_1: 13549	2	49.6	-135.5	C_{86} C_1: 63755	0	33.5	-132.0	34.6	-124.4	C_{88} C_1: 81729	0	63.3	-131.5	86.9	-123.8
C_{72} C_1: 10615	2	66.5	-136.1	C_{74} C_1: 13410	2	74.9	-135.3	C_{86} C_1: 63291	1	51.3	-131.9	54.9	-124.2	C_{88} C_1: 80982	1	57.2	-131.6	78.3	-124.0
C_{72} C_2: 10554	2	148.1	-135.3	C_{74} C_1: 13393	1	65.7	-135.5	C_{86} C_2: 63339	1	48.0	-132.0	56.2	-124.4	C_{88} C_2: 81731	0	86.1	-131.3	86.9	-123.9
C_{72} C_1: 10849	2	132.1	-135.5	C_{74} C_1: 13334	2	72.7	-135.4	C_{86} C_2: 63229	1	87.9	-131.7	69.5	-124.3	C_{88} C_1: 69747	1	80.1	-131.4	75.5	-124.0
C_{72} C_1: 10538	2	51.2	-136.4	C_{74} C_1: 14049	1	47.1	-135.7	C_{86} C_2: 63756	0	44.9	-132.2	84.5	-124.2	C_{88} C_s: 81712	0	43.2	-131.8	76.1	-124.0
								C_{86} C_s: 63750	0	80.6	-131.8	87.7	-124.2	C_{88} C_1: 70333	1	105.0	-131.2	79.3	-124.0

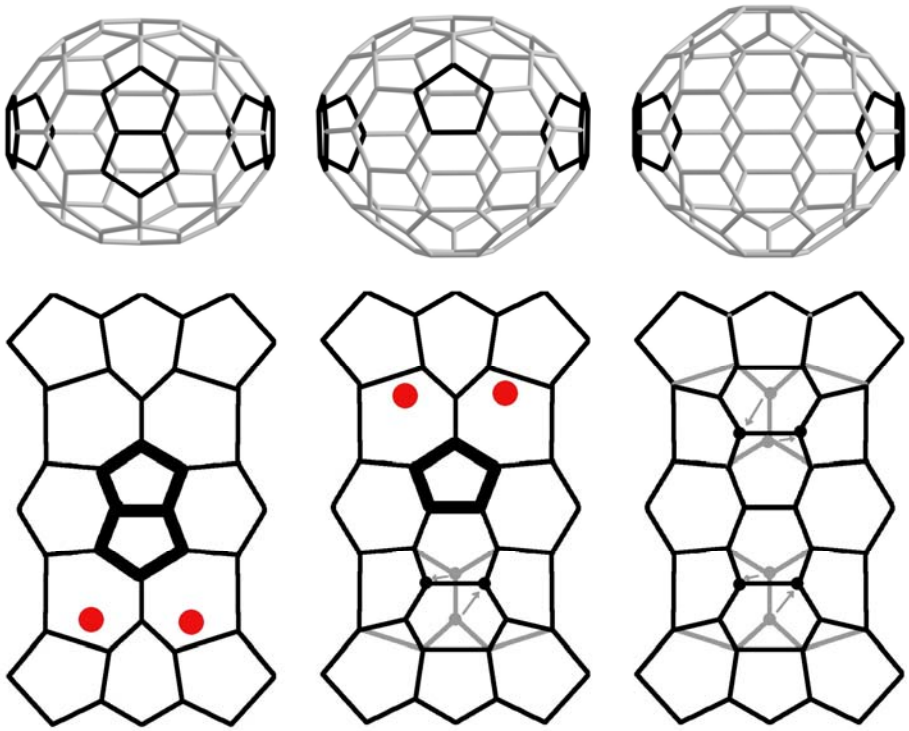

Figure S1. Structural correlation between C_{70} (C_{2v}: 7854, left), C_{72} (C_s: 10528, middle), and C_{74} (C_{2v}: 14239, right) cages, all corresponding to the most stable $Sc_3N@C_{2n}$ isomers. Red dots show approximate positions of carbon atoms to be added to C_{70} to form C_{72} and to C_{72} to form C_{74}. Grey lines show the bonds in the predecessors, which are broken after addition of two carbon atoms. Gray and black dots and gray arrows show the atoms involved in Stones-Wales rearrangements.

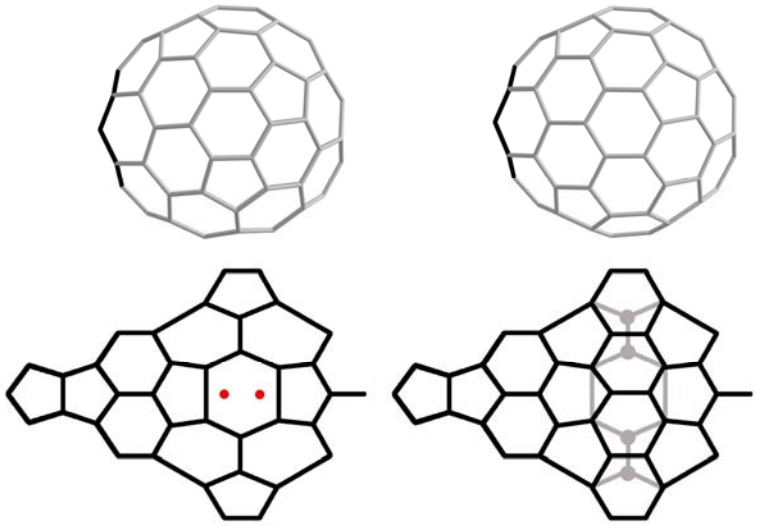

Figure S2a. Correlation between C_{82} (C_s: 39663, left) and C_{84} (C_s: 51365, right). Red dots show where carbon atoms should be added to C_{82} to form C_{84}. Two Stone-Wales rearrangements are also required to complete trnsformation.

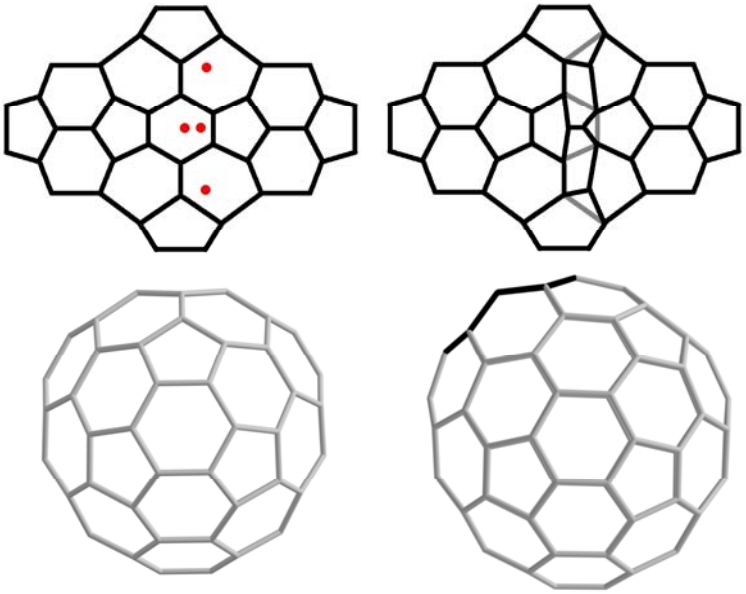

Figure S2b. Correlation between C_{78} (D_{3h}: 24109, left) and C_{82} (C_s: 39663, right). Red dots show where carbon atoms should be added to C_{78} to form C_{82}.