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Supporting Information

Vibrational Spectra and Structures of Si_nC clusters (n=3–8)

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Table S1: Natural bond orbital charge distributions of the Si_nC (n=3–8) isomers calculated at the B3LYP/cc-pVTZ level.

Cluster	Isomer	Atom	Charge	Cluster	Isomer	Atom	Charge	Cluster	Isomer	Atom	Charge
Si_3C				**Si_6C**					**7d**	1C	**-1.932**
	3a	1C	**-1.828**		**6a**	1C	**-1.887**			2Si	0.583
		(2, 4)Si	0.757			(2–4,6,7)Si	0.360			3Si	-0.020
		3Si	0.314			5Si	0.087			4Si	0.002
	3b	1C	**-2.049**		**6b**	1C	**-1.900**			(5, 6)Si	0.352
		2Si	0.822			2Si	0.162			(7, 8)Si	0.331
		(3, 4)Si	0.614			3Si	0.118	**Si_8C**			
	3c	1C	**-1.514**			(4, 5)Si	0.678		**8a**	1C	**-1.838**
		(2, 4)Si	0.732			(6, 7)Si	0.132			2Si	0.962
		3Si	0.050		**6c**	1C	**-1.963**			3Si	0.037
Si_4C						2Si	-0.051			4Si	0.490
	4a	1C	**-1.860**			3Si	0.577			5Si	-0.129
		(2, 3)Si	0.196			4Si	0.815			(6, 7)Si	0.195
		(4, 5)Si	0.734			5Si	0.189			(8, 9)Si	0.043
	4b	1C	**-1.748**			6Si	0.247		**8b**	1C	**-1.884**
		2Si	-0.189			7Si	0.185			2Si	0.193
		(3–5)Si	0.646		**6d**	1C	**-1.790**			3Si	0.080
	4c	1C	**-1.929**			2Si	0.742			4Si	0.087
		2Si	0.254			3Si	0.670			5Si	-0.119
		3Si	0.590			4Si	-0.010			6Si	0.593
		(4,5)Si	0.543			5Si	0.086			7Si	0.804
	4d	1C	**-1.844**			(6, 7)Si	0.151			8Si	-0.073
		2Si	0.870	**Si_7C**						9Si	0.320
		3Si	0.472		**7a**	1C	**-1.777**		**8c**	1C	**-1.902**
		4Si	0.584			2Si	-0.130			2Si	0.451
		5Si	-0.081			3Si	0.924			3Si	0.280
Si_5C						4Si	0.005			4Si	-0.051
	5a	1C	**-1.959**			5Si	0.628			5Si	0.101
		2Si	-0.012			6Si	0.294			6Si	0.027
		(3, 5)Si	0.532			7Si	-0.062			7Si	0.788
		(4, 6)Si	0.454			8Si	0.117			8Si	0.058
	5b	1C	**-1.958**		**7b**	1C	**-1.778**			9Si	0.249
		2Si	-0.018			2Si	0.114		**8d**	1C	**-1.836**
		(3–6)Si	0.494			3Si	0.909			2Si	0.669
	5c	1C	**-1.776**			4Si	0.561			3Si	0.120
		2Si	0.690			5Si	0.350			4Si	0.024
		3Si	0.654			6Si	-0.091			5Si	0.052
		4Si	0.041			7Si	-0.017			(6, 7)Si	0.564
		(5, 6)Si	0.196			8Si	-0.047			(8, 9)Si	-0.079
	5d	1C	**-1.832**		**7c**	1C	**-1.824**		**8e**	1C	**-1.856**
		2Si	0.574			3Si	0.046			2Si	0.526
		3Si	0.624			(2, 4, 5)Si	0.651			3Si	0.076
		4Si	0.098			(6–8)Si	-0.058			4Si	0.014
		(5, 6)Si	0.268							5Si	0.393
										(6, 7)Si	0.474
										(8, 9)Si	-0.050

Table S2: Vibrational frequencies in cm^{-1} of the low-energy Si_nC (n=3–8) structures calculated at the B3LYP/cc-pVTZ level.

Structure	Frequency[a]
3a	180.5 (0.04), 297.2 (5.2), 337.6 (10.9), 508.6 (21.8), 651.6 (49.9), 1109.1 (71.6)
3b	68.1 (0.01), 268.7 (6.0), 300.1 (0.12), 498.2 (0.38), 534.7 (0.39), 967.7 (22.7)
3c	166.9 (11.5), 209.3 (21.0), 229.7 (0.005), 310.2 (4.7), 726.6 (24.5), 986.4 (21.4)
4a	132. 4(1.05), 163.4 (0.41), 325.0 (1.2), 328.3 (17.0), 345.6 (3.3), 377.9 (11.3), 489.5 (55.4), 517.3 (2.9), 1046.8 (26.6)
4b	240.2 (2.1), 296.6 (8.6), 316.5 (18.3), 395.3 (6.8), 659.9 (27.5), 721.3 (24.2)
4c	115.7 (6.1), 158.4 (1.2), 186.7 (0.37), 276.1 (0.2), 295.5 (0.11), 431.8 (9.5), 622.2 (17.2), 715.1 (117.9), 848.1 (2.6)
4d	111.4 (0.27), 123.4 (3.2), 268.5 (1. 5), 284.4 (4.5), 372.6 (8.7), 467.2 (19.2), 478.1 (6.8), 616.6 (12.1), 1140.5 (80.5)
5a	47.2 (0.03), 118.3 (0.06), 131.9 (0.23), 301.9 (0.00), 311.6 (5.1), 324.4 (1.3), 372.1 (3.0), 397.3 (2.7), 424.1 (33.7), 564.6 (26.2), 725.9 (63.3), 846.9 (50.7)
5b	*i*33.9 (0.00), 125.2 (0.28), 310.9 (0.00), 333.5 (1.4), 340.8 (8. 3), 392.9 (0.00), 420.2 (34.8), 567.2 (27.9), 785.4 (113.5)
5c	155.1 (1.37), 188.2 (3.5), 214.7 (0.36), 256.1 (2.5), 277.1 (1.1), 337.9 (0.48), 353.8 (15.3) 433.4 (11.5), 448.6 (9.4), 465.8 (30.9), 598.0 (23.5), 1006.7 (4.4)
5d	56.1 (0.28), 185.2 (0.07), 195.5 (0.16), 228.8 (4.0), 270.4 (0.76), 300.5 (3.0), 374.2 (0.43), 396.2 (1.9), 448.8 (32.9), 563.9 (30.2), 569.8 (13.7), 926.4 (19.1)
6a	103.9 (0.00), 226.1 (3.8), 256.5 (1.5), 269.1 (0.00), 350.4 (0.46), 415.7 (0.00), 424.9 (8.9), 543.7 (48.4), 549.6 (70.2)
6b	78.2 (0.05), 97.9 (1.04), 153.3 (0.45), 161.2 (5.0), 191.6 (0.56), 262.0 (1.9), 272.0 (0.005), 309.9 (0.01), 342.9 (3.7), 362.4 (0.55), 441.0 (9.8), 486.8 (35.3), 498.1 (0.07), 581.4 (50.5), 879.1 (48.3)
6c	50.8 (2.2), 137.4 (2.8), 167.7 (1.6), 194.5 (0.08), 248.1 (0.14), 301.1(0.5), 325.9 (0.33), 338.3 (4.6), 340.1 (9.9), 366.9 (2.1), 370.9 (3.8), 427.5 (5.4), 445.6, (3.6), 478.5 (33.9), 886.2 (58.8)
6d	37.6 (1.2), 39.8 (1.6), 136.8 (0.009), 192.7 (1.7), 222.9 (1.8), 260.8 (19.4), 276.6 (0.29), 305.0 (5.7), 313.6 (8.8), 394.4 (0.44), 395.0 (6.4), 428.8 (8.7), 466.4 (19.2), 557.7 (18.1), 985.4 (19.3)
7a	68.7 (0.34), 89.1 (0.41), 128.7 (2.0), 149.9 (3.5), 186.1 (0.23), 227.8 (0.51), 252.1 (1.24), 267.8 (0.88), 287.5 (0.82), 306.9 (4.4), 332.7 (1.7), 359.5 (0.77), 361.0 (2.1), 403.0 (6.2), 446.4 (0.75), 456.8 (13.6), 679.5 (63.5), 1103.2 (95.7)
7b	50.4 (0.10), 98.7 (0.45), 127.2 (4.0), 194.9 (2.3), 213.1 (2.2), 230.1 (2.6), 262.2 (1.5), 272.5 (1.8), 289.8 (1.8), 307.9 (5.0), 315.1 (3.4), 339.9 (3.4), 361.7 (4.6), 383.7 (2.1), 449.9 (1.8), 460.5 (50.8), 610.2 (5.8), 1194.8 (96.4)
7c	133.1 (0.05), 143.2 (0.00), 160.0 (2.0), 241.5 (4.5), 271.2 (0.005), 271.6 (2.4), 293.9 (0.18), 359.9 (21.2), 377.5 (4.1), 476.1 (8.8), 488.7 (0.83), 767.7 (33.0)
7d	117.5 (0.34), 135.8 (0.53), 185.3 (1.5), 193.3 (1.4), 220.7 (0.51), 247.7 (0.02), 256.1 (0.48), 291.4 (0.03), 291.7 (0.7), 306.2 (0.13), 327.1 (2.2), 334.6 (1.8), 362.0 (1.5), 387.3 (7.1), 466.3 (5.4), 475.3 (14.2), 525.5 (46.6), 793.3 (22.3)
8a	105.3 (0.52), 110.5 (6.2), 156.5 (7.8), 173.2 (0.63), 225.5 (1.3), 239.9 (0.36), 241.8 (0.43), 258.1 (2.27), 276.1 (1.8), 293.7 (1.5), 297.4 (0.06), 311.1 (1.2), 321.9 (2.0), 367.6 (2.1), 387.5 (2.0), 391.2 (6.5), 433.3 (6.6), 437.0 (0.4), 446.3 (32.8), 478.6 (7.5), 1051.7 (4.8)
8b	63.7 (0.82), 74.4 (0.22), 101.5 (1.8), 140.2 (0.36), 166.1 (1.1), 190.6 (0.92), 217.8 (0.67), 219.6 (1.2), 236.6 (0.65), 249.6 (1.5), 256.6 (6.5), 317.9 (1.4), 342.1 (1.2), 364.2 (1.4), 385.5 (1.4), 422.1 (0.81), 452.3 (32.3), 465.4 (7.7), 513.9 (7.0), 563.0 (20.8), 961.9 (11.4)
8c	93.1 (0.14), 107.7 (1.1), 131.1 (0.50), 156.2 (5.7), 171.3 (3.0), 191.0 (0.48), 218.9 (0.26), 232.5 (5.0), 251.4 (0.21), 268.7 (2.3), 278.4 (2.9), 308.7 (11.9), 324.8 (0.22), 350.4 (2.5), 388.4 (9.5), 405.9 (8.2), 434.2 (14.4), 459.5 (9.9), 484.7 (1.3), 541.6 (13.8), 928.5 (23.1)
8d	51.9 (0.62), 119.9 (0.13), 143.5 (0.41), 164.5 (1.0), 187.7 (0.02), 211.5 (0.33), 231.6 (2.2), 231.8 (0.08), 242.9 (0.29), 256.9 (0.13), 301.0 (0.77), 308.9 (0.06), 312.2 (0.02), 367.5 (2.19), 381.7 (17.9), 389.7 (0.04), 402.1 (8.7), 434.6 (2.8), 475.0 (0.2), 602.5 (14.0), 796.7 (3.3)
8e	89.1 (0.30), 103.9 (0.98), 141.8 (0.05), 151.8 (0.46), 197.1 (0.5), 213.7 (0.04), 230.2 (0.11), 249.8 (1.4), 255.5 (2.2), 255.7 (0.31), 277.8 (1.2), 303.7 (0.21), 333.06 (0.11), 354.9 (7.4), 364.4 (0.2), 369.3 (11.9), 420.6 (1.9), 443.8 (7.0), 471.5 (8.8), 587.6 (43.1), 638.6 (12.5)

[a] Intensities (in km/mol) are given in parentheses.

Table S3: Cartesian coordinates in Å of the low-energy Si_nC (n=3–8) structures calculated at the B3LYP/cc-pVTZ level.

Structure					Structure				
3a	C	0.00000	0.00000	0.70242	**3b**	C	0.00000	0.00000	0.31586
	Si	0.00000	0.00000	-1.24162		Si	0.00000	0.00000	2.06888
	Si	0.00000	-1.74854	0.47029		Si	0.00000	1.17876	-1.10213
	Si	0.00000	1.74854	0.47029		Si	0.00000	-1.17876	-1.10213
3c	C	-0.69718	-0.95481	0.00000					
	Si	0.09960	-0.50393	1.49539					
	Si	0.09960	1.41707	0.00000					
	Si	0.09960	-0.50393	-1.49539					
4a	C	0.00000	0.00000	0.00000	**4b**	C	0.00000	0.00000	-1.09648
	Si	0.00000	0.00000	2.15352		Si	0.00000	0.00000	1.40921
	Si	1.95913	0.00000	0.89411		Si	0.00000	-1.67100	-0.31310
	Si	-0.84411	-1.48698	0.48319		Si	1.44713	0.83550	-0.31310
	Si	0.79004	1.48698	-0.56731		Si	-1.44713	0.83550	-0.31310
4c	C	-0.64459	-0.17442	0.00000	**4d**	C	0.99000	-0.63614	0.00000
	Si	0.47757	-1.74018	0.00000		Si	2.56054	0.05486	0.00000
	Si	-1.15646	1.53445	0.00000		Si	0.00000	0.98998	0.00000
	Si	0.47757	0.14024	1.51376		Si	-0.72700	-1.24720	0.00000
	Si	0.47757	0.14024	-1.51376		Si	-2.25783	0.47499	0.00000
5a	C	0.00000	0.00000	-0.83687	**5b**	C	0.00000	0.00000	-0.83844
	Si	0.00000	0.00000	1.43093		Si	0.00000	0.00000	1.43001
	Si	0.00000	1.80175	-0.35683		Si	0.00000	1.80674	-0.26767
	Si	-1.81315	0.00000	-0.17931		Si	-1.80674	0.00000	-0.26767
	Si	0.00000	-1.80175	-0.35683		Si	0.00000	-1.80674	-0.26767
	Si	1.81315	0.00000	-0.17931		Si	1.80674	0.00000	-0.26767
5c	C	-0.30873	1.16058	0.00000	**5d**	C	-1.03187	-0.40219	0.00000
	Si	-2.07568	0.77695	0.00000		Si	0.04752	-1.86933	0.00000
	Si	1.46965	1.06229	0.00000		Si	-1.48848	1.35407	0.00000
	Si	1.35581	-1.51874	0.00000		Si	1.78815	0.34172	0.00000
	Si	-0.30873	-0.40895	1.29655		Si	0.04752	0.17295	1.59274
	Si	-0.30873	-0.40895	-1.29655		Si	0.04752	0.17295	-1.59274
6a	C	0.00000	0.00000	-0.66223	**6b**	C	-0.69490	-0.90070	0.00000
	Si	0.00000	2.01131	-0.23669		Si	1.41271	-0.40903	0.00000
	Si	1.91287	0.62153	-0.23669		Si	0.59984	2.33019	0.00000
	Si	1.18222	-1.62718	-0.23669		Si	-0.42868	-1.51679	1.72510
	Si	0.00000	0.00000	1.46733		Si	-0.42868	-1.51679	-1.72510
	Si	-1.91287	0.62153	-0.23669		Si	-0.42868	0.74922	1.33516
	Si	-1.18222	-1.62718	-0.23669		Si	-0.42868	0.74922	-1.33516
6c	C	-0.63006	0.73221	-0.22055	**6d**	C	1.01960	0.00000	-0.50451
	Si	2.41978	-0.37072	0.14915		Si	1.57145	-1.72510	-0.12259
	Si	1.03691	1.64556	-0.12451		Si	0.12376	-0.00000	1.46555
	Si	-2.41275	0.91976	0.05568		Si	1.57144	1.72511	-0.12259
	Si	-1.50803	-1.35880	-0.04085		Si	-2.40267	-0.00001	0.13058
	Si	0.46279	-0.67674	-1.21990		Si	-0.65048	-1.33516	-0.56736

	Si	0.27133	-0.47286	1.27495		Si	-0.65049	1.33516	-0.56736
7a	C	2.16516	-0.55234	-0.12359	**7b**	C	2.06761	0.75029	0.06758
	Si	-0.96098	-0.42127	-1.29060		Si	-1.86101	1.53427	-0.13430
	Si	3.38880	0.63422	0.04656		Si	3.59536	-0.00941	-0.07272
	Si	-2.83032	-0.14767	0.10092		Si	0.36637	1.20455	0.26364
	Si	0.77024	-1.78427	-0.20315		Si	1.26012	-1.08530	-0.10810
	Si	0.79508	0.70624	0.21537		Si	-0.77721	-0.46896	-1.32329
	Si	-0.90113	-0.55554	1.37215		Si	-2.68808	-0.84774	-0.00776
	Si	-1.18963	1.80501	-0.18829		Si	-0.78167	-0.64896	1.35357
7c	C	0.00000	0.00000	1.58319	**7d**	C	-1.06434	-0.14629	0.00000
	Si	0.00000	1.82557	1.26359		Si	-2.10034	-1.64728	0.00000
	Si	0.00000	0.00000	-2.46510		Si	1.57869	-0.21682	0.00000
	Si	1.58099	-0.91279	1.26359		Si	1.70699	2.06290	0.00000
	Si	-1.58099	-0.91279	1.26359		Si	-0.18230	-1.23174	1.52981
	Si	0.00000	-1.51829	-0.66806		Si	-0.18230	-1.23174	-1.52981
	Si	-1.31487	0.75914	-0.66806		Si	-0.18230	1.16369	1.32720
	Si	1.31487	0.75914	-0.66806		Si	-0.18230	1.16369	-1.32720
8a	C	1.50775	0.55726	0.00000	**8b**	C	1.81110	0.21047	0.61936
	Si	1.70567	2.28914	0.00000		Si	1.00312	-1.29473	-0.52352
	Si	-1.95895	1.32010	0.00000		Si	-1.40228	-1.96105	-0.69283
	Si	1.28009	-1.28603	0.00000		Si	-1.79312	1.82561	0.36563
	Si	-1.45516	-1.07318	0.00000		Si	-1.43194	-0.39017	1.09131
	Si	-0.05446	0.79287	1.38170		Si	2.39012	0.54109	-1.15126
	Si	-0.05446	0.79287	-1.38170		Si	1.15572	-0.64887	2.02328
	Si	-0.05446	-1.53730	1.98225		Si	-1.26789	0.26704	-1.35480
	Si	-0.05446	-1.53730	-1.98225		Si	0.57008	1.57088	-0.02324
8c	C	1.02244	-0.31923	0.85579	**8d**	C	-0.62455	-1.56821	0.00000
	Si	0.17207	-1.67753	-0.13144		Si	-1.96595	-0.19452	0.00000
	Si	-1.01936	0.28638	1.35017		Si	1.53423	-1.02331	0.00000
	Si	-1.73176	0.16611	-1.09572		Si	1.77047	1.51970	0.00000
	Si	0.82058	1.12693	-0.66888		Si	-1.21950	2.16515	0.00000
	Si	-2.17827	-1.59773	0.37850		Si	0.03710	-1.72466	1.73807
	Si	2.65684	0.34714	1.07491		Si	0.03710	-1.72466	-1.73807
	Si	-1.24365	2.22799	-0.09050		Si	0.03710	0.82720	1.48450
	Si	2.08537	-0.74248	-1.18381		Si	0.03710	0.82720	-1.48450
8e	C	-0.89700	0.99185	0.00000					
	Si	-2.15495	-0.55196	0.00000					
	Si	1.54554	-2.13280	0.00000					
	Si	1.48974	0.25963	0.00000					
	Si	0.60875	2.46675	0.00000					
	Si	-0.27616	1.15696	1.82631					
	Si	-0.27616	1.15696	-1.82631					
	Si	-0.27616	-1.39031	1.30919					
	Si	-0.27616	-1.39031	-1.30919					