

Supporting Information:

Vibrational spectra and structures of neutral Si_6X clusters

($X = \text{Be, B, C, N, O}$)

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In this Supporting Information, we provide the predicted vibrational spectra of the first five low-energy Si_6X isomers ($X=\text{Be}, \text{B}, \text{C}, \text{N}, \text{O}$) in Fig. S1–S5, the natural electronic configurations and natural populations (Table S1) of the most stable structures, and the Cartesian coordinates (section SII) of the Si_6X clusters shown in the paper.

SI. CALCULATED VIBRATIONAL SPECTRA

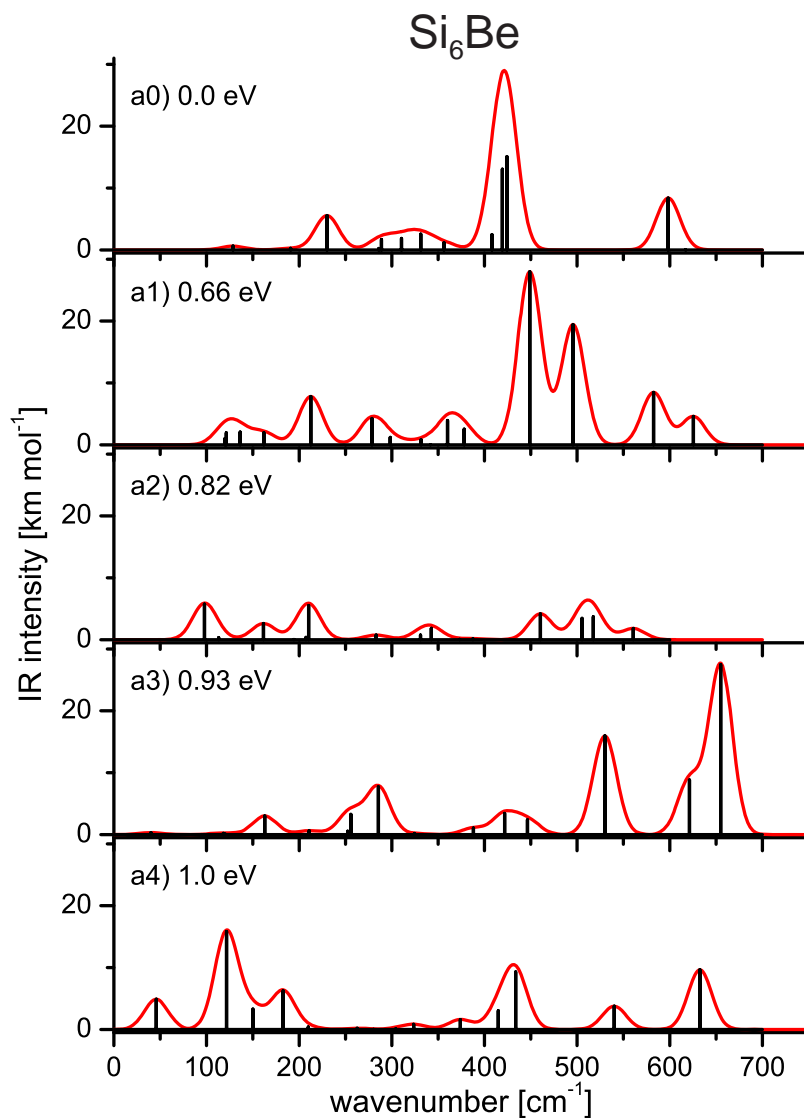


FIG. S1. Calculated vibrational spectra of the first five low-energy Si_6Be isomers (**a0–a4**) as shown in Fig. 2.

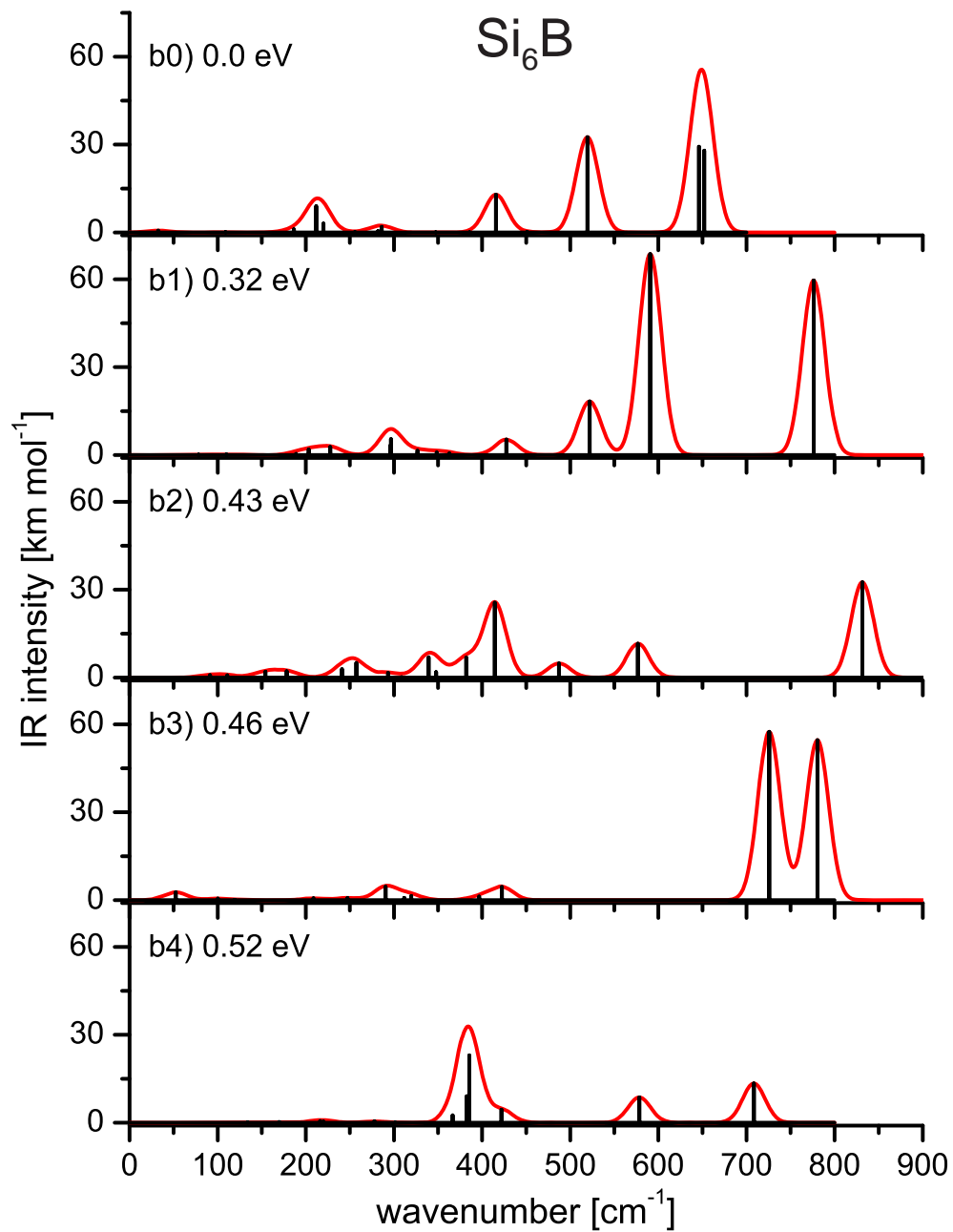


FIG. S2. Calculated vibrational spectra of the first five low-energy Si_6B isomers (b0–b4) as shown in Fig. 2.

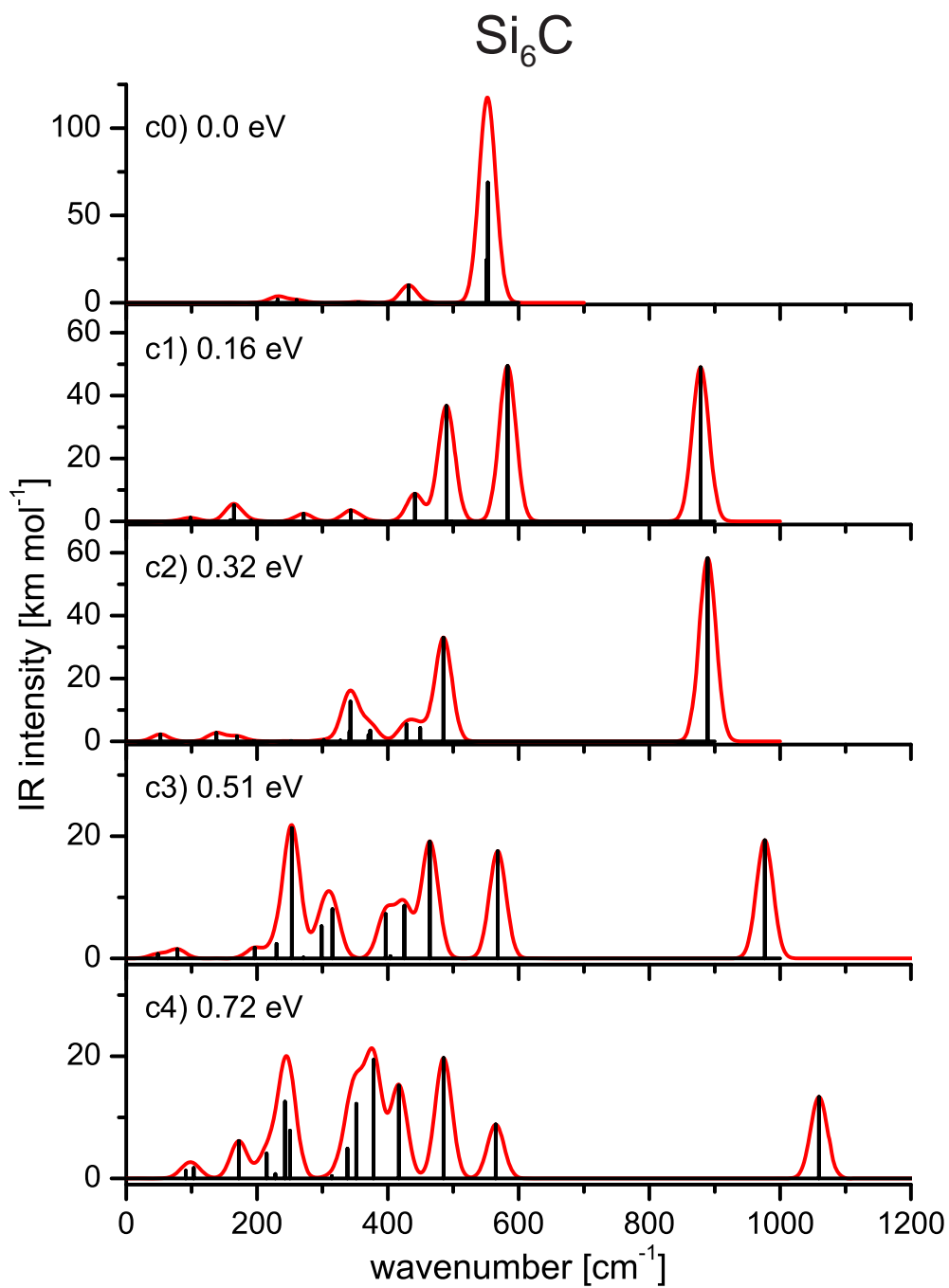


FIG. S3. Calculated vibrational spectra of the first five low-energy Si_6C isomers (c0–c4) as shown in Fig. 2.

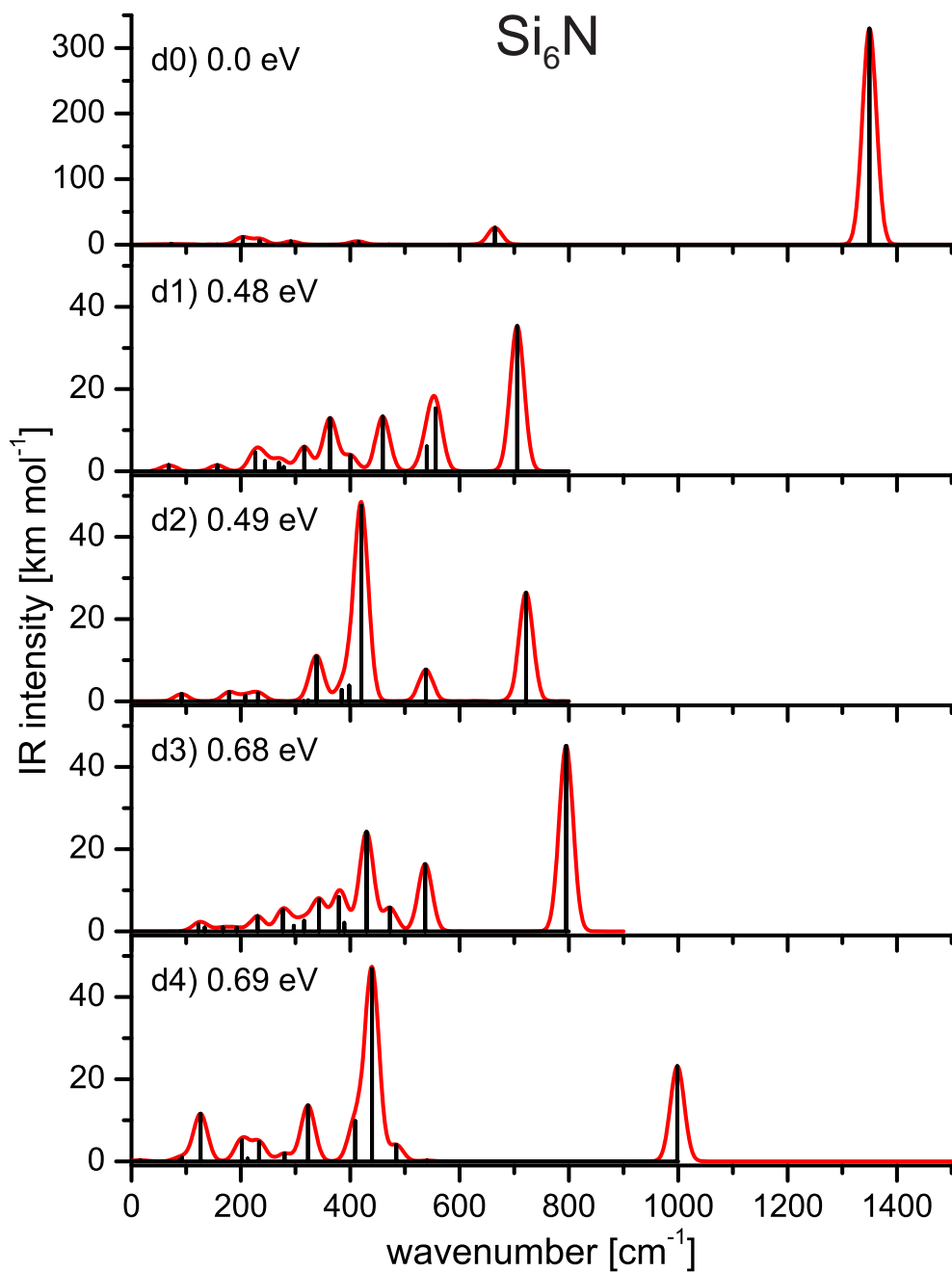


FIG. S4. Calculated vibrational spectra of the first five low-energy Si_6N isomers (d0–d4) as shown in Fig. 2.

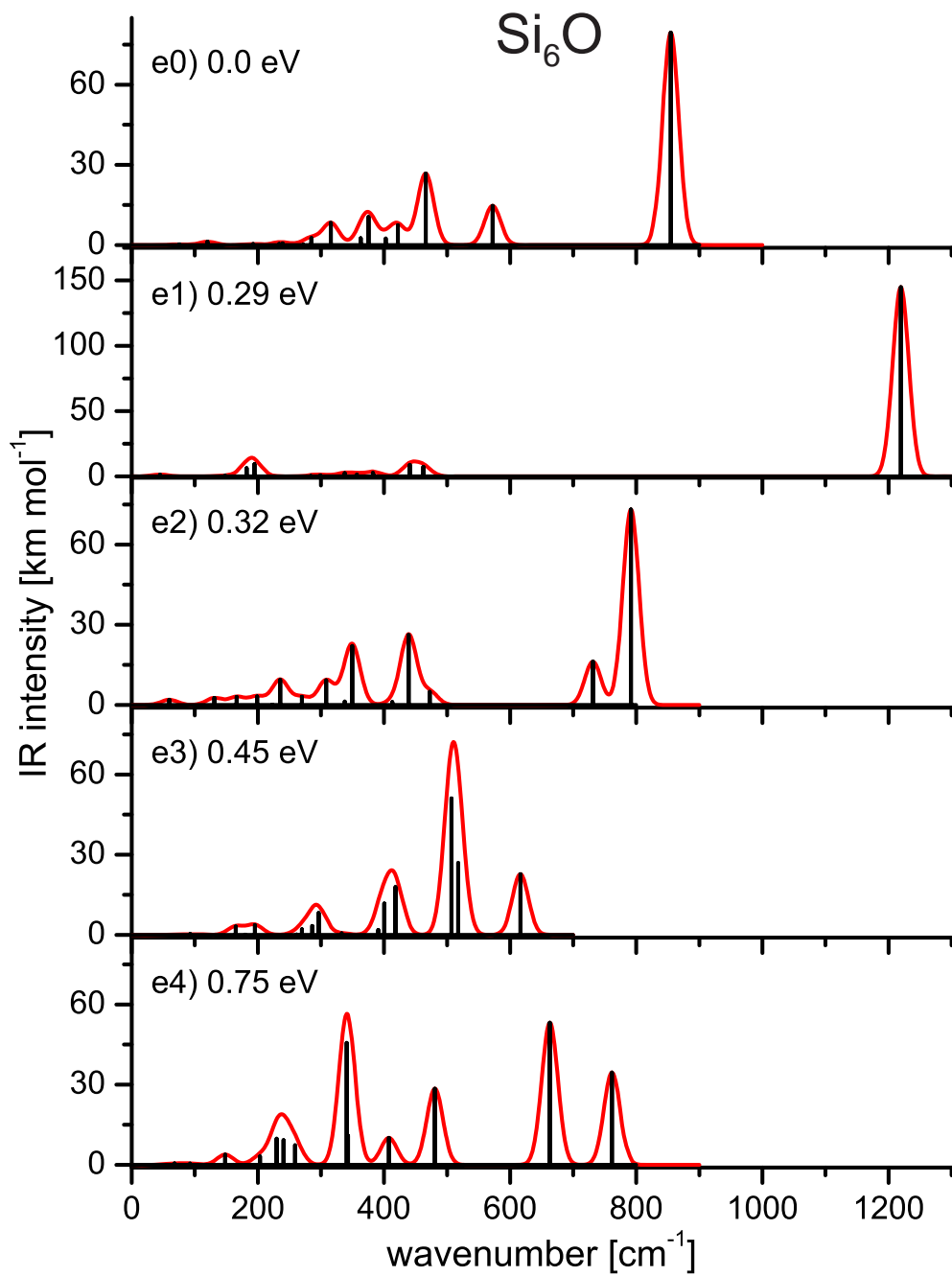


FIG. S5. Calculated vibrational spectra of the first five low-energy Si_6O isomers (e0–e4) as shown in Fig. 2.

TABLE S1. Natural electronic configurations and natural populations of the most stable Si_6X ($X=\text{Si, Be, B, C, N, O}$) clusters found at the B3LYP/cc-pVTZ level. The numbers assigned to the Si atoms are the same as those provided in section SII.

Cluster	Atom	Natural electronic configuration	Natural population
Si_7	Si(1-5)	[core]3s ^{1.69} 3p ^{2.16} 3d ^{0.06} 4p ^{0.01}	0.079
	Si(6,7)	[core]3s ^{1.52} 3p ^{2.52} 4s ^{0.01} 3d ^{0.14} 4p ^{0.01}	-0.198
Si_6Be	Be	[core]2s ^{0.66} 2p ^{1.45} 3p ^{0.01} 3d ^{0.04}	-0.166
	Si(1,6)	[core]3s ^{1.49} 3p ^{2.49} 3d ^{0.11} 4p ^{0.01}	-0.113
	Si(2,4)	[core]3s ^{1.61} 3p ^{2.27} 3d ^{0.05} 4p ^{0.01}	0.066
	Si(3,5)	[core]3s ^{1.72} 3p ^{2.09} 3d ^{0.05} 4p ^{0.01}	0.130
Si_6B	B	[core]2s ^{1.07} 2p ^{3.16} 3s ^{0.01} 3p ^{0.02} 3d ^{0.19} 4f ^{0.01}	-1.449
	Si(1,3)	[core]3s ^{1.64} 3p ^{1.99} 3d ^{0.04} 4p ^{0.01}	0.321
	Si(2)	[core]3s ^{1.74} 3p ^{2.16} 3d ^{0.05} 4p ^{0.01}	0.033
	Si(4,5)	[core]3s ^{1.57} 3p ^{2.10} 3d ^{0.04} 4p ^{0.01}	0.277
	Si(6)	[core]3s ^{1.45} 3p ^{2.27} 3d ^{0.05} 4p ^{0.01}	0.219
	Si_6C	C	[core]2s ^{1.46} 2p ^{4.29} 3s ^{0.02} 3p ^{0.01} 3d ^{0.10}
Si(1-5)		[core]3s ^{1.64} 3p ^{1.94} 3d ^{0.04} 4p ^{0.01}	0.359
Si(6)		[core]3s ^{1.70} 3p ^{2.14} 3d ^{0.05} 4p ^{0.01}	0.087
Si_6N	N	[core]2s ^{1.61} 2p ^{5.05} 3p ^{0.01}	-1.673
	Si(1,6)	[core]3s ^{1.61} 3p ^{2.35} 3d ^{0.05} 4p ^{0.01}	-0.024
	Si(2)	[core]3s ^{1.73} 3p ^{1.14} 4s ^{0.01} 3d ^{0.02}	1.105
	Si(3)	[core]3s ^{0.99} 3p ^{2.37} 3d ^{0.07} 4p ^{0.01} 4d ^{0.01}	0.053
	Si(4,5)	[core]3s ^{1.69} 3p ^{2.20} 3d ^{0.05} 4p ^{0.01}	0.043
	Si_6O	O	[core]2s ^{1.81} 2p ^{5.39} 3d ^{0.03}
Si(1)		[core]3s ^{1.55} 3p ^{2.57} 3d ^{0.11} 4p ^{0.01}	-0.242
Si(2)		[core]3s ^{1.68} 3p ^{2.19} 3d ^{0.05} 4p ^{0.01}	0.067
Si(3)		[core]3s ^{1.62} 3p ^{2.41} 3d ^{0.08} 4p ^{0.01}	-0.125
Si(4)		[core]3s ^{1.25} 3p ^{1.90} 3d ^{0.08} 4p ^{0.01} 4d ^{0.01}	0.749
Si(5)		[core]3s ^{1.69} 3p ^{2.22} 3d ^{0.05} 4p ^{0.01}	0.029
Si(6)		[core]3s ^{1.65} 3p ^{1.54} 3d ^{0.03} 4p ^{0.01} 4d ^{0.01}	0.763

SII. CARTESIAN COORDINATES

Si₆Be-a0:			
Be	0.00000000	-1.91864300	-0.00000400
Si1	0.00000100	-0.12095400	-1.31489500
Si2	1.95743800	-1.00454300	0.00000000
Si3	-1.40901500	1.39959100	0.00000300
Si4	-1.95743800	-1.00454300	-0.00000400
Si5	1.40901500	1.39959100	0.00000300
Si6	-0.00000100	-0.12095900	1.31489500

Si₆Be-a1:			
Be	0.91772900	-0.00000600	-1.39328600
Si	1.68750700	1.42868100	0.13240800
Si	0.04916300	-0.00004300	1.20749600
Si	-0.70195700	1.26207100	-0.82013000
Si	-0.70204200	-1.26188700	-0.82022000
Si	1.68745800	-1.42877300	0.13231900
Si	-2.28233700	-0.00004800	0.56620900

Si₆Be-a2:			
Be	-0.00002300	0.06797900	-1.32490900
Si	-1.39785500	1.43314100	-0.31089800
Si	0.00007500	0.35939200	1.51506600
Si	0.00000800	-1.62639800	0.05406300
Si	-2.11990500	-0.80936700	-0.28435400
Si	1.39779600	1.43316400	-0.31092800
Si	2.11988800	-0.80935500	-0.28440300

Si₆Be-a3:			
Be	0.37781500	2.20225600	0.00000400
Si	1.16056200	0.65623000	-1.25478700
Si	-0.35331300	-1.08041500	-0.00000700
Si	1.16049100	0.65619600	1.25483600
Si	-2.62324600	-0.77668300	-0.00001100
Si	-1.42139400	1.18381000	-0.00001900
Si	1.96895100	-1.26835400	-0.00001300

Si₆Be-a4:			
Be	2.53449900	1.17428900	-0.00000200
Si	-1.72813300	-1.32110800	0.00000200
Si	0.08029500	-0.42219000	1.28901700
Si	2.08535800	-0.94608300	-0.00000600
Si	0.48570100	1.67319200	0.00000700
Si	0.08028700	-0.42218200	-1.28901600
Si	-1.72765000	1.10286000	-0.00000200

Si₆B-b0:			
B	0.00000000	0.04080600	-0.78739400
Si1	-1.26898800	1.59394300	-0.22369500
Si2	-0.00000200	0.06826200	1.50291900
Si3	1.26893600	1.59398100	-0.22367000
Si4	-1.92368700	-0.67794000	-0.34794500
Si5	1.92371100	-0.67788300	-0.34796000
Si6	0.00003000	-1.91493600	-0.07843800

Si₆B-b1:			
B	-0.00000600	0.00002100	-0.64970600
Si	2.00865700	0.57056200	-0.94569800
Si	-0.76266900	-0.92945200	1.16960600
Si	-1.22442700	1.51493400	-0.10789000
Si	1.22441700	-1.51492000	-0.10793100
Si	0.76270300	0.92940900	1.16963200
Si	-2.00867900	-0.57054000	-0.94568200

Si₆B-b2:			
B	0.65406600	0.51769300	-0.79173100
Si	2.31049100	0.97570900	0.12366100
Si	-0.03520800	0.01150900	1.26619500
Si	-2.34101100	-0.23453200	0.55835300
Si	-1.03860100	1.48574400	-0.64121300
Si	-0.63622700	-1.05964100	-0.99311700
Si	1.50696100	-1.36367900	-0.03111800

Si₆B-b3:			
B	0.00002300	-0.00001700	-0.85868400
Si	-1.97373800	-0.00006100	-1.02125200
Si	-0.00000800	1.85904800	-0.09215100
Si	-1.17912300	0.00006900	1.26664900
Si	1.97376700	-0.00007700	-1.02124900
Si	-0.00003500	-1.85902600	-0.09199000
Si	1.17912800	0.00005300	1.26666600

Si₆B-b4:			
B	-0.00004000	-1.74186700	-0.00000400
Si	-0.00000100	-0.08946000	1.29838500
Si	1.89594200	-1.09222100	-0.00000200
Si	-1.89599700	-1.09216300	0.00000000
Si	1.33851100	1.49266900	0.00000100
Si	0.00000000	-0.08945700	-1.29838100
Si	-1.33844200	1.49272800	-0.00000100

Si ₆ C-c0:			
C	0.00003500	0.00004500	-0.66437600
Si1	1.02445300	1.72751100	-0.23545500
Si2	0.18658900	-1.99966600	-0.23593600
Si3	1.95952800	-0.44046300	-0.23562200
Si4	-1.84422400	-0.79536300	-0.23597500
Si5	-1.32636300	1.50815800	-0.23555400
Si6	0.00000000	-0.00019600	1.46327500

Si ₆ C-c1:			
C	1.00742900	0.00002800	-0.51564300
Si	-2.39581000	-0.00010000	0.14215300
Si	1.57067300	-1.71818000	-0.11302600
Si	1.57054900	1.71826900	-0.11302500
Si	-0.64726700	-1.33342100	-0.57688500
Si	0.11749800	-0.00000500	1.45862900
Si	-0.64739800	1.33342500	-0.57685600

Si ₆ C-c2:			
C	0.63148700	0.72598500	-0.22627000
Si	-0.27023000	-0.46782600	1.27592500
Si	-2.41834600	-0.36660600	0.15215300
Si	-1.03119400	1.64364100	-0.12814600
Si	-0.46555700	-0.67888400	-1.21855900
Si	1.50248500	-1.35675800	-0.04057100
Si	2.41220400	0.91529700	0.05617000

Si ₆ C-c3:			
C	-1.31847000	0.79526600	0.00000800
Si	1.36800700	-1.71989300	-0.00001300
Si	-0.17567800	-0.32062800	1.25922800
Si	-0.17570600	-0.32063400	-1.25922600
Si	1.90989400	0.62890800	0.00000800
Si	-0.10788100	2.15503900	-0.00001300
Si	-2.25357700	-0.76361900	0.00001300

Si ₆ C-c4:			
C	1.08739300	-0.70223800	0.64982600
Si	0.01475500	-0.62174500	-1.04082200
Si	-2.20740800	-0.94841400	-0.22538000
Si	-1.34252300	1.46255400	-0.33736800
Si	1.00622200	1.40801300	0.20635400
Si	-0.52234900	-0.44197500	1.39583900
Si	2.58527900	-0.55747400	-0.27712000

Si₆N-d0:			
N	2.12900000	-0.00000600	0.00000700
Si1	-1.03035100	1.78061700	-0.00003600
Si2	3.70797200	-0.00000200	-0.00000200
Si3	0.43182800	-0.00000500	0.00001000
Si4	-1.57178600	-0.00002400	-1.50072000
Si5	-1.57179200	0.00003300	1.50073200
Si6	-1.03037000	-1.78061500	0.00001300

Si₆N-d1:			
N	2.01738400	-0.64962800	-0.00002000
Si	0.74794200	-0.68110500	-1.28790100
Si	-1.22626900	-1.28327600	-0.00001000
Si	0.74797300	-0.68112100	1.28791200
Si	-2.75106200	0.61186600	-0.00000100
Si	-0.48576800	1.15994300	0.00002600
Si	1.95849200	1.19850700	-0.00001600

Si₆N-d2:			
N	0.00018100	-1.51420600	-0.00006800
Si	-1.77453600	-1.11175600	-0.00002400
Si	-1.20920600	1.59474000	0.00000500
Si	0.00004700	-0.10477800	-1.41815500
Si	0.00003100	-0.10484500	1.41821600
Si	1.20876900	1.59509400	0.00000300
Si	1.77480500	-1.11135400	-0.00001100

Si₆N-d3:			
N	-0.96548400	0.50289900	-0.61319700
Si	-2.37447200	-0.32488200	0.26348200
Si	1.96521400	0.81587900	-0.04191800
Si	-0.51236300	-1.29432100	-0.84605300
Si	-0.12213100	0.01828200	1.25521500
Si	-0.13171000	2.05471600	-0.37391500
Si	1.65820400	-1.52112300	0.04978800

Si₆N-d4:			
N	-1.85414500	0.63665400	-0.00008500
Si	1.12907300	-0.24217400	1.29130700
Si	-0.75306600	-0.97255800	0.00012400
Si	-3.10734900	-0.48071000	0.00004200
Si	-0.48569600	1.70591900	-0.00017800
Si	3.01502600	-0.08625400	0.00000600
Si	1.12908400	-0.24254900	-1.29125800

Si ₆ O-e0:			
O	2.40591100	0.63869200	0.02396600
Si1	-0.29985200	-0.43313900	-1.27613800
Si2	-1.31395000	1.53837600	-0.20842200
Si3	-0.27147600	-0.76290500	1.32427400
Si4	0.85905900	1.09585100	0.43154000
Si5	-2.23696600	-0.79264100	0.03940800
Si6	1.88837900	-1.01051100	-0.32435800

Si ₆ O-e1:			
O	3.27388700	-0.37763700	0.00003000
Si	-1.33949600	-1.77269500	0.00008100
Si	1.75350700	-0.23192600	-0.00003800
Si	-1.92915000	0.58220800	-0.00006600
Si	-0.13153000	-0.17330600	-1.40816100
Si	-0.09258800	1.98469100	0.00000100
Si	-0.13153500	-0.17317900	1.40816700

Si ₆ O-e2:			
O	-1.62001900	-1.30970600	-0.77094200
Si	1.31242700	1.12499700	-1.09880500
Si	-0.01605300	-0.73272300	-0.68219100
Si	2.05585400	-1.17816400	0.26918700
Si	0.64532800	0.22103900	1.51265800
Si	-2.39872200	-0.26818600	0.29910500
Si	-0.67310800	1.58144200	0.14058400

Si ₆ O-e3:			
O	1.91260000	-0.68632300	0.00001500
Si	-1.17267600	-1.21588900	-0.00002600
Si	0.76328400	-0.63361900	1.39934100
Si	0.76330800	-0.63362100	-1.39931600
Si	-0.54808600	1.15286700	-0.00000200
Si	1.86038400	1.22866800	-0.00001100
Si	-2.75912700	0.49377800	0.00000500

Si ₆ O-e4:			
O	2.16430900	0.00002200	-0.60868500
Si	-0.15065900	0.00005600	1.29536600
Si	1.61922400	-1.47573900	0.02651900
Si	1.61917200	1.47576000	0.02650700
Si	-0.84204200	-1.38337900	-0.49484400
Si	-0.84217600	1.38336500	-0.49488400
Si	-2.64026800	-0.00007500	-0.01084400

Si₇-f0:			
Si1	-1.34813300	1.65424400	0.00022700
Si2	1.15668700	1.79334800	0.00002700
Si3	2.06308300	-0.54591300	-0.00021100
Si4	0.11831200	-2.13072000	-0.00015700
Si5	-1.98989500	-0.77097100	0.00011300
Si6	-0.00012800	0.00009000	-1.28485200
Si7	0.00007400	-0.00007700	1.28485300

Si₇-f1:			
Si	0.00000	0.00000	1.37981
Si	0.73082	1.26581	-0.71558
Si	-1.22072	-2.11434	0.25564
Si	-1.46163	0.00000	-0.71558
Si	2.44143	-0.00000	0.25564
Si	0.73082	-1.26581	-0.71558
Si	-1.22071	2.11434	0.25564

Si₇-f2:			
Si	0.00000	0.00000	-2.83354
Si	0.00000	-1.27246	-0.92073
Si	0.00000	1.27246	-0.92073
Si	0.00000	2.08551	1.27652
Si	0.00000	-2.08551	1.27652
Si	1.22440	0.00000	1.06098
Si	-1.22440	0.00000	1.06098

Si₇-f3:			
Si	1.97095	0.61003	-1.10403
Si	-1.97321	1.09839	0.61291
Si	-1.97430	-1.10115	-0.60439
Si	3.87801	0.00272	-0.00837
Si	-3.87801	-0.00272	0.00837
Si	0.00000	0.00000	0.00000
Si	1.97656	-0.60726	1.09551

Si₇-f4:			
Si	0.00000	0.00000	-2.55120
Si	0.00000	1.43767	-0.57712
Si	-1.24506	-0.71884	-0.57712
Si	1.24506	-0.71884	-0.57712
Si	1.30198	0.75170	1.42751
Si	0.00000	-1.50339	1.42751
Si	-1.30198	0.75170	1.42751