Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: An Investigation into Transition States of Cyclic Tetra-Atomic Silicon and Germanium Interstellar Dust Compounds: Si_xC_{4-x}, Ge_xC_{4-x}, and Ge_xSi_{4-x} ($x \in \{1, 2, 3\}$)

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Supporting Data

Table S1: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family relative energies (in kJ mol^{-1}) of optimized geometries with inclusion of harmonic zero-point vibrational energy (ZPVE). Relative energies are taken with respect to the lowest energy isomer in each group. Results calculated using the B3LYP-D3BJ, M06-2X, and ωB97X-D4 functionals, all using the aug-cc-pVTZ basis set.

Structure	SiC	GeC	GeSi	SiC	GeC	GeSi	SiC	GeC	GeSi
	B3LYP-D3BJ			M06-2X			ωB97X-D4		
XY_3									
d	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
r	14.9	-0.5	13.9	31.7	22.1	15.8	31.7	20.8	21.5
TS	152.9	148.0	83.7	196.3	179.1	139.4	206.6	186.5	151.5
X_2Y_2									
r	0.0	25.8	0.0	0.0	15.9	0.0	0.0	17.6	0.0
t	19.4	0.0	10.5	32.4	0.0	11.3	30.0	0.0	18.4
d	345.6	395.6	26.9	376.9	435.5	30.1	384.1	425.9	41.7
TS r-t	136.8	176.1	81.5	188.8	163.6	141.9	196.4	170.7	143.9
TS d-r	336.2	420.3	88.1	405.4	460.7	146.7	424.9	468.4	158.1
X_3Y									
r	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
d	216.1	199.2	13.2	232.0	225.0	13.5	232.2	217.6	20.3
TS	219.2	238.1	106.3	272.2	265.8	135.5	283.1	266.6	138.3

Table S2: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family barrier heights (in kJ mol^{-1}) of optimized geometries with inclusion of harmonic zero-point vibrational energy (ZPVE). Each barrier height is shown as going from either structure to its respective transition state. All results at the B2GP-PLYP/AVTZ level of theory.

Structure	SiC	GeC	GeSi
XY_3			
r-d	164.1	155.2	127.6
d-r	187.9	166.2	138.8
X_2Y_2			
t-r	155.4	158.3	138.7
r-t	181.3	142.4	147.5
d-r	15.2	21.4	118.3
r-d	351.9	371.4	139.5
X_3Y			
d-r	48.6	47.9	120.3
r-d	258.7	241.2	130.5

Table S3: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family zero-point energy contributions in kJ mol^{-1}. Results calculated using the B3LYP-D3BJ and M06-2X functionals, all using the aug-cc-pVTZ basis set.

Structure	SiC	GeC	GeSi	SiC	GeC	GeSi
	B3LYP-D3BJ			M06-2X		
XY_3						
d	28.5	26.2	11.0	30.3	28.2	11.8
r	27.6	26.3	10.7	28.5	27.1	11.4
TS	23.5	22.6	9.5	24.8	23.4	9.7
X_2Y_2						
r	24.6	20.9	9.7	25.8	22.1	10.5
t	23.4	20.5	9.5	24.2	21.5	10.2
d	18.4	14.9	9.2	19.0	15.5	9.8
TS r-t	19.9	17.4	9.1	21.0	17.8	9.4
TS d-r	18.1	14.0	8.1	18.4	14.6	8.5
X_3Y						
r	18.4	13.5	8.3	19.1	14.3	9.7
d	15.6	11.0	8.0	16.2	11.7	8.6
TS	15.1	10.4	7.0	15.3	11.0	7.3

Table S4: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family zero-point energy contributions in kJ mol^{-1}. Results calculated using the ωB97X-D4 and B2GP-PLYP functionals, all using the aug-cc-pVTZ basis set.

Structure	SiC	GeC	GeSi	SiC	GeC	GeSi
	ωB97X-D4			B2GP-PLYP		
XY_3						
d	30.3	28.3	12.3	28.9	26.8	11.4
r	29.0	27.5	12.0	28.3	26.9	11.1
TS	24.9	23.4	9.7	24.0	22.5	9.9
X_2Y_2						
r	26.2	22.4	11.0	24.8	21.3	10.2
t	24.7	21.6	10.7	23.7	20.9	9.8
d	19.3	16.0	10.4	18.8	15.5	9.6
TS r-t	21.7	18.9	10.2	20.1	17.7	9.0
TS d-r	18.5	14.7	8.9	23.9	18.4	8.6
X_3Y						
r	19.7	14.7	9.4	18.7	14.0	8.7
d	16.7	12.3	9.1	15.8	11.4	8.5
TS	15.6	11.0	7.8	15.2	10.5	7.5

Table S5: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family Gibbs energy contributions (at T = 298.15K) in kJ mol^{-1}. Results calculated using the B3LYP-D3BJ and M06-2X functionals, all using the aug-cc-pVTZ basis set.

Structure	SiC	GeC	GeSi	SiC	GeC	GeSi
	B3LYP-D3BJ			M06-2X		
XY_3						
d	-38.0	-43.9	-68.6	-36.0	-41.5	-69.1
r	-39.9	-44.8	-70.5	-38.6	-43.5	-69.5
TS	-44.9	-51.3	-72.8	-43.1	-48.1	-70.0
X_2Y_2						
r	-44.7	-55.1	-72.7	-43.4	-53.7	-71.5
t	-48.9	-58.6	-74.6	-47.8	-57.0	-73.5
d	-50.2	-61.6	-73.0	-49.5	-60.9	-72.0
TS r-t	-51.9	-60.9	-74.6	-50.8	-61.1	-73.1
TS d-r	-50.8	-60.8	-72.6	-50.4	-60.2	-72.1
X_3Y						
r	-55.0	-69.4	-76.8	-54.1	-68.2	-77.4
d	-60.1	-73.7	-78.7	-59.4	-72.6	-77.6
TS	-59.7	-73.0	-78.3	-58.8	-71.1	-77.7

Table S6: X_xY_{4-x} ($x \in \{1, 2, 3\}$) family Gibbs energy contributions (at T = 298.15K) in kJ mol^{-1}. Results calculated using the ωB97X-D4, and B2GP-PLYP functionals, all using the aug-cc-pVTZ basis set.

Structure	SiC	GeC	GeSi	SiC	GeC	GeSi
	ωB97X-D4			B2GP-PLYP		
XY_3						
d	-35.8	-41.3	-66.5	-37.5	-42.9	-69.6
r	-38.0	-42.9	-66.8	-38.9	-43.7	-69.7
TS	-43.0	-48.0	-71.3	-44.3	-49.5	-73.0
X_2Y_2						
r	-42.9	-53.1	-70.6	-44.4	-54.5	-71.8
t	-47.2	-56.7	-72.5	-48.5	-57.7	-74.0
d	-49.1	-60.2	-71.0	-49.7	-60.8	-72.2
TS r-t	-49.8	-58.7	-71.5	-51.8	-60.4	-74.1
TS d-r	-50.3	-60.1	-71.3	-44.7	-55.9	-72.0
X_3Y						
r	-53.2	-67.3	-76.5	-54.6	-68.5	-77.7
d	-58.6	-71.6	-74.9	-60.0	-73.0	-77.7
TS	-58.4	-71.9	-76.9	-59.0	-71.8	-77.2

Table S7: Harmonic fundamental vibrational frequencies (in cm^{-1}) of SiC isomers at the B3LYP-D3BJ/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-SiC_3		r-SiC_3		TS-SiC_3	
6	1406.2	203.2	1592.4	52.6	-813.4	n/a
5	1037.4	1.6	1155.9	3.5	1464.1	34.2
4	1007.2	54.7	784.8	20.1	1053.6	33.6
3	674.1	49.5	499.2	50.6	726.8	60.1
2	398.9	40.6	384.9	3.5	427.5	5.3
1	236.8	10.6	198.4	52.6	263.8	11.8
	r-Si_2C_2		t-Si_2C_2		d-Si_2C_2	
6	1126.6	0.0	1588.8	14.3	-214.4	n/a
5	973.5	310.6	710.0	26.4	757.1	0.0
4	957.9	0.0	628.9	70.4	662.3	17.1
3	503.1	0.0	494.3	5.2	600.7	0.0
2	357.7	58.8	283.8	1.2	547.0	0.0
1	196.4	3.7	204.0	11.4	506.1	0.0
	TS-r-t-Si_2C_2		TS-d-rSi_2C_2		r-Si_3C	
6	-479.7	n/a	-607.9	n/a	1107.3	74.8
5	1171.1	13.1	771.9	1.7	648.7	52.7
4	902.9	113.6	720.4	8.4	507.2	23.0
3	609.7	15.3	620.0	10.6	336.1	10.7
2	474.6	54.8	599.8	12.5	296.1	5.5
1	171.9	2.5	308.9	13.3	179.1	0.1
	d-Si_3C		TS-Si_3C			
6	745.1	4.7	-543.5	n/a		
5	658.4	0.2	851.5	13.7		
4	454.4	1.8	267.3	33.3		
3	397.9	29.1	394.6	5.7		
2	262.7	0.2	731.5	5.4		
1	91.3	47.0	851.5	1.0		

Table S8: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeC isomers at the B3LYP-D3BJ/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-GeC_3		r-GeC_3		TS-SiC_3	
6	1403.6	169.0	1612.6	87.4	-714.3	n/a
5	1009.8	1.3	1141.7	4.4	1449.5	37.1
4	933.6	28.6	704.3	29.2	1141.8	51.2
3	510.2	43.2	397.1	22.3	590.8	40.5
2	325.3	33.2	311.3	4.5	381.9	10.4
1	199.7	11.8	210.9	44.4	132.7	8.8
	r-Ge_2C_2		t-Ge_2C_2		d-Ge_2C_2	
6	1165.4	0.0	1622.4	25.7	643.6	6.4
5	856.0	0.0	561.2	32.7	550.8	6.0
4	796.0	212.6	505.7	48.4	457.1	0.0
3	279.3	0.0	374.8	13.1	396.5	3.2
2	258.7	58.3	184.1	7.7	313.3	0.2
1	145.3	8.0	170.9	1.0	123.6	56.1
	TS-r-t-Ge_2C_2		TS-d-rGe_2C_2		r-Ge_3C	
6	-467.8	n/a	-496.8	n/a	959.2	94.5
5	1258.0	35.4	586.4	17.7	506.5	71.5
4	720.4	86.4	551.0	13.3	295.8	6.0
3	456.2	25.9	488.4	3.4	185.9	3.3
2	363.3	43.6	467.2	14.4	169.2	1.1
1	112.7	0.6	250.7	7.0	148.3	0.8
	d-Ge_3C		TS-Ge_3C			
6	637.3	0.5	-420.4	n/a		
5	499.3	4.4	674.2	28.3		
4	270.1	1.3	533.7	39.6		
3	224.4	10.8	213.3	2.5		
2	142.8	0.4	191.1	2.0		
1	65.9	36.2	123.9	0.2		

Table S9: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeSi isomers at the B3LYP-D3BJ/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-$GeSi_3$		r-$GeSi_3$		TS-SiC_3	
6	475.9	47.2	483.3	54.6	-410.7	n/a
5	410.4	15.0	416.1	0.5	449.1	0.1
4	400.2	0.0	315.0	6.7	396.4	1.2
3	268.7	3.6	300.7	0.7	297.0	2.3
2	202.9	1.3	194.7	0.1	269.0	1.5
1	74.9	1.2	80.0	2.8	152.1	0.0
	r-Ge_2Si_2		t-Ge_2Si_2		d-Ge_2Si_2	
6	407.6	0.0	463.8	42.6	381.8	43.1
5	392.7	59.8	358.4	3.5	375.7	0.0
4	368.4	0.0	298.7	3.5	294.6	0.0
3	214.5	0.0	238.6	4.5	231.8	0.0
2	178.4	1.2	162.2	0.1	177.3	0.0
1	66.7	0.8	72.2	1.7	75.5	2.3
	TS-r-t-Ge_2Si_2		TS-d-rGe_2Si_2		r-Ge_3Si	
6	-129.5	n/a	-365.8	n/a	398.5	39.2
5	456.1	31.0	357.8	5.6	340.6	1.0
4	404.6	5.2	323.1	0.1	242.0	7.4
3	272.2	0.3	282.3	0.2	204.6	0.1
2	261.6	2.4	265.4	3.2	141.0	0.1
1	91.7	0.6	134.6	0.0	63.0	0.7
	d-Ge_3Si		TS-Ge_3Si			
6	379.9	24.3	-335.0	n/a		
5	272.2	0.1	343.5	4.9		
4	267.0	8.9	299.9	2.0		
3	211.0	1.5	221.0	1.7		
2	144.1	0.0	191.1	0.7		
1	65.8	1.4	114.5	0.0		

Table S10: Harmonic fundamental vibrational frequencies (in cm^{-1}) of SiC isomers at the M06-2X/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-SiC_3		r-SiC_3		TS-SiC_3	
6	1455.4	221.9	1582.6	81.2	-834.0	n/a
5	1110.4	1.6	1180.0	0.5	1534.1	31.8
4	1099.2	69.8	826.0	48.4	1061.4	39.6
3	709.3	61.8	534.3	26.6	752.0	77.6
2	425.6	43.5	424.2	1.8	437.8	2.7
1	257.9	7.1	224.1	47.5	468.3	11.4
	r-Si_2C_2		t-Si_2C_2		d-Si_2C_2	
6	1182.9	0.0	1623.3	14.9	-139.9	n/a
5	1011.1	356.6	729.8	28.2	784.9	0.0
4	1008.9	0.0	657.5	67.0	675.7	33.9
3	534.2	0.0	514.7	8.5	636.0	0.0
2	380.9	59.9	313.1	0.7	561.6	0.0
1	198.8	4.6	215.7	9.9	512.1	1.1
	TS-r-t-Si_2C_2		TS-d-rSi_2C_2		r-Si_3C	
6	-507.2	n/a	-664.2	n/a	1128.6	85.8
5	1209.7	18.2	800.9	1.8	679.0	57.5
4	943.2	115.0	726.4	6.1	526.3	23.1
3	650.9	17.3	642.7	9.6	362.2	15.3
2	531.9	58.7	610.2	15.9	311.9	5.5
1	167.6	5.6	300.6	15.8	178.5	0.3
	d-Si_3C		TS-Si_3C			
6	773.5	5.2	-561.4	n/a		
5	674.9	0.5	874.0	17.3		
4	477.9	0.7	755.0	35.7		
3	419.4	38.3	417.3	10.1		
2	275.8	0.7	279.6	6.5		
1	81.6	48.2	235.5	1.6		

Table S11: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeC isomers at the M06-2X/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-GeC_3		r-GeC_3		TS-SiC_3	
6	1457.9	188.3	1597.3	111.6	-785.9	n/a
5	1082.7	0.8	1168.0	3.5	1537.9	29.6
4	1028.0	48.3	754.7	28.5	1080.9	51.8
3	541.6	49.3	432.4	25.7	599.4	53.4
2	360.7	36.9	350.3	3.7	408.5	4.5
1	242.4	7.7	227.3	41.4	283.8	11.0
	r-Ge_2C_2		t-Ge_2C_2		d-Ge_2C_2	
6	1202.2	0.0	1676.0	24.2	674.5	7.7
5	911.8	0.0	593.4	34.1	571.6	14.3
4	841.2	223.9	534.2	41.0	481.8	0.0
3	297.7	0.0	400.4	16.8	411.3	0.0
2	280.9	60.1	202.0	8.0	323.5	0.2
1	153.2	8.0	193.3	1.0	120.6	62.7
	TS-r-t-Ge_2C_2		TS-d-rGe_2C_2		r-Ge_3C	
6	-471.6	n/a	-492.2	n/a	996.5	85.8
5	1290.5	65.9	634.7	13.7	542.1	72.7
4	763.7	51.4	554.7	7.7	311.0	6.2
3	502.5	19.6	512.6	6.0	202.8	5.9
2	404.5	62.2	493.5	18.3	184.9	1.2
1	111.0	4.2	245.6	9.2	152.9	0.9
	d-Ge_3C		TS-Ge_3C			
6	672.3	0.1	-378.2	n/a		
5	516.1	1.4	719.3	34.4		
4	284.0	1.2	559.3	42.2		
3	236.7	14.9	228.7	4.7		
2	150.0	0.1	192.4	2.7		
1	96.5	39.4	136.3	0.5		

Table S12: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeSi isomers at the M06-2X/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-$GeSi_3$		r-$GeSi_3$		TS-SiC_3	
6	511.8	58.1	508.6	75.5	-450.9	n/a
5	439.6	20.6	441.0	0.7	473.5	0.0
4	435.2	0.0	341.8	9.5	414.4	1.7
3	286.2	4.5	324.2	1.1	309.7	3.3
2	214.6	2.2	207.3	0.4	273.5	1.4
1	80.3	1.6	77.0	2.6	150.6	0.2
	r-Ge_2Si_2		t-Ge_2Si_2		d-Ge_2Si_2	
6	436.1	0.0	495.6	56.0	407.1	64.0
5	423.4	77.3	382.6	5.4	400.9	0.0
4	401.6	0.0	323.8	5.5	316.1	0.0
3	229.7	0.0	254.5	6.0	250.4	0.0
2	187.6	2.0	173.0	0.4	187.0	0.2
1	70.6	0.7	74.2	1.6	75.7	2.2
	TS-r-t-Ge_2Si_2		TS-d-rGe_2Si_2		r-Ge_3Si	
6	-150.5	n/a	-381.0	n/a	425.6	53.6
5	473.5	36.6	379.2	6.2	364.0	1.5
4	433.4	8.6	337.2	0.1	262.6	10.8
3	289.8	1.0	294.2	1.0	219.7	0.2
2	276.4	3.3	273.1	2.0	150.8	0.3
1	106.2	1.6	132.7	0.0	66.7	0.7
	d-Ge_3Si		TS-Ge_3Si			
6	408.4	34.8	-336.1	n/a		
5	292.2	0.0	365.5	5.4		
4	284.7	13.3	308.7	3.2		
3	226.1	2.2	231.1	1.9		
2	151.4	0.1	202.2	0.4		
1	68.5	1.4	112.4	0.1		

Table S13: Harmonic fundamental vibrational frequencies (in cm^{-1}) of SiC isomers at the ωB97X-D4/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-SiC_3		r-SiC_3		TS-SiC_3	
6	1461.8	231.1	1594.9	69.4	-908.0	n/a
5	1099.0	1.4	1193.3	0.4	1561.1	33.1
4	1087.3	74.6	831.1	47.9	1026.3	42.5
3	719.5	62.2	553.7	27.9	749.2	89.5
2	432.1	46.0	436.9	1.9	444.3	0.9
1	272.0	7.4	245.6	46.1	380.7	12.8
	r-Si_2C_2		t-Si_2C_2		d-Si_2C_2	
6	1170.7	0.0	1627.1	17.1	-45.6	n/a
5	1036.0	378.3	746.2	26.8	811.7	0.0
4	1024.8	0.0	662.6	64.6	693.2	39.7
3	548.6	0.0	524.4	9.1	641.4	0.0
2	393.0	59.9	343.8	0.4	570.5	0.0
1	203.0	3.3	218.3	10.7	512.0	9.6
	TS-r-t-Si_2C_2		TS-d-rSi_2C_2		r-Si_3C	
6	-487.4	n/a	-747.1	n/a	1150.3	86.0
5	1201.2	25.3	826.3	2.1	702.7	51.5
4	981.6	118.0	716.2	5.3	539.7	26.1
3	673.1	16.6	644.8	8.2	391.6	20.9
2	565.3	58.6	613.2	34.1	334.6	6.6
1	198.8	8.6	299.8	14.4	177.2	0.1
	d-Si_3C		TS-Si_3C			
6	798.7	5.9	-600.9	n/a		
5	673.0	4.0	907.0	34.8		
4	502.3	0.5	745.5	36.3		
3	441.5	49.3	436.3	17.0		
2	288.2	3.3	293.8	6.8		
1	91.6	58.9	233.2	2.6		

Table S14: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeC isomers at the ωB97X-D4/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-GeC_3		r-GeC_3		TS-SiC_3	
6	1462.5	202.7	1609.4	93.5	-853.8	n/a
5	1070.1	1.1	1180.1	3.4	1544.9	32.2
4	1025.6	48.6	755.8	28.5	1050.7	49.0
3	552.3	57.2	441.3	32.2	603.3	63.2
2	368.4	38.8	357.6	3.4	410.8	3.7
1	249.4	7.1	247.0	40.4	303.1	10.5
	r-Ge_2C_2		t-Ge_2C_2		d-Ge_2C_2	
6	1179.8	0.0	1671.7	26.8	741.0	0.0
5	932.6	0.0	604.3	36.1	582.5	35.1
4	873.0	295.0	536.7	44.4	495.0	0.0
3	312.5	0.0	399.6	19.4	399.1	0.0
2	297.5	61.7	208.0	0.6	341.6	0.0
1	155.4	7.5	197.7	7.8	116.7	85.9
	TS-r-t-Ge_2C_2		TS-d-rGe_2C_2		r-Ge_3C	
6	-472.7	n/a	-601.4	n/a	1015.4	112.5
5	1254.7	37.7	648.0	19.7	564.4	80.9
4	800.6	78.5	559.6	8.3	320.3	8.3
3	539.7	23.7	514.7	2.4	221.0	6.9
2	432.1	58.9	494.8	16.1	195.4	1.1
1	138.4	4.3	236.5	8.0	149.0	0.8
	d-Ge_3C		TS-Ge_3C			
6	700.2	0.4	-469.4	n/a		
5	528.5	0.9	727.5	51.6		
4	296.6	0.3	558.1	47.7		
3	253.9	19.9	236.7	5.8		
2	162.7	0.0	185.6	2.2		
1	107.8	37.6	138.3	0.4		

Table S15: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeSi isomers at the ωB97X-D4/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-$GeSi_3$		r-$GeSi_3$		TS-SiC_3	
6	533.0	71.6	535.7	88.9	-501.7	n/a
5	464.0	30.0	469.6	1.2	525.3	0.2
4	451.4	0.1	361.3	11.7	433.2	2.8
3	299.3	6.1	334.3	1.5	324.3	3.4
2	224.8	4.7	214.0	1.3	271.9	1.2
1	82.3	1.9	88.3	2.8	149.0	0.9
	r-Ge_2Si_2		t-Ge_2Si_2		d-Ge_2Si_2	
6	465.8	0.0	517.0	68.6	431.1	73.7
5	440.8	99.9	406.6	6.7	428.5	0.0
4	418.3	0.0	340.3	7.3	336.8	0.0
3	240.1	0.0	267.6	7.6	256.7	0.0
2	200.4	4.0	181.4	1.0	196.4	0.5
1	72.1	0.8	78.9	1.7	83.8	2.4
	TS-r-t-Ge_2Si_2		TS-d-rGe_2Si_2		r-Ge_3Si	
6	-161.1	n/a	-446.3	n/a	445.7	65.0
5	496.0	34.9	420.9	7.5	388.5	2.2
4	464.8	16.3	350.4	0.1	279.5	13.7
3	313.7	1.6	308.2	0.1	230.1	0.2
2	289.1	3.9	261.3	1.3	159.3	0.8
1	148.3	2.3	150.8	0.5	68.1	0.7
	d-Ge_3Si		TS-Ge_3Si			
6	432.2	40.1	-400.1	n/a		
5	311.1	0.0	405.1	6.7		
4	304.5	17.3	320.8	3.0		
3	235.2	2.5	248.7	3.1		
2	162.4	0.3	199.5	0.4		
1	72.6	1.5	121.8	0.1		

Table S16: Harmonic fundamental vibrational frequencies (in cm^{-1}) of SiC isomers at the B2GP-PLYP/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-SiC_3		r-SiC_3		TS-SiC_3	
6	1409.2	205.8	1614.9	59.8	-888.4	n/a
5	1052.2	1.9	1146.9	0.2	1462.8	49.4
4	989.2	44.1	800.3	51.6	1078.8	39.8
3	683.4	49.8	516.8	19.2	734.6	71.0
2	428.4	40.0	411.5	3.9	422.2	6.1
1	261.1	8.5	233.9	53.8	309.0	12.6
	r-Si_2C_2		t-Si_2C_2		d-Si_2C_2	
6	1091.3	0.0	1572.8	18.9	-165.9	n/a
5	993.9	316.0	724.5	27.3	747.8	0.0
4	969.2	0.0	639.9	66.8	688.5	6.3
3	512.6	0.0	511.9	6.3	622.9	0.0
2	373.3	61.4	299.5	1.2	553.0	0.0
1	206.1	3.7	208.3	10.6	534.3	1.5
	TS-r-t-Si_2C_2		TS-d-rSi_2C_2		r-Si_3C	
6	-509.0	n/a	-744.7	n/a	1118.5	79.4
5	1163.0	12.3	1503.3	1225.5	654.4	48.9
4	913.5	99.5	761.6	29.1	507.1	20.6
3	628.2	14.4	742.2	24.8	358.8	11.3
2	489.8	65.9	649.3	28.7	307.1	5.8
1	163.6	3.1	333.8	6.8	175.0	0.1
	d-Si_3C		TS-Si_3C			
6	755.0	1.3	-591.5	n/a		
5	668.1	0.1	847.9	23.7		
4	473.5	1.1	754.5	52.0		
3	403.4	24.3	413.9	6.0		
2	282.3	0.1	286.9	5.9		
1	54.3	59.8	238.5	3.0		

Table S17: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeC isomers at the B2GP-PLYP/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-GeC_3		r-GeC_3		TS-SiC_3	
6	1404.6	177.2	1633.3	81.5	-791.5	n/a
5	1031.2	1.7	1135.0	2.9	1453.0	41.5
4	919.0	21.0	725.9	31.6	1123.9	59.9
3	524.7	43.4	420.0	21.9	603.3	48.8
2	366.6	33.2	339.7	4.7	387.9	10.4
1	242.1	9.9	236.2	47.0	200.6	10.0
	r-Ge_2C_2		t-Ge_2C_2		d-Ge_2C_2	
6	1118.3	0.0	1593.4	25.5	630.8	6.2
5	880.6	0.0	587.9	31.4	589.3	0.3
4	830.1	218.2	530.7	48.9	500.7	0.0
3	288.5	0.0	402.1	16.1	447.5	7.0
2	277.1	58.7	200.2	8.8	315.2	0.4
1	163.6	7.3	183.7	0.9	113.1	50.8
	TS-r-t-Ge_2C_2		TS-d-rGe_2C_2		r-Ge_3C	
6	-498.1	n/a	-896.5	n/a	982.6	97.7
5	1232.7	40.5	1121.1	58.0	529.4	64.8
4	748.0	80.2	607.0	24.4	297.6	5.8
3	486.3	24.0	536.7	24.0	203.2	3.5
2	384.4	51.5	525.5	61.4	180.3	1.1
1	111.9	0.8	283.1	4.6	149.2	0.4
	d-Ge_3C		TS-Ge_3C			
6	649.7	0.4	-419.3	n/a		
5	523.2	5.6	682.6	20.3		
4	281.8	0.9	578.3	66.0		
3	231.2	8.2	235.8	2.7		
2	158.5	0.3	200.8	2.3		
1	66.7	40.7	149.7	0.2		

Table S18: Harmonic fundamental vibrational frequencies (in cm^{-1}) of GeSi isomers at the B2GP-PLYP/AVTZ level of theory. Intensities in km mol^{-1}.

Mode	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
	d-$GeSi_3$		r-$GeSi_3$		TS-SiC_3	
6	486.7	42.6	490.3	47.4	-359.9	n/a
5	421.1	1.6	421.4	0.5	448.7	0.2
4	412.0	0.0	332.4	5.6	406.2	0.7
3	272.5	2.7	308.2	0.4	327.8	4.5
2	225.0	1.1	212.9	0.1	309.1	0.5
1	88.6	2.3	94.6	3.4	156.3	0.0
	r-Ge_2Si_2		t-Ge_2Si_2		d-Ge_2Si_2	
6	418.3	0.0	470.1	36.9	396.7	37.2
5	406.2	53.5	367.9	2.7	381.8	0.0
4	381.2	0.0	314.1	3.4	303.2	0.0
3	218.0	0.0	242.7	3.3	237.2	0.0
2	200.9	1.2	177.6	0.1	196.5	0.3
1	83.2	1.6	65.7	2.4	96.2	3.0
	TS-r-t-Ge_2Si_2		TS-d-rGe_2Si_2		r-Ge_3Si	
6	-140.0	n/a	-315.3	n/a	405.6	34.9
5	462.3	22.2	367.1	2.9	352.0	0.7
4	416.7	4.4	345.3	0.2	259.1	7.2
3	291.7	0.1	310.7	5.6	208.9	0.1
2	271.0	2.3	295.9	1.4	156.3	0.1
1	86.6	0.6	149.0	0.1	75.2	1.0
	d-Ge_3Si		TS-Ge_3Si			
6	390.8	22.1	-277.1	n/a		
5	283.4	0.0	350.9	3.1		
4	276.9	7.0	313.3	2.0		
3	217.2	1.2	247.3	2.3		
2	162.2	0.0	219.7	0.7		
1	86.1	1.4	127.2	0.0		