

Interaction of SiCl₂ with CO₂ in Ar matrices

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1. Experimental setup

Matrices were formed on a mirror copper plate located inside a vacuum cryostat (APD Cryogenics, Inc.) equipped with a KBr window for IR measurements and a CaF₂ window for irradiation of matrices with UV and visible light. The plate was cooled by a CSW-208R Displex closed-cycle refrigeration system (APD Cryogenics, Inc.). The temperature of the copper plate during deposition of matrices and recording spectra was kept at ca. 10—12 K. The procedure of annealing of matrices consisted in their heating (with a rate of 2 - 3 K min⁻¹) to a preselected temperature in the range of 24—42 K, their holding at this temperature for 2—3 min, and subsequent cooling by turning off the supply of power to the heating elements. A Lake Shore Model 330-11 temperature controller (Lake Shore Cryotronics, Inc.) in combination with a DT-470-SD12 silicon diode fixed on the copper plate was used to control the temperature. The residual pressure in the cryostat was ca. 10⁻⁶ Torr.

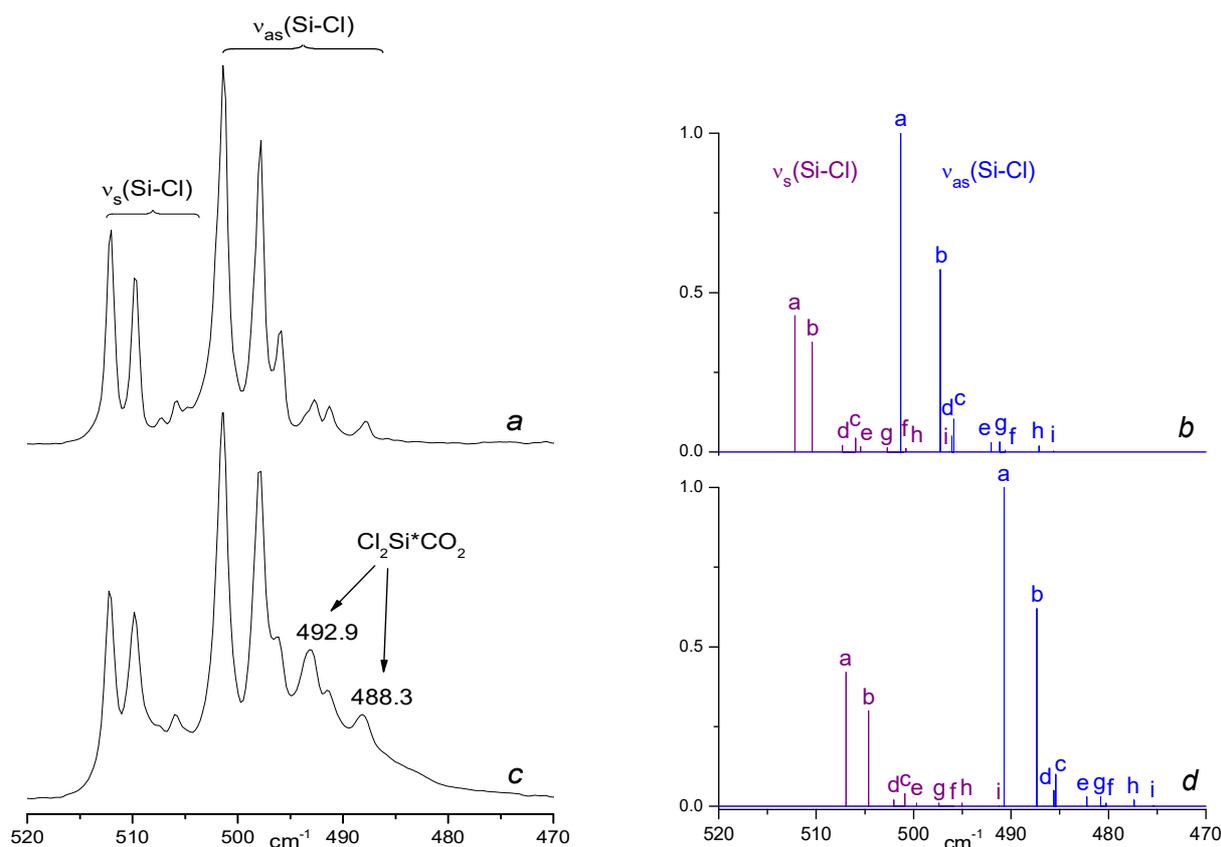
Mixtures of Ar (99.998%, Mechel Mining, Moscow Coke and Gas Plant) and CO₂ (99.995%, Linde Gas Rus) were prepared using the standard manometric procedure in a glass vessel for about an hour before an experiment. The component pressures were measured by a vacuum gauge CAP 100 (Ilmvac). The CO₂:Ar molar ratio was varied from 1 : 20 to 1 : 500 in different experiments. The mixtures were passed over P₂O₅ powder to remove traces of water and fed into the cryostat through a stainless steel line with a rate of 7—9 mmol h⁻¹. The outlet of the line was located at a distance of ca. 40 mm from the copper plate surface.

Pyrolysis of precursors was carried out in a quartz reactor (a quartz tube) with outer and inner diameters of 6 and 4 mm and the length of the heated zone of 100 mm. The reactor was attached directly to the cryostat, its outlet was located in front of the copper plate at a distance of ca. 50 mm from it. The reactor was heated by a nichrome heating coil to ca. 900 (Si₂Cl₆) or 1000 °C (1,1-dichloro-1-silacyclopent-3-ene, SCP). The temperature was measured with a chromel-alumel thermocouple. The pressure of a precursor in a flow in the reactor was controlled by a manometric transducer PMT-4M. It was typically kept at ca. 10⁻² Torr.

The typical time of deposition of matrices was 1—2 h. Taking into account the equimolar formation of SiCl₂ and SiCl₄ upon Si₂Cl₆ decomposition (Refs. 17, 19 and Refs. cited therein), the concentrations of SiCl₂ in matrices were assumed to be equal to those of SiCl₄ when Si₂Cl₆ was used as a precursor. The SiCl₄ concentrations in matrices were determined from its band intensities on the basis of data obtained in separate experiments on deposition of mixtures of SiCl₄ (99%, Impulse, RF) with Ar of known compositions. In the experiments with the use of SCP as a precursor, the SiCl₂ concentration in matrices was estimated based on intensities of its bands using the correlation between the band intensities and SiCl₂ concentration obtained in the experiments, in which Si₂Cl₆ was used as a precursor. The SiCl₂/Ar molar ratio was varied from 1 : 400 to 1 : 1000 in different experiments.

A DRSh-500 high pressure Hg arc lamp (500 W) equipped with a water filter and suitable cut-off filters (with 50% transmission at the wavelengths specified in the text) were used as a light source to irradiate matrices. IR spectra were recorded using a Bruker IFS 113v FTIR spectrometer (with a DTGS/KBr detector) in the range of 4000—400 cm⁻¹ with a resolution of 0.5 cm⁻¹ by the reflection scheme.

2. Isotopic splitting of the $\nu(\text{Si-Cl})$ bands of SiCl_2 and $\text{Cl}_2\text{Si}^*\text{CO}_2$



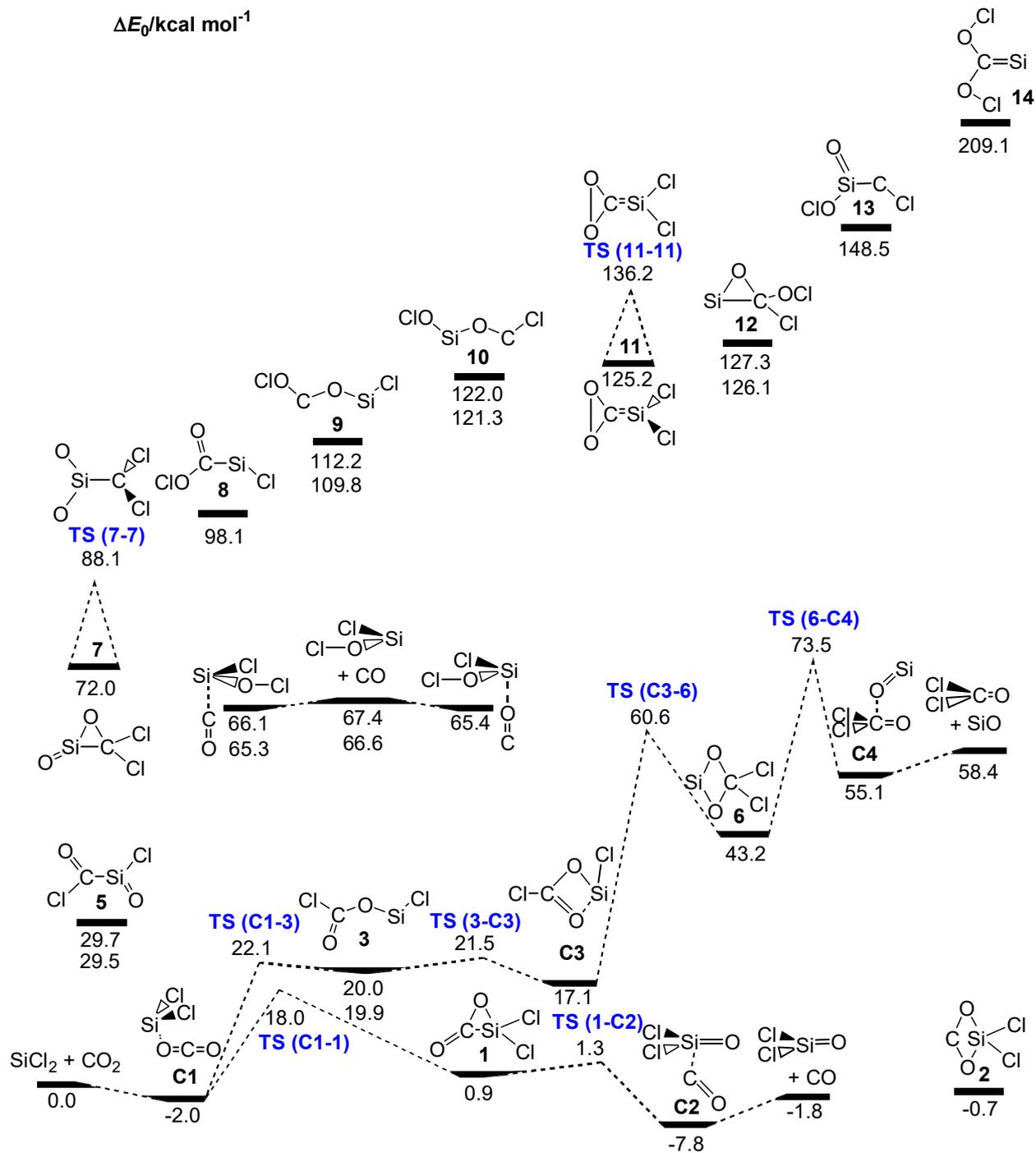
a) IR spectrum of SiCl_2 in an Ar matrix, 10 K, $\text{SiCl}_2 : \text{Ar} \sim 1 : 500$;

b) the B3LYP/ 6-31G(2df) calculated isotopic splitting of the $\nu(\text{Si-Cl})$ bands of SiCl_2 for a sample with the natural isotopic abundance; bands of different isotopomers are marked with different letters: a (28-35-35), b (28-35-37), c (28-37-37), d (29-35-35), e (29-35-37), f (29-37-37), g (30-35-35), h (30-35-37), i (30-37-37); calculated $\nu_s(\text{Si-Cl})$ and $\nu_{as}(\text{Si-Cl})$ frequencies were multiplied by 1.0188 and 1.0075, respectively, to match them with the experimentally observed frequencies;

c) IR bands of $\text{Cl}_2\text{Si}^*\text{CO}_2$ (indicated) on the background of SiCl_2 bands; Ar matrix, 10 K, $\text{SiCl}_2:\text{CO}_2:\text{Ar} \sim 1 : 10 : 500$;

d) the B3LYP/ 6-31G(2df) calculated isotopic splitting of the $\nu(\text{Si-Cl})$ bands of $\text{Cl}_2\text{Si}^*\text{CO}_2$ for a sample with the natural isotopic abundance; the isotopomer designations are the same as in figure *b*; calculated $\nu_s(\text{Si-Cl})$ and $\nu_{as}(\text{Si-Cl})$ frequencies were multiplied by 1.0188 and 1.0075, respectively, by analogy with the SiCl_2 frequencies.

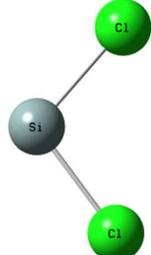
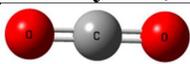
3. Diagram of energies of the [C, 2O, Si, 2Cl] isomers and some transition states connecting them according to the G4(MP2) calculations

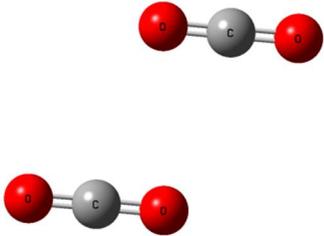
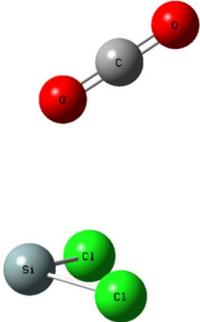


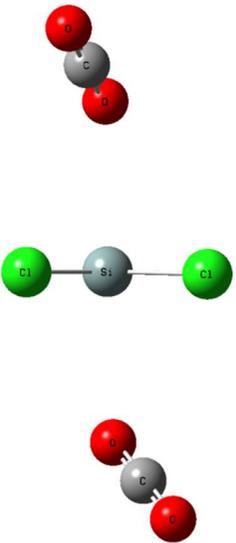
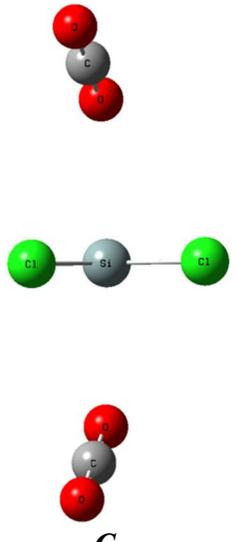
4. Stationary points found in the [2C, 4O, Si, 2Cl] system in the G4(MP2) calculations, their energies (G4(MP2)) and spectral characteristics (B3LYP/6-31G(2df))

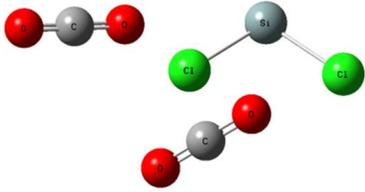
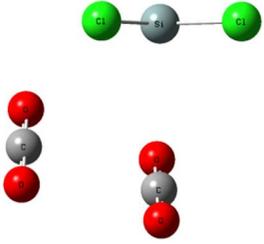
Note. Wavefunctions of all stationary points were passed the RHF/UHF stability tests and T1 diagnostics.

4.1. Reactants and their complexes

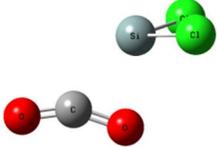
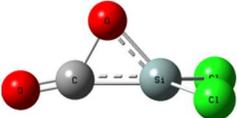
Structure	Energies ($\Delta E_0 = \Delta E + \text{ZPE}$, ΔH^0 , and ΔG^0 in kcal mol ⁻¹) relative to free SiCl ₂ + 2CO ₂ and absolute energies including ZPE (E/Hartree)			Frequencies (ν) and IR intensities (I) of fundamental vibrations		Electronic transition in the UV region	
	ΔE_0 E	ΔH^0_{298}	ΔG^0_{298}	ν/cm^{-1}	$I/\text{km mol}^{-1}$	λ/nm	f
 <p>C_{2v} Dichlorosilylene, SiCl₂</p>	-1208.683756			503 498 191	83 194 2	327 269 227 210 200	0.029 0.000 0.024 0.009 0.001
 <p>$D_{\infty h}$ Carbon dioxide, CO₂</p>	-188.408754			2436 1379 688 688	550 0 31 31	n/a	

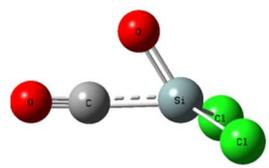
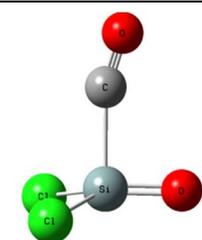
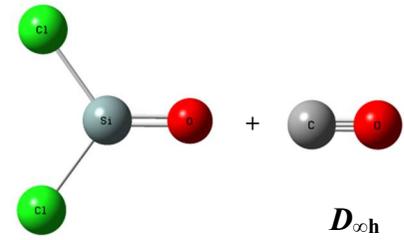
 <p style="text-align: center;">C_{2h} Dimer of carbon dioxide, $(CO_2)_2$</p>	-1.1 -376.819274	-0.8	3.3	2435 2435 1379 1379 690 687 686 686 103 36 23 22	1105 0 0 0 60 0 0 76 0 0 0 0	n/a	
 <p style="text-align: center;">C_s $Cl_2Si^*CO_2$</p>	-2.0 -1397.095759	-1.4 -0.5 (600 K) 0.4 (900 K) 1.3 (1200 K)	2.8 6.6 (600 K) 10.0 (900 K) 13.1 (1200 K)	2432 1379 686 683 498 487 191 77 70 54 22 3	667 2 31 29 78 185 1 4 5 0 0 0	315 260 223 205	0.040 0.000 0.018 0.013

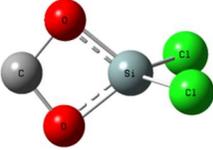
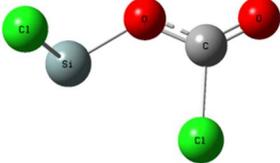
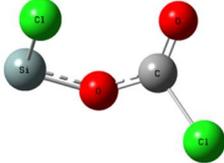
 <p style="text-align: center;">C₂ CO₂*Cl₂Si*CO₂-1</p>	-4.2 -1585.507987	-3.0	6.9	2434 2429 1378 1378 686 685 683 683 492 477 191 100 75 74 53 44 34 22 14 6 5	501 820 1 3 20 49 47 7 72 175 1 17 0 6 0 0 0 0 0 0 0 0	304 251 218	0.053 0.000 0.012
 <p style="text-align: center;">C₁ CO₂*Cl₂Si*CO₂-2</p>	-4.2 -1585.507973	-3.0	5.8	2434 2430 1378 1378 686 685 683 683 494 475 191 99 76 71 54 45 34 22 14 4 2	641 677 1 3 20 45 57 2 83 164 1 16 6 0 1 0 0 0 0 0 0 0	304 251 218	0.052 0.000 0.013

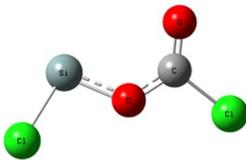
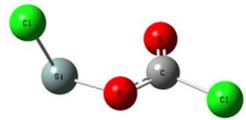
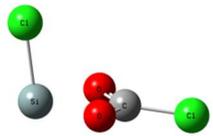
 <p style="text-align: center;">C₁</p> <p style="text-align: center;">Cl₂Si*(CO₂)₂-1</p>	-4.2 -1585.507937	-3.0	8.3	2430 2433 1379 1378 688 686 683 680 499 479 191 91 86 81 59 53 36 23 20 18 13	795 462 1 2 31 47 26 32 112 161 1 8 2 0 0 1 0 0 0 0 0	314 258 222 204	0.042 0.000 0.016 0.015
 <p style="text-align: center;">C₁</p> <p style="text-align: center;">Cl₂Si*(CO₂)₂-2</p>	-4.1 -1585.507834	-2.9	7.8	2433 2430 1378 1378 688 687 684 682 496 484 191 98 75 67 48 41 34 23 20 15 13	1137 13 2 1 41 46 3 46 83 183 0 1 6 0 0 0 0 0 0 0	317 262 223 206	0.039 0.000 0.019 0.012

4.2. Low-energy [C, 2O, Si, 2Cl] isomers and transition states

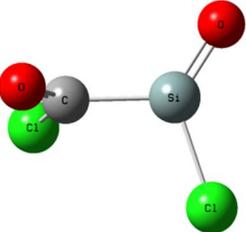
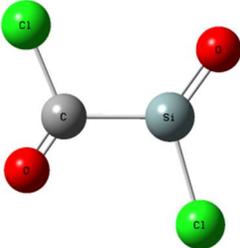
Structure	Energies ($\Delta E_0 = \Delta E + \text{ZPE}$, ΔH^0 , and ΔG^0 in kcal mol ⁻¹) relative to free SiCl ₂ + CO ₂ and absolute energies including ZPE (E/Hartree)			Frequencies (ν) and IR intensities (I) of fundamental vibrations		Electronic transition in the UV region	
	ΔE_0 E	ΔH^0_{298}	ΔG^0_{298}	ν/cm^{-1}	$I/\text{km mol}^{-1}$	λ/nm	f
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">TS (Cl₂Si*CO₂ - 1)</p>	18.0 -1397.063903	17.5 17.9 (600 K) 18.3 (900 K) 18.6 (1200 K)	27.4 37.3 (600 K) 47.0 (900 K) 56.5 (1200 K)	2155 1201 609 591 540 526 260 174 154 154 75 360 (i)	602 141 324 5 167 198 13 19 0 1 1 123		
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">1,1-Dichloro-1-siloxirane (1)</p>	0.9 -1397.091035	0.4 1.1 (600 K) 2.1 (900 K) 3.1 (1200 K)	10.8 21.2 (600 K) 31.0 (900 K) 40.5 (1200 K)	1975 1025 773 625 614 495 447 397 214 181 169 107	426 153 42 187 174 11 10 5 8 1 3 4	264 225 210	0.011 0.150 0.009

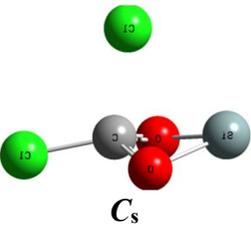
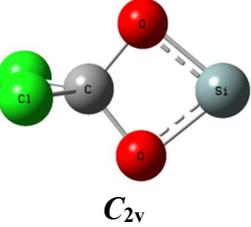
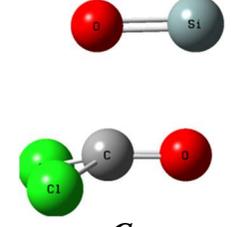
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">TS (1 - $Cl_2Si=O*CO$)</p>	<p style="text-align: center;">1.3 -1397.090460</p>	<p style="text-align: center;">0.6 0.9 (600 K) 1.3 (900 K) 1.7 (1200 K)</p>	<p style="text-align: center;">11.4 22.3 (600 K) 32.9 (900 K) 43.4 (1200 K)</p>	<p>2079 1075 713 621 463 436 416 274 232 180 103 251 (i)</p>	<p>278 141 100 202 43 6 3 62 15 4 2 118</p>		
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">$Cl_2Si=O*CO$</p>	<p style="text-align: center;">-7.8 -1397.105009</p>	<p style="text-align: center;">-7.8 -6.8 (600 K) -5.8 (900 K) -4.8 (1200 K)</p>	<p style="text-align: center;">1.3 10.2 (600 K) 18.5 (900 K) 26.4 (1200 K)</p>	<p>2244 1227 594 495 396 362 339 251 236 187 85 78</p>	<p>220 105 208 57 13 0 42 25 13 4 7 0</p>	<p>306 304 249 226 224 214 212 207 203 202</p>	<p>0.000 0.002 0.079 0.000 0.008 0.000 0.024 0.067 0.001 0.001</p>
 <p style="text-align: center;">C_{2v}</p> <p style="text-align: center;">$D_{\infty h}$</p> <p style="text-align: center;">$Cl_2Si=O + CO$</p>	<p style="text-align: center;">-1.8 CO -113.207664 $Cl_2Si=O$ -1283.887733</p>	<p style="text-align: center;">-1.4 -1.1 (600 K) -1.0 (900 K) -0.8 (1200 K)</p>	<p style="text-align: center;">-1.7 -2.1 (600 K) -2.7 (900 K) -3.3 (1200 K)</p>	<p>CO 2205 $Cl_2Si=O$ 1278 622 489 285 267 198</p>	<p>63 91 227 20 34 27 2</p>	<p>n/a 246 236 226</p>	<p>0.025 0.000 0.016</p>

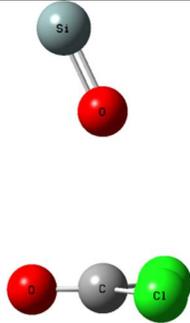
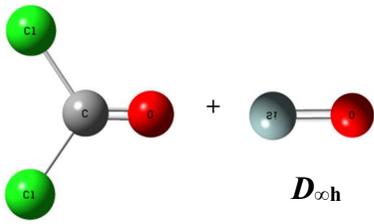
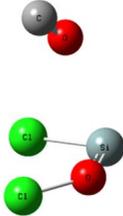
 <p style="text-align: center;">C_{2v}</p> <p style="text-align: center;">3,3-Dichloro-3-sila-2,4-dioxetan-1-ylidene (2)</p>	-0.7 -1397.093638	-1.4	10.0	1135 1052 996 731 648 611 434 411 232 177 175 165	14 194 45 200 244 6 0 2 7 2 0 16	262 217 209	0.008 0.007 0.138
 <p style="text-align: center;">C_1</p> <p style="text-align: center;">TS ($Cl_2Si^*CO_2 - 3c$)</p>	22.1 -1397.057258	21.3 21.5 (600 K) 21.8 (900 K) 22.2 (1200 K)	31.9 42.7 (600 K) 53.2 (900 K) 63.6 (1200 K)	1948 1151 837 670 515 500 439 408 228 94 73 47 (i)	621 420 214 18 103 192 6 19 1 4 1 1		
 <p style="text-align: center;">C_1</p> <p style="text-align: center;"><i>gauche</i>-Chloroformoxy(chloro)silylene (3g)</p>	19.9 -1397.060756	19.6 20.3 (600 K) 21.2 (900 K) 22.1 (1200 K)	28.6 37.5 (600 K) 45.9 (900 K) 54.0 (1200 K)	1887 1115 847 641 708 505 474 349 273 93 85 26	322 1014 76 120 64 120 24 28 9 1 0 0		

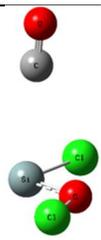
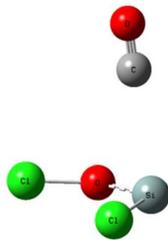
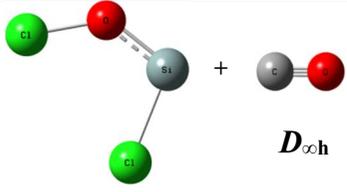
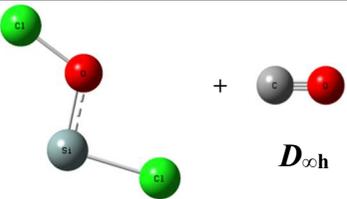
 <p style="text-align: center;">C_1</p> <p style="text-align: center;"><i>cis</i>-Chloroformoxy(chloro)silylene (3c)</p>	20.0 -1397.060582	19.7 20.4 (600 K) 21.3 (900 K) 22.3 (1200 K)	28.7 37.6 (600 K) 46.1 (900 K) 54.2 (1200 K)	1855 1137 816 735 683 517 472 348 201 100 85 34	318 1018 60 137 66 181 12 35 1 2 0 2		
 <p style="text-align: center;">C_1</p> <p style="text-align: center;">TS (3c – 3C)</p>	21.5 -1397.058194	20.7 20.8 (600 K) 21.1 (900 K) 21.5 (1200 K)	31.2 41.7 (600 K) 52.1 (900 K) 62.4 (1200 K)	1770 1210 824 706 684 515 468 354 221 77 57 75 (i)	247 763 132 59 104 163 19 50 1 3 4 6		
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">Chloroformoxy(chloro)silylene, intramolecular complex (3C)</p>	17.1 -1397.065205	16.6 17.2 (600 K) 18.1 (900 K) 19.1 (1200 K)	27.0 37.4 (600 K) 47.4 (900 K) 57.0 (1200 K)	1578 1399 909 722 564 502 446 394 226 204 155 77	135 618 151 25 56 119 5 181 1 8 1 0		

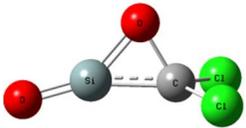
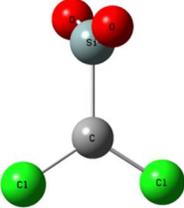
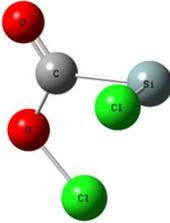
4.3. High-energy [C, 2O, Si, 2Cl] isomers and transition states

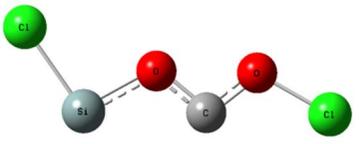
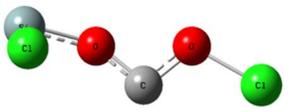
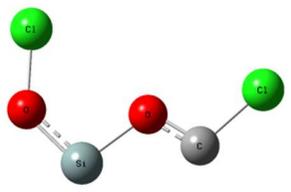
Structure	Energies ($\Delta E_0 = \Delta E + \text{ZPE}$, ΔH^0 , and ΔG^0 in kcal mol ⁻¹) relative to free SiCl ₂ + CO ₂ and absolute energies including ZPE (E/Hartree)			Frequencies (ν) and IR intensities (I) of fundamental vibrations	
	ΔE_0 E	ΔH^0_{298}	ΔG^0_{298}	ν/cm^{-1}	$I/\text{km mol}^{-1}$
 <p style="text-align: center;">C₁ <i>gauche</i>-Dichlorosilaglyoxal (5g)</p>	29.5 -1397.045569	29.3	38.1	1893 1279 791 575 514 438 374 289 229 123 79 32	248 77 123 151 52 76 15 29 21 6 6 1
 <p style="text-align: center;">C_s <i>trans</i>-Dichlorosilaglyoxal (5t)</p>	29.7 -1397.045244	29.5	38.1	1849 1277 838 570 497 478 385 276 216 195 116 11	199 69 113 295 0 12 22 27 38 2 4 1

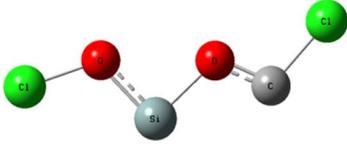
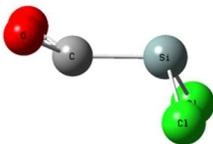
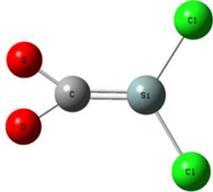
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">TS (3C - 6)</p>	60.6 -1396.995952	59.4	71.5	1207 1168 898 699 620 493 432 386 285 265 198 292 (i)	416 99 114 193 167 6 41 1 98 4 19 45
 <p style="text-align: center;">C_{2v}</p> <p style="text-align: center;">3,3-Dichloro-1-sila-2,4-dioxetan-1-ylidene (6)</p>	43.2 -1397.023626	42.2	54.4	1053 1023 904 837 751 663 432 420 376 301 250 140	430 73 165 311 101 11 5 44 3 0 2 1
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">TS (6 - Cl₂C=O*SiO)</p>	73.5 -1396.975441	72.8	83.6	1524 1088 859 594 552 421 328 264 215 197 89 469 (i)	505 41 391 76 107 1 47 206 17 2 2 89

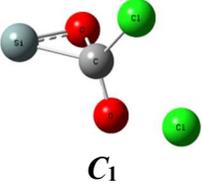
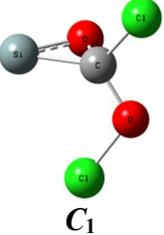
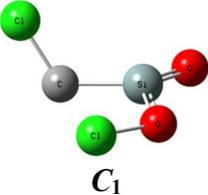
 <p>C₁ Si=O*O=CCl₂</p>	55.1 -1397.004781	55.5	61.3	1904 1265 817 576 561 434 297 91 64 62 27 20	308 54 467 21 16 2 0 2 3 1 6 9
 <p>C_{2v} Cl₂C=O + SiO</p>	58.4 SiO -364.254254 Cl₂C=O -1032.745194	58.3	58.4	SiO 1268 Cl₂C=O 1902 817 588 562 435 297	30 318 490 7 16 2 0
 <p>C₁ cis-Cl(CIO)Si*OC</p>	65.4 -1396.988268	66.6	70.5	2199 855 554 504 325 183 118 71 52 48 22 21	88 37 62 115 4 10 0 1 0 0 0 0

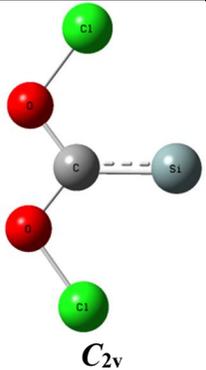
 <p style="text-align: center;">C_1 <i>trans</i>-Cl(ClO)Si*CO</p>	66.1 -1396.987126	67.2	71.9	2231 843 636 502 232 169 140 129 88 58 33 19	74 119 43 140 1 4 2 3 1 4 1 0
 <p style="text-align: center;">C_1 <i>cis</i>-Cl(ClO)Si*CO</p>	65.3 -1396.988498	66.3	71.2	2231 847 553 499 325 196 138 116 92 56 29 21	74 35 58 115 4 16 2 0 1 4 0 0
 <p style="text-align: center;">C_s <i>cis</i>-Cl(ClO)Si + CO</p>	66.6 c-Cl(ClO)Si -1283.778740	67.1	65.9	c-Cl(ClO)Si 860 554 505 324 178 117	c-Cl(ClO)Si 40 64 117 4 6 0
 <p style="text-align: center;">C_s <i>trans</i>-Cl(ClO)Si + CO</p>	67.4 t-Cl(ClO)Si -1283.777404	68.1	66.8	t-Cl(ClO)Si 853 636 511 231 117 150	t-Cl(ClO)Si 127 44 146 1 0 1

 <p style="text-align: center;">C_s</p> <p style="text-align: center;">3,3-Dichloro-1-siloxiranone (7)</p>	72.0 -1396.977706	71.4	82.2	1373 957 944 785 603 449 402 331 299 262 192 104	68 68 108 164 104 4 40 4 25 6 7 7
 <p style="text-align: center;">C_{2v} TS (7-7)</p>	88.1 -1396.952097	87.4	98.2	1358 1010 933 889 473 450 361 340 219 130 53 92 (i)	23 1 150 258 1 32 36 33 10 10 0 2
 <p style="text-align: center;">C_1</p> <p style="text-align: center;">Chloro(chloroxycarbonyl)silylene (8)</p>	98.1 -1396.936141	98.0	107.2	1840 1017 738 595 546 493 390 315 153 117 94 69	181 215 1 27 13 100 6 30 1 3 4 0

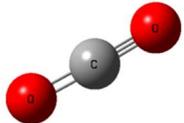
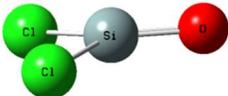
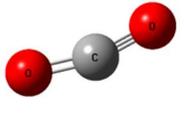
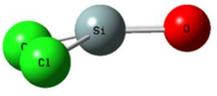
 <p style="text-align: center;">C_s</p> <p><i>trans</i>-Chloroxy(chlorosilylidenyloxy)carbene (9t)</p>	109.8 -1396.917612	109.7	118.6	1245 1103 905 677 508 408 359 239 191 139 80 48	139 452 249 95 205 7 34 1 2 2 1 0
 <p style="text-align: center;">C_1</p> <p><i>gauche</i>-Chloroxy(chlorosilylidenyloxy)carbene (9g)</p>	112.2 -1396.913690	112.2	120.4	1244 1067 892 683 498 391 326 295 189 109 60 30	268 615 156 82 146 9 1 10 2 2 1 0
 <p style="text-align: center;">C_s</p> <p><i>cis</i>-Chloroxy(chloromethylidenyloxy)silylene (10c)</p>	121.3 -1396.899263	121.4	129.5	1281 889 766 719 563 387 289 194 164 96 59 57	530 63 397 5 76 72 47 6 8 0 2 4

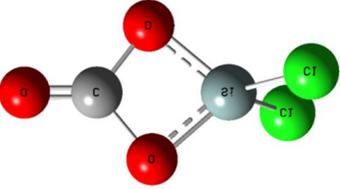
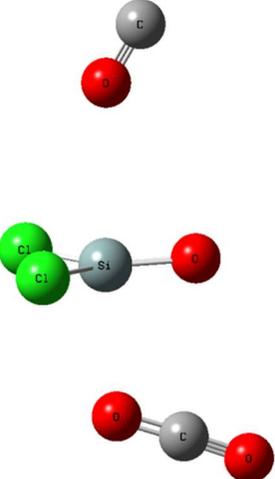
 <p style="text-align: center;">C_s</p> <p><i>trans</i>-Chloroxy(chloromethylidenoxy)silylene (10t)</p>	<p style="text-align: center;">122.0 -1396.898053</p>	<p style="text-align: center;">122.2</p>	<p style="text-align: center;">130.3</p>	<p style="text-align: center;">1286 890 762 722 655 361 222 190 147 103 72 42</p>	<p style="text-align: center;">616 148 486 6 70 110 22 1 0 3 3 2</p>
 <p style="text-align: center;">C_s</p> <p>3-(Dichlorosilylidene)-dioxirane (11)</p>	<p style="text-align: center;">125.2 -1396.892953</p>	<p style="text-align: center;">125.1</p>	<p style="text-align: center;">134.4</p>	<p style="text-align: center;">1487 867 815 542 525 428 339 323 172 125 120 77</p>	<p style="text-align: center;">454 19 59 151 74 13 19 0 14 0 5 1</p>
 <p style="text-align: center;">C_{2v} TS (11-11)</p>	<p style="text-align: center;">136.2 -1396.875449</p>	<p style="text-align: center;">135.5</p>	<p style="text-align: center;">146.5</p>	<p style="text-align: center;">1570 950 891 672 658 406 362 281 172 159 95 241 (i)</p>	<p style="text-align: center;">252 1 1 100 159 4 2 2 0 1 4 1</p>

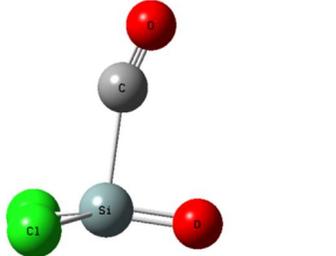
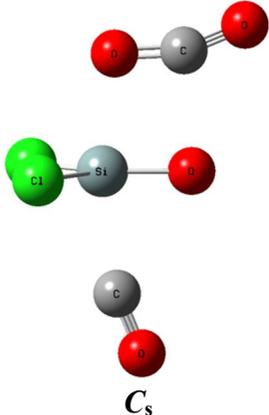
 <p><i>cis</i>-3-Chloro-3-chloroxy-2-silaoxiran-2-ylidene (12)</p>	126.1 -1396.891505	125.6	135.9	1184 1003 837 687 659 455 420 374 262 143 135 105	108 110 89 96 29 2 121 1 144 14 15 1
 <p><i>trans</i>-3-Chloro-3-chloroxy-2-silaoxiran-2-ylidene (12)</p>	127.3 -1396.889615	126.7	137.3	1105 995 881 698 668 589 416 398 305 213 120 93	70 52 112 30 41 25 10 8 1 4 5 0
 <p>Chloroxy(chloromethyldeny)silanone (13)</p>	148.5 -1396.855824	148.6	157.3	1265 978 862 664 502 348 286 238 137 128 96 65	76 39 114 60 20 32 5 23 8 12 0 0

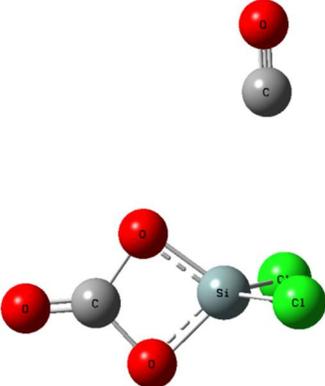
 <p style="text-align: center;">C_{2v}</p> <p><i>cis</i>-2,2-Dichloroxy-1-silavinylidene (14)</p>	209.1 -1396.759228	208.8	218.7	1260 1146 838 716 623 492 475 326 158 142 82 62	180 237 0 0 22 1 5 0 0 5 2
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4.4. Low-energy [2C, 4O, Si, 2Cl] isomers and transition states

Structure	Energies ($\Delta E_0 = \Delta E + \text{ZPE}$, ΔH^0 , and ΔG^0 in kcal mol ⁻¹) relative to free SiCl ₂ + 2CO ₂ and absolute energies including ZPE (E/Hartree)			Frequencies (ν) and IR intensities (I) of fundamental vibrations		Electronic transition in the UV region	
	ΔE_0 E	ΔH^0_{298}	ΔG^0_{298}	ν/cm^{-1}	$I/\text{km mol}^{-1}$	λ/nm	f
Cl₂Si=O + CO₂ (+ CO)	0.0	0.0	0.0				
  C _s Cl₂Si=O*CO₂	-5.5 -1472.305214	-5.1	2.4	2426 1369 679 672 1266 615 485 289 273 207 152 101 76 59 35	745 15 41 42 104 208 29 92 23 2 19 0 28 1 0		
  C _s TS (Cl₂Si=O*CO₂ - 4)	-3.7 -1472.302330	-4.2	6.2	2343 1274 1191 658 627 610 497 362 287 276 206 163 160 63 256 (i)	676 76 83 73 186 182 136 139 16 11 8 0 2 0 46		

 <p style="text-align: center;">C_{2v}</p> <p style="text-align: center;">1,1-Dichloro-1-sila-2,4-dioxetan-3-one (4)</p>	-30.1 -1472.344460	-31.0	-19.2	1984 1101 985 898 781 707 687 646 524 414 306 219 177 173 99	595 244 60 274 62 135 5 195 0 0 6 6 2 0 5	n/a	
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">Cl₂Si=O*CO₂*OC</p>	-7.1 -1585.515445	-6.2	7.0	2427 2198 1371 1267 681 673 618 485 282 272 204 146 91 87 65 64 57 52 34 24 21	718 109 10 103 40 44 202 25 114 23 2 17 0 3 15 1 4 8 0 0 0		

 <p style="text-align: center;">C_s</p> <p style="text-align: center;">$Cl_2Si=O*CO_2*CO$</p>	<p>-9.9</p> <p>-1585.519883</p>	<p>-9.7</p>	<p>5.7</p>	<p>2432</p> <p>2247</p> <p>1378</p> <p>1217</p> <p>691</p> <p>671</p> <p>599</p> <p>497</p> <p>398</p> <p>363</p> <p>337</p> <p>253</p> <p>240</p> <p>187</p> <p>129</p> <p>89</p> <p>78</p> <p>57</p> <p>29</p> <p>21</p> <p>14</p>	<p>530</p> <p>228</p> <p>0</p> <p>114</p> <p>32</p> <p>70</p> <p>197</p> <p>54</p> <p>18</p> <p>0</p> <p>55</p> <p>23</p> <p>17</p> <p>4</p> <p>2</p> <p>6</p> <p>0</p> <p>1</p> <p>0</p> <p>1</p> <p>1</p>		
 <p style="text-align: center;">C_s</p> <p style="text-align: center;">TS ($Cl_2Si=O*CO_2*CO - 4*CO$)</p>	<p>-3.1</p> <p>-1585.509027</p>	<p>-3.8</p>	<p>16.2</p>	<p>2290</p> <p>2241</p> <p>1270</p> <p>1124</p> <p>674</p> <p>640</p> <p>596</p> <p>475</p> <p>430</p> <p>359</p> <p>341</p> <p>277</p> <p>266</p> <p>200</p> <p>163</p> <p>162</p> <p>143</p> <p>76</p> <p>67</p> <p>65</p> <p>318 (i)</p>	<p>702</p> <p>203</p> <p>67</p> <p>108</p> <p>53</p> <p>185</p> <p>176</p> <p>22</p> <p>276</p> <p>0</p> <p>108</p> <p>112</p> <p>12</p> <p>15</p> <p>3</p> <p>7</p> <p>4</p> <p>0</p> <p>1</p> <p>0</p> <p>67</p>		

 <p style="text-align: center;">C_s 4*CO</p>	-32.0 -1585.555135	-32.4	-14.6	2224 1980 1105 984 901 783 706 688 645 522 412 307 214 178 173 124 110 97 52 30 25	78 611 277 48 282 60 131 6 185 1 0 5 11 2 0 0 0 4 1 0 1		
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4.5. The B3LYP/ 6-31G(2df) calculated frequencies (ν/cm^{-1}) and IR intensities ($I/\text{km mol}^{-1}$) of fundamental vibrations of SiCl_2 and $\text{Cl}_2\text{Si}^*\text{CO}_2$ isotopomers

SiCl_2

28-35-35 ^a		28-35-37		28-37-37		29-35-35		29-35-37		29-37-37		30-35-35		30-35-37		30-37-37	
ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I
503	83	501	103	497	82	498	81	496	100	492	80	493	80	492	96	487	78
498	194	494	172	492	190	492	190	488	169	487	186	488	186	484	167	482	182
191	2	189	1	187	1	190	2	188	2	186	1	190	2	188	2	186	1

^a Rounded atomic masses of Si and two Cl isotopes composing an isotopomer are given in this row.

$\text{Cl}_2\text{Si}^*\text{CO}_2$

28-35-35 ^a		28-35-37		28-37-37		29-35-35		29-35-37		29-37-37		30-35-35		30-35-37		30-37-37	
ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I	ν	I
2432	667	2432	667	2432	667	2432	667	2432	667	2432	667	2432	667	2432	667	2432	667
1379	2	1379	2	1379	2	1379	2	1379	2	1379	2	1379	2	1379	2	1379	2
686	31	686	31	686	31	686	31	686	31	686	31	686	31	686	31	686	31
683	29	683	29	683	29	683	29	683	29	683	29	683	29	683	29	683	29
498	78	495	84	492	77	493	76	490	82	487	75	488	75	486	81	482	73
487	185	484	176	482	181	482	181	479	172	477	177	477	177	474	169	472	174
191	1	189	1	187	1	191	1	189	1	187	1	190	1	188	1	186	1
77	4	77	4	77	4	77	4	76	4	76	4	76	3	76	3	76	3
70	5	70	5	70	5	69	6	69	6	69	5	69	6	69	6	69	6
54	0	54	0	54	0	54	0	54	0	54	0	54	0	54	0	54	0
22	0	21	0	21	0	22	0	21	0	21	0	22	0	21	0	21	0
3	0	3	0	3	0	3	0	3	0	3	0	3	0	3	0	3	0

^a Rounded atomic masses of Si and two Cl isotopes are given in this row; all isotopomers include ^{12}C and ^{16}O isotopes.

5. Cartesian coordinates

SiCl₂ Si 0.00000000 0.00000000 0.93694600 Cl 0.00000000 1.63137500 -0.38580100 Cl 0.00000000 -1.63137500 -0.38580100	CO₂ C 0.00000000 0.00000000 0.00000000 O 0.00000000 0.00000000 1.16287900 O 0.00000000 0.00000000 -1.16287900
(CO₂)₂ C 0.56138900 1.74766400 0.00000000 O -0.56138900 1.43998100 0.00000000 O 1.67922100 2.06329600 0.00000000 C -0.56138900 -1.74766400 0.00000000 O -1.67922100 -2.06329600 0.00000000 O 0.56138900 -1.43998100 0.00000000	Cl₂Si*CO₂ C -0.26566600 -2.56266600 0.00000000 O -1.05121300 -1.70105300 0.00000000 O 0.50884700 -3.42545500 0.00000000 Si -0.81199500 1.31224200 0.00000000 Cl 0.50884700 1.11813800 1.63207200 Cl 0.50884700 1.11813800 -1.63207200
CO₂*Cl₂Si*CO₂-1 Si 0.00000000 0.00000000 1.01880400 Cl -1.61464500 -0.24448700 -0.32812700 Cl 1.61464500 0.24448700 -0.32812700 O -0.34330500 3.01496500 0.77775200 C 0.00000000 3.73312700 -0.07409500 O 0.33846100 4.45474400 -0.91636500 O 0.34330500 -3.01496500 0.77775200 C 0.00000000 -3.73312700 -0.07409500 O -0.33846100 -4.45474400 -0.91636500	CO₂*Cl₂Si*CO₂-2 Si -0.00000100 0.43840500 0.96415000 Cl -0.00000700 -1.44067900 -0.02237700 Cl 0.00000900 1.75744400 -0.68459600 O -3.03329900 0.28744500 0.74234600 C -3.70264900 -0.26389600 -0.03685300 O -4.37605200 -0.80968000 -0.80718300 O 3.03329700 0.28742300 0.74235800 C 3.70264700 -0.26390300 -0.03685000 O 4.37605200 -0.80967300 -0.80718900

Cl₂Si*(CO₂)₂-1 C -2.96809500 0.86310200 -0.45165500 O -2.26154600 0.14876500 -1.04167600 O -3.67669200 1.57451500 0.12991000 C -0.89530700 -2.19000500 0.23337000 O -1.88459400 -2.38900600 0.80527000 O 0.10278000 -2.00127200 -0.33826100 Si 1.45809400 0.62304400 -0.79504300 Cl 0.52084700 1.32130100 0.97310300 Cl 3.27489000 -0.11102000 -0.03202200	Cl₂Si*(CO₂)₂-2 C -1.08054300 2.12879200 0.05130300 O -0.72895500 1.27897400 0.76953300 O -1.42918800 2.97880400 -0.65447400 C -2.69861900 -1.12017600 0.33120200 O -3.25010800 -0.28013800 -0.25547800 O -2.15106000 -1.95978700 0.91959000 Si 1.46756500 -0.90490900 0.61813500 Cl 2.89935800 0.61778700 0.35133800 Cl 0.78320400 -1.17812800 -1.36206000
TS (Cl₂Si*CO₂ - 1) C 0.30250900 -1.91377700 0.00000000 O -0.10439900 -3.00532200 0.00000000 O 1.20136500 -1.06694600 0.00000000 Si -0.50294500 0.08088800 0.00000000 Cl -0.10439900 1.26259900 -1.65942500 Cl -0.10439900 1.26259900 1.65942500	
1,1-Dichloro-1-siloxiranone (1) C -0.13908200 -1.74552700 0.00000000 O 1.15367800 -1.13473600 0.00000000 Si -0.01798800 0.06435400 0.00000000 Cl -0.13908200 1.22754900 1.66073600 Cl -0.13908200 1.22754900 -1.66073600 O -0.42678900 -2.88582200 0.00000000	TS (1 - Cl₂Si=O*CO) O 1.37581400 -0.95775500 0.00000000 Cl -0.29084700 1.17167800 1.65067600 Cl -0.29084700 1.17167800 -1.65067600 O -0.29084700 -2.86406000 0.00000000 C -0.14962600 -1.71658100 0.00000000 Si 0.15048700 0.07406800 0.00000000

Cl₂Si=O*CO O 0.61121800 1.80886500 0.00000000 Si 0.37873600 0.30246200 0.00000000 Cl 0.61121800 -0.89339800 1.64387400 Cl 0.61121800 -0.89339800 -1.64387400 C -1.62797800 0.56479800 0.00000000 O -2.65069700 1.03517000 0.00000000	Cl₂Si=O O 0.00000000 0.00000000 2.01524800 Si 0.00000000 0.00000000 0.50506200 Cl 0.00000000 1.64025100 -0.68214200 Cl 0.00000000 -1.64025100 -0.68214200
CO C 0.00000000 0.00000000 -0.64623500 O 0.00000000 0.00000000 0.48467600	3,3-Dichloro-3-sila-2,4-dioxetan-1-ylidene (2) C 0.00000000 0.00000000 2.23488500 O 0.00000000 1.06682400 1.38358300 O 0.00000000 -1.06682400 1.38358300 Cl -1.66397300 0.00000000 -1.07624000 Cl 1.66397300 0.00000000 -1.07624000 Si 0.00000000 0.00000000 0.07468100
TS (Cl₂Si*CO₂ – 3c) Si 0.01657500 -0.07821600 0.01909300 Cl -0.06461900 0.11532200 2.10224600 O 1.74301200 -0.05464000 -0.14077100 Cl 1.48451500 -2.50070000 -0.96872200 C 2.47692100 -0.96217900 -0.73439100 O 3.59980000 -0.90842300 -1.08523700	<i>gauche</i>-Chloroformoxy(chloro)silylene (3g) C -1.03935100 -0.16551700 -0.48785300 Cl 2.10768300 -0.79300500 0.45747200 O -0.94423700 -1.07974800 -1.23096200 Cl -2.40941400 0.04663000 0.62201400 O -0.19440900 0.86807500 -0.36972800 Si 1.46248000 1.09820500 -0.18704300
<i>cis</i>-Chloroformoxy(chloro)silylene (3c) C -1.31219000 0.40982700 -0.13252800 Cl 2.71394700 -0.62495600 -0.17313700 O -1.59738600 1.54228900 -0.34843400 Cl -2.52579100 -0.86111800 0.09859300 O -0.08600800 -0.11145700 -0.03987100 Si 1.29583200 0.81125900 0.36920300	TS (3c – 3C) C -1.10041200 0.26430400 -0.15113600 O -0.90652600 1.18348300 -0.90102000 O -0.18346300 -0.27572400 0.62252500 Si 1.26936000 0.70366900 0.65794900 Cl -2.67415400 -0.50557600 0.03319400 Cl 2.53011400 -0.59438100 -0.39063600

Chloroformoxy(chloro)silylene, intramolecular complex (3C) C -0.26142500 0.91997800 0.00000000 Si 1.36587400 -0.68625200 0.00000000 Cl 0.16628500 -2.42051400 0.00000000 Cl -1.35535800 2.25664600 0.00000000 O 0.16628500 0.42958900 1.08032000 O 0.16628500 0.42958900 -1.08032000	<i>gauche</i>-Dichlorosilaglyoxal (5g) C -1.00322900 0.31905300 0.56489700 O -1.50826000 0.66526600 1.56978400 Cl -1.92649600 -0.61826200 -0.72621600 Si 0.75969100 0.56879800 -0.11178700 Cl 1.78196700 -1.14087300 0.24552100 O 1.23834700 1.83820900 -0.77635400
<i>trans</i>-Dichlorosilaglyoxal (5t) C -0.09479800 -1.06408000 0.00000000 O 0.84699700 -1.78036000 0.00000000 Cl -1.77942000 -1.67968800 0.00000000 Si 0.00000000 0.86357500 0.00000000 Cl 1.97013100 1.33205300 0.00000000 O -1.18116100 1.80588900 0.00000000	TS (3C - 6) C 0.35851800 0.24730900 0.00000000 O 0.68043500 -0.48152300 1.07954100 Si 0.34012900 -1.84982100 0.00000000 Cl 0.68043500 1.95258800 0.00000000 Cl -1.72748700 -0.06329400 0.00000000 O 0.68043500 -0.48152300 -1.07954100
3,3-Dichloro-1-sila-2,4-dioxetan-1-ylidene (6) O 0.00000000 1.08198900 0.74339500 O 0.00000000 -1.08198900 0.74339500 Cl -1.46307900 0.00000000 -1.17844700 Cl 1.46307900 0.00000000 -1.17844700 C 0.00000000 0.00000000 -0.13278800 Si 0.00000000 0.00000000 2.06925700	TS (6 - Cl₂C=O*SiO) O -0.58553500 1.46507800 0.00000000 O 1.36091900 -0.08461100 0.00000000 Cl -0.58553500 -1.04969500 1.45256500 Cl -0.58553500 -1.04969500 -1.45256500 C 0.17728100 -0.43763100 0.00000000 Si 0.90296000 1.94797700 0.00000000

Si=O*O=CCl₂ C -1.17617000 0.22124800 0.00000000 O 1.72776600 0.21419600 0.00000000 O -1.19457900 1.39562100 0.00000000 Si 3.10051500 0.85282700 0.00000000 Cl -1.19457900 -0.76898800 1.45567700 Cl -1.19457900 -0.76898800 -1.45567700	Cl₂C=O C 0.00000000 0.00000000 0.50518900 Cl 0.00000000 1.45631000 -0.48447000 Cl 0.00000000 -1.45631000 -0.48447000 O 0.00000000 0.00000000 1.68010500
SiO O 0.00000000 0.00000000 -0.96270800 Si 0.00000000 0.00000000 0.55011900	<i>cis</i>-Cl(ClO)Si*OC C 3.18042000 -0.74383300 -0.39653600 O 2.24213400 -1.06222800 0.15033900 Si -0.82435300 -0.55874800 1.10524100 Cl -1.40263600 -1.18409000 -0.81209400 O -0.22416500 0.97369700 0.92799400 Cl 0.00938100 1.94842700 -0.46560100
<i>trans</i>-Cl(ClO)Si*CO C 0.00000000 0.00000000 0.00000000 O 0.00000000 0.00000000 1.12815300 Cl 2.14297600 0.00000000 -3.10261700 O -0.10610300 -1.66242400 -2.95024300 Si 0.03374700 0.02025300 -3.09353900 Cl -1.71945100 -2.22276700 -2.85388700	<i>cis</i>-Cl(ClO)Si*CO O -0.00023100 -0.00021700 0.00000100 Cl 0.00025700 -0.00068400 1.71763200 Cl 3.01852800 0.00038600 0.03668900 O 1.10944200 4.24663400 -0.26005200 C 1.17362800 3.14154100 -0.47771400 Si 1.24379000 0.11018900 -1.08936100
<i>cis</i>-Cl(ClO)Si Si 1.32553900 0.25942200 0.00000000 O 0.00000000 1.24910800 0.00000000 Cl 0.58925400 -1.70307300 0.00000000 Cl -1.68087500 0.90161600 0.00000000	<i>trans</i>-Cl(ClO)Si Si -0.35075100 -0.86463400 0.00000000 O 0.00000000 0.78740500 0.00000000 Cl 1.65973100 -1.46890700 0.00000000 Cl -1.37087800 1.81041500 0.00000000

3,3-Dichloro-1-siloxiranone (7) O 1.29072500 -0.35821500 0.00000000 Cl -0.27047400 1.30904400 1.45737300 Cl -0.27047400 1.30904400 -1.45737300 O -0.27047400 -2.92032700 0.00000000 C -0.03466200 0.35384600 0.00000000 Si 0.08871900 -1.45730300 0.00000000	TS (7-7) Cl 0.00000000 1.42727300 -1.36082700 Cl 0.00000000 -1.42727300 -1.36082700 O -1.47777300 0.00000100 1.81201600 O 1.47777300 -0.00000100 1.81201600 C 0.00000000 0.00000000 -0.46028600 Si 0.00000000 0.00000000 1.43125600
Chloro(chloroxycarbonyl)silylene (8) C -0.47494100 1.09360900 -0.02019900 O -0.39559900 2.26587500 0.18521500 Si 0.79026100 -0.01118100 -1.06351000 Cl 2.06152900 -0.45541300 0.54769300 O -1.64544800 0.46454800 0.44415000 Cl -1.58421400 -1.20626300 0.03909600	trans-Chloroxy(chlorosilylidenyloxy)carbene (9t) O 0.00000000 0.33447100 0.00000000 C 0.13534100 -0.99265500 0.00000000 O 1.45371700 -1.15319400 0.00000000 Cl 1.92904600 -2.80929700 0.00000000 Si -1.64764400 0.80966000 0.00000000 Cl -1.30403200 2.87814800 0.00000000
gauche-Chloroxy(chlorosilylidenyloxy)carbene (9g) O -0.29234100 0.92714500 -0.06319500 C 0.77211900 0.34789800 -0.60309500 O 1.62098100 0.27397100 0.42400500 Cl 3.14212800 -0.39904500 -0.01565500 Si -1.95665100 0.96712300 0.06179100 Cl -2.42852300 -1.08542800 0.00783300	cis-Chloroxy(chloromethylidenyloxy)silylene (10c) O 0.00000000 0.58658800 0.00000000 O -1.30771600 -1.65416700 0.00000000 Cl 0.18060600 -2.50310800 0.00000000 Cl 1.76104600 2.37035500 0.00000000 C 0.03988000 1.88547900 0.00000000 Si -1.62754500 -0.03681800 0.00000000
trans-Chloroxy(chloromethylidenyloxy)silylene (10t) O 0.00000000 0.85951800 0.00000000 O -0.62304600 -1.48336000 0.00000000 Cl -0.49871400 -3.18082800 0.00000000 Cl -0.19153800 3.35979000 0.00000000 C 0.80811600 1.87545400 0.00000000 Si 0.84785300 -0.66459600 0.00000000	3-(Dichlorosilylidene)-dioxirane (11) C -0.18805900 1.36710300 0.00000000 Si 0.65241500 -0.32844500 0.00000000 O -0.16010900 2.44547400 0.77191100 O -0.16010900 2.44547400 -0.77191100 Cl -0.16010900 -1.25682300 1.68842100 Cl -0.16010900 -1.25682300 -1.68842100

TS (11-11) C 0.00000000 0.00000000 -1.42249300 Si 0.00000000 0.00000000 0.27469800 O 0.00000000 0.76133300 -2.54241100 O 0.00000000 -0.76133300 -2.54241100 Cl 0.00000000 1.72730100 1.33434600 Cl 0.00000000 -1.72730100 1.33434600	<i>cis</i>-3-Chloro-3-chloroxy-2-silaoxiran-2-ylidene (12) O 0.87954100 -0.60983100 0.98493600 Cl 0.34019300 1.79807400 -0.00036500 O -0.63417800 -0.53625800 -0.80527100 Cl -2.24701500 -0.47705100 0.13865600 C 0.37628500 0.02937700 -0.19461200 Si 2.01395500 -0.96178200 -0.18718500
<i>trans</i>-3-Chloro-3-chloroxy-2-silaoxiran-2-ylidene (12) O -0.40864700 0.96591300 1.04282500 Cl -2.00383400 -0.78558900 -0.19267400 O 0.46424200 -1.07842000 0.25230300 Cl 2.07878500 -0.59486000 -0.10514500 C -0.41963200 -0.01160800 0.02561000 Si 0.05706200 1.74552400 -0.38941200	Chloroxy(chloromethylidanyl)silanone (13) O 0.09891000 2.55411200 0.06671700 O 1.70754500 0.27527400 0.13890400 Cl 1.56293600 -1.42704400 0.00345700 Cl -2.26368500 -0.72228000 0.16787800 C -0.99319400 -0.12702500 -0.74501700 Si 0.24430400 1.04754200 -0.00625400
<i>cis</i>-2,2-Dichloroxy-1-silavinylidene (14) C 0.00000000 0.00000000 -0.24149600 Si 0.00000000 0.00000000 1.54300400 O 0.00000000 1.09322600 -1.08467700 O 0.00000000 -1.09322600 -1.08467700 Cl 0.00000000 2.47005800 -0.08230100 Cl 0.00000000 -2.47005800 -0.08230100	

Cl₂Si=O*CO₂ O -1.76207300 0.07246100 0.00000000 Si -0.36685900 0.65898500 0.00000000 Cl 0.64735300 1.28615700 1.64295200 Cl 0.64735300 1.28615700 -1.64295200 C -0.14232600 -2.43014200 0.00000000 O -0.88778500 -3.30874300 0.00000000 O 0.64735300 -1.56050300 0.00000000	TS (Cl₂Si=O*CO₂ - 4) Si -0.22802500 0.42618200 0.00000000 Cl 0.63419400 1.25699200 1.64638300 Cl 0.63419400 1.25699200 -1.64638300 O 0.63419400 -1.35474900 0.00000000 C -0.34222700 -2.07161600 0.00000000 O -1.04862200 -2.97303000 0.00000000 O -1.62518300 -0.20654300 0.00000000
1,1-Dichloro-1-sila-2,4-dioxetan-3-one (4) O 0.00000000 1.08700300 -1.00788900 O 0.00000000 -1.08700300 -1.00788900 Cl -1.65830100 0.00000000 1.41515200 Cl 1.65830100 0.00000000 1.41515200 C 0.00000000 0.00000000 -1.87914700 Si 0.00000000 0.00000000 0.26658700 O 0.00000000 0.00000000 -3.05578400	
Cl₂Si=O*CO₂*OC O -1.27651200 0.76224700 0.00000000 Si 0.09229300 0.11741100 0.00000000 Cl 1.20953800 -0.28973400 1.64344200 Cl 1.20953800 -0.28973400 -1.64344200 C -2.19209200 -2.07690600 0.00000000 O -3.34471600 -2.02304100 0.00000000 O -1.02303400 -2.16938900 0.00000000 C 1.03566000 4.07551600 0.00000000 O 1.20953800 2.95712400 0.00000000	Cl₂Si=O*CO₂*CO O -0.93261500 0.77966200 0.00000000 Si 0.48227900 0.20586500 0.00000000 Cl 1.39317300 -0.59154000 1.64632000 Cl 1.39317300 -0.59154000 -1.64632000 C -2.96382900 -1.21282900 0.00000000 O -3.83843600 -0.44992400 0.00000000 O -2.11862400 -2.01540000 0.00000000 C 1.27253100 2.07442700 0.00000000 O 1.39317300 3.19324300 0.00000000

TS (Cl₂Si=O*CO₂*CO – 4*CO)

Si	0.14717300	0.04826500	0.00000000
Cl	1.17196200	-0.54531100	1.67930400
Cl	1.17196200	-0.54531100	-1.67930400
O	-1.07957500	-1.60512200	0.00000000
C	-2.14680100	-1.03078400	0.00000000
O	-3.28800000	-0.86772100	0.00000000
O	-1.19300300	0.84350200	0.00000000
C	1.01376500	2.01194700	0.00000000
O	1.17196200	3.12657700	0.00000000

4*CO

Si	0.56122100	-0.14877500	0.00000000
Cl	1.06134100	0.87953400	1.66266400
Cl	1.06134100	0.87953400	-1.66266400
O	1.06134100	-1.75244000	0.00000000
C	-0.27434000	-2.12940000	0.00000000
O	-0.73865300	-3.21134700	0.00000000
O	-0.93576500	-0.90145600	0.00000000
C	-2.08322000	2.01080000	0.00000000
O	-3.11158900	2.47652900	0.00000000