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Formation of 1,1-dichloro-2-vinyl-1-silacyclopropane by a photoinduced reaction between dichlorosilylene and 1,3-butadiene

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Abbreviation used: 1,3-butadiene is hereinafter abbreviated as BD.

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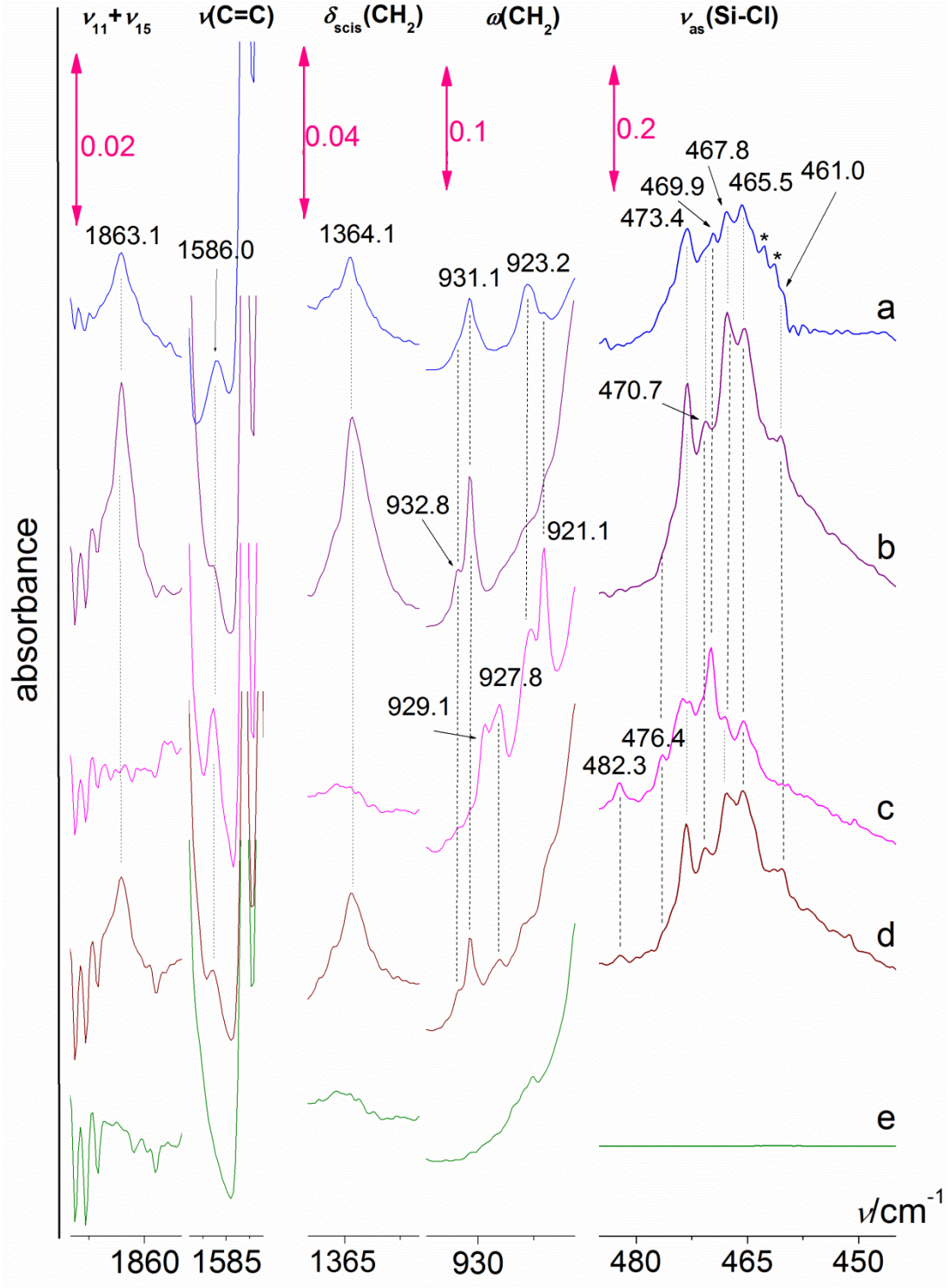


Figure S1 Bands of conformers of the BD•$SiCl_2$ complex observed upon deposition (*a*; $SiCl_2$: BD : Ar = 1 : 1 : 400) and their behaviour upon annealing (*b*; 37 K, 3 min), subsequent photolysis (*c*; λ > 450 nm, 20 min), subsequent annealing (*d*; 37 K, 2 min) and final photolysis (*e*; λ > 300 nm, 15 min). Fragments of the spectra in the ν_{as}(Si–Cl) vibration region were obtained by the subtraction of spectrum recorded after the final photolysis from the original spectra; residual bands of Si_2Cl_6 are marked with asterisks. Other fragments represent fragments of originally recorded spectra. The ν_s(Si–Cl) bands of the conformers could not be revealed because they were hidden by the isotopically split (due to Cl and Si isotopes) ν_{as}(Si–Cl) band of starting $SiCl_2$.

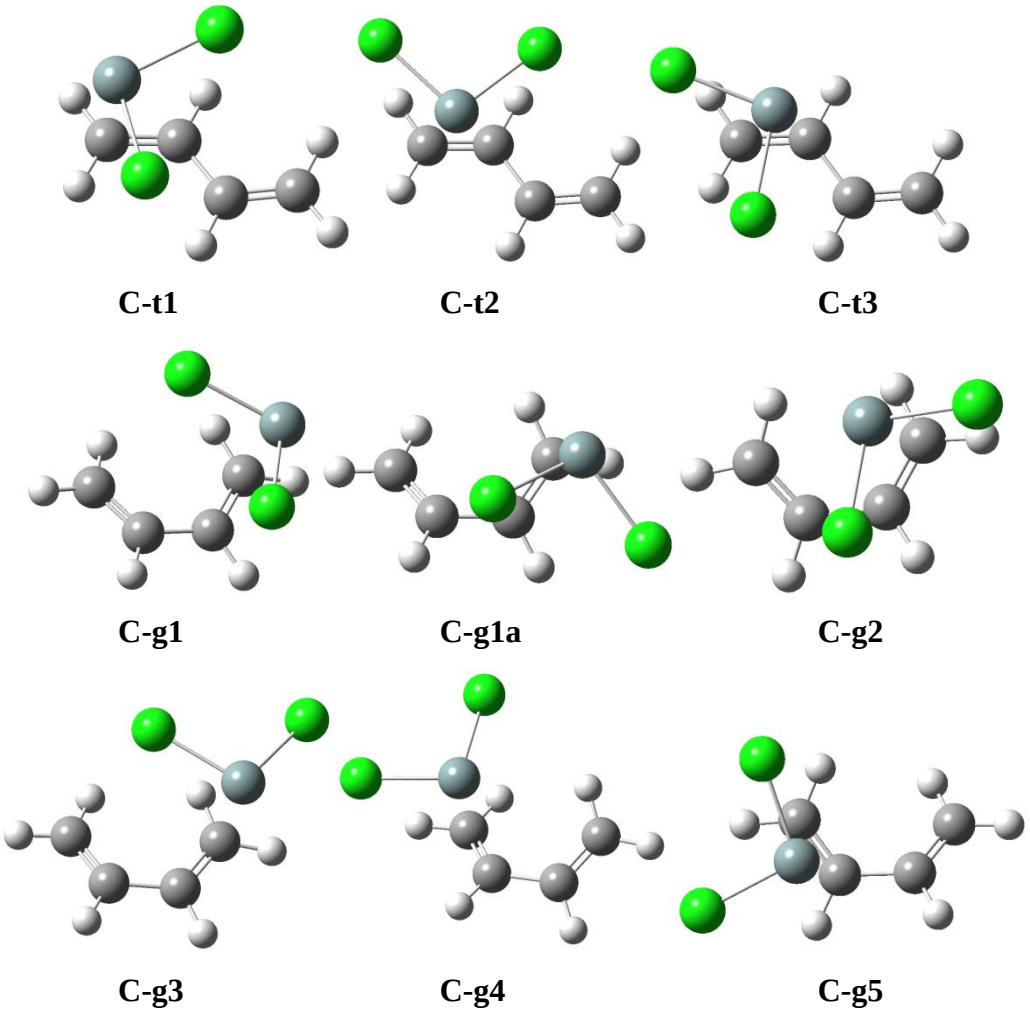


Figure S2 Conformers of the BD•$SiCl_2$ complex revealed in the M06-2X/6-311++G(d,p) and G3(MP2)//B3LYP calculations.

Table S1 Energies ($\Delta E_0 = \Delta E$+ZPE /kcal mol^{-1}), enthalpies (ΔH^0/kcal mol^{-1}) and the Gibbs free energies (ΔG^0/kcal mol^{-1}) of conformers of the BD•$SiCl_2$ complex (relative to free $SiCl_2$ and trans-BD) obtained by the M06-2X/6-311++G(d,p) and G3(MP2)//B3LYP (in parentheses) calculations.[a]

	C-t1	**C-t2**	**C-t3**	**C-g1**	**C-g1a**	**C-g2**	**C-g3**	**C-g4**	**C-g5**
ΔE_0	-7.5 (-5.4)	-6.0 (-4.2)	-6.1 (-4.3)	-5.0 (-2.6)	-4.3	-3.7 (-1.6)	-3.2 (-1.3)	-3.5 (-1.9)	-2.9
ΔH^0	-7.4 (-5.1)	-5.6 (-3.7)	-5.7 (-3.8)	-4.9 (-2.3)	-4.2	-3.3 (-1.1)	-2.6 (-0.7)	-3.0 (-1.2)	-2.4
ΔG^0	3.2 (4.1)	3.6 (3.8)	3.7 (4.0)	6.0 (7.5)	6.2	6.4 (7.1)	6.2 (7.5)	6.3 (6.2)	6.3

[a] including BSSE corrections in the case of M06-2X/6-311++G(d,p) calculations.

Table S2 Fundamental frequencies (ν/cm^{-1}), their shifts relative to those of starting reactants[a] ($\Delta\nu$/cm^{-1}) and IR intensities (I/km mol^{-1}) of corresponding vibrations of the BD•$SiCl_2$ conformers according to the M06-2X/6-311++G(d,p) calculations.

C-t1			**C-t2**			**C-t3**			**C-g1**			**C-g1a**			**C-g2**			**C-g3**			**C-g4**			**C-g5**		
ν	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***
3266		2	3263		0	3266		0	3269		1	3265		2	3267		3	3268		2	3257		4	3264		0
3258		0	3264		3	3264		3	3259		0	3252		1	3264		1	3261		0	3267		0	3262		3
3201		2	3186		3	3191		1	3186		4	3180		4	3191		4	3178		4	3173		0	3169		2
3181		1	3178		0	3170		2	3205		2	3197		1	3206		2	3198		6	3188		5	3185		2
3170		1	3168		1	3167		1	3164		2	3172		1	3169		3	3167		3	3162		5	3169		0
3158		3	3161		2	3164		2	3177		1	3157		2	3175		2	3178		2	3161		1	3162		4
1710	*-33*	28	1726	*-17*	21	1729	*-15*	15	1643	*-68*	43	1655	*-56*	53	1661	*-50*	22	1668	*-43*	80	1683	*-28*	18	1682	*-29*	44
1638	***-41***	**52**	**1660**	***-20***	**45**	**1660**	***-19***	**41**	1702	*-17*	5	1707	*-12*	3	1704	*-15*	2	1710	*-9*	5	1713	*-6*	1	1716	*-3*	4
1476	*3*	3	1477	*4*	2	1476	*3*	1	1473	*8*	27	1465	*0*	23	1473	*8*	21	1472	*7*	23	1471	*6*	16	1467	*2*	19
1413	*-5*	9	1418	*1*	11	1418	*1*	11	1438	*5*	4	1432	*-2*	2	1438	*5*	5	1437	*3*	4	1439	*5*	5	1435	*1*	3
1325	*9*	2	1320	*4*	2	1320	*4*	2	1309	*-1*	1	1307	*-3*	0	1311	*1*	1	1313	*3*	1	1308	*-2*	1	1309	*-1*	0
1315	*-2*	7	1318	*1*	4	1318	*1*	3	1352	*11*	5	1344	*3*	4	1352	*11*	2	1356	*15*	6	1344	*3*	2	1343	*2*	3
1245	*15*	4	1233	*3*	2	1233	*2*	1	1114	*12*	9	1106	*3*	8	1109	*7*	12	1109	*6*	12	1106	*4*	12	1102	*-1*	6
1068	***11***	**50**	**1064**	***7***	**59**	**1064**	***8***	**61**	1049	*9*	26	1043	*3*	25	1045	*6*	16	1048	*8*	27	1045	*5*	39	1048	*8*	43
1020	*11*	0	1014	*5*	2	1016	*7*	3	1024	*2*	10	1024	*2*	6	1028	*6*	10	1031	*9*	11	1030	*8*	7	1027	*5*	4
1001	*2*	16	1001	*2*	6	1003	*4*	2	1082	*10*	0	1087	*14*	2	1072	*-1*	2	1076	*4*	0	1065	*-7*	1	1078	*5*	5
987	*30*	25	**987**	***29***	**51**	**980**	***22***	**33**	981	*10*	76	990	*19*	123	970	*-1*	8	979	*8*	106	988	*17*	37	988	*17*	51
975	***13***	**80**	**975**	***14***	**82**	**987**	***25***	**92**	994	*21*	42	995	*22*	11	981	*8*	109	996	*23*	69	1007	*34*	66	1005	*33*	77
913	*9*	5	907	*3*	1	904	*1*	1	906	*11*	10	902	*7*	6	899	*4*	2	899	*4*	5	894	*-1*	1	894	*-1*	1
823	*40*	1	793	*10*	1	787	*4*	2	813	*50*	1	822	*60*	5	782	*19*	5	785	*22*	2	765	*2*	6	771	*8*	8
610	*76*	8	576	*41*	12	570	*35*	16	553	*82*	11	634	*163*	10	543	*72*	15	541	*70*	21	508	*37*	19	502	*31*	22
520	*1*	1	516	*-3*	2	517	*-1*	1	593	*-34*	6	529	*-99*	22	599	*-28*	26	578	*-49*	5	625	*-3*	15	630	*3*	14
471	***-41***	**84**	**489**	***-23***	**108**	**488**	***-24***	**91**	469	*-43*	80	472	*-40*	90	482	*-30*	121	484	*-28*	87	485	*-27*	94	487	*-25*	83
457	***-42***	**142**	**464**	***-35***	**158**	**467**	***-32***	**182**	456	*-43*	147	458	*-41*	168	464	*-35*	158	461	*-38*	173	464	*-36*	180	465	*-34*	182
304		1	300		2	302		1	313		0	314		1	311		0	318		0	295		0	290		0
264		5	221		12	166		3	284		3	207		3	251		12	179		5	221		2	247		3
215		1	196		2	201		1	214		3	294		4	196		3	199		2	196		1	198		3
206		15	153		31	189		3	191		38	131		2	161		26	149		40	146		32	153		63
180		23	141		6	147		44	166		5	183		38	136		7	128		34	121		18	111		4
132		3	97		16	98		19	139		2	159		6	107		7	95		1	110		5	101		1
127		9	80		5	85		1	117		2	115		4	93		1	91		0	84		1	76		5
75		1	58		5	58		1	97		0	71		0	85		2	81		1	74		3	60		0
38		1	26		0	34		0	49		1	37		0	35		0	5		0	31		0	15		0

[a] Relative to the frequencies of free $SiCl_2$ and *trans*- or *gauche*-BD for conformers containing the BD moiety in the *trans*- or *gauche*-conformation, respectively, $\Delta\nu = \nu_{complex} - \nu_{reactant}$. The parameters for vibrations of the $SiCl_2$ moiety are shown on a green background. The parameters of vibrations, which are characterized by large intensities and large frequency shifts for conformers with the *trans*-BD moiety, are underlined and set off in bold. The parameters of vibrational modes observed in the experiment are in red.

Table S3 Fundamental frequencies (ν/cm^{-1}), their shifts relative to those of starting reactants[a] ($\Delta\nu$/cm^{-1}) and IR intensities (I/km mol^{-1}) of corresponding vibrations of the BD•$SiCl_2$ conformers according to the B3LYP/6-31G(d) calculations.

C-t1			**C-t2**			**C-t3**			**C-g1**			**C-g2**			**C-g3**			**C-g4**		
ν	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***	***ν***	***Δν***	***I***
3261		6	3256		8	3256		8	3268		5	3258		8	3263		6	3255		10
3248		1	3260		2	3258		2	3243		0	3262		2	3258		2	3265		2
3183		7	3176		8	3180		5	3184		6	3177		7	3177		15	3174		4
3176		2	3172		4	3170		2	3193		6	3189		7	3185		8	3180		3
3170		3	3162		2	3158		4	3159		2	3175		1	3173		2	3168		15
3160		1	3167		4	3168		7	3176		9	3172		8	3160		10	3155		8
1694	*-36*	28	**1708**	***-22***	**40**	**1707**	***-23***	**46**	1609	*-86*	25	1645	*-50*	42	1648	*-48*	82	1669	*-26*	45
1621	***-56***	**51**	**1649**	***-28***	**73**	**1649**	***-28***	**77**	1684	*-37*	8	1699	*-22*	2	1700	*-20*	3	1708	*-12*	3
1495	*-1*	3	1497	*1*	2	1496	*0*	3	1489	*3*	23	1489	*3*	16	1489	*3*	18	1489	*3*	11
1422	*-13*	5	1431	*-5*	6	1430	*-5*	4	1460	*2*	3	1461	*3*	4	1461	*3*	3	1462	*4*	4
1336	*4*	3	1335	*3*	2	1335	*3*	2	1312	*-12*	0	1322	*-2*	2	1324	*0*	4	1325	*1*	2
1317	*-12*	10	1326	*-4*	11	1325	*-5*	13	1362	*4*	7	1365	*7*	5	1369	*11*	10	1364	*6*	4
1255	*14*	3	1246	*6*	3	1248	*7*	2	1133	*18*	8	1121	*6*	15	1122	*7*	13	1119	*4*	12
1065	*0*	32	1066	*1*	37	1068	*3*	39	1038	*1*	2	1044	*7*	6	1052	*14*	10	1044	*7*	21
1019	*8*	3	1014	*3*	2	1014	*3*	2	1088	*12*	1	1079	*3*	1	1082	*5*	1	1076	*-1*	3
993	*-11*	5	1003	*-1*	1	1004	*0*	1	1017	*-9*	25	1028	*3*	19	1027	*2*	22	1031	*5*	15
968	*36*	16	963	*31*	19	960	*28*	17	965	*30*	31	957	*22*	56	963	*28*	43	961	*26*	60
947	***19***	**88**	**947**	***19***	**135**	**947**	***18***	**140**	951	*16*	45	945	*9*	60	939	*4*	104	952	*17*	54
917	*10*	4	911	*4*	4	912	*4*	4	908	*16*	9	897	*5*	6	899	*6*	7	891	*-1*	1
825	*43*	2	800	*18*	2	802	*20*	2	817	*60*	2	778	*20*	7	782	*24*	3	764	*6*	5
615	*75*	9	580	*40*	12	579	*39*	9	588	*110*	11	543	*65*	11	547	*68*	4	510	*31*	11
517	*1*	1	517	*1*	0	517	*1*	0	569	*-45*	3	594	*-20*	19	581	*-33*	10	606	*-7*	11
461	***-38***	**123**	**475**	***-25***	**113**	**475**	***-25***	**103**	451	*-49*	95	470	*-29*	123	470	*-29*	87	476	*-23*	101
457	***-38***	**129**	**463**	***-33***	**166**	**464**	***-32***	**170**	459	*-37*	155	462	*-34*	165	460	*-35*	166	463	*-33*	168
305		3	296		3	298		2	320		1	298		0	303		0	282		0
261		2	214		3	198		2	121		0	145		31	161		1	166		5
191		1	186		1	188		1	204		0	185		2	189		1	187		1
179		11	155		35	143		34	279		4	239		5	147		37	129		40
163		13	118		15	130		18	177		21	105		10	116		15	92		5
102		17	87		10	87		8	150		8	85		0	89		1	77		0
94		3	69		2	70		2	102		1	71		5	69		1	58		0
65		0	39		0	46		0	85		3	51		0	66		3	46		0
21		0	7		0	10		0	32		1	17		0	17		0	14		0

[a] Relative to the frequencies of free $SiCl_2$ and *trans*- or *gauche*-BD for conformers containing the BD moiety in the *trans*- or *gauche*-conformation, respectively, $\Delta\nu = \nu_{complex} - \nu_{reactant}$. The parameters for vibrations of the $SiCl_2$ moiety are shown on a green background. The parameters of vibrations, which are characterized by large intensities and large frequency shifts for conformers with the *trans*-BD moiety, are underlined and set off in bold. The parameters of vibrational modes observed in the experiment are in red.

Table S4 Experimentally obtained frequencies (ν_{exp}/cm^{-1}) of conformers of the BD•$SiCl_2$ complex and the comparison of their shifts relative to the corresponding frequencies of starting reactants (*trans*-BD and $SiCl_2$) with the shifts obtained in the performed calculations.

ν_{exp}	$\Delta\nu_{exp}$	$\Delta\nu_{calc}$[a]	$\Delta\nu_{calc}$[b]	**Vibration mode**
1863.1	47.4	-	-	combination band (ω(CH_2) in-phase + ω(CH_2) antiphase)
1586.0	-10.0	-19 - -41	-28 - -56	ν_{as}(C=C)
1364.1	-15.5	1 - -5	-5 - -13	δ_{sciss}(CH_2) antiphase
932.8 931.1 929.1 927.8 923.2 921.1	26.8 25.1 23.1 21.8 17.2 15.1	13 – 26[c]	18 – 35[c]	ω(CH_2)
482.3 476.4 473.4 470.7 469.9 467.8 465.5 461.0	-19.0 -24.9 -27.9 -30.6 -31.4 -33.5 -35.8 -40.3	-32 - -42	-32 - -38	ν_{as}(Si–Cl)

[a] the M06-2X/6-311++G(d,p) calculations; [b] the B3LYP/6-31G(d) calculations; [c] for both the in-phase and antiphase modes relative to the only experimentally observable band of *trans*-BD corresponding to the in-phase mode.

Table S5 The M06-2X/6-311++G(d,p) calculated energies ($\Delta E_0 = \Delta E$ + ZPE /kcal mol^{-1}, counterpoise corrected) of TSs for interconversions of selected conformers of the BD•$SiCl_2$ complex.

Connected conformers	**C-t1 – C-t2**	**C-t2 – C-t3**	**C-t1 – C-t3**	**C-t1 – C-g1**	**C-t1 – C-g1**	**C-t1 – C-g1a**	**C-t2 – C-g1**
ΔE_0 (relative to $SiCl_2$ + *trans*-BD)	-6.0	-5.5	-5.5	-0.7	-0.4	-0.5	-0.5
ΔE_0 (relative to the more stable conformer)	1.5	0.6	2.0	6.8	7.9	7.1	6.5
ΔE_0 (relative to the less stable conformer)	0.0	0.5	0.6	4.3	5.4	3.9	5.5

ΔE_0 for *gauche*-BD and TS(gauche-BD – trans-BD) relative to *trans*-BD are 2.8 and 5.8 kcal mol^{-1}, respectively.

Table S6 The experimentally observed and calculated bands of 1,1-dichloro-1-silacyclopent-3-ene (**1**).

bands of authentic sample		**bands observed upon photolysis of the complex**	**the B3LYP/ 6-31G(d) calculations**		**the M06-2X/ 6-311++G(d,p) calculations**		**approximate description**
ν/cm^{-1}	**I**	**ν/cm^{-1}**	**ν/cm^{-1}**	**I/ km mol^{-1}**	**ν/cm^{-1}**	**I/ km mol^{-1}**	
3055	w						
3052	w		3185	36	3206	17	CH sym. stretch
3049	m-w		3163	5	3184	1	CH antisym. stretch
3043	w		3087	9	3121	1	CH_2 stretch
3041	w		3087	0	3120	0	CH_2 stretch
2955	w		3053	2	3076	1	CH_2 stretch
2909	w		3053	14	3076	4	CH_2 stretch
2905	w						
1615	w						
1610	sh	1610.2					
1609	m-w	1609.0	1696	16	1702	18	C=C stretch
1607	sh						
1606	sh						
1603	w						
1404	w						
1400	m-w		1475	11	1443	0	CH_2 antisym. scissoring
1397	w		1474	0	1442	19	CH_2 sym. scissoring
1391	w						
1388	w						
1350	w		1391	0	1375	0	CH antisym. ip bend

1215 1209 1206 1204	w m-w vw w	1214.2 1208.7 1205.6 1204.1	1258	12	1248	20	CH_2 sym. wag + CH ip bend
1182 1181 1180 1173	w w sh w w	1182.4 1173.0	1227	7	1220	10	CH_2 sym. wag
1116 1108 1105 1104 1103 1099 1097 1096	w sh vs sh m s w s	 1108.2 1105.3 1104.0 1102.6 1098.8 1097.3 1096.1	 1146 1142 1132	 29 20 0	 1135 1131 1130	 31 32 0	 CH_2 wag + CH ip bend CH_2 twist + CH ip bend CH_2 twist
1085	vw		986	0	998	0	CH oop bend
949 946 945 944	m-w sh m sh	 944.7 943.6	965	11	966	17	C-C assym. stretch
909 907	vw vw		921	0	929	0	C-C sym. stretch
823 821 817	m m s	823.2 821.5 817.1	848 830 785	34 16 0	839 836 769	21 17 0	CH_2 rock Si-C assym. stretch + cycle ip deformation CH_2 rock
733 731[x] 729 723	s w s w	732.5 731.2 728.9 726.0	718	48	741	50	Si-C sym. stretch
664 662 661[x] 659 654	vs s sh s vs	 660.8 659.3 654.5	668	133	667	159	CH oop bend
645 644 642 639 637	w w m w vw		642	22	657	20	Si-C assym. stretch
577 574 571 568 566 563	vs sh vs m sh w br	576.5 573.7 571.5 568.1	552	106	564	123	SiCl sym. stretch

553 552 542 539	m-w sh m-w w						
521 519 517 515 512 510	w sh sh s w sh w sh w sh	517.5 514.4	537	90	536	76	SiCl assym. stretch
			377	0	371	0	
			351	0	359	0	
			226	9	225	9	
			225	1	221	2	
			167	3	169	3	
			156	0	156	0	
			35	1	3	1	

[x] appears on annealing

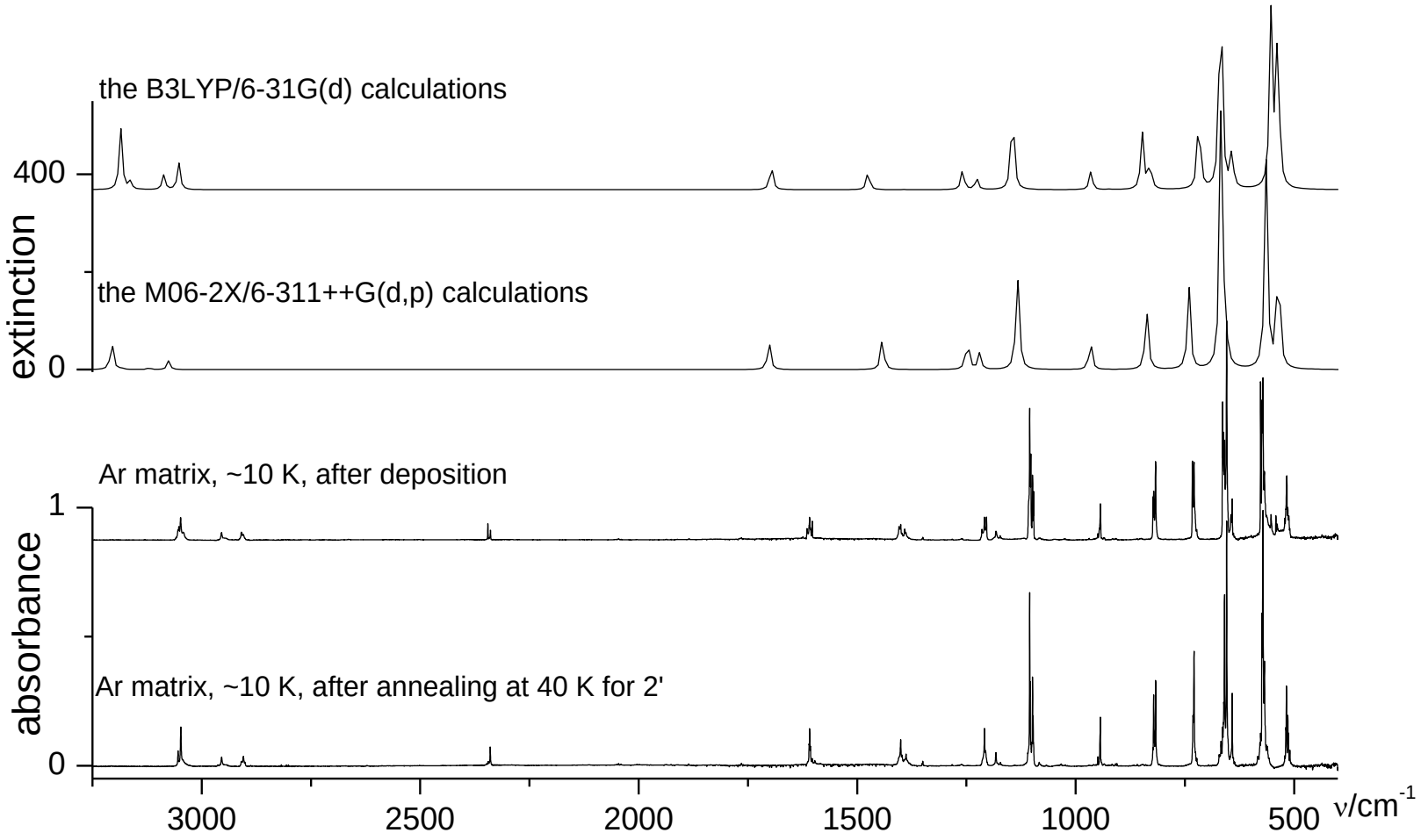


Figure S3 Calculated and experimental IR spectra of 1,1-dichloro-1-silacyclopent-3-ene (**1**).

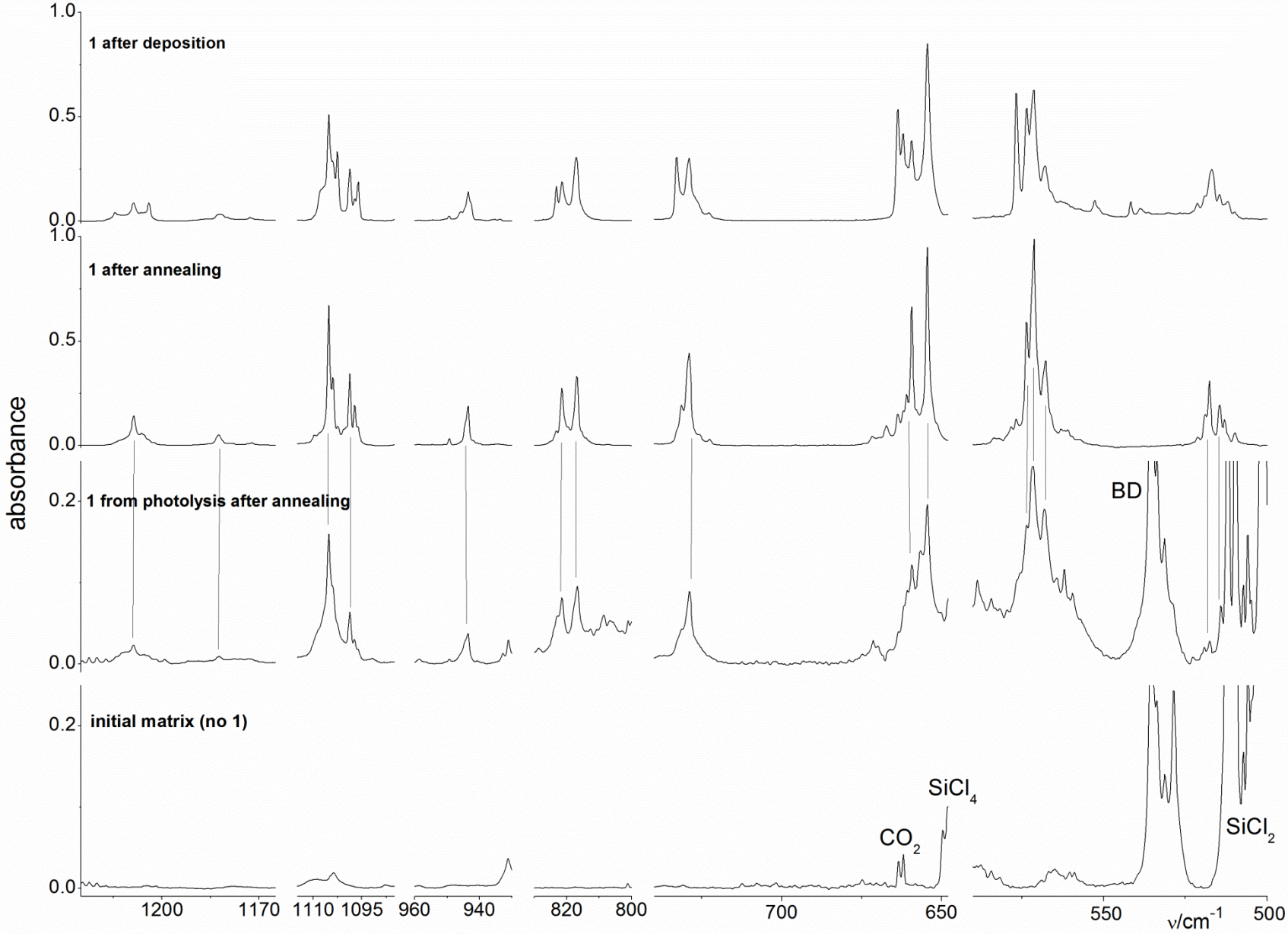
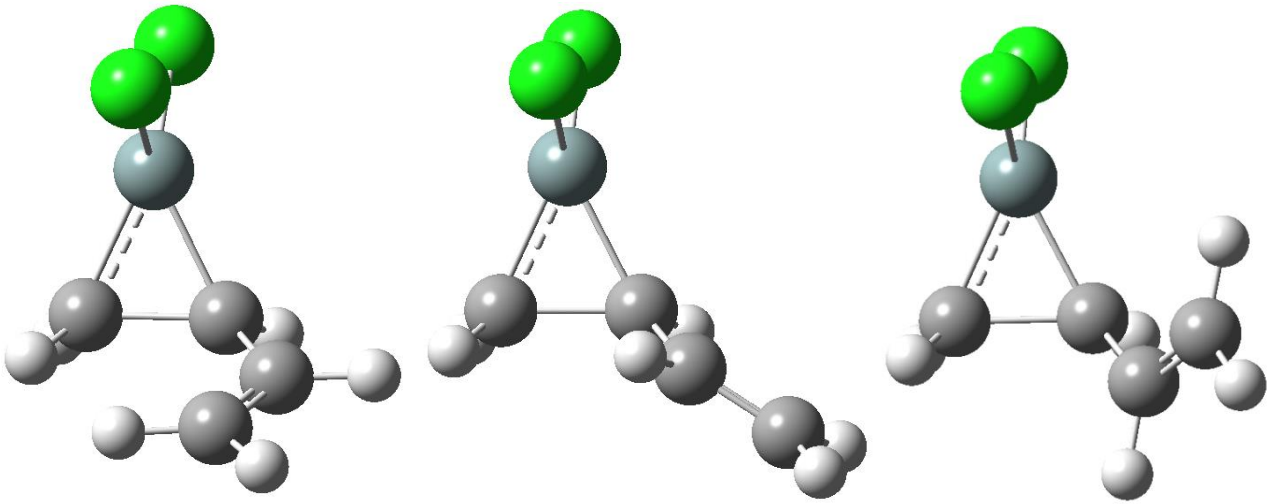


Figure S4 Comparison of the IR spectrum of **1** formed upon photolysis of the BD•$SiCl_2$ complex with the matrix IR spectrum of an authentic sample of **1**.



	cis-2	**trans-2**	**gauche-2**
ΔE_0	-19.2 (-17.1)	-18.8 (-17.0)	-17.8 (-16.0)
ΔH^0	-19.8 (-17.6)	-19.4 (-17.4)	-18.3 (-16.4)
ΔG^0	-7.3 (-5.7)	-7.0 (-5.6)	-5.8 (-4.6)

Figure S5 Conformers of 1,1-dichloro-2-vinylsilirane (**2**) and their energies ($\Delta E_0 = \Delta E$+ZPE /kcal mol^{-1}), enthalpies (ΔH^0/kcal mol^{-1}) and the Gibbs free energies (ΔG^0/kcal mol^{-1}) relative to starting $SiCl_2$ and *trans*-BD according to the M06-2X/6-311++G(d,p) and G3(MP2)//B3LYP (in parentheses) calculations.

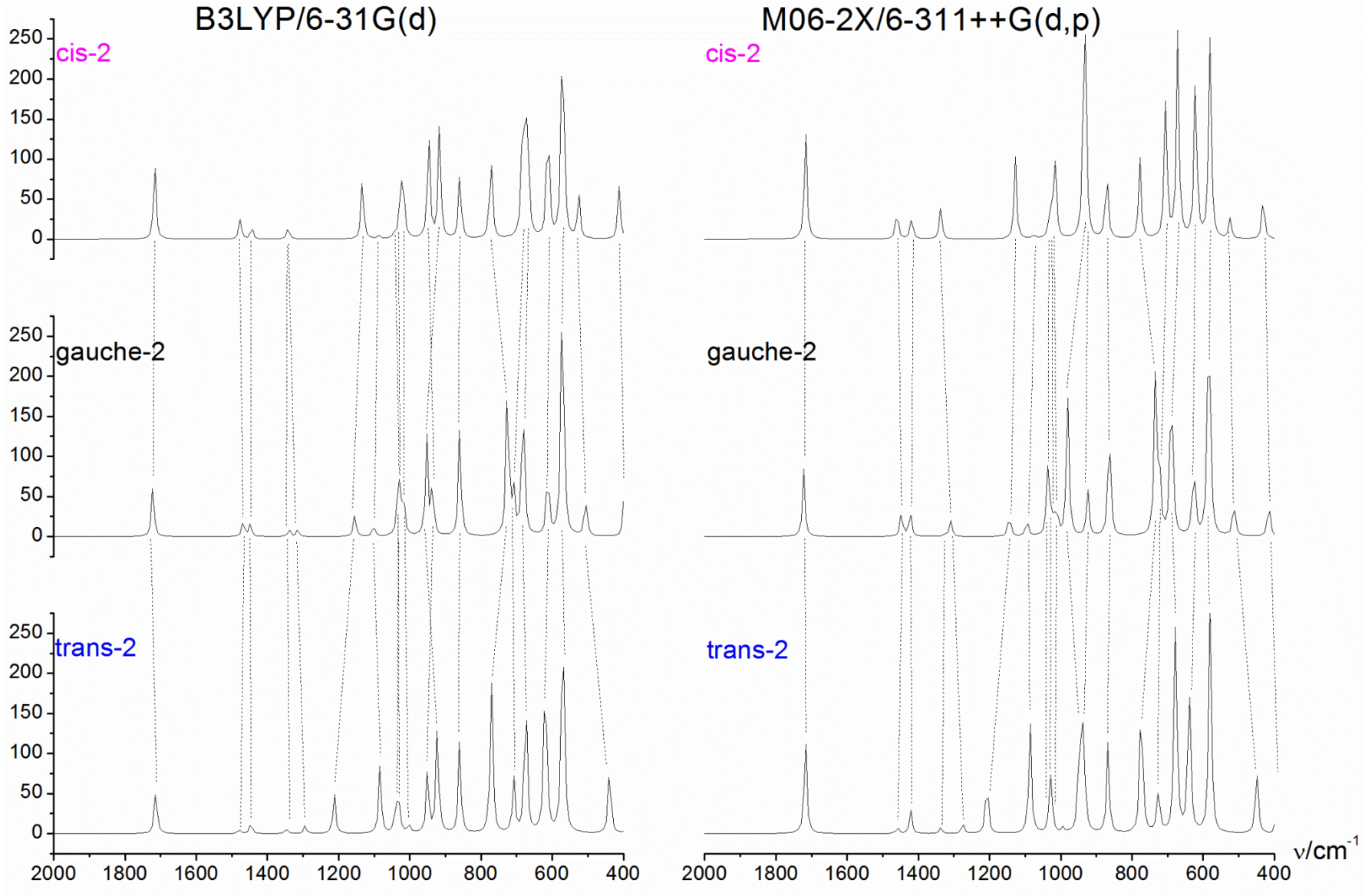


Figure S6 Theoretical IR spectra of conformers of 1,1-dichloro-2-vinylsilirane (**2**).

Table S7 Experimentally observed and calculated bands of 1,1-dichloro-2-vinylsilirane (**2**).

experiment			calculations										
			cis-**2**				*trans*-**2**				*gauche*-**2**				approximate description
			B3LYP/6-31G(d)		M06-2X/ 6-311++G(d,p)		B3LYP/6-31G(d)		M06-2X/ 6-311++G(d,p)		B3LYP/6-31G(d)		M06-2X/ 6-311++G(d,p)		
ν /cm^{-1}	I_{rel}/ %	annealing behaviour[a]	ν /cm^{-1}	I/ km mol^{-1}	ν /cm^{-1}	I/ km mol^{-1}	ν /cm^{-1}	I/ km mol^{-1}	ν /cm^{-1}	I/ km mol^{-1}	ν /cm^{-1}	I/ km mol^{-1}	ν /cm^{-1}	I/ km mol^{-1}	
			3248	17	3263	7	3244	16	3259	7	3246	17	3256	8	=CH_2 antisym. stretch
			3211	1	3232	0	3204	1	3225	0	3203	2	3224	0	CH_2 antisym. stretch
			3173	4	3182	1	3163	6	3169	2	3167	5	3167	2	=CH_2 sym. stretch
			3150	20	3170	11	3147	14	3157	6	3119	25	3141	14	=CH stretch
			3135	3	3151	1	3126	3	3139	1	3123	5	3135	1	CH_2 sym. stretch
			3110	4	3149	0	3124	2	3147	1	3091	5	3128	3	CH stretch
1632.0[b]	24	1631.5	1716	26	1717	43	1713	18	1717	39	1721	18	1722	24	C=C stretch
			1476	7	1460	12	1479	1	1458	2	1468	6	1447	9	=CH_2 scissoring
			1444	5	1419	9	1446	4	1421	8	1449	4	1423	9	CH_2 scissoring
			1340	3	1329	0	1347	2	1337	2	1339	3	1326	1	=CH bend
			1345	2	1337	11	1294	3	1276	4	1315	2	1309	6	CH bend
1179.9[c]		1179.9					1212	15	1207	22					=CH_2 rock
1172.7[c]		dec	1133	22	1128	31					1154	8	1145	8	=CH_2 rock
1064.3	3	1064.4	1087	1	1075	1	1084	26	1086	42	1102	4	1095	6	CH_2 rock + CH bend
			1042	2	1025	8	1039	13	1027	16	1032	17	1026	9	CH_2 wag
982.7	6	982.6	1026	12	1031	7	1029	9	1030	9	1030	9	1037	25	CH_2=CH twist
		977.9	1019	25	1016	28	1003	3	994	2	1018	17	1012	10	CH_2 wag + CH_2=CH rock
896.4[b]		896.5													
895.0	33	?	947	43	932	54	950	26	936	42	936	19	924	17	CH(H)-CH wag
893.2		893.6													
889.3[b]		dis													
886.7	16	886.3	916	40	935	47	922	42	948	38	953	37	980	50	=CH_2 wag
		884.3													

845.9 843.2	29	849.7 846.5 843.3	859	26	871	28	860	34	868	33	860	42	864	45	c-Si-C(H_2)-C(H) bend
754.1 751.9 749.2 742.9	55	755.5 754.3 dis ? 751.3 dis ? 747.5 743.4	772	34	778	30	771	56	774	59	726	63	734	59	Si-C assym. stretch
698.9	5	699	682	55	705	56	708	21	726	18	708	17	723	24	Si-C sym. stretch
658.0[c]	100	657.8	670	50	671	75	674	55	677	86	682	57	689	67	CH_2-CH rock
612.5[d]	27	612.5	612	48	622	61	620	72	639	62	613	26	626	29	CH_2=CH twist
577.6[c]	57	577.4 574.9	571	95	582	74	570	95	581	84	571	108	584	101	Si-Cl assym. stretch
			526	16	524	8	439	26	450	26	507	15	514	14	CCCC deformation
			412	20	431	18	385	6	398	3	399	14	416	13	Si-Cl sym. stretch
			299	1	322	1	303	4	309	4	325	2	331	3	
			278	6	275	7	278	4	277	5	241	8	245	9	
			188	2	189	2	203	4	207	5	185	2	187	3	
			166	5	167	5	168	4	169	4	171	3	172	3	
			147	2	146	2	137	1	136	2	128	1	138	1	
			99	1	97	1	90	1	86	1	88	0	93	0	
			58	0	53	0	70	1	69	1	67	0	74	0	

[a] dec = decay, dis = disappearance, numbers = appearing or remaining bands; [b] contributed by BD bands; [c] contributed by bands of **1**; [d] hidden by $SiCl_4$ bands, observed only when **1** was used as the precursor.

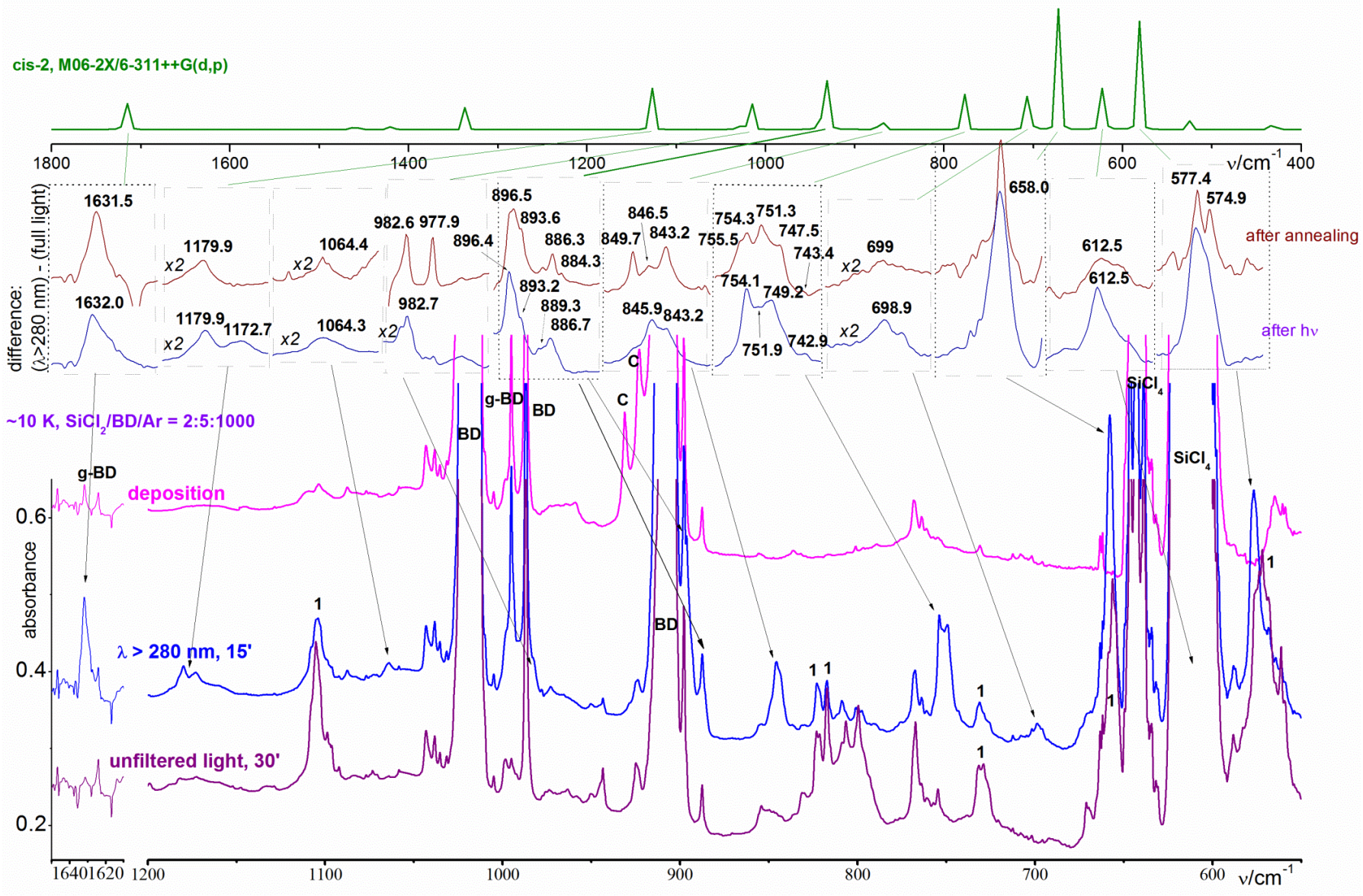


Figure S7 Calculated (for *cis*-**2**) and experimental IR spectra of 1,1-dichloro-2-vinylsilirane (**2**). The bands of complex are marked with "**C**".

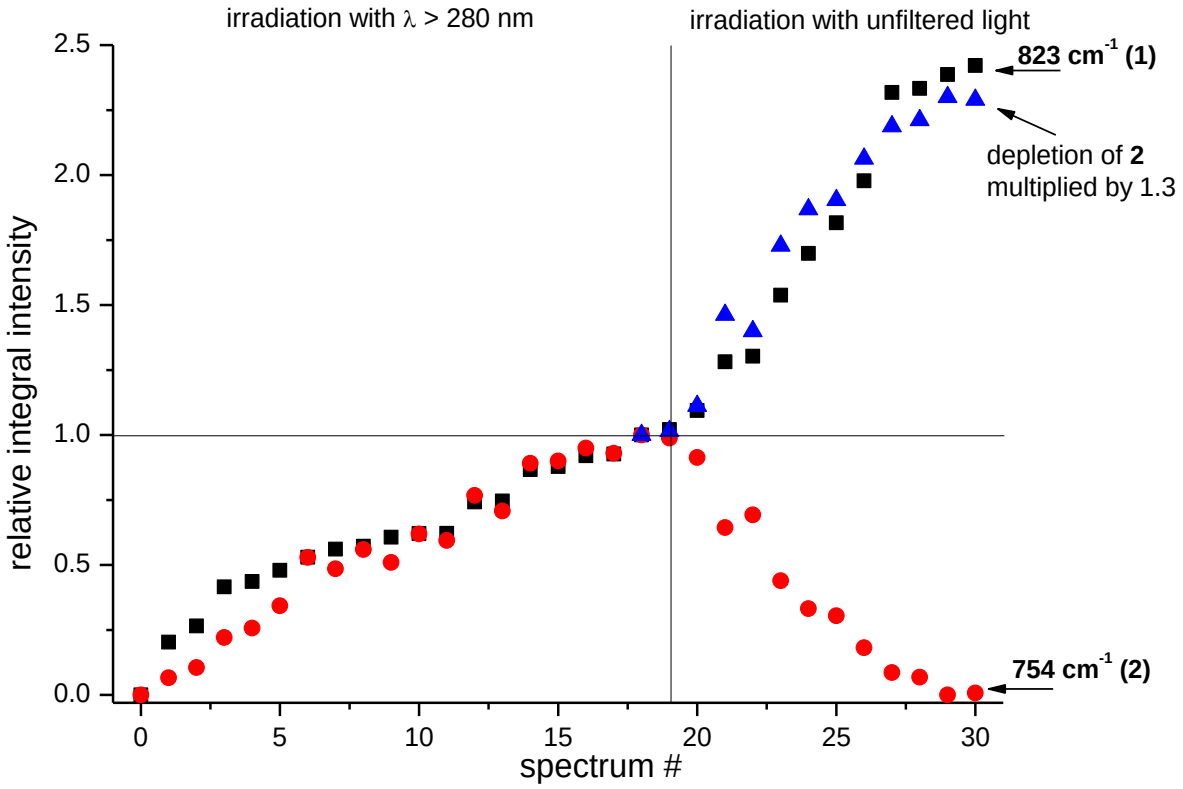


Figure S8 Curves of accumulation of **1** (black squares) and accumulation and decay of **2** (red circles) under irradiation with light with different λ based on the relative integral intensities of the bands at 823 (a band of **1**) and 754 cm^{-1} (a band of **2**) measured in several series of experiments. Integral intensities of bands measured in each series after irradiation of a matrix with light of λ > 280 nm (which resulted in complete transformation of the $SiCl_2$ + BD complex into **1** and **2**, but not gave rise to transformation of **2** into **1**) are taken as 1. Blue triangles correspond to depletion of **2** multiplied by 1.3 (ordinate = 1 + 1.3 * (1 – I_{rel}(754 cm^{-1})) and, hence, to the increment of **1** due to its formation from **2**. The coefficient 1.3 (1.3 ± 0.3) indicates that **1** and **2** are formed under irradiation at λ > 280 nm in a ratio of *ca.* 1 : 1.3 (actually, > 1 : 1.3 as **1** is not the only product of photoinduced transformation of **2**).

Series 1 ($SiCl_2$: BD : Ar = 5 : 2 : 1000): deposition (sp. 0), >450 nm, 19 min (sp. 1), > 400 nm, 16 min (sp. 4), > 400 nm, 15 min (sp. 5), > 350 nm, 15 min (sp. 7), > 350 nm, 15 min (sp. 11), > 300 nm, 15 min (sp. 12), >280 nm, 14 min (sp. 18), unfiltered, 10 min (sp. 22);

Series 2 ($SiCl_2$: BD : Ar = 1.25 : 2 : 1000): deposition (sp. 0), > 450, 15 min (sp. 2), > 400 nm, 15 min (sp. 3), > 350 nm, 15 min (sp. 8), >300 nm, 18 min (sp. 15), >280 nm, 10 min (sp. 18), > 350 nm, 30 min (sp. 19), > 250 nm, 15 min (sp. 20), unfiltered, 18 min (sp. 28), unfiltered, 15 min (sp. 30);

Series 3 ($SiCl_2$: BD : Ar = 5 : 2 : 1000): deposition (sp. 0), >330 nm, 3 min (sp. 9), >330 nm, 11 min (sp. 13), >330 nm, 31 min (sp. 14), >330 nm, 63 min (sp. 16), >280 nm, 10 min (sp. 18), unfiltered, 4 min (sp. 23), unfiltered, 4 min (sp. 25), unfiltered, 22 min (sp. 27);

Series 4 ($SiCl_2$: BD : Ar = 7 : 2 : 1000): deposition (sp. 0), >330 nm, 3 min (sp. 6), >300 nm, 3 min (sp. 10), >280 nm, 3 min (sp. 17), >280 nm, 7 min (sp. 18), unfiltered, 3 min (sp. 21), unfiltered, 7 min (sp. 24), unfiltered, 21 min (sp. 26), unfiltered, 51 min (sp. 29).

Total energies and Cartesian coordinates of atoms for stationary points found on PES of the $SiCl_2$ + BD system at the M06-2X/6-311++G(d,p) level of theory

***trans*-BD**
E(au) = -155.951054

Coordinates/Å	X	Y	Z
C	-1.72860400	-0.63482100	-0.00002000
C	-0.39568500	-0.61384500	-0.00002000
H	-2.30357500	0.28556400	0.00000900
H	-2.28255800	-1.56508700	-0.00005000
H	0.16046600	-1.54833900	-0.00005000
C	0.39568500	0.61384500	0.00002000
C	1.72860400	0.63482100	0.00002000
H	-0.16046600	1.54833900	0.00005000
H	2.28255800	1.56508700	0.00005000
H	2.30357500	-0.28556400	-0.00000900

***gauche*-BD**
E(au) = -155.946683

Coordinates/Å	X	Y	Z
C	0.000000	0.000000	2.056953
C	1.287776	0.000000	1.717296
H	-0.491885	-0.945849	2.269440
H	1.862767	-0.917333	1.687320
H	1.796948	0.918039	1.443573
C	-0.837386	1.207017	2.144570
C	-0.410690	2.389147	2.585351
H	-1.875711	1.097840	1.841732
H	-1.065759	3.251280	2.610283
H	0.602921	2.521010	2.948919

TS (*trans*-BD – *gauche*-BD)
E(au) = -155.941121

Coordinates/Å	X	Y	Z
C	0.67319900	0.37036100	-0.31439900
C	1.70534700	-0.32731600	0.14611600
H	0.80047700	0.99295100	-1.19765400
H	2.67079400	-0.29555500	-0.34479600
H	1.61286900	-0.95566800	1.02576500
C	-0.67319900	0.37036100	0.31439900

C	-1.70534700	-0.32731600	-0.14611600
H	-0.80047700	0.99295100	1.19765400
H	-2.67079400	-0.29555500	0.34479600
H	-1.61286900	-0.95566800	-1.02576500

$SiCl_2$

E(au) = -1209.934219

Coordinates/Å

	X	Y	Z
Si	0.00000000	0.00000000	0.94296200
Cl	0.00000000	1.60921300	-0.38827800
Cl	0.00000000	-1.60921300	-0.38827800

C-t1

E(au) = -1365.899400 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	1.36844700	-0.04078400	0.69070100
C	-1.53663400	0.04000100	1.00069400
C	-0.79745300	-0.68771700	1.86777600
Cl	1.10569900	-1.41264400	-0.90993600
Cl	0.86147600	1.77230000	-0.30485200
C	-2.05297000	-0.45693700	-0.25967200
H	-1.72126000	1.08938000	1.21668900
H	-0.50690200	-0.28422700	2.82971100
H	-0.63612000	-1.74932400	1.70548200
H	-1.92172500	-1.51250300	-0.47558000
C	-2.62764700	0.35591300	-1.14955800
H	-2.98714600	-0.01024900	-2.10284000
H	-2.73886000	1.41618100	-0.94732300

C-t2

E(au) = -1365.896273 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-0.80649100	0.16979100	0.88759300
C	1.54681100	-0.98377800	-0.63769000
C	0.69023200	-1.99528600	-0.43067600
Cl	-2.50219800	-0.62808900	-0.09059300
Cl	-0.38161600	1.79690200	-0.39631600
C	2.53695600	-0.54514600	0.34030000
H	1.49682400	-0.41990800	-1.56582300
H	-0.03587000	-2.28590900	-1.17953100
H	0.72583000	-2.58201400	0.48244400

H	2.63456000	-1.14229800	1.24338700
C	3.27928300	0.54956300	0.17284500
H	3.99632300	0.86843200	0.91879600
H	3.17835400	1.16266900	-0.71677600

C-t3

E(au) = -1365.896469 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-0.75000800	0.19533300	-0.90198700
C	1.64630800	-1.23914500	0.18250900
C	0.68127600	-1.52309600	1.06994800
Cl	-0.55334100	1.76051800	0.50871200
Cl	-2.45522500	-0.78306100	-0.12182600
C	2.49359500	-0.05130700	0.24609900
H	1.82645100	-1.91806300	-0.64828700
H	0.08372200	-2.42245900	0.98826100
H	0.48109900	-0.86796000	1.91214600
H	2.34026600	0.61705300	1.08878800
C	3.40243600	0.23553900	-0.68624100
H	4.01373700	1.12701000	-0.62626300
H	3.55877300	-0.41895700	-1.53776700

C-g1

E(au) = -1365.895428 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-1.21383100	0.19652700	0.83837200
Cl	-1.61938700	-1.12063800	-0.79122900
Cl	-0.39988000	1.84258100	-0.22511700
C	1.04273300	-0.53606500	1.65031100
C	1.31590900	-1.25071800	0.53259500
H	0.69639900	-1.03733100	2.54538400
H	1.35607600	0.49742100	1.75782800
C	1.90513700	-0.74497100	-0.69966100
H	1.01381500	-2.29413300	0.51739600
C	2.54215200	0.42351300	-0.81249200
H	1.78694900	-1.37547800	-1.57441400
H	2.92722500	0.75790600	-1.76752800
H	2.70511700	1.07665600	0.03749100

C-g1a

E(au) = -1365.894211 (counterpoise corrected)

Coordinates/Å

	X	Y	Z

Si	-1.04959400	0.11576300	0.95538800
C	1.21275700	-1.01339000	-0.48329100
C	0.86042300	-1.51862100	0.71826600
Cl	-2.21623600	-0.79352500	-0.57914400
Cl	-0.36678500	1.85040300	-0.06673400
C	2.27991900	-0.03504500	-0.69320400
H	0.64023400	-1.30902800	-1.35888800
H	0.14647400	-2.33183200	0.78879600
H	1.40044800	-1.24890500	1.62010600
H	2.12949300	0.67397600	-1.50153800
C	3.40125900	0.00152600	0.02675800
H	4.16263700	0.74822300	-0.16074500
H	3.60023600	-0.72686100	0.80558800

C-g2

E(au) = -1365.892801 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-0.66390600	0.06156200	0.82852100
C	1.53484500	-0.69396500	-0.99352100
C	0.87325300	-1.74504000	-0.47416600
Cl	-2.41687600	-0.77663300	-0.01500900
Cl	-0.51556200	1.81874700	-0.34898400
C	2.61226200	0.04617000	-0.33180700
H	1.22870200	-0.32275100	-1.96723600
H	0.08328100	-2.23331700	-1.03118000
H	1.18427300	-2.21311200	0.45354500
H	3.17747600	0.72640300	-0.95992900
C	2.88915100	-0.01765900	0.97251800
H	3.68562000	0.57739400	1.40097500
H	2.32970600	-0.64944600	1.65427200

C-g3

E(au) = -1365.891572 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	0.85878200	0.13920900	0.91902400
C	-1.59790300	-1.41770600	0.14834200
C	-0.85943500	-1.39025900	-0.97063300
Cl	0.43705400	1.79697400	-0.32063500
Cl	2.43349700	-0.75227500	-0.17501800
C	-2.52630600	-0.36317500	0.58354400
H	-1.50634600	-2.27651200	0.80859100
H	-0.21757400	-2.22113300	-1.23582400
H	-0.88477200	-0.54587400	-1.65174900
H	-2.71947100	-0.30733100	1.65095800

C	-3.13353200	0.49326500	-0.23593600
H	-3.79024500	1.26406600	0.14722100
H	-3.00085300	0.44523200	-1.31135200

C-g4

E(au) = -1365.892186 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	0.69812300	0.13008200	-0.88819800
C	-2.74304700	-0.56756200	-0.38847400
C	-2.89239900	0.75624000	-0.39455900
Cl	2.20605500	-1.10749900	-0.07250900
Cl	0.86478300	1.81344700	0.38761800
C	-1.63190100	-1.27393700	0.26954300
H	-3.45755000	-1.18860500	-0.92050700
H	-3.73527900	1.22177200	-0.88976300
H	-2.17375400	1.41580400	0.08295100
H	-1.31976200	-2.21441700	-0.17988100
C	-1.02308500	-0.86040600	1.38920200
H	-0.20446200	-1.42037500	1.82512500
H	-1.34457100	0.03755000	1.90573900

C-g5

E(au) = -1365.891221 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
C	-2.72511300	-0.44202200	-0.48700100
H	-2.71958300	-1.00112900	-1.41855800
C	-3.66699000	0.47500000	-0.27565400
H	-3.73323100	1.01128200	0.66495800
H	-4.41050400	0.70008800	-1.03002100
C	-1.67798900	-0.78624700	0.48744100
H	-1.35090600	-1.82373200	0.50511600
C	-1.10359100	0.08501100	1.32885900
H	-1.36905500	1.13716100	1.31954400
H	-0.35929600	-0.23524000	2.04848800
Si	0.80558500	0.03085400	-0.89912800
Cl	1.83845100	-1.50483200	0.13066600
Cl	1.55604800	1.72772500	0.11500500

TS (C-t1 – C-t2)

E(au) = -1365.896234 (counterpoise corrected)

Coordinates/Å

	X	Y	Z

Si	-0.89093000	0.14757700	0.91202200
C	1.49911800	-1.04494300	-0.56000000
C	0.66574600	-2.03113300	-0.19204200
Cl	-0.30052200	1.79821700	-0.27394100
Cl	-2.50353000	-0.57012200	-0.25419300
C	2.56313000	-0.52466700	0.29027800
H	1.37418700	-0.57048300	-1.53035800
H	-0.10795800	-2.39676900	-0.85539500
H	0.78034100	-2.53119600	0.76485200
H	2.72744400	-1.03099800	1.23804100
C	3.29879000	0.53579900	-0.04406200
H	4.07474600	0.91667100	0.60791700
H	3.13243400	1.05874600	-0.98013200

TS (C-t2 – C-t3)

E(au) = -1365.895237 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-0.69218000	0.02058500	-0.88862300
C	1.76015500	-0.57904700	0.71721900
C	0.91417800	-0.17430400	1.67516200
Cl	-1.47681300	1.72476600	0.08408400
Cl	-1.89868600	-1.49281300	-0.03601900
C	2.72484900	0.30085800	0.06175500
H	1.75316600	-1.61971100	0.39795900
H	0.21745100	-0.85805200	2.14434300
H	0.90882800	0.85502900	2.01846400
H	2.74538200	1.33541800	0.39525800
C	3.54517700	-0.10943500	-0.90497800
H	4.24836100	0.56540600	-1.37627300
H	3.53464900	-1.13791400	-1.25108700

TS (C-t1 – C-t3)

E(au) = -1365.895406 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	1.14552000	0.16107600	0.94231300
C	-1.69295000	-1.16860000	0.40170900
C	-0.62554000	-1.91914600	0.08472000
Cl	0.23934400	1.76612200	-0.08170200
Cl	2.43247000	-0.56642400	-0.57397100
C	-2.40979700	-0.33508900	-0.55178300
H	-2.05572500	-1.15713900	1.42755000
H	-0.14903500	-2.56478800	0.81308200
H	-0.25688800	-1.96546100	-0.93491100
H	-2.04092500	-0.32931300	-1.57374100
C	-3.46232500	0.40914300	-0.21026000

H	-3.97824800	1.02765700	-0.93354400
H	-3.83362700	0.42127800	0.80931300

TS (C-t1 – C-g1), *syn*

E(au) = -1365.885401 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	1.30639400	0.06816600	0.86154600
C	-1.89883400	0.53220900	0.78772200
C	-1.37313800	-0.20167100	1.77509200
Cl	1.19181300	-1.63702300	-0.37205600
Cl	1.15199100	1.60007100	-0.59011700
C	-2.55937500	-0.03545400	-0.41322900
H	-1.89848700	1.61729200	0.88033600
H	-1.00106500	0.26299000	2.68116000
H	-1.38209700	-1.28655000	1.73301700
H	-3.62242900	-0.24025300	-0.29941200
C	-1.96645900	-0.27944700	-1.57546000
H	-2.52802100	-0.69624300	-2.40295000
H	-0.91523000	-0.07719400	-1.74159900

TS (C-t1 – C-g1), *anti*

E(au) = -1365.887490 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-1.41477900	0.02816400	0.76940800
C	1.53337300	-0.54181400	0.77108400
C	1.06582900	0.23878000	1.75769400
Cl	-1.09425600	1.65169400	-0.55471900
Cl	-1.26189000	-1.57989600	-0.60860300
C	2.01579100	-0.03899700	-0.53543000
H	1.54531700	-1.62051700	0.91587200
H	0.78857900	-0.18153200	2.71751000
H	1.06957000	1.32033400	1.66392000
H	1.25383400	0.22903700	-1.26590600
C	3.30301600	0.07341400	-0.84054900
H	3.61469100	0.43867100	-1.81127200
H	4.08134100	-0.18915500	-0.13217100

TS (C-t1 – C-g1a)

E(au) = -1365.887018 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-1.26830200	0.08924200	0.88623800

C	1.38225400	-0.85579400	-0.11951500
C	0.91375700	-1.35444000	1.03625100
Cl	-2.03816100	-1.01410600	-0.75773200
Cl	-0.64312500	1.85823200	-0.10534000
C	2.40383900	0.21280600	-0.20186800
H	0.98586800	-1.24018600	-1.05778600
H	0.24042600	-2.20533400	1.04235800
H	1.30564400	-1.01890900	1.99080000
H	2.05202800	1.23174300	-0.05240000
C	3.68352400	-0.02348000	-0.46573200
H	4.39883800	0.78773300	-0.52267800
H	4.05504500	-1.02912700	-0.63022000

TS (C-t2 – C-g1)

E(au) = -1365.885051 (counterpoise corrected)

Coordinates/Å

	X	Y	Z
Si	-0.84822700	0.20782800	0.87969700
C	1.67374300	-0.94883400	-0.74661400
C	0.90675000	-1.89523400	-0.19749700
Cl	-2.45299600	-0.80611700	-0.04051600
Cl	-0.54550400	1.75461300	-0.53041400
C	2.89390500	-0.40204400	-0.10178200
H	1.42539700	-0.57164900	-1.73696500
H	0.05881500	-2.31107500	-0.72933300
H	1.14361800	-2.31205900	0.77651200
H	3.80633400	-0.97221300	-0.26556700
C	2.93954200	0.70746400	0.62616700
H	3.86959500	1.04295000	1.06893300
H	2.06226600	1.32190000	0.79482900

1

E(au) = -1365.982613

Coordinates/Å

	X	Y	Z
Si	-0.19507800	-0.02555200	0.00000000
C	1.02328700	-0.13951800	1.41661500
C	1.02328700	-0.13951800	-1.41661500
Cl	-1.21400200	1.76662700	0.00000000
Cl	-1.60066300	-1.53176500	0.00000000
C	2.33991100	-0.08942500	0.66772000
C	2.33991100	-0.08942500	-0.66772000
H	0.91623000	-1.07130300	1.97912000
H	0.92597500	0.68429900	2.12771500
H	3.26879900	-0.05680200	1.22788100
H	3.26879900	-0.05680200	-1.22788100
H	0.92597500	0.68430000	-2.12771400

H	0.91622900	-1.07130200	-1.97912100

***cis*-2**

E(au) = -1365.918619

Coordinates/Å

	X	Y	Z
Si	-0.48516200	-0.08292400	0.13226100
C	0.95358000	-1.14630300	-0.28782700
C	0.57169600	-1.05220200	1.24580400
Cl	-0.31526700	1.94391300	0.05130200
Cl	-2.39607000	-0.66626000	-0.28366200
C	2.22618700	-0.57179900	-0.77994900
H	0.69948100	-2.10572000	-0.73249300
H	0.20405500	-1.97842800	1.67450400
H	1.28985600	-0.54773300	1.88340400
H	2.39580800	-0.70329400	-1.84553300
C	3.12597200	0.10243200	-0.06768900
H	4.01157900	0.50755300	-0.54027600
H	3.01959700	0.27568900	0.99682300

***trans*-2**

E(au) = -1365.917850

Coordinates/Å

	X	Y	Z
Si	-0.52419600	-0.06442800	0.18888500
C	1.17976200	-0.74096500	0.13877700
C	0.48793900	-0.63906900	1.57731600
Cl	-0.83934600	1.93202300	-0.08701400
Cl	-2.11112200	-1.15117900	-0.48904000
C	2.36952100	0.10175700	-0.10034200
H	1.27662900	-1.76376400	-0.21828300
H	0.29305900	-1.59044200	2.06059700
H	0.94629500	0.09020300	2.23909600
H	2.34059300	1.10422500	0.32361100
C	3.43915800	-0.27789900	-0.79488700
H	4.27543100	0.39237900	-0.94835300
H	3.50640600	-1.26791100	-1.23333800

***gauche*-2**

E(au) = -1365.916142

Coordinates/Å

	X	Y	Z
Si	-0.45907600	-0.10690900	0.18596500
C	2.78956400	0.38014200	-0.92013300

C	0.38760400	-1.17718000	1.38581400
Cl	-2.26873800	-0.63674200	-0.59568900
Cl	-0.31588800	1.92310700	0.32210500
C	2.40630900	-0.68208300	-0.22036700
C	1.00242700	-1.16261000	-0.08975000
H	3.83190500	0.67086700	-0.97427000
H	2.07293800	0.98781600	-1.46263400
H	3.15324700	-1.26633900	0.31617900
H	0.80617100	-2.09805500	-0.61259100
H	1.02212300	-0.69751500	2.12649700
H	-0.03611300	-2.11787300	1.72086300

Total energies and Cartesian coordinates of atoms for stationary points found on PES of the $SiCl_2$ + BD system at the G3(MP2)//B3LYP level of theory

***trans*-BD**

E_0(au) = -155.707316

Coordinates/Å	X	Y	Z
C	0.60193100	1.75134900	0.00000000
C	0.60193100	0.41079300	0.00000000
C	-0.60193100	-0.41079300	0.00000000
C	-0.60193100	-1.75134900	0.00000000
H	1.52443400	2.32401800	0.00000000
H	-0.32521100	2.32054200	0.00000000
H	1.55157100	-0.12522000	0.00000000
H	-1.55157100	0.12522000	0.00000000
H	-1.52443400	-2.32401800	0.00000000
H	0.32521100	-2.32054200	0.00000000

***gauche*-BD**

E_0(au) = -155.702652

Coordinates/Å	X	Y	Z
C	-0.24971000	1.52498800	-0.49359300
C	-0.24971000	0.69135600	0.55446400
C	0.24971000	-0.69135600	0.55446400
C	0.24971000	-1.52498800	-0.49359300
H	-0.65587400	2.52958300	-0.41892700
H	0.16605900	1.23611200	-1.45575300
H	-0.63018800	1.05543900	1.50945400
H	0.63018800	-1.05543900	1.50945400
H	0.65587400	-2.52958300	-0.41892700
H	-0.16605900	-1.23611200	-1.45575300

$SiCl_2$

E_0(au) = -1208.648406

Coordinates/Å	X	Y	Z
Cl	0.00000000	1.64238700	-0.38609100
Si	0.00000000	0.00000000	0.93765000
Cl	0.00000000	-1.64238700	-0.38609100

C-t1

E_0(au) = -1364.364361

Coordinates/Å	X	Y	Z
C	2.44314600	-0.11456400	0.08805900
H	2.68492800	0.49044800	0.96019800
C	3.09358000	0.08847200	-1.07078000
H	2.86576300	-0.49448800	-1.95984300
H	3.86875000	0.84223900	-1.16543700
C	1.41166300	-1.11413600	0.24059300
H	1.17636000	-1.71112400	-0.63932400
C	0.68567200	-1.31429900	1.37951300
H	0.94823100	-0.80492400	2.30422600
H	0.03566300	-2.17929600	1.47579400
Si	-1.28220800	0.11795300	0.81375700
Cl	-1.92390900	-0.90048000	-0.96742200
Cl	-0.39568800	1.89653700	0.01492100

C-t2

E_0(au) = -1364.362442

Coordinates/Å	X	Y	Z
C	1.83503600	-0.64001500	-0.67699200
H	1.84329400	0.09629300	-1.47982300
C	0.84716800	-1.56443600	-0.64551700
H	0.82457500	-2.34403300	0.11276200
H	0.11683400	-1.63991200	-1.44472800
C	2.88958800	-0.52791800	0.31472300
H	2.89202900	-1.26498300	1.11705300
C	3.83326800	0.42597600	0.28015400
H	3.85437600	1.17647900	-0.50652900
H	4.61189900	0.48684500	1.03414200
Si	-0.91486900	0.08478700	0.85007500
Cl	-2.58229000	-0.91337300	-0.04278600
Cl	-0.81566400	1.86282300	-0.33181000

C-t3

E_0(au) = -1364.362617

Coordinates/Å	X	Y	Z
C	-2.69300800	-0.12543100	-0.41437700
H	-2.36269600	0.31108200	-1.35535800
C	-3.81345000	0.32077600	0.17513900
H	-4.16594500	-0.09469300	1.11653700
H	-4.41271000	1.11254700	-0.26329500
C	-1.87161500	-1.18380300	0.14384700

H	-2.20093200	-1.60013800	1.09619800
C	-0.73964300	-1.66187800	-0.42275100
H	-0.39939600	-1.30998100	-1.39373400
H	-0.20340300	-2.50276500	0.00611300
Si	1.05288600	0.11136800	0.91166500
Cl	0.53931400	1.82570400	-0.25369100
Cl	2.62015500	-0.74177400	-0.26753900

C-g1

E_0(au) = -1364.359806

Coordinates/Å

	X	Y	Z
C	2.12407700	-0.77860600	-0.73883400
H	2.22955900	-1.24851000	-1.71412800
C	2.80472700	0.35800600	-0.49480200
H	2.75507300	0.87882100	0.45617700
H	3.44229100	0.80091200	-1.25340700
C	1.22252000	-1.44465200	0.17751300
H	0.77330300	-2.36196900	-0.19780900
C	0.81552600	-1.02178700	1.42037700
H	1.31087900	-0.19539200	1.92561800
H	0.29386500	-1.71868900	2.07002700
Si	-1.12857100	0.24603600	0.85964500
Cl	-2.00947400	-0.83553200	-0.77928900
Cl	-0.15558900	1.87803600	-0.13288900

C-g2

E_0(au) = -1364.358297

Coordinates/Å

	X	Y	Z
C	1.74712400	-0.46384600	-1.03121000
H	1.51828000	0.02973200	-1.97394800
C	0.96198700	-1.50714200	-0.66053200
H	1.18809700	-2.11739600	0.20950500
H	0.19292400	-1.88467700	-1.32692400
C	2.84945500	0.11640700	-0.26950900
H	3.44167400	0.86129700	-0.79712600
C	3.14895300	-0.15612200	1.01148400
H	2.58102500	-0.86635200	1.60622800
H	3.97653300	0.33808800	1.51078000
Si	-0.72178000	0.00636800	0.78506000
Cl	-2.46456800	-0.95341100	-0.00528700
Cl	-0.77300400	1.87190400	-0.26063900

C-g3

E_0(au) = -1364.357754

Coordinates/Å

	X	Y	Z
C	2.85007600	-0.16887500	-0.08096000
H	3.68923500	0.07427300	-0.72984200
C	2.73430800	0.48400600	1.08751800
H	1.91934400	0.30364200	1.78218600
H	3.46059200	1.23498900	1.38229000
C	1.93547100	-1.18064600	-0.59857200
H	2.17063900	-1.54970300	-1.59643100
C	0.83301800	-1.68767100	0.00752800
H	0.56728200	-1.43541600	1.03030300
H	0.28833100	-2.51324100	-0.44045400
Si	-1.13704200	-0.01387800	-0.93379600
Cl	-2.39599800	-0.65372300	0.68006600
Cl	-0.32718300	1.79483200	-0.14171300

C-g4

E_0(au) = -1364.358768

Coordinates/Å

	X	Y	Z
C	1.86478800	-1.31298800	0.17164900
H	1.70065600	-2.27198500	-0.31993800
C	1.08632700	-1.00524600	1.23034900
H	1.23425700	-0.09857200	1.81001500
H	0.32296100	-1.69105100	1.58397200
C	2.94873800	-0.49622400	-0.38666300
H	3.67900500	-1.03915100	-0.98510400
C	3.08570900	0.83018700	-0.24893300
H	2.36486400	1.43644400	0.29368300
H	3.92447000	1.35663100	-0.69419200
Si	-0.80027500	0.08790800	-0.85059100
Cl	-0.91228900	1.85183000	0.35318300
Cl	-2.37804800	-1.08814800	-0.02251100

1

E_0(au) = -1364.446529

Coordinates/Å

	X	Y	Z
Si	0.00000000	0.00000000	0.19594100
C	0.00000000	1.42781300	-1.04075700
C	0.00000000	-1.42781300	-1.04075700
Cl	-1.68184700	0.00000000	1.42202400
Cl	1.68184700	0.00000000	1.42202400
C	0.00000000	0.67066200	-2.35602600
C	0.00000000	-0.67066200	-2.35602600

H	0.88039300	2.07495400	-0.93828800
H	-0.88039300	2.07495400	-0.93828800
H	0.00000000	1.23255800	-3.28872200
H	0.00000000	-1.23255800	-3.28872200
H	-0.88039300	-2.07495400	-0.93828800
H	0.88039300	-2.07495400	-0.93828800

***cis*-2**

E_0(au) = -1364.383017

Coordinates/Å

	X	Y	Z
Si	-0.49211600	-0.07144600	0.12940600
C	1.01187400	-1.08739200	-0.26480400
C	0.61979800	-0.97213400	1.27350100
Cl	-0.45154100	1.98426800	0.03300700
Cl	-2.38339300	-0.79006000	-0.28217200
C	2.28790200	-0.53103100	-0.77977900
H	0.76957200	-2.06735500	-0.68349900
H	0.31159500	-1.90547500	1.74213900
H	1.31091300	-0.40643600	1.89621600
H	2.42052400	-0.64441600	-1.85608300
C	3.24058700	0.09161300	-0.07941300
H	4.13061800	0.47738000	-0.56709300
H	3.17930700	0.23868000	0.99540900

***trans*-2**

E_0(au) = -1364.382767

Coordinates/Å

	X	Y	Z
Si	-0.52668700	-0.05587300	0.18504400
C	1.21638600	-0.68999500	0.15715900
C	0.51046900	-0.56877500	1.59884300
Cl	-0.93416400	1.94303600	-0.11865700
Cl	-2.08518500	-1.23782200	-0.47165200
C	2.41545300	0.13453300	-0.11071700
H	1.31622800	-1.72594700	-0.17273500
H	0.35395000	-1.51294500	2.11849200
H	0.94032500	0.19507100	2.24701600
H	2.39479400	1.15386200	0.27694600
C	3.49084000	-0.27789300	-0.78914400
H	4.33638000	0.38035700	-0.96548500
H	3.56199700	-1.28404200	-1.19644700

***gauche*-2**

E_0(au) = -1364.381170

Coordinates/Å

	X	Y	Z
Si	-0.46214200	-0.09664300	0.18879500
C	2.85700800	0.37685500	-0.93045900
C	0.41321000	-1.12386100	1.42864500
Cl	-2.26186300	-0.72277700	-0.60602400
Cl	-0.40052600	1.96075500	0.29329900
C	2.45106100	-0.66987300	-0.20957700
C	1.04159000	-1.13265400	-0.05256100
H	3.90848500	0.64209000	-1.00011700
H	2.15706700	1.00132500	-1.47953100
H	3.19539500	-1.26643500	0.32404500
H	0.84581700	-2.08849400	-0.54847800
H	1.02918800	-0.61262600	2.16890100
H	0.01743500	-2.07129000	1.79208500