# The conformational behavior and structure of monosubstituted 1,3,5-trisilacyclohexanes. Part II: 1-Methoxy-1,3,5-trisilacyclohexane

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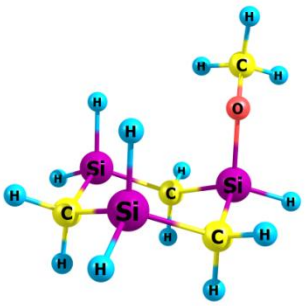
## Оглавление

**Cartesian coordinates (Å) and absolute energies (a.u.) for** 1-Methoxy-1,3,5-trisilacyclohexane **of computed structures. The structures were confirmed to be minima through vibrational analysis.**

**M062X/6-311G****

**I** (*g*-Ax)

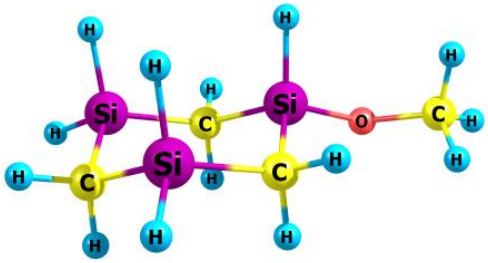


E(RM062X) = -1104.54563839

| | | | |
|---|---|---|---|
| 14 | -1.325074000 | 0.645559000 | 0.158682000 |
| 6 | -0.121519000 | 0.885250000 | 1.559368000 |
| 6 | -0.494075000 | 1.060906000 | -1.469308000 |
| 14 | 1.429141000 | -0.170160000 | 1.367781000 |
| 14 | 1.028793000 | -0.006142000 | -1.775047000 |
| 6 | 2.199955000 | 0.181034000 | -0.315525000 |
| 1 | -2.571099000 | 1.438335000 | 0.326174000 |
| 8 | -1.702191000 | -0.973006000 | 0.178185000 |
| 6 | -2.495750000 | -1.571285000 | -0.825211000 |
| 1 | -3.458080000 | -1.057537000 | -0.936520000 |
| 1 | -2.686048000 | -2.605721000 | -0.540104000 |
| 1 | -1.979782000 | -1.566956000 | -1.792240000 |
| 1 | -0.611674000 | 0.653451000 | 2.509345000 |
| 1 | 0.176260000 | 1.939145000 | 1.600632000 |
| 1 | -1.200230000 | 0.958627000 | -2.299476000 |
| 1 | -0.186058000 | 2.112859000 | -1.450715000 |
| 1 | 1.084187000 | -1.606236000 | 1.472415000 |
| 1 | 2.400705000 | 0.154459000 | 2.442636000 |
| 1 | 0.616292000 | -1.425753000 | -1.909699000 |
| 1 | 1.701421000 | 0.393659000 | -3.036749000 |
| 1 | 3.071350000 | -0.465095000 | -0.458437000 |
| 1 | 2.573933000 | 1.211588000 | -0.310804000 |

**M062X/6-311G****

**III** (*g*-Eq)




E(RM062X) = -1104.54495110

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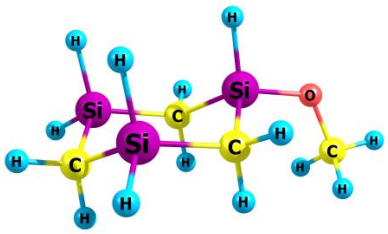
| 6 | -0.231910000 | -0.229366000 | 1.588498000 |
| 6 | -0.183329000 | 0.788258000 | -1.292383000 |
| 14 | 1.614368000 | -0.595607000 | 1.531221000 |
| 14 | 1.665131000 | 0.460601000 | -1.426511000 |
| 6 | 2.428924000 | 0.560514000 | 0.290636000 |
| 8 | -2.646038000 | 0.157192000 | -0.012342000 |
| 1 | -1.008999000 | -1.742278000 | -0.550388000 |
| 6 | -3.577918000 | -0.470539000 | 0.843935000 |
| 1 | -3.345453000 | -0.272699000 | 1.896189000 |
| 1 | -3.600552000 | -1.555679000 | 0.687852000 |
| 1 | -4.567407000 | -0.069267000 | 0.625718000 |
| 1 | -0.711622000 | -0.917015000 | 2.292604000 |
| 1 | -0.370192000 | 0.783527000 | 1.985518000 |
| 1 | -0.650451000 | 0.703156000 | -2.277830000 |
| 1 | -0.331023000 | 1.822269000 | -0.959913000 |
| 1 | 1.820143000 | -1.999166000 | 1.091841000 |
| 1 | 2.221006000 | -0.441686000 | 2.876325000 |
| 1 | 1.885272000 | -0.902291000 | -1.973313000 |
| 1 | 2.301579000 | 1.434974000 | -2.346078000 |
| 1 | 3.499393000 | 0.342524000 | 0.231473000 |
| 1 | 2.335632000 | 1.589266000 | 0.656566000 |

**M062X/6-311G****

**IV** (*tr*-Eq)




E(RM062X) = -1104.54447475

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| 6 | -0.094300000 | -0.290128000 | 1.760936000 |
| 6 | -0.467413000 | 0.075113000 | -1.219698000 |
| 14 | 1.780721000 | -0.254507000 | 1.589570000 |
| 14 | 1.393276000 | 0.125881000 | -1.505344000 |
| 6 | 2.231150000 | 0.746650000 | 0.061156000 |
| 8 | -2.607327000 | -1.021414000 | 0.449774000 |
| 1 | -0.567422000 | -2.386458000 | 0.027308000 |
| 6 | -3.381955000 | 0.133829000 | 0.687087000 |
| 1 | -4.424845000 | -0.168087000 | 0.781822000 |
| 1 | -3.301850000 | 0.847456000 | -0.141143000 |
| 1 | -3.080918000 | 0.635091000 | 1.614327000 |
| 1 | -0.373135000 | -0.871181000 | 2.645394000 |
| 1 | -0.433042000 | 0.738892000 | 1.933318000 |
| 1 | -0.969275000 | -0.287490000 | -2.122088000 |
| 1 | -0.807829000 | 1.104870000 | -1.055197000 |
| 1 | 2.284798000 | -1.641462000 | 1.425918000 |
| 1 | 2.408146000 | 0.324560000 | 2.802747000 |
| 1 | 1.881030000 | -1.244014000 | -1.805277000 |
| 1 | 1.723609000 | 0.996748000 | -2.660017000 |
| 1 | 3.316658000 | 0.743802000 | -0.075095000 |
| 1 | 1.936605000 | 1.789256000 | 0.226176000 |

**NMR Spectrum of 1-Methoxy-1,3,5-trisilacyclohexane**

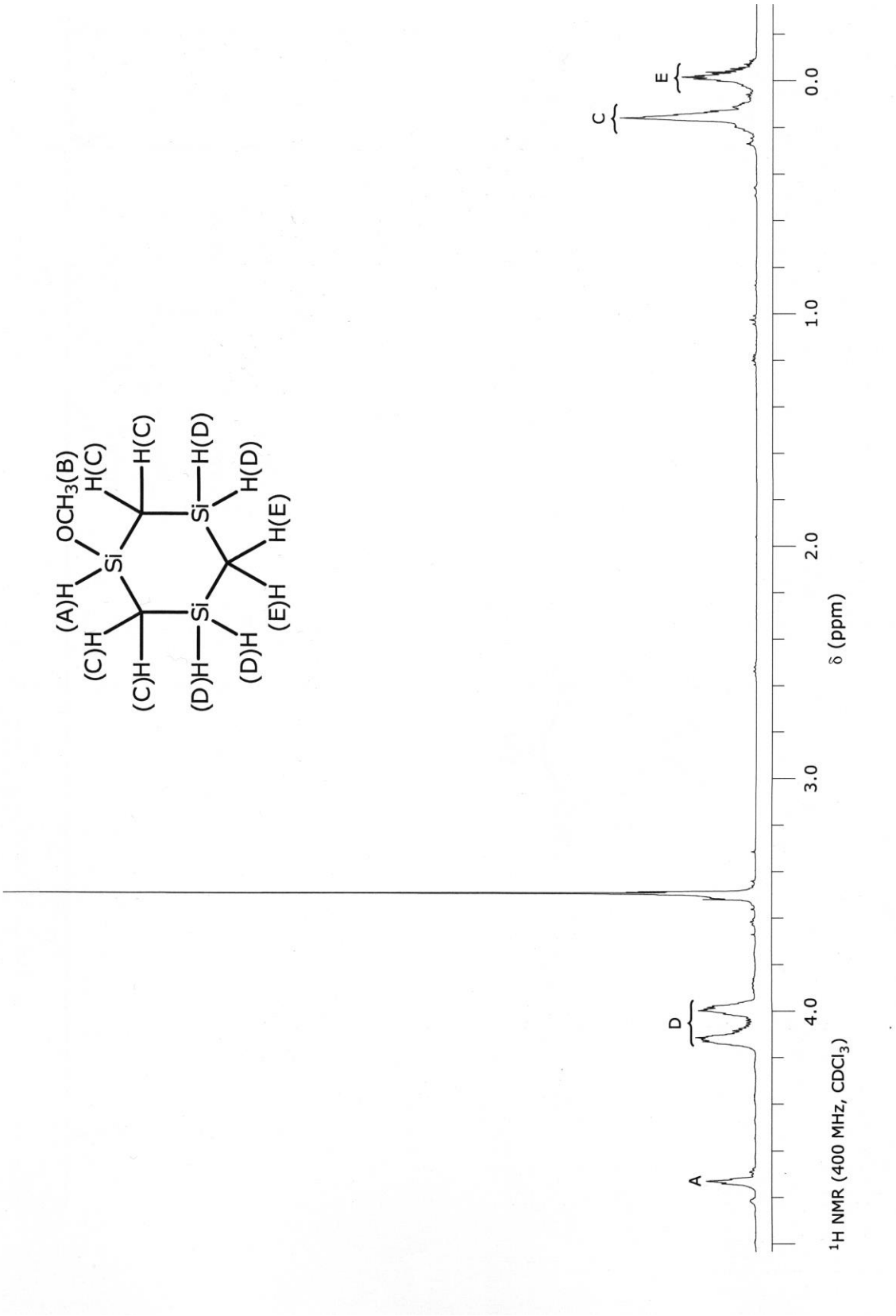



Figure S1. $^{1}$H NMR Spectrum of compound 1

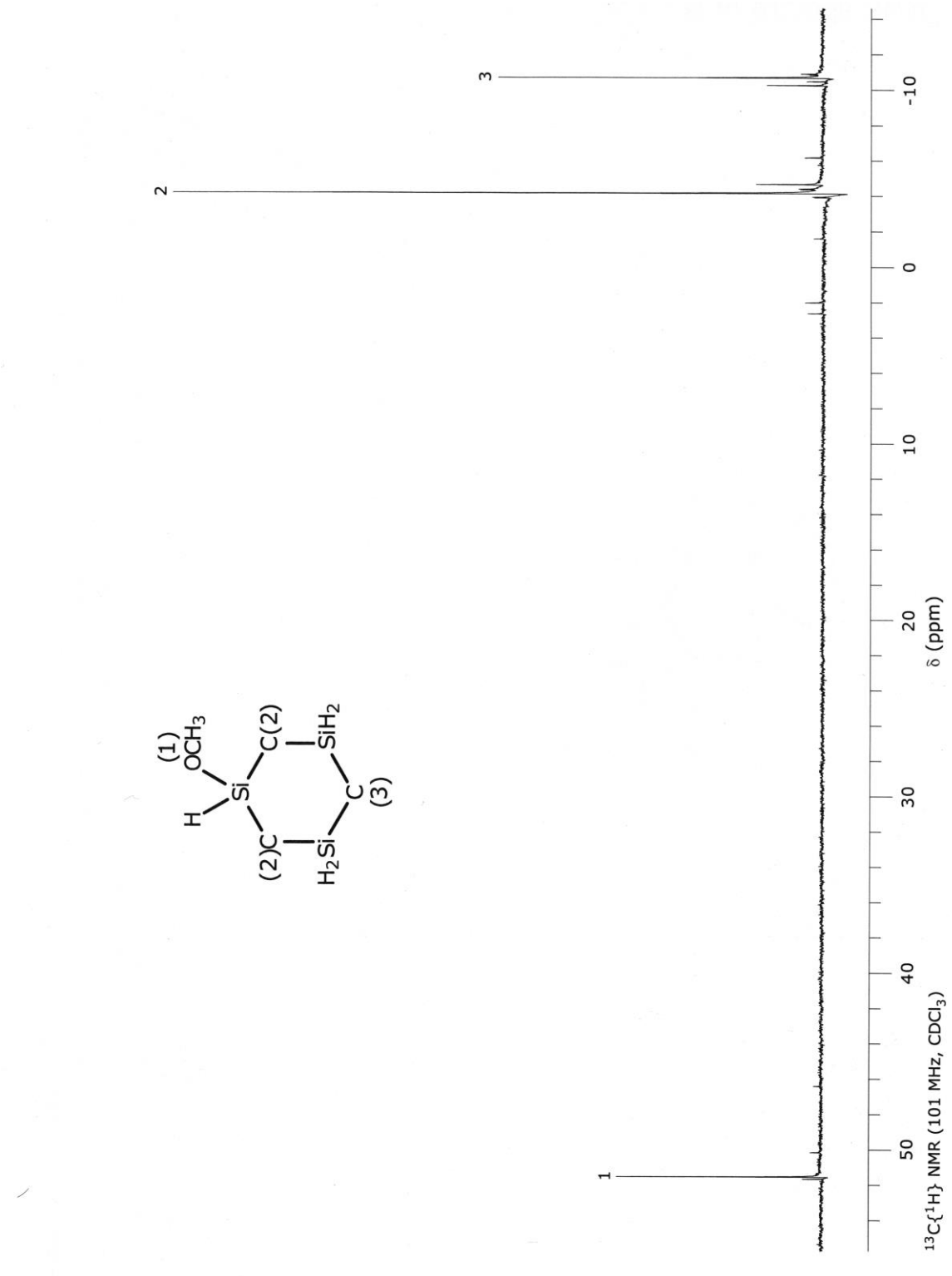



Figure S2. $^{13}C$ NMR Spectrum of compound 1

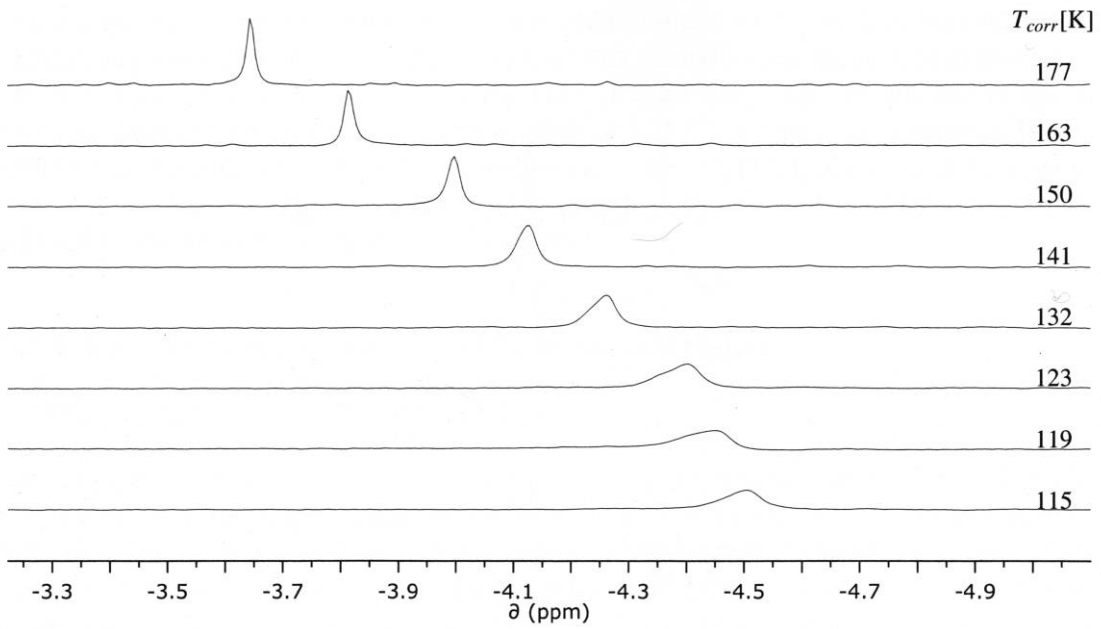



Figure S3. $^{13}$C NMR Spectra of compound 1 at low temperatures

**Experimental Section**

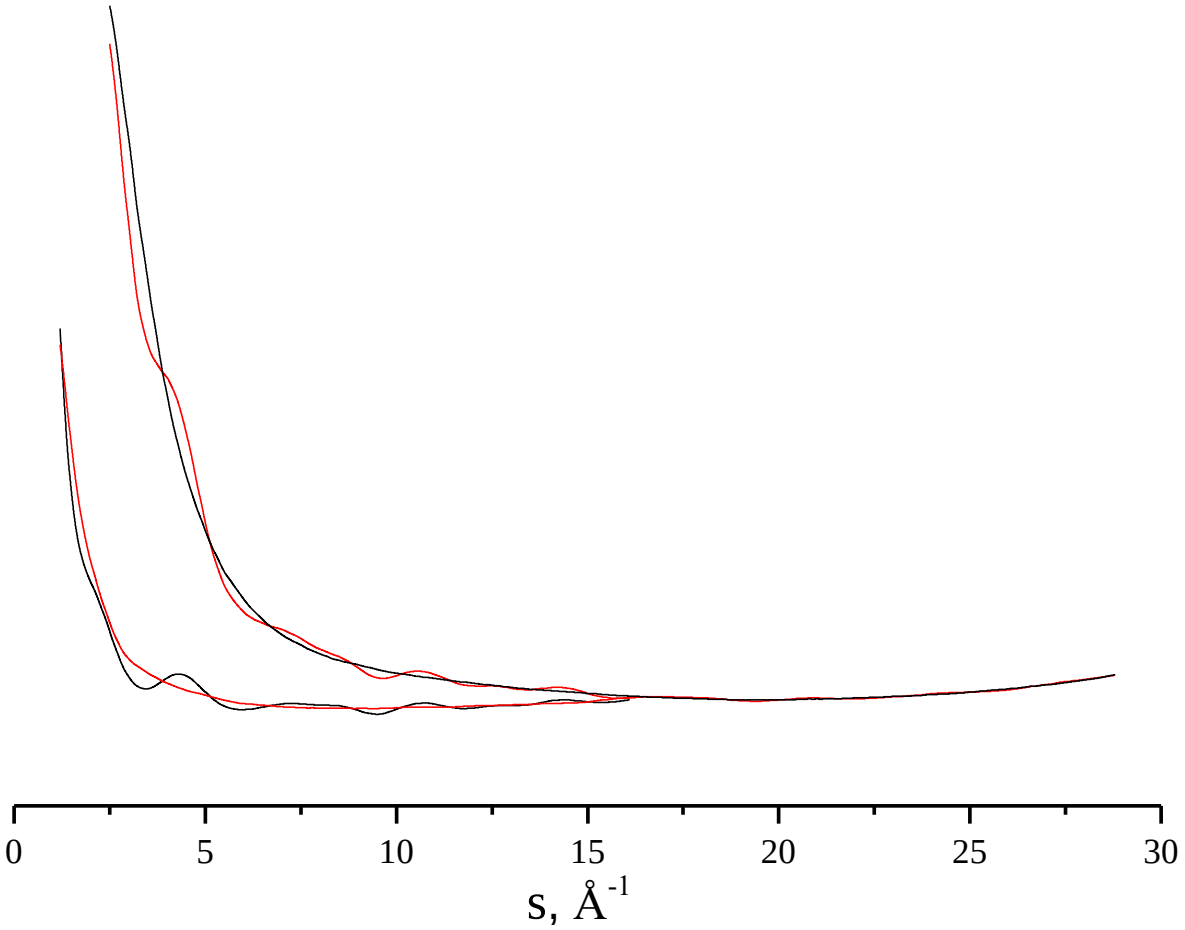



Figure S4. Total electron scattering intensity curves and experimental background lines of 1-Methoxy-1,3,5-trisilacyclohexane for short and long nozzle-to-plate distances GED/MS

The diffraction patterns of compounds **1** were obtained in a synchronous gas-phase electron diffraction and mass-spectrometric experiment carried out using the *EMR-100/APDM-1* unit [1, 2]. The conditions of the GED/MS experiments are listed in **Ошибка! Источник ссылки не найден.**.

Inlet system with dosing valve was applied though which a vapour flow of the compound passed into a stainless steel outlet effusion cell filled with shavings of the same material. The cell had a cylindrical nozzle of 0.6×1.2 $mm^2$ size (diameter × length) and were kept at 287 (3) K in the course of the experiments for compounds **1**. Diffraction patterns were recorded on MACO EM/EMS photographic films of 9x12 $cm^2$.

Accurate wavelengths of the electrons were calibrated using polycrystalline ZnO. The two camera distances resulted in diffraction patterns in the s-range for compounds of 1.9 to 13.8 $Å^{-1}$ and 3.3 to 25.7 $Å^{-1}$ with a step size of 0.1 $Å^{-1}$, where $s=(4\pi/\lambda)\sin(\theta/2)$, $\lambda$ is electron wavelength and $\theta$ is scattering angle, respectively. The optical densities of the diffraction patterns were measured by a computer controlled MD-100 (Carl Zeiss, Jena) microdensitometer [3] with a step size of 0.1 mm. The molecular scattering function, sM(s), was evaluated as

$$sM(s)=(I(s)/G(s)-1)s, \quad (1)$$

where I(s) is the total electron scattering intensity, G(s) the experimental background. A least-squares analysis of the scattering intensities was performed using a modified in Ivanovo version of the program KCED-35 [4] by minimizing an agreement functional $R_f$ expressed as:

$$R_f = 100\left[\frac{\sum_i^n \omega_i \left[s_i M_{\text{exp.}}(s_i) - k s_i M_{\text{theor.}}(s_i)\right]^2}{\sum_i^n \omega_i \left[s_i M_{\text{exp.}}(s_i)\right]^2}\right]^{1/2}, \quad (2)$$

where: $\omega_i$ – weight function; k– scale coefficient, $k=s_iM_{exp.}(s_i)/s_iM_{theor.}(s_i)$, $s_iM_{exp.}(s_i)$, $s_iM_{theor.}(s_i)$ – experimental and theoretical molecular scattering intensities, respectively.

**Table S1(a): Conditions of the synchronous GED/MS experiments**

| Compound | 1-Methoxy-1,3,5-trisilacyclohexane | |
|---|---|---|
| Camera distance | Long | Short |
| Nozzle-to-plate distance, mm | 598 | 338 |
| Number of recorded films | 6[c] | 6[c] |
| Primary electron beam current, μA | 0.7 | 1.3 |
| Accelerating voltage [a], kV | 80.5 | 81.9 |
| Temperature of effusion cell, K | 288(4) | 285(3) |
| Wavelength of electrons [b], Å | 0.04161(5) | 0.04123(5) |
| Exposure time, s | 80 | 120 |
| Residual gas pressure, Torr, in<br>–diffraction chamber<br>–mass spectrometric block | <br>$1.5\cdot10^{-6}$<br>$5.5\cdot10^{-7}$ | <br>$1.5\cdot10^{-6}$<br>$5.3\cdot10^{-7}$ |

[a] Approximate value

[b] Accurate wavelengths of electrons were calibrated using diffractions pattern of polycrystalline ZnO

[c] 6 for and 3 photographic films for the long and short camera distances, respectively, were taken for further procedures

**Table S1(b): Relative ion currents of major peaks in the mass spectra (EI, 50 eV) recorded during synchronous GED/MS experiments**

| m/z, Da | Relative intensity, % | | Assignment |
|---|---|---|---|
| | Long camera | Short camera | |
| 162 | 100 | 100 | $Si_3C_4H_{14}O^+$, $[M]^+$ |
| 147 | 57 | 62 | $Si_3C_3H_{11}O^+$, $[M\text{-}Me]^+$ |
| 131 | 72 | 53 | $Si_3C_3H_{11}^+$, $[M\text{-}OMe]^+$ |
| 101 | 30 | 23 | $Si_2C_3H_9^+$ |
| 85 | 26 | 19 | $Si_2C_2H_5^+$ |
| 69 | 22 | 16 | $SiC_3H_5^+$ |
| 58 | 45 | 49 | $SiC_2H_6^+$ |
| 43 | 22 | 20 | $SiCH_3^+$ |

**Computational details**

All calculations of molecule **1** were performed with Gaussian 09 program suite [5]. The geometry and vibrational calculations were performed using DFT (with B3LYP, B3LYP-D3 and M062X functionals) and MP2 methods with the 6-311G**, cc-pVTZ basic sets. The potential energy surface (PES) were obtained by scanning of ring conversion were performed at the M062X/6-311G** level from equatorial and axial forms.

**Table S2: Experimental total intensities and background for 1-Methoxy-1,3,5-trisilacyclohexane**

**I(s) long camera s= 1.2 to 16.1 Å$^{-1}$; step 0.1 Å$^{-1}$; λ=** 0.04160859 **Å, sequence in rows**

1.68184 1.44682 1.24436 1.09361 0.98826 0.91488 0.85651 0.82042
0.78955 0.75921 0.72643 0.69203 0.65429 0.61513 0.57438 0.53703
0.50173 0.47412 0.45166 0.43374 0.42346 0.41616 0.41218 0.41224
0.41606 0.42258 0.43177 0.44108 0.45005 0.45798 0.46297 0.46436
0.46321 0.45816 0.44989 0.43938 0.42754 0.41447 0.40084 0.38787
0.37637 0.36607 0.35743 0.35092 0.34546 0.34221 0.33947 0.33823
0.33889 0.33946 0.34100 0.34281 0.34528 0.34748 0.35033 0.35331
0.35493 0.35718 0.35851 0.36000 0.36059 0.36048 0.36006 0.35933
0.35814 0.35613 0.35606 0.35483 0.35451 0.35454 0.35418 0.35402
0.35379 0.35243 0.35028 0.34760 0.34449 0.33967 0.33621 0.33186
0.32798 0.32498 0.32296 0.32256 0.32396 0.32625 0.33016 0.33443
0.33984 0.34506 0.35014 0.35396 0.35772 0.35980 0.36119 0.36184
0.36161 0.35990 0.35827 0.35524 0.35270 0.34976 0.34713 0.34493
0.34413 0.34272 0.34297 0.34370 0.34455 0.34596 0.34760 0.34916
0.35056 0.35179 0.35239 0.35314 0.35351 0.35310 0.35310 0.35300
0.35365 0.35415 0.35507 0.35611 0.35891 0.36116 0.36380 0.36635
0.36883 0.37111 0.37230 0.37307 0.37355 0.37283 0.37162 0.37059
0.36941 0.36751 0.36583 0.36590 0.36439 0.36449 0.36425 0.36444
0.36545 0.36676 0.36858 0.36965 0.37151 0.37345

**I(s) short camera s= 2.5 to 28.8 Å$^{-1}$; step 0.1 Å$^{-1}$; λ=** 0.04122798 **Å, sequence in rows**

2.68315 2.58520 2.44349 2.29785 2.16278 2.03765 1.91853 1.80204
1.73062 1.66648 1.62295 1.58594 1.56255 1.54248 1.52308 1.50987
1.48229 1.45686 1.41440 1.36891 1.31632 1.25380 1.19122 1.12402
1.06128 0.99551 0.93955 0.88936 0.84642 0.80908 0.77355 0.75085
0.73058 0.71331 0.69642 0.68315 0.67210 0.66136 0.65482 0.64881
0.64343 0.63671 0.63308 0.62907 0.62523 0.62094 0.61536 0.60965
0.60382 0.59734 0.58898 0.58096 0.57166 0.56536 0.55761 0.55167
0.54643 0.54132 0.53516 0.52976 0.52532 0.51831 0.51206 0.50378
0.49471 0.48563 0.47579 0.46744 0.45997 0.45421 0.45041 0.44834
0.44950 0.45111 0.45500 0.45873 0.46311 0.46776 0.47102 0.47304
0.47363 0.47424 0.47221 0.47090 0.46769 0.46212 0.45765 0.45162
0.44666 0.44063 0.43580 0.43072 0.42746 0.42529 0.42316 0.42270
0.42150 0.42110 0.42205 0.42256 0.42228 0.42141 0.42086 0.41828
0.41701 0.41397 0.41199 0.41007 0.40958 0.40852 0.40873 0.40960
0.41156 0.41310 0.41440 0.41592 0.41697 0.41799 0.41732 0.41645
0.41406 0.41160 0.40805 0.40461 0.40057 0.39553 0.39237 0.38895
0.38535 0.38317 0.38171 0.37950 0.37863 0.37845 0.37851 0.38010
0.38000 0.38111 0.38244 0.38258 0.38391 0.38365 0.38469 0.38437
0.38415 0.38412 0.38398 0.38373 0.38208 0.38282 0.38230 0.38268
0.38187 0.38164 0.38128 0.38058 0.37992 0.37881 0.37804 0.37769
0.37640 0.37519 0.37375 0.37235 0.37130 0.37015 0.36924 0.36878
0.36818 0.36839 0.36867 0.36895 0.37011 0.37089 0.37136 0.37287
0.37395 0.37472 0.37588 0.37669 0.37825 0.37853 0.37953 0.38038
0.38013 0.38032 0.37900 0.37969 0.37921 0.37803 0.37753 0.37699
0.37756 0.37746 0.37728 0.37733 0.37771 0.37775 0.37830 0.37854

0.37953 0.37982 0.38026 0.38167 0.38244 0.38363 0.38421 0.38498
0.38672 0.38736 0.38851 0.39009 0.39078 0.39233 0.39395 0.39472
0.39570 0.39702 0.39728 0.39778 0.39857 0.39918 0.39930 0.39958
0.40033 0.40040 0.40118 0.40177 0.40281 0.40303 0.40335 0.40506
0.40524 0.40601 0.40706 0.40873 0.41063 0.41184 0.41376 0.41550
0.41830 0.42043 0.42181 0.42349 0.42622 0.42734 0.42928 0.43098
0.43327 0.43549 0.43715 0.43769 0.44059 0.44223 0.44399 0.44479
0.44607 0.44871 0.45029 0.45173 0.45380 0.45586 0.45789 0.46011

**Background G(s) long camera, sequence in rows**

1.62374 1.52144 1.38972 1.26405 1.15595 1.06456 0.98032 0.91819
0.86298 0.81242 0.76501 0.72217 0.68176 0.64471 0.60941 0.57953
0.55220 0.53239 0.51640 0.50273 0.49434 0.48538 0.47606 0.46735
0.45940 0.45176 0.44535 0.43865 0.43238 0.42694 0.42143 0.41589
0.41159 0.40729 0.40321 0.39967 0.39668 0.39349 0.38984 0.38619
0.38279 0.37906 0.37538 0.37231 0.36886 0.36650 0.36361 0.36141
0.36050 0.35888 0.35776 0.35651 0.35561 0.35422 0.35339 0.35272
0.35090 0.35004 0.34877 0.34827 0.34755 0.34682 0.34637 0.34606
0.34556 0.34435 0.34493 0.34421 0.34414 0.34427 0.34399 0.34405
0.34438 0.34416 0.34384 0.34372 0.34389 0.34289 0.34355 0.34329
0.34308 0.34298 0.34278 0.34294 0.34356 0.34375 0.34447 0.34470
0.34562 0.34621 0.34689 0.34684 0.34745 0.34726 0.34730 0.34754
0.34778 0.34736 0.34769 0.34716 0.34746 0.34751 0.34780 0.34824
0.34961 0.34974 0.35084 0.35171 0.35206 0.35248 0.35283 0.35304
0.35322 0.35353 0.35361 0.35426 0.35491 0.35502 0.35563 0.35606
0.35699 0.35736 0.35767 0.35760 0.35882 0.35912 0.35959 0.35995
0.36039 0.36097 0.36099 0.36121 0.36182 0.36194 0.36220 0.36317
0.36436 0.36509 0.36608 0.36873 0.36954 0.37160 0.37286 0.37405
0.37556 0.37688 0.37825 0.37846 0.37917 0.37976

**Background G(s) short camera, sequence in rows**

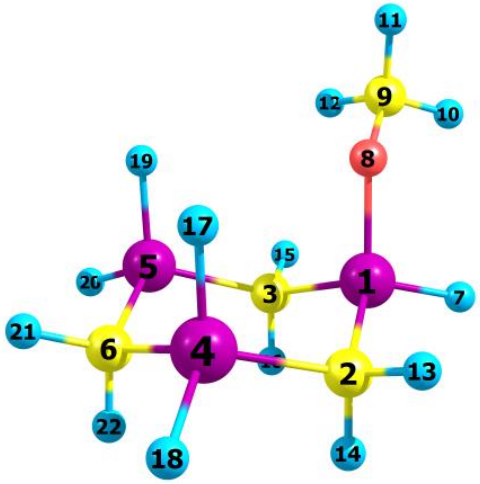
2.81751 2.74942 2.64509 2.53902 2.44037 2.34290 2.23762 2.11755
2.03172 1.93651 1.84962 1.75831 1.67497 1.59298 1.51436 1.44837
1.37816 1.32148 1.26162 1.21108 1.16507 1.11917 1.07972 1.03994
1.00556 0.96717 0.93532 0.90513 0.87769 0.85140 0.82266 0.80386
0.78462 0.76615 0.74616 0.72856 0.71215 0.69521 0.68204 0.66901
0.65641 0.64250 0.63199 0.62165 0.61225 0.60343 0.59455 0.58677
0.58008 0.57377 0.56641 0.55979 0.55204 0.54702 0.54028 0.53493
0.53000 0.52515 0.51951 0.51514 0.51252 0.50842 0.50614 0.50287
0.49958 0.49667 0.49284 0.48984 0.48650 0.48324 0.48005 0.47660
0.47462 0.47147 0.46955 0.46685 0.46472 0.46326 0.46118 0.45893
0.45649 0.45532 0.45284 0.45221 0.45078 0.44795 0.44685 0.44465
0.44368 0.44152 0.44015 0.43785 0.43657 0.43544 0.43343 0.43228
0.42975 0.42769 0.42693 0.42589 0.42445 0.42292 0.42225 0.42000
0.41936 0.41705 0.41571 0.41409 0.41344 0.41164 0.41051 0.40949
0.40915 0.40814 0.40688 0.40603 0.40514 0.40481 0.40355 0.40288
0.40150 0.40077 0.39956 0.39888 0.39783 0.39581 0.39552 0.39466
0.39317 0.39259 0.39218 0.39043 0.38949 0.38877 0.38789 0.38825
0.38668 0.38622 0.38599 0.38465 0.38466 0.38330 0.38346 0.38250
0.38183 0.38150 0.38118 0.38079 0.37903 0.37964 0.37897 0.37919
0.37825 0.37791 0.37752 0.37690 0.37643 0.37565 0.37535 0.37560
0.37502 0.37462 0.37404 0.37352 0.37333 0.37296 0.37272 0.37276

0.37246 0.37275 0.37289 0.37280 0.37338 0.37340 0.37299 0.37353
0.37361 0.37342 0.37370 0.37375 0.37471 0.37457 0.37535 0.37620
0.37613 0.37669 0.37591 0.37724 0.37748 0.37708 0.37736 0.37756
0.37882 0.37933 0.37965 0.38011 0.38078 0.38101 0.38164 0.38187
0.38277 0.38289 0.38308 0.38419 0.38461 0.38539 0.38552 0.38581
0.38703 0.38712 0.38770 0.38871 0.38883 0.38984 0.39098 0.39135
0.39205 0.39321 0.39347 0.39413 0.39523 0.39629 0.39699 0.39795
0.39944 0.40027 0.40179 0.40309 0.40475 0.40550 0.40623 0.40822
0.40854 0.40934 0.41029 0.41175 0.41335 0.41417 0.41564 0.41688
0.41916 0.42076 0.42162 0.42281 0.42510 0.42584 0.42746 0.42891
0.43101 0.43311 0.43474 0.43531 0.43828 0.44006 0.44201 0.44306
0.44463 0.44761 0.44957 0.45143 0.45393 0.45644 0.45891 0.46156

**Table S3: Z-matrix used in the refinement of 1-Methoxy-1,3,5-trisilacyclohexane**

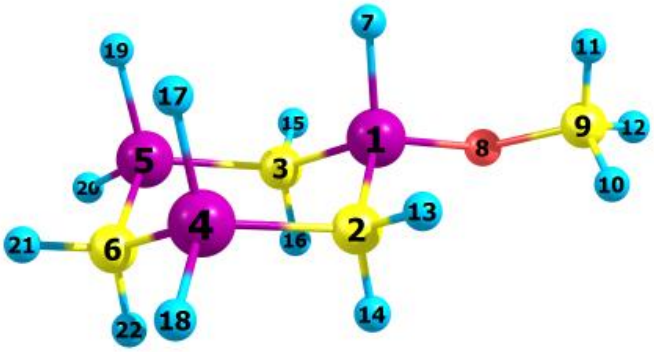
**I** (*g*-Ax) conformer

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | Si | | | | | | | |
| 2 | C | 1 | rCSi1 | | | | | |
| 3 | C | 1 | rCSi2 | 2 | aCSiC | | | |
| 4 | Si | 2 | rCSi3 | 1 | aSiCSi1 | 3 | -dSiCSiC1 | |
| 5 | Si | 3 | rCSi4 | 1 | aSiCSi2 | 2 | dSiCSiC2 | |
| 6 | C | 4 | rCSi5 | 5 | rCSi6 | 3 | -dCSiSiC | 4 |
| 7 | H | 1 | rHSi1 | 2 | aHSiC1 | 4 | tHSiCSi1 | |
| 8 | O | 1 | rOSi | 2 | aOSiC | 4 | tOSiCSi | |
| 9 | C | 8 | rCO | 1 | aCOSi | 3 | -tCOSiC | |
| 10 | H | 9 | rCH1 | 8 | aHCO1 | 1 | -tHCOSi | |
| 11 | H | 9 | rCH2 | 10 | aHCH1 | 8 | dHCHO1 | |
| 12 | H | 9 | rCH3 | 10 | aHCH2 | 8 | -dHCHO2 | |
| 13 | H | 2 | rCH4 | 4 | aHCSi1 | 6 | dHCSiC1 | |
| 14 | H | 2 | rCH5 | 13 | aHCH3 | 4 | -dHCHSi1 | |
| 15 | H | 3 | rCH6 | 5 | aHCSi2 | 6 | -dHCSiC2 | |
| 16 | H | 3 | rCH7 | 15 | aHCH4 | 5 | dHCHSi2 | |
| 17 | H | 4 | rHSi2 | 2 | aHSiC2 | 1 | -dHSiCSi2 | |
| 18 | H | 4 | rHSi3 | 17 | aHSiH1 | 2 | dHSiHC1 | |
| 19 | H | 5 | rHSi4 | 3 | aHSiC3 | 1 | dHSiCSi3 | |
| 20 | H | 5 | rHSi5 | 19 | aHSiH2 | 3 | -dHSiHC2 | |
| 21 | H | 6 | rCH8 | 4 | aHCSi3 | 2 | -dHCSiC3 | |
| 22 | H | 6 | rCH9 | 21 | aHCH5 | 4 | dHCHSi3 | |



**III** (*g*-Eq) conformer

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1 | Si | | | | | | |
| 2 | C | 1 | rCSi1 | | | | |
| 3 | C | 1 | rCSi2 | 2 | aCSiC | | |
| 4 | Si | 2 | rCSi3 | 1 | aSiCSi1 | 3 | -dSiCSiC1 |
| 5 | Si | 3 | rCSi4 | 1 | aSiCSi2 | 2 | dSiCSiC2 |
| 6 | C | 4 | rCSi5 | 5 | rCSi6 | 3 | -dCSiSiC 4 |
| 7 | H | 1 | rHSi1 | 2 | aHSiC1 | 4 | tHSiCSi1 |
| 8 | O | 1 | rOSi | 2 | aOSiC | 4 | tOSiCSi |
| 9 | C | 8 | rCO | 1 | aCOSi | 3 | -tCOSiC |
| 10 | H | 9 | rCH1 | 8 | aHCO1 | 1 | -tHCOSi |
| 11 | H | 9 | rCH2 | 10 | aHCH1 | 8 | dHCHO1 |
| 12 | H | 9 | rCH3 | 10 | aHCH2 | 8 | -dHCHO2 |
| 13 | H | 2 | rCH4 | 4 | aHCSi1 | 6 | dHCSiC1 |
| 14 | H | 2 | rCH5 | 13 | aHCH3 | 4 | -dHCHSi1 |
| 15 | H | 3 | rCH6 | 5 | aHCSi2 | 6 | -dHCSiC2 |
| 16 | H | 3 | rCH7 | 15 | aHCH4 | 5 | dHCHSi2 |
| 17 | H | 4 | rHSi2 | 2 | aHSiC2 | 1 | -dHSiCSi2 |
| 18 | H | 4 | rHSi3 | 17 | aHSiH1 | 2 | dHSiHC1 |
| 19 | H | 5 | rHSi4 | 3 | aHSiC3 | 1 | dHSiCSi3 |
| 20 | H | 5 | rHSi5 | 19 | aHSiH2 | 3 | -dHSiHC2 |
| 21 | H | 6 | rCH8 | 4 | aHCSi3 | 2 | -dHCSiC3 |
| 22 | H | 6 | rCH9 | 21 | aHCH5 | 4 | dHCHSi3 |



**IV** (*tr*-Eq) conformer

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1 | Si | | | | | | |
| 2 | C | 1 | rCSi1 | | | | |
| 3 | C | 1 | rCSi2 | 2 | aCSiC | | |
| 4 | Si | 2 | rCSi3 | 1 | aSiCSi1 | 3 | -dSiCSiC1 |
| 5 | Si | 3 | rCSi4 | 1 | aSiCSi2 | 2 | dSiCSiC2 |
| 6 | C | 4 | rCSi5 | 5 | rCSi6 | 3 | -dCSiSiC 4 |
| 7 | H | 1 | rHSi1 | 2 | aHSiC1 | 4 | tHSiCSi1 |
| 8 | O | 1 | rOSi | 2 | aOSiC | 4 | tOSiCSi |
| 9 | C | 8 | rCO | 1 | aCOSi | 3 | -tCOSiC |
| 10 | H | 9 | rCH1 | 8 | aHCO1 | 1 | -tHCOSi |
| 11 | H | 9 | rCH2 | 10 | aHCH1 | 8 | dHCHO1 |
| 12 | H | 9 | rCH3 | 10 | aHCH2 | 8 | -dHCHO2 |
| 13 | H | 2 | rCH4 | 4 | aHCSi1 | 6 | dHCSiC1 |
| 14 | H | 2 | rCH5 | 13 | aHCH3 | 4 | -dHCHSi1 |
| 15 | H | 3 | rCH6 | 5 | aHCSi2 | 6 | -dHCSiC2 |
| 16 | H | 3 | rCH7 | 15 | aHCH4 | 5 | dHCHSi2 |
| 17 | H | 4 | rHSi2 | 2 | aHSiC2 | 1 | -dHSiCSi2 |
| 18 | H | 4 | rHSi3 | 17 | aHSiH1 | 2 | dHSiHC1 |
| 19 | H | 5 | rHSi4 | 3 | aHSiC3 | 1 | dHSiCSi3 |
| 20 | H | 5 | rHSi5 | 19 | aHSiH2 | 3 | -dHSiHC2 |
| 21 | H | 6 | rCH8 | 4 | aHCSi3 | 2 | -dHCSiC3 |
| 22 | H | 6 | rCH9 | 21 | aHCH5 | 4 | dHCHSi3 |

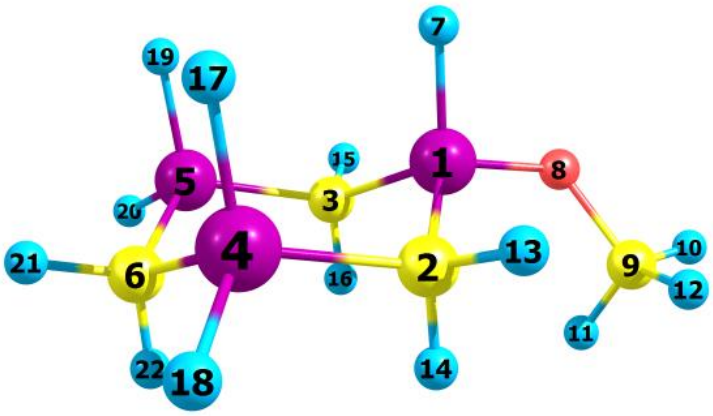


**Table S4: Interatomic $r_a$ distances in 1-methoxy-1,3,5-trisilacyclohexane with corresponding refined amplitudes and vibrational corrections. Numbers in the last column indicate groups in which scale factors for the corresponding amplitudes have been refined. All values of parameters are in Å. Internal numeration (see Table S3) of atoms is used.**

**I** (*g*-Ax) conformer

| At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu | At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C9 | H11 | 1.078592 | 0.078601 | 0.001500 | 100 | C3 | Si4 | 3.648193 | 0.103212 | 0.012100 | 105 |
| C2 | H13 | 1.082260 | 0.078807 | 0.001900 | 100 | H17 | H22 | 3.629776 | 0.153962 | 0.027800 | 105 |
| C6 | H21 | 1.082624 | 0.078807 | 0.001900 | 100 | H19 | H22 | 3.616027 | 0.153748 | 0.027600 | 105 |
| C3 | H15 | 1.083108 | 0.078910 | 0.001900 | 100 | H16 | H19 | 3.640460 | 0.153748 | 0.026200 | 105 |
| C2 | H14 | 1.084275 | 0.079116 | 0.002000 | 100 | H14 | H17 | 3.645032 | 0.154176 | 0.026700 | 105 |
| C9 | H12 | 1.085019 | 0.079528 | 0.001400 | 100 | C3 | H10 | 3.645461 | 0.464135 | 0.074800 | 105 |
| C3 | H16 | 1.084619 | 0.079116 | 0.002000 | 100 | H7 | H12 | 3.430213 | 0.375804 | 0.061500 | 105 |
| C6 | H22 | 1.084764 | 0.079116 | 0.001900 | 100 | O8 | H14 | 3.801755 | 0.120664 | 0.025800 | 105 |
| C9 | H10 | 1.085584 | 0.079631 | 0.001300 | 100 | H11 | H19 | 3.834502 | 0.633086 | 0.103600 | 105 |
| O8 | C9 | 1.431041 | 0.059701 | 0.000600 | 101 | O8 | H16 | 3.720692 | 0.121200 | 0.024000 | 105 |
| Si4 | H17 | 1.498308 | 0.111586 | 0.001700 | 101 | Si1 | H22 | 3.891324 | 0.234262 | 0.033300 | 105 |
| Si5 | H19 | 1.502229 | 0.112099 | 0.001600 | 101 | Si4 | H16 | 3.939974 | 0.232549 | 0.027900 | 105 |
| Si5 | H20 | 1.502323 | 0.112355 | 0.001700 | 101 | Si5 | C9 | 4.098733 | 0.282121 | 0.032100 | 105 |
| Si4 | H18 | 1.502580 | 0.112355 | 0.001600 | 101 | Si5 | H14 | 3.956169 | 0.240044 | 0.029600 | 105 |
| Si1 | H7 | 1.504094 | 0.112611 | 0.001600 | 101 | C3 | H13 | 3.979406 | 0.123769 | 0.023800 | 105 |
| Si1 | O8 | 1.668949 | 0.072412 | -0.000400 | 102 | C2 | H15 | 3.987011 | 0.124519 | 0.022300 | 105 |
| H21 | H22 | 1.728953 | 0.127713 | 0.010700 | 103 | C3 | H21 | 3.953814 | 0.124733 | 0.024700 | 105 |
| H15 | H16 | 1.728956 | 0.127713 | 0.010900 | 103 | C2 | H21 | 3.962969 | 0.124947 | 0.025100 | 105 |
| H13 | H14 | 1.734339 | 0.127612 | 0.010700 | 103 | C6 | H15 | 3.965584 | 0.124733 | 0.024100 | 105 |
| H11 | H12 | 1.748635 | 0.124667 | 0.009300 | 103 | C6 | H13 | 3.965166 | 0.124626 | 0.025200 | 105 |
| H10 | H11 | 1.749957 | 0.124769 | 0.009200 | 103 | C6 | O8 | 4.123209 | 0.217271 | 0.037900 | 106 |
| H10 | H12 | 1.757447 | 0.124769 | 0.009300 | 103 | H12 | H16 | 4.020782 | 0.369487 | -0.019300 | 105 |
| Si1 | C2 | 1.862141 | 0.052385 | 0.000400 | 103 | H7 | H11 | 3.907429 | 0.299787 | 0.082700 | 105 |
| Si1 | C3 | 1.874319 | 0.053197 | 0.000400 | 103 | C2 | C9 | 4.255570 | 0.078911 | 0.025300 | 106 |
| Si5 | C6 | 1.880360 | 0.053400 | 0.000600 | 103 | H10 | H19 | 4.402420 | 0.379321 | 0.109700 | 106 |
| Si4 | C6 | 1.884019 | 0.053603 | 0.000700 | 103 | C2 | H19 | 4.230261 | 0.199921 | 0.029700 | 106 |
| C3 | Si5 | 1.884468 | 0.053704 | 0.000300 | 103 | H13 | H16 | 4.180823 | 0.196574 | 0.036900 | 106 |
| C2 | Si4 | 1.885315 | 0.053704 | 0.000500 | 103 | H11 | H15 | 4.006268 | 0.335012 | 0.077800 | 105 |
| O8 | H11 | 2.041263 | 0.102536 | 0.005300 | 103 | H14 | H15 | 4.190995 | 0.201330 | 0.035600 | 106 |
| O8 | H12 | 2.081396 | 0.102434 | 0.004700 | 103 | C9 | H17 | 4.549934 | 0.331586 | 0.056600 | 106 |
| O8 | H10 | 2.086213 | 0.102333 | 0.004800 | 103 | H16 | H21 | 4.193950 | 0.199745 | 0.039700 | 106 |
| H19 | H20 | 2.421413 | 0.140493 | 0.009500 | 104 | C3 | H17 | 4.271203 | 0.196750 | 0.029100 | 106 |
| H17 | H18 | 2.424950 | 0.140112 | 0.009500 | 104 | H15 | H22 | 4.186889 | 0.200185 | 0.038600 | 106 |
| Si1 | H14 | 2.420176 | 0.117267 | 0.010300 | 104 | H14 | H21 | 4.218049 | 0.200713 | 0.040200 | 106 |
| Si5 | H22 | 2.416400 | 0.117267 | 0.010300 | 104 | H13 | H22 | 4.219870 | 0.198952 | 0.039800 | 106 |
| Si1 | H13 | 2.449194 | 0.116411 | 0.009100 | 104 | H12 | H20 | 4.609861 | 0.383284 | -0.060700 | 106 |
| Si4 | H22 | 2.440492 | 0.117458 | 0.010300 | 104 | C3 | H11 | 4.237131 | 0.188383 | 0.072300 | 106 |
| Si1 | H16 | 2.426431 | 0.118790 | 0.010600 | 104 | H11 | H17 | 4.741329 | 0.457616 | 0.051900 | 106 |
| Si5 | H16 | 2.447218 | 0.117743 | 0.010400 | 104 | C9 | H16 | 4.286095 | 0.166013 | 0.033000 | 106 |
| Si4 | H14 | 2.447704 | 0.117553 | 0.010300 | 104 | Si1 | H18 | 4.398884 | 0.106654 | 0.021300 | 106 |
| Si5 | H21 | 2.446713 | 0.115078 | 0.009100 | 104 | Si1 | H20 | 4.409977 | 0.106830 | 0.021200 | 106 |
| Si4 | H21 | 2.458013 | 0.115554 | 0.009200 | 104 | Si5 | H7 | 4.409598 | 0.106213 | 0.022300 | 106 |
| Si4 | H13 | 2.463443 | 0.115078 | 0.009300 | 104 | C9 | H13 | 4.516241 | 0.188736 | 0.038100 | 106 |
| Si1 | H15 | 2.474064 | 0.116030 | 0.008800 | 104 | Si4 | H7 | 4.435503 | 0.105861 | 0.023100 | 106 |
| Si5 | H15 | 2.469128 | 0.115173 | 0.009200 | 104 | Si5 | H18 | 4.470475 | 0.107622 | 0.023900 | 106 |
| H7 | O8 | 2.521596 | 0.114507 | 0.006300 | 104 | Si4 | H20 | 4.481319 | 0.107534 | 0.024000 | 106 |
| H12 | H19 | 3.079671 | 0.460884 | -0.037400 | 104 | H12 | H17 | 4.889117 | 0.398520 | 0.053500 | 106 |
| H12 | H15 | 2.537915 | 0.397777 | -0.038900 | 104 | C2 | H12 | 4.669478 | 0.160377 | 0.019000 | 106 |
| Si1 | C9 | 2.680260 | 0.077290 | 0.010900 | 104 | Si1 | H21 | 4.508412 | 0.119336 | 0.034900 | 106 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C3 | H19 | 2.765594 | 0.124026 | 0.008200 | 104 | H10 | H16 | 4.458860 | 0.410146 | 0.083200 | 106 |
| C6 | H19 | 2.762322 | 0.124311 | 0.008600 | 104 | C2 | H10 | 4.570056 | 0.161522 | 0.038500 | 106 |
| C6 | H17 | 2.763712 | 0.124502 | 0.008900 | 104 | Si5 | H13 | 4.617848 | 0.112907 | 0.032500 | 106 |
| C6 | H18 | 2.796325 | 0.122788 | 0.007000 | 104 | Si4 | H15 | 4.636375 | 0.110353 | 0.030300 | 106 |
| C2 | H17 | 2.776054 | 0.124311 | 0.008400 | 104 | Si5 | H10 | 4.776029 | 0.337135 | 0.103800 | 106 |
| C2 | H18 | 2.779021 | 0.122027 | 0.006700 | 104 | Si5 | H11 | 4.710272 | 0.376062 | 0.096800 | 106 |
| C3 | H7 | 2.777219 | 0.121551 | 0.005900 | 104 | Si4 | C9 | 4.926097 | 0.241822 | 0.045500 | 107 |
| C6 | H20 | 2.805670 | 0.122122 | 0.006900 | 104 | C6 | H12 | 5.080630 | 0.403146 | -0.014700 | 107 |
| C3 | H20 | 2.787468 | 0.122122 | 0.006700 | 104 | H10 | H13 | 4.739547 | 0.297432 | 0.039400 | 107 |
| C2 | H7 | 2.807797 | 0.121360 | 0.005500 | 104 | C2 | H11 | 4.918437 | 0.169143 | 0.048500 | 107 |
| C2 | O8 | 2.926245 | 0.086523 | 0.005700 | 104 | O8 | H18 | 4.978788 | 0.248209 | 0.037600 | 107 |
| C3 | O8 | 2.819276 | 0.083001 | 0.005100 | 104 | O8 | H22 | 4.812854 | 0.256908 | 0.051900 | 107 |
| H7 | H10 | 2.718242 | 0.349137 | -0.011700 | 104 | H7 | H19 | 4.828332 | 0.206878 | 0.036500 | 106 |
| Si1 | H10 | 2.909994 | 0.229395 | 0.015600 | 104 | O8 | H21 | 4.850095 | 0.365706 | 0.060600 | 107 |
| H18 | H22 | 2.976764 | 0.211405 | 0.014400 | 104 | Si4 | H12 | 5.185000 | 0.330578 | 0.019000 | 107 |
| H14 | H18 | 2.974887 | 0.202458 | 0.013700 | 104 | H13 | H15 | 4.816394 | 0.165509 | 0.038200 | 107 |
| H20 | H22 | 2.971427 | 0.209977 | 0.014600 | 104 | H13 | H21 | 4.796222 | 0.132635 | 0.040300 | 106 |
| H17 | H21 | 2.985772 | 0.213214 | 0.017100 | 104 | H15 | H21 | 4.792745 | 0.131754 | 0.039400 | 106 |
| H7 | H15 | 3.000319 | 0.189608 | 0.008000 | 104 | O8 | H20 | 4.838547 | 0.241051 | 0.036700 | 107 |
| H16 | H20 | 3.006547 | 0.202553 | 0.014500 | 104 | H14 | H19 | 4.844576 | 0.263515 | 0.046500 | 107 |
| H19 | H21 | 2.988172 | 0.212452 | 0.017200 | 104 | H7 | H17 | 4.889620 | 0.260101 | 0.037900 | 107 |
| H13 | H17 | 3.006277 | 0.214451 | 0.018200 | 104 | H16 | H17 | 4.861464 | 0.261643 | 0.045300 | 107 |
| Si1 | H12 | 3.000801 | 0.205599 | 0.007100 | 104 | H11 | H13 | 5.062519 | 0.309765 | 0.048500 | 107 |
| H15 | H19 | 3.019925 | 0.212167 | 0.018000 | 104 | C3 | H18 | 4.959117 | 0.159673 | 0.027500 | 107 |
| C3 | H12 | 3.033303 | 0.313538 | -0.041300 | 104 | H18 | H19 | 4.983493 | 0.277610 | 0.042400 | 107 |
| H7 | H13 | 3.043356 | 0.188180 | 0.006600 | 104 | C2 | H20 | 4.976804 | 0.158131 | 0.028500 | 107 |
| H18 | H21 | 3.063849 | 0.188180 | 0.010300 | 104 | H17 | H20 | 4.992357 | 0.281244 | 0.043200 | 107 |
| H20 | H21 | 3.051502 | 0.188180 | 0.009800 | 104 | C6 | H7 | 4.933556 | 0.150863 | 0.032400 | 107 |
| O8 | H13 | 3.187389 | 0.203029 | 0.017300 | 104 | H12 | H13 | 5.113701 | 0.256578 | 0.056600 | 107 |
| H15 | H20 | 3.036591 | 0.188561 | 0.010400 | 104 | C9 | H14 | 5.031595 | 0.135777 | 0.043600 | 107 |
| H7 | H16 | 3.027349 | 0.208645 | 0.014600 | 104 | H13 | H19 | 5.012704 | 0.326283 | 0.051000 | 107 |
| H13 | H18 | 3.044125 | 0.187894 | 0.010200 | 104 | C6 | C9 | 5.181741 | 0.289063 | 0.050800 | 107 |
| C2 | C3 | 3.056406 | 0.087855 | 0.007500 | 104 | H16 | H18 | 5.041634 | 0.320777 | 0.041600 | 107 |
| C3 | C6 | 3.032325 | 0.089854 | 0.009100 | 104 | H15 | H17 | 5.081565 | 0.313069 | 0.048000 | 107 |
| C2 | C6 | 3.037745 | 0.090045 | 0.009500 | 104 | H14 | H20 | 5.091806 | 0.329697 | 0.044200 | 107 |
| H7 | H14 | 3.052239 | 0.208645 | 0.013200 | 104 | C9 | H20 | 5.218216 | 0.342801 | 0.042400 | 107 |
| H14 | H16 | 3.020088 | 0.313538 | 0.026700 | 104 | Si4 | H11 | 5.385082 | 0.398301 | 0.065200 | 107 |
| Si1 | Si5 | 3.112748 | 0.079479 | 0.009700 | 104 | H10 | H17 | 5.295003 | 0.415149 | 0.118500 | 107 |
| Si1 | Si4 | 3.113613 | 0.079003 | 0.010100 | 104 | H7 | H22 | 5.114352 | 0.320227 | 0.049300 | 107 |
| H16 | H22 | 3.044490 | 0.318202 | 0.031900 | 104 | H12 | H14 | 5.352132 | 0.255917 | 0.030600 | 107 |
| O8 | H17 | 3.295470 | 0.325341 | 0.034000 | 104 | H12 | H21 | 5.705073 | 0.497298 | 0.004800 | 107 |
| H14 | H22 | 3.090632 | 0.320487 | 0.032100 | 104 | H10 | H14 | 5.237947 | 0.270343 | 0.049100 | 107 |
| O8 | H19 | 3.126663 | 0.313919 | 0.030500 | 104 | H11 | H16 | 5.223377 | 0.231581 | 0.102200 | 107 |
| Si4 | Si5 | 3.197433 | 0.086713 | 0.010800 | 104 | Si4 | H10 | 5.540809 | 0.240941 | 0.092000 | 107 |
| O8 | H15 | 3.055300 | 0.187038 | 0.014800 | 104 | H18 | H20 | 5.567503 | 0.194801 | 0.039000 | 107 |
| C9 | H15 | 3.082464 | 0.282032 | 0.012300 | 104 | H12 | H22 | 5.738402 | 0.398191 | -0.002400 | 107 |
| H7 | C9 | 3.022285 | 0.201696 | 0.024200 | 104 | H7 | H20 | 5.535004 | 0.183899 | 0.031700 | 107 |
| C2 | H16 | 3.216436 | 0.203410 | 0.020500 | 104 | H7 | H18 | 5.554950 | 0.184670 | 0.032500 | 107 |
| C3 | H14 | 3.227430 | 0.209882 | 0.021100 | 104 | C6 | H11 | 5.724229 | 0.493664 | 0.102600 | 107 |
| C6 | H16 | 3.224479 | 0.206836 | 0.023300 | 104 | C9 | H21 | 5.850789 | 0.403477 | 0.076400 | 107 |
| C3 | H22 | 3.220066 | 0.209406 | 0.023800 | 104 | H10 | H20 | 5.829510 | 0.525599 | 0.122000 | 107 |
| C6 | H14 | 3.245530 | 0.210072 | 0.024000 | 104 | H11 | H14 | 5.782723 | 0.174869 | 0.084100 | 107 |
| C2 | H22 | 3.247404 | 0.208645 | 0.024000 | 104 | C9 | H22 | 5.863590 | 0.271774 | 0.066600 | 107 |
| C9 | H19 | 3.517831 | 0.371315 | 0.035800 | 104 | C6 | H10 | 5.862005 | 0.320667 | 0.111100 | 107 |
| H10 | H15 | 3.256642 | 0.555022 | 0.098300 | 104 | H11 | H20 | 5.821641 | 0.524718 | 0.117900 | 107 |
| C3 | C9 | 3.331379 | 0.167906 | 0.011600 | 104 | H7 | H21 | 5.935371 | 0.166280 | 0.056300 | 107 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Si5 | H12 | 3.697367 | 0.411244 | -0.052000 | 105 | H15 | H18 | 5.990326 | 0.169143 | 0.049200 | 107 |
| H17 | H19 | 3.409476 | 0.439081 | 0.049400 | 105 | H13 | H20 | 5.994337 | 0.167712 | 0.052200 | 107 |
| Si4 | O8 | 3.585680 | 0.231800 | 0.026400 | 105 | C9 | H18 | 6.348612 | 0.261203 | 0.064700 | 107 |
| Si5 | O8 | 3.478589 | 0.221521 | 0.024500 | 105 | H11 | H21 | 6.261727 | 0.651685 | 0.131200 | 107 |
| Si1 | H19 | 3.509344 | 0.223877 | 0.020900 | 105 | H12 | H18 | 6.653869 | 0.346325 | 0.044800 | 107 |
| Si1 | H17 | 3.546197 | 0.223877 | 0.021600 | 105 | H10 | H22 | 6.427542 | 0.370771 | 0.122500 | 107 |
| Si1 | C6 | 3.542300 | 0.108137 | 0.015900 | 105 | H11 | H22 | 6.513540 | 0.427262 | 0.124000 | 107 |
| Si1 | H11 | 3.540621 | 0.118630 | 0.050000 | 105 | H11 | H18 | 6.773442 | 0.421096 | 0.081400 | 107 |
| Si4 | H19 | 3.617013 | 0.258887 | 0.027700 | 105 | H10 | H21 | 6.619384 | 0.388060 | 0.146900 | 107 |
| Si5 | H17 | 3.635243 | 0.258138 | 0.028100 | 105 | H10 | H18 | 6.909876 | 0.257128 | 0.110300 | 107 |
| C2 | Si5 | 3.643681 | 0.103534 | 0.012800 | 105 | | | | | | |

**Table S2: Interatomic $r_a$ distances in 1-methoxy-1,3,5-trisilacyclohexane with corresponding refined amplitudes and vibrational corrections. Numbers in the last column indicate groups in which scale factors for the corresponding amplitudes have been refined. All values of parameters are in Å. Internal numeration (see Table S3) of atoms is used.**
**III** (*g*-Eq) conformer

| At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu | At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C9 | H12 | 1.078770 | 0.078395 | 0.001400 | 100 | H7 | H14 | 3.608463 | 0.153427 | 0.026600 | 105 |
| C3 | H15 | 1.082311 | 0.078807 | 0.001900 | 100 | H19 | H22 | 3.613609 | 0.153427 | 0.027000 | 105 |
| C6 | H21 | 1.082482 | 0.078807 | 0.001900 | 100 | H17 | H22 | 3.627844 | 0.153320 | 0.027000 | 105 |
| C2 | H13 | 1.083316 | 0.078910 | 0.001900 | 100 | H7 | H16 | 3.621659 | 0.153748 | 0.027000 | 105 |
| C9 | H10 | 1.084578 | 0.079322 | 0.001400 | 100 | H14 | H17 | 3.634340 | 0.153748 | 0.027300 | 105 |
| C6 | H22 | 1.084315 | 0.079116 | 0.001900 | 100 | H16 | H19 | 3.637228 | 0.153641 | 0.027500 | 105 |
| C3 | H16 | 1.084584 | 0.079116 | 0.001900 | 100 | H7 | H10 | 3.551250 | 0.408460 | 0.069000 | 105 |
| C9 | H11 | 1.085583 | 0.079425 | 0.001300 | 100 | C2 | H11 | 3.771654 | 0.488332 | 0.079500 | 105 |
| C2 | H14 | 1.085118 | 0.079219 | 0.001900 | 100 | Si1 | H22 | 3.896326 | 0.233834 | 0.031900 | 105 |
| O8 | C9 | 1.431459 | 0.059701 | 0.000600 | 101 | Si4 | H16 | 3.944550 | 0.232870 | 0.032400 | 105 |
| Si5 | H20 | 1.500946 | 0.112099 | 0.001700 | 101 | Si5 | H14 | 3.952501 | 0.230836 | 0.031000 | 105 |
| Si4 | H18 | 1.501260 | 0.112227 | 0.001700 | 101 | C2 | H15 | 3.977114 | 0.124305 | 0.024300 | 105 |
| Si5 | H19 | 1.502682 | 0.112227 | 0.001600 | 101 | C3 | H13 | 3.983359 | 0.124305 | 0.024000 | 105 |
| Si4 | H17 | 1.502832 | 0.112227 | 0.001600 | 101 | C6 | H13 | 3.959872 | 0.125161 | 0.024400 | 105 |
| Si1 | H7 | 1.505433 | 0.112739 | 0.001500 | 101 | C3 | H21 | 3.957038 | 0.124947 | 0.024700 | 105 |
| Si1 | O8 | 1.666697 | 0.072083 | -0.000300 | 102 | C2 | H21 | 3.964502 | 0.125054 | 0.024300 | 105 |
| H21 | H22 | 1.731467 | 0.127612 | 0.010700 | 103 | C6 | H15 | 3.964921 | 0.124947 | 0.024800 | 105 |
| H15 | H16 | 1.732016 | 0.127713 | 0.010700 | 103 | H7 | H12 | 3.942755 | 0.306853 | 0.075300 | 105 |
| H13 | H14 | 1.735228 | 0.127612 | 0.010700 | 103 | C3 | H17 | 4.172299 | 0.215421 | 0.034200 | 106 |
| H11 | H12 | 1.749509 | 0.124464 | 0.009100 | 103 | H11 | H14 | 4.207575 | 0.445374 | 0.129400 | 106 |
| H10 | H12 | 1.748860 | 0.124363 | 0.009900 | 103 | C2 | H19 | 4.191194 | 0.213396 | 0.033800 | 106 |
| H10 | H11 | 1.755592 | 0.124464 | 0.009500 | 103 | C3 | C9 | 4.124836 | 0.080497 | 0.033800 | 106 |
| Si1 | C3 | 1.861390 | 0.052385 | 0.000700 | 103 | C6 | H7 | 4.173397 | 0.211282 | 0.031300 | 106 |
| Si1 | C2 | 1.873445 | 0.053298 | 0.000700 | 103 | H13 | H16 | 4.206396 | 0.195341 | 0.038700 | 106 |
| Si4 | C6 | 1.881274 | 0.053400 | 0.000300 | 103 | H13 | H22 | 4.201161 | 0.199040 | 0.039300 | 106 |
| Si5 | C6 | 1.881915 | 0.053501 | 0.000400 | 103 | H14 | H21 | 4.201376 | 0.198864 | 0.039200 | 106 |
| C3 | Si5 | 1.881867 | 0.053501 | 0.000500 | 103 | H14 | H15 | 4.209743 | 0.195957 | 0.039000 | 106 |
| C2 | Si4 | 1.882930 | 0.053704 | 0.000500 | 103 | H16 | H21 | 4.198855 | 0.200097 | 0.040100 | 106 |
| O8 | H12 | 2.042060 | 0.102130 | 0.004600 | 103 | H15 | H22 | 4.190745 | 0.199745 | 0.040100 | 106 |
| O8 | H10 | 2.082180 | 0.102333 | 0.004900 | 103 | H12 | H13 | 4.424548 | 0.267119 | 0.054700 | 106 |
| O8 | H11 | 2.087600 | 0.102130 | 0.004000 | 103 | C9 | H16 | 4.300590 | 0.197455 | 0.047100 | 106 |
| H17 | H18 | 2.424220 | 0.140493 | 0.009400 | 104 | Si1 | H20 | 4.415406 | 0.107446 | 0.024200 | 106 |
| H19 | H20 | 2.425122 | 0.140397 | 0.009400 | 104 | Si1 | H18 | 4.422818 | 0.107975 | 0.024300 | 106 |
| Si1 | H16 | 2.401122 | 0.117743 | 0.011100 | 104 | Si4 | H20 | 4.465163 | 0.107006 | 0.022700 | 106 |
| Si1 | H14 | 2.421581 | 0.118315 | 0.010900 | 104 | Si5 | H18 | 4.466004 | 0.107006 | 0.022900 | 106 |
| Si1 | H15 | 2.447413 | 0.114793 | 0.008800 | 104 | C9 | H15 | 4.278809 | 0.170681 | 0.040500 | 106 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| Si4 | H14 | 2.442095 | 0.117553 | 0.010600 | 104 | C2 | H12 | 4.530656 | 0.203884 | 0.067400 | 106 |
| Si5 | H16 | 2.444028 | 0.117648 | 0.010600 | 104 | H12 | H14 | 4.610432 | 0.352723 | 0.087100 | 106 |
| Si4 | H22 | 2.444913 | 0.116982 | 0.010200 | 104 | Si5 | O8 | 4.487593 | 0.075212 | 0.020500 | 106 |
| Si5 | H22 | 2.425810 | 0.117172 | 0.010300 | 104 | C3 | H11 | 4.478625 | 0.174732 | 0.046700 | 106 |
| Si4 | H13 | 2.453143 | 0.115554 | 0.008900 | 104 | Si4 | O8 | 4.655911 | 0.074420 | 0.020300 | 106 |
| Si4 | H21 | 2.459364 | 0.115364 | 0.008600 | 104 | C3 | H10 | 4.552350 | 0.182483 | 0.040100 | 106 |
| Si5 | H21 | 2.450276 | 0.115269 | 0.008600 | 104 | Si4 | H15 | 4.600716 | 0.116077 | 0.033300 | 106 |
| Si1 | H13 | 2.471164 | 0.115364 | 0.008700 | 104 | Si1 | H21 | 4.555014 | 0.113876 | 0.032800 | 106 |
| Si5 | H15 | 2.463833 | 0.115649 | 0.008700 | 104 | Si5 | H13 | 4.607420 | 0.115813 | 0.032600 | 106 |
| O8 | H7 | 2.522263 | 0.114793 | 0.006200 | 104 | H10 | H16 | 4.601186 | 0.301554 | 0.045400 | 106 |
| Si1 | C9 | 2.675599 | 0.076624 | 0.010500 | 104 | H11 | H15 | 4.579511 | 0.274605 | 0.048700 | 106 |
| C2 | H7 | 2.740089 | 0.123264 | 0.007600 | 104 | H16 | H17 | 4.799354 | 0.214188 | 0.050700 | 106 |
| H10 | H13 | 3.041563 | 0.408342 | -0.077900 | 104 | H13 | H15 | 4.812597 | 0.165509 | 0.038300 | 107 |
| C6 | H19 | 2.749226 | 0.124311 | 0.008400 | 104 | H13 | H21 | 4.792208 | 0.132458 | 0.039000 | 106 |
| C6 | H17 | 2.749753 | 0.124121 | 0.008300 | 104 | H14 | H19 | 4.817087 | 0.213043 | 0.049700 | 106 |
| C2 | H17 | 2.761549 | 0.124216 | 0.008500 | 104 | C3 | H12 | 4.750646 | 0.135189 | 0.053300 | 106 |
| C3 | H19 | 2.763560 | 0.124121 | 0.008500 | 104 | H15 | H21 | 4.792140 | 0.132282 | 0.039300 | 106 |
| C3 | H7 | 2.768380 | 0.123454 | 0.007300 | 104 | H7 | H22 | 4.796261 | 0.214276 | 0.048200 | 106 |
| C3 | H20 | 2.784144 | 0.121836 | 0.006600 | 104 | H18 | H19 | 4.907741 | 0.272215 | 0.039500 | 107 |
| C2 | H18 | 2.787135 | 0.122217 | 0.006700 | 104 | H17 | H20 | 4.907773 | 0.271774 | 0.039300 | 107 |
| C6 | H20 | 2.812100 | 0.122217 | 0.006600 | 104 | H7 | H18 | 4.879563 | 0.278161 | 0.039800 | 107 |
| C6 | H18 | 2.812234 | 0.122027 | 0.006600 | 104 | H12 | H16 | 4.831047 | 0.260161 | 0.057200 | 106 |
| C3 | O8 | 2.778202 | 0.084810 | 0.003100 | 104 | H7 | H20 | 4.918975 | 0.278932 | 0.040100 | 107 |
| H7 | H11 | 2.796454 | 0.369031 | -0.019700 | 104 | H12 | H15 | 4.746003 | 0.229160 | 0.046500 | 106 |
| C2 | O8 | 3.038507 | 0.083477 | 0.003400 | 104 | C2 | H20 | 4.972639 | 0.157250 | 0.031100 | 107 |
| Si1 | H11 | 2.897967 | 0.221590 | 0.011800 | 104 | C3 | H18 | 4.971904 | 0.156479 | 0.032100 | 107 |
| H7 | H13 | 2.981703 | 0.211215 | 0.016100 | 104 | H15 | H17 | 4.950665 | 0.347096 | 0.054000 | 107 |
| H16 | H20 | 3.001324 | 0.207978 | 0.014500 | 104 | H11 | H16 | 4.856841 | 0.249750 | 0.082700 | 107 |
| H14 | H18 | 3.001926 | 0.208835 | 0.015200 | 104 | Si4 | H10 | 5.177383 | 0.405349 | -0.013100 | 107 |
| H19 | H21 | 2.982168 | 0.212642 | 0.016900 | 104 | H13 | H19 | 4.969832 | 0.343462 | 0.053400 | 107 |
| H13 | H17 | 3.002366 | 0.212262 | 0.017000 | 104 | H7 | H21 | 4.956009 | 0.339167 | 0.050600 | 107 |
| O8 | H16 | 2.948831 | 0.197984 | 0.013300 | 104 | O8 | H19 | 4.958476 | 0.255697 | 0.037200 | 107 |
| H20 | H22 | 3.000807 | 0.206741 | 0.014500 | 104 | H10 | H15 | 4.896504 | 0.234003 | 0.069200 | 107 |
| H17 | H21 | 2.994954 | 0.212357 | 0.017000 | 104 | O8 | H17 | 5.104541 | 0.256798 | 0.036800 | 107 |
| H18 | H22 | 3.033004 | 0.207217 | 0.014700 | 104 | C6 | O8 | 5.077018 | 0.132804 | 0.028400 | 107 |
| H7 | H15 | 3.018369 | 0.210072 | 0.015300 | 104 | H14 | H20 | 5.098898 | 0.321768 | 0.047200 | 107 |
| H15 | H19 | 3.015338 | 0.212547 | 0.016600 | 104 | H16 | H18 | 5.099873 | 0.324191 | 0.049200 | 107 |
| Si1 | H10 | 3.003117 | 0.207788 | 0.010500 | 104 | O8 | H22 | 5.190422 | 0.320337 | 0.045700 | 107 |
| H13 | H18 | 3.018433 | 0.189513 | 0.009500 | 104 | Si4 | C9 | 5.332196 | 0.206694 | 0.031800 | 107 |
| H18 | H21 | 3.064671 | 0.188466 | 0.009100 | 104 | Si4 | H11 | 5.382065 | 0.495096 | 0.070700 | 107 |
| H15 | H20 | 3.033079 | 0.189417 | 0.009300 | 104 | H11 | H17 | 5.454329 | 0.582751 | 0.044200 | 107 |
| H20 | H21 | 3.054685 | 0.188275 | 0.009200 | 104 | H10 | H17 | 5.623836 | 0.467126 | 0.019200 | 107 |
| C2 | C3 | 3.053763 | 0.088331 | 0.009300 | 104 | H18 | H20 | 5.594141 | 0.187092 | 0.034900 | 107 |
| C3 | C6 | 3.034937 | 0.090330 | 0.009800 | 104 | C9 | H17 | 5.659670 | 0.316593 | 0.040200 | 107 |
| C2 | C6 | 3.036673 | 0.090330 | 0.009300 | 104 | O8 | H20 | 5.538140 | 0.166390 | 0.033900 | 107 |
| O8 | H15 | 2.932988 | 0.167715 | 0.005400 | 104 | H10 | H18 | 5.938792 | 0.482432 | -0.031100 | 107 |
| O8 | H14 | 3.210431 | 0.192559 | 0.012900 | 104 | O8 | H18 | 5.785619 | 0.163747 | 0.034100 | 107 |
| H14 | H22 | 3.060260 | 0.316489 | 0.032200 | 104 | Si5 | C9 | 5.722932 | 0.111441 | 0.053100 | 107 |
| H14 | H16 | 3.060210 | 0.309636 | 0.030700 | 104 | H15 | H18 | 5.987941 | 0.167161 | 0.054700 | 107 |
| H16 | H22 | 3.049745 | 0.319059 | 0.033900 | 104 | H13 | H20 | 5.989854 | 0.167381 | 0.053500 | 107 |
| C2 | H10 | 3.352442 | 0.353325 | -0.038100 | 104 | Si5 | H11 | 5.908021 | 0.295230 | 0.063100 | 107 |
| Si1 | Si5 | 3.133283 | 0.085476 | 0.011100 | 104 | C6 | H10 | 6.140183 | 0.389602 | 0.024800 | 107 |
| Si1 | Si4 | 3.134948 | 0.086047 | 0.011100 | 104 | Si5 | H10 | 6.046502 | 0.276509 | 0.051200 | 107 |
| Si4 | Si5 | 3.167669 | 0.083953 | 0.010000 | 104 | H10 | H22 | 6.199331 | 0.537051 | 0.038300 | 107 |
| H10 | H14 | 3.398871 | 0.490772 | -0.008500 | 104 | C6 | C9 | 6.113450 | 0.188194 | 0.055500 | 107 |
| H7 | C9 | 3.090304 | 0.223113 | 0.022200 | 104 | H11 | H19 | 5.988959 | 0.494655 | 0.055000 | 107 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| O8 | H13 | 3.332037 | 0.161338 | 0.005300 | 104 | C9 | H18 | 6.291446 | 0.295560 | 0.041400 | 107 |
| C9 | H13 | 3.453121 | 0.304391 | -0.012400 | 105 | O8 | H21 | 6.095237 | 0.141944 | 0.050800 | 107 |
| H17 | H19 | 3.258102 | 0.359988 | 0.037300 | 104 | C9 | H19 | 6.047031 | 0.318355 | 0.068500 | 107 |
| C2 | H16 | 3.234667 | 0.203410 | 0.023600 | 104 | C9 | H22 | 6.253853 | 0.368789 | 0.076800 | 107 |
| C6 | H14 | 3.231317 | 0.206646 | 0.023700 | 104 | Si4 | H12 | 6.291178 | 0.220679 | 0.098200 | 107 |
| H7 | H17 | 3.256369 | 0.371315 | 0.038800 | 104 | H11 | H18 | 6.365009 | 0.588036 | 0.099000 | 107 |
| C2 | H22 | 3.232788 | 0.207407 | 0.023800 | 104 | C6 | H11 | 6.318523 | 0.373304 | 0.085100 | 107 |
| C6 | H16 | 3.232423 | 0.208740 | 0.024800 | 104 | H10 | H19 | 6.466413 | 0.391584 | 0.082700 | 107 |
| C3 | H14 | 3.244872 | 0.202934 | 0.023300 | 104 | Si5 | H12 | 6.455847 | 0.155709 | 0.091600 | 107 |
| C3 | H22 | 3.220178 | 0.207788 | 0.024500 | 104 | H12 | H17 | 6.642460 | 0.329697 | 0.116100 | 107 |
| H7 | H19 | 3.304221 | 0.376550 | 0.040500 | 104 | H11 | H22 | 6.611863 | 0.440036 | 0.122200 | 107 |
| H11 | H13 | 3.461802 | 0.632015 | 0.086800 | 105 | C9 | H20 | 6.861918 | 0.162536 | 0.076400 | 107 |
| C2 | C9 | 3.580735 | 0.230515 | 0.012100 | 105 | H12 | H19 | 6.809885 | 0.340819 | 0.116400 | 107 |
| Si5 | H17 | 3.541168 | 0.249144 | 0.025000 | 105 | C6 | H12 | 6.964247 | 0.222220 | 0.109300 | 107 |
| Si4 | H19 | 3.545975 | 0.248074 | 0.025000 | 105 | H10 | H21 | 7.138147 | 0.395658 | 0.047300 | 107 |
| Si1 | H17 | 3.524401 | 0.253962 | 0.026500 | 105 | H12 | H22 | 7.041455 | 0.428364 | 0.124500 | 107 |
| Si4 | H7 | 3.532740 | 0.253213 | 0.024600 | 105 | C9 | H21 | 7.111254 | 0.195572 | 0.079300 | 107 |
| Si1 | H19 | 3.534573 | 0.253855 | 0.026900 | 105 | H12 | H18 | 7.238546 | 0.333991 | 0.115400 | 107 |
| Si5 | H7 | 3.564499 | 0.255568 | 0.024900 | 105 | H10 | H20 | 7.228484 | 0.308664 | 0.080200 | 107 |
| Si1 | H12 | 3.538221 | 0.118309 | 0.047100 | 105 | H11 | H20 | 7.130007 | 0.283447 | 0.095100 | 107 |
| Si1 | C6 | 3.578239 | 0.105568 | 0.014700 | 105 | H11 | H21 | 7.251423 | 0.408652 | 0.104100 | 107 |
| C3 | Si4 | 3.625936 | 0.106746 | 0.014900 | 105 | H12 | H20 | 7.482623 | 0.230259 | 0.105800 | 107 |
| C2 | Si5 | 3.632838 | 0.106853 | 0.014300 | 105 | H12 | H21 | 7.975210 | 0.220679 | 0.139700 | 107 |
| C9 | H14 | 3.774831 | 0.379766 | 0.043900 | 105 | | | | | | |

**Table S6: Interatomic ra distances in 1-methoxy-1,3,5-trisilacyclohexane with corresponding refined amplitudes and vibrational corrections. Numbers in the last column indicate groups in which scale factors for the corresponding amplitudes have been refined. All values of parameters are in Å. Internal numeration (see Table S3) of atoms is used.**
**IV** (*tr*-Eq) conformer

| At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu | At1 | At2 | $r_a$ | l | $r_{h1}$-$r_a$ | Gu |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C9 | H10 | 1.078680 | 0.079322 | 0.001500 | 100 | C2 | Si5 | 3.617582 | 0.106853 | 0.014000 | 105 |
| C6 | H21 | 1.082471 | 0.078807 | 0.001900 | 100 | C3 | Si4 | 3.617608 | 0.106853 | 0.014000 | 105 |
| C2 | H13 | 1.082808 | 0.078807 | 0.001900 | 100 | Si1 | C6 | 3.591236 | 0.105782 | 0.014700 | 105 |
| C3 | H15 | 1.082815 | 0.078807 | 0.001900 | 100 | H16 | H19 | 3.630085 | 0.153427 | 0.027400 | 105 |
| C6 | H22 | 1.084350 | 0.079116 | 0.001900 | 100 | H14 | H17 | 3.630323 | 0.153427 | 0.027200 | 105 |
| C9 | H11 | 1.084837 | 0.081485 | 0.001700 | 100 | H17 | H22 | 3.628108 | 0.153534 | 0.026900 | 105 |
| C9 | H12 | 1.084844 | 0.081485 | 0.001700 | 100 | H19 | H22 | 3.614674 | 0.153534 | 0.026900 | 105 |
| C3 | H16 | 1.085411 | 0.079219 | 0.001900 | 100 | H7 | H14 | 3.636770 | 0.152998 | 0.025800 | 105 |
| C2 | H14 | 1.085412 | 0.079219 | 0.001900 | 100 | H7 | H16 | 3.634400 | 0.152998 | 0.025900 | 105 |
| O8 | C9 | 1.429793 | 0.059701 | 0.000600 | 101 | C9 | H15 | 3.999155 | 0.404391 | 0.049800 | 105 |
| Si1 | H7 | 1.495318 | 0.111202 | 0.001500 | 101 | C9 | H13 | 3.406404 | 0.403856 | 0.050500 | 105 |
| Si4 | H18 | 1.501184 | 0.112099 | 0.001700 | 101 | H7 | C9 | 3.686892 | 0.131692 | 0.043700 | 105 |
| Si5 | H20 | 1.501191 | 0.112227 | 0.001700 | 101 | C3 | H12 | 4.237081 | 0.605784 | 0.123800 | 105 |
| Si5 | H19 | 1.502529 | 0.112227 | 0.001600 | 101 | C2 | H11 | 3.351177 | 0.605141 | 0.124600 | 105 |
| Si4 | H17 | 1.502544 | 0.112227 | 0.001600 | 101 | Si5 | H14 | 3.908108 | 0.232549 | 0.031000 | 105 |
| Si1 | O8 | 1.665937 | 0.072083 | -0.000300 | 102 | Si4 | H16 | 3.908885 | 0.233406 | 0.031200 | 105 |
| H21 | H22 | 1.731150 | 0.127612 | 0.010700 | 103 | C3 | H13 | 3.959239 | 0.123983 | 0.023100 | 105 |
| H13 | H14 | 1.735298 | 0.127713 | 0.010700 | 103 | C2 | H15 | 3.959059 | 0.123983 | 0.023300 | 105 |
| H15 | H16 | 1.735302 | 0.127713 | 0.010700 | 103 | Si1 | H22 | 3.934386 | 0.230087 | 0.031200 | 105 |
| H10 | H12 | 1.748648 | 0.126190 | 0.008900 | 103 | C2 | H21 | 3.962371 | 0.124733 | 0.024400 | 105 |
| H10 | H11 | 1.748651 | 0.126089 | 0.008900 | 103 | C3 | H21 | 3.956687 | 0.124840 | 0.024400 | 105 |
| H11 | H12 | 1.756016 | 0.126901 | 0.010300 | 103 | C6 | H13 | 3.963086 | 0.125268 | 0.024100 | 105 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Si1 | C3 | 1.873996 | 0.053298 | 0.000600 | 103 | C6 | H15 | 3.962978 | 0.125268 | 0.024300 | 105 |
| Si1 | C2 | 1.874001 | 0.053298 | 0.000600 | 103 | C3 | H17 | 4.180324 | 0.210137 | 0.032200 | 106 |
| Si4 | C6 | 1.881727 | 0.053501 | 0.000400 | 103 | C2 | H19 | 4.181228 | 0.210930 | 0.032400 | 106 |
| Si5 | C6 | 1.881743 | 0.053501 | 0.000400 | 103 | C6 | H7 | 4.152116 | 0.205205 | 0.031600 | 106 |
| C3 | Si5 | 1.882978 | 0.053704 | 0.000500 | 103 | H14 | H15 | 4.155844 | 0.195781 | 0.037600 | 106 |
| C2 | Si4 | 1.882979 | 0.053704 | 0.000500 | 103 | H13 | H16 | 4.156151 | 0.195869 | 0.037400 | 106 |
| O8 | H10 | 2.037123 | 0.102637 | 0.007500 | 103 | H7 | H11 | 4.220707 | 0.188383 | 0.056800 | 106 |
| O8 | H11 | 2.085834 | 0.106698 | 0.003100 | 103 | H7 | H12 | 3.861254 | 0.188295 | 0.056900 | 106 |
| O8 | H12 | 2.085897 | 0.106698 | 0.003100 | 103 | H10 | H16 | 4.369270 | 0.293716 | 0.085700 | 106 |
| H17 | H18 | 2.425341 | 0.140397 | 0.009400 | 104 | H10 | H14 | 4.227712 | 0.294244 | 0.086300 | 106 |
| H19 | H20 | 2.425396 | 0.140397 | 0.009400 | 104 | H14 | H21 | 4.183298 | 0.198776 | 0.039600 | 106 |
| Si4 | H14 | 2.433471 | 0.117648 | 0.010900 | 104 | H16 | H21 | 4.178558 | 0.199128 | 0.039800 | 106 |
| Si5 | H16 | 2.433504 | 0.117743 | 0.010900 | 104 | H13 | H22 | 4.204114 | 0.199745 | 0.039000 | 106 |
| Si4 | H22 | 2.444958 | 0.117172 | 0.010400 | 104 | H15 | H22 | 4.187567 | 0.199656 | 0.039300 | 106 |
| Si5 | H22 | 2.425720 | 0.117172 | 0.010400 | 104 | H12 | H15 | 4.629316 | 0.542076 | 0.186000 | 106 |
| Si1 | H16 | 2.432708 | 0.117934 | 0.010500 | 104 | H11 | H13 | 3.589598 | 0.540755 | 0.186500 | 106 |
| Si1 | H14 | 2.432721 | 0.117934 | 0.010500 | 104 | Si1 | H18 | 4.423080 | 0.108063 | 0.023800 | 106 |
| Si1 | H13 | 2.462855 | 0.115745 | 0.008800 | 104 | Si1 | H20 | 4.422951 | 0.108063 | 0.024000 | 106 |
| Si1 | H15 | 2.462860 | 0.115745 | 0.008800 | 104 | Si4 | H20 | 4.464232 | 0.106830 | 0.022800 | 106 |
| Si4 | H21 | 2.459987 | 0.115173 | 0.008800 | 104 | Si5 | H18 | 4.464473 | 0.106830 | 0.022700 | 106 |
| Si5 | H21 | 2.449989 | 0.115173 | 0.008800 | 104 | C3 | H10 | 4.497891 | 0.212251 | 0.080200 | 106 |
| Si5 | H15 | 2.461114 | 0.115554 | 0.008900 | 104 | C2 | H10 | 4.358620 | 0.212867 | 0.080500 | 106 |
| Si4 | H13 | 2.461465 | 0.115364 | 0.008800 | 104 | H7 | H10 | 4.381213 | 0.147695 | 0.046400 | 106 |
| O8 | H7 | 2.445298 | 0.114983 | 0.006000 | 104 | H10 | H13 | 4.344996 | 0.323660 | 0.083900 | 106 |
| H11 | H16 | 3.313228 | 0.426237 | -0.173600 | 104 | H10 | H15 | 4.566177 | 0.323836 | 0.083500 | 106 |
| H12 | H14 | 3.155819 | 0.426332 | -0.173500 | 104 | Si4 | O8 | 4.661368 | 0.076093 | 0.018400 | 106 |
| Si1 | C9 | 2.690121 | 0.073387 | 0.009000 | 104 | Si5 | O8 | 4.539514 | 0.076181 | 0.018500 | 106 |
| C6 | H17 | 2.750864 | 0.124406 | 0.008300 | 104 | Si4 | H15 | 4.603091 | 0.113876 | 0.031800 | 106 |
| C6 | H19 | 2.750855 | 0.124502 | 0.008400 | 104 | Si5 | H13 | 4.603606 | 0.113787 | 0.031600 | 106 |
| C3 | H19 | 2.763285 | 0.123930 | 0.008300 | 104 | Si1 | H21 | 4.558054 | 0.115461 | 0.032900 | 106 |
| C2 | H17 | 2.763334 | 0.123835 | 0.008300 | 104 | H16 | H17 | 4.782967 | 0.212867 | 0.048700 | 106 |
| C2 | H7 | 2.768685 | 0.123264 | 0.007700 | 104 | H14 | H19 | 4.783109 | 0.213131 | 0.048700 | 106 |
| C3 | H7 | 2.765585 | 0.123264 | 0.007800 | 104 | H13 | H15 | 4.803216 | 0.130609 | 0.036800 | 106 |
| C3 | H20 | 2.787784 | 0.122217 | 0.006800 | 104 | H15 | H21 | 4.789997 | 0.132018 | 0.039000 | 106 |
| C6 | H20 | 2.810085 | 0.122122 | 0.006800 | 104 | H13 | H21 | 4.798041 | 0.131930 | 0.038800 | 106 |
| C2 | H18 | 2.787955 | 0.122217 | 0.006800 | 104 | H7 | H22 | 4.797488 | 0.210577 | 0.047900 | 106 |
| C6 | H18 | 2.810249 | 0.122027 | 0.006800 | 104 | H7 | H18 | 4.884312 | 0.271884 | 0.039600 | 107 |
| C3 | O8 | 2.861645 | 0.082906 | 0.002800 | 104 | H7 | H20 | 4.881714 | 0.272435 | 0.040000 | 107 |
| C2 | O8 | 3.043407 | 0.082906 | 0.003000 | 104 | H17 | H20 | 4.920369 | 0.271113 | 0.038900 | 107 |
| Si1 | H12 | 2.977418 | 0.217687 | 0.002800 | 104 | H18 | H19 | 4.920619 | 0.271774 | 0.038900 | 107 |
| Si1 | H11 | 2.977926 | 0.217497 | 0.003000 | 104 | Si5 | H11 | 5.336847 | 0.391804 | -0.050600 | 107 |
| H16 | H20 | 2.999127 | 0.208074 | 0.015700 | 104 | Si4 | H12 | 5.043332 | 0.392134 | -0.050700 | 107 |
| H14 | H18 | 3.000009 | 0.207598 | 0.015600 | 104 | C2 | H20 | 4.956168 | 0.157581 | 0.030800 | 107 |
| H20 | H22 | 2.994359 | 0.207312 | 0.015000 | 104 | C3 | H18 | 4.956820 | 0.157470 | 0.030700 | 107 |
| H19 | H21 | 2.980457 | 0.212262 | 0.016900 | 104 | H7 | H21 | 4.917189 | 0.331128 | 0.050900 | 107 |
| H18 | H22 | 3.022506 | 0.206836 | 0.014900 | 104 | H15 | H17 | 4.977887 | 0.335093 | 0.051000 | 107 |
| H17 | H21 | 2.989217 | 0.212167 | 0.016900 | 104 | H13 | H19 | 4.979707 | 0.335533 | 0.051000 | 107 |
| H15 | H19 | 3.021483 | 0.211500 | 0.017000 | 104 | O8 | H17 | 5.052681 | 0.261863 | 0.034700 | 107 |
| H13 | H17 | 3.022503 | 0.210834 | 0.016900 | 104 | O8 | H19 | 4.936570 | 0.262854 | 0.034900 | 107 |
| C2 | C3 | 3.024765 | 0.087760 | 0.008800 | 104 | H14 | H20 | 5.049601 | 0.321878 | 0.047000 | 107 |
| H7 | H15 | 3.032314 | 0.210453 | 0.016500 | 104 | H16 | H18 | 5.051250 | 0.322649 | 0.047200 | 107 |
| H7 | H13 | 3.037085 | 0.210072 | 0.016400 | 104 | C6 | O8 | 5.143656 | 0.118158 | 0.025200 | 107 |
| H13 | H18 | 3.022306 | 0.189513 | 0.009700 | 104 | Si5 | C9 | 5.463959 | 0.222441 | 0.028300 | 107 |
| H15 | H20 | 3.022336 | 0.189513 | 0.009700 | 104 | Si4 | C9 | 5.191520 | 0.222771 | 0.028600 | 107 |
| H14 | H16 | 2.974383 | 0.304496 | 0.029100 | 104 | H12 | H22 | 5.861809 | 0.690337 | 0.003100 | 107 |
| H18 | H21 | 3.069875 | 0.188180 | 0.009700 | 104 | H11 | H22 | 5.309248 | 0.690667 | 0.004400 | 107 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| H20 | H21 | 3.055753 | 0.188180 | 0.009700 | 104 | O8 | H22 | 5.313399 | 0.297102 | 0.040900 | 107 |
| C2 | C6 | 3.034054 | 0.090235 | 0.009300 | 104 | Si5 | H12 | 5.803224 | 0.569757 | 0.088600 | 107 |
| C3 | C6 | 3.034256 | 0.090235 | 0.009400 | 104 | Si4 | H11 | 5.126088 | 0.569206 | 0.089300 | 107 |
| H14 | H22 | 3.043231 | 0.315727 | 0.032800 | 104 | C6 | H12 | 5.889091 | 0.524057 | 0.005900 | 107 |
| H16 | H22 | 3.030025 | 0.316203 | 0.033000 | 104 | C6 | H11 | 5.539321 | 0.524167 | 0.006800 | 107 |
| C3 | H11 | 3.668510 | 0.352659 | -0.091700 | 104 | H18 | H20 | 5.589047 | 0.187643 | 0.035500 | 107 |
| C2 | H12 | 3.201797 | 0.397325 | -0.091300 | 105 | C9 | H22 | 5.742157 | 0.408652 | 0.021100 | 107 |
| O8 | H13 | 3.277596 | 0.166288 | 0.006200 | 104 | H11 | H20 | 6.219932 | 0.485736 | -0.081600 | 107 |
| O8 | H15 | 3.005722 | 0.166573 | 0.005800 | 104 | H12 | H18 | 5.757349 | 0.485846 | -0.081400 | 107 |
| Si1 | Si4 | 3.133005 | 0.085761 | 0.011000 | 104 | C6 | C9 | 5.784670 | 0.225854 | 0.022600 | 107 |
| Si1 | Si5 | 3.133196 | 0.085952 | 0.011100 | 104 | O8 | H20 | 5.623297 | 0.158461 | 0.031400 | 107 |
| Si4 | Si5 | 3.168307 | 0.084048 | 0.009800 | 104 | O8 | H18 | 5.797140 | 0.158241 | 0.031300 | 107 |
| O8 | H16 | 3.115485 | 0.181803 | 0.010700 | 104 | H11 | H19 | 6.161607 | 0.402816 | 0.014200 | 107 |
| O8 | H14 | 3.281557 | 0.181803 | 0.010900 | 104 | H12 | H17 | 5.643727 | 0.402816 | 0.014100 | 107 |
| C3 | H14 | 3.185453 | 0.201791 | 0.022700 | 104 | C9 | H19 | 6.078353 | 0.273426 | 0.063900 | 107 |
| C2 | H16 | 3.185847 | 0.202172 | 0.022700 | 104 | C9 | H17 | 5.824520 | 0.273096 | 0.063900 | 107 |
| C6 | H14 | 3.207451 | 0.206931 | 0.024100 | 104 | H13 | H20 | 5.981949 | 0.167491 | 0.052500 | 107 |
| C9 | H16 | 3.652755 | 0.317060 | -0.011700 | 104 | H15 | H18 | 5.982093 | 0.167491 | 0.052600 | 107 |
| C6 | H16 | 3.208313 | 0.207503 | 0.024300 | 104 | C9 | H20 | 6.472324 | 0.343131 | 0.038800 | 107 |
| C9 | H14 | 3.251886 | 0.357389 | -0.010700 | 105 | C9 | H18 | 6.063469 | 0.343021 | 0.039200 | 107 |
| H7 | H17 | 3.238403 | 0.360274 | 0.038500 | 104 | O8 | H21 | 6.146900 | 0.134786 | 0.047400 | 107 |
| H11 | H15 | 3.953064 | 0.542933 | -0.028700 | 104 | Si5 | H10 | 6.274196 | 0.229048 | 0.104600 | 107 |
| H7 | H19 | 3.236824 | 0.361892 | 0.039100 | 104 | Si4 | H10 | 6.170404 | 0.229598 | 0.104600 | 107 |
| H12 | H13 | 2.904887 | 0.610816 | -0.027700 | 105 | H12 | H19 | 6.387117 | 0.466905 | 0.112200 | 107 |
| H17 | H19 | 3.281632 | 0.361511 | 0.037300 | 104 | H11 | H17 | 5.999676 | 0.466134 | 0.112200 | 107 |
| C2 | H22 | 3.238274 | 0.207027 | 0.023900 | 104 | H12 | H20 | 6.900797 | 0.737358 | 0.137000 | 107 |
| C3 | H22 | 3.225000 | 0.207027 | 0.024000 | 104 | H11 | H18 | 5.893113 | 0.736037 | 0.137700 | 107 |
| C3 | C9 | 3.758602 | 0.236819 | 0.014100 | 104 | H12 | H21 | 6.906857 | 0.520203 | 0.030400 | 107 |
| C2 | C9 | 3.369166 | 0.266917 | 0.014700 | 105 | H11 | H21 | 6.599108 | 0.520203 | 0.031100 | 107 |
| Si1 | H17 | 3.506899 | 0.250322 | 0.026100 | 105 | H10 | H22 | 6.658228 | 0.432108 | 0.136700 | 107 |
| Si1 | H19 | 3.507740 | 0.251500 | 0.026400 | 105 | C6 | H10 | 6.717674 | 0.242152 | 0.119700 | 107 |
| Si4 | H7 | 3.528499 | 0.245397 | 0.024800 | 105 | C9 | H21 | 6.827255 | 0.230479 | 0.050900 | 107 |
| Si5 | H7 | 3.526564 | 0.245825 | 0.025000 | 105 | H10 | H17 | 6.751379 | 0.294569 | 0.112700 | 107 |
| Si5 | H17 | 3.554393 | 0.248074 | 0.024500 | 105 | H10 | H19 | 6.851060 | 0.294899 | 0.113000 | 107 |
| H12 | H16 | 4.093486 | 0.716931 | 0.165700 | 104 | H10 | H20 | 7.201061 | 0.348858 | 0.124400 | 107 |
| Si4 | H19 | 3.554817 | 0.248930 | 0.024600 | 105 | H10 | H18 | 7.041323 | 0.349078 | 0.124300 | 107 |
| H11 | H14 | 2.858395 | 0.806320 | 0.167200 | 105 | H10 | H21 | 7.760114 | 0.243584 | 0.147400 | 107 |
| Si1 | H10 | 3.544048 | 0.115311 | 0.051400 | 105 | | | | | | |

**Table S7: Matrix of correlation coefficients between refined parameters.**
The order of parameters was as follows: two scale factors for sMs(s) curves, conformational composition, groups of geometrical parameters (1-10), groups of scale factors for amplitudes (100-107, see Table S4-6).

```
 1.0000
 0.5321  1.0000
-0.0577 -0.0744  1.0000
-0.0206 -0.0266 -0.4910  1.0000
-0.1939 -0.1925 -0.1360  0.4953  1.0000
-0.3091 -0.3298  0.0883 -0.0522  0.2778  1.0000
-0.4836 -0.4548  0.0417  0.0295  0.3806  0.4632  1.0000
-0.0988 -0.1276  0.0521 -0.1810 -0.0373  0.2917  0.2030  1.0000
 0.1419  0.1460  0.3035 -0.6435 -0.7099 -0.0836 -0.1662  0.0952
-0.0234  0.0027  0.2054 -0.6761 -0.3293  0.1171  0.0518  0.1526
```

0.2063 0.2093 -0.2575 0.2213 -0.0407 -0.4780 -0.4325 -0.0391
0.1880 0.1962 -0.3139 -0.2859 -0.1767 0.0229 -0.0423 0.0966
0.1304 0.1155 0.0620 0.1103 0.0239 -0.0637 -0.0554 -0.0263
0.0823 0.1022 0.1067 -0.7574 -0.3967 0.0492 -0.0319 0.1360
0.1525 0.1580 -0.0239 0.0282 0.0327 0.0837 -0.0865 -0.0447
0.0465 0.0422 -0.0133 0.0016 0.1390 0.0813 -0.3137 -0.1692
-0.1230 -0.0697 0.0073 0.0146 0.2236 0.1946 -0.0315 -0.0096
0.5613 0.7367 -0.0772 -0.0462 -0.2168 -0.3859 -0.5129 -0.1404
0.1778 0.2062 -0.3358 0.3362 0.3423 -0.0432 -0.0251 -0.0840
0.1030 0.0936 -0.3483 0.4045 0.2465 -0.0614 -0.0583 -0.0542
0.1083 0.1126 -0.5816 0.5695 0.2092 -0.0883 -0.1304 -0.1227
-0.0865 -0.0920 0.2645 0.0313 0.0157 0.0249 -0.0145 -0.0295

1.0000
0.3998 1.0000
-0.1991 -0.0295 1.0000
0.2785 0.1033 -0.0365 1.0000
0.0029 -0.2128 0.0186 -0.0974 1.0000
0.5452 0.5741 -0.1360 0.5243 -0.3151 1.0000
-0.0174 -0.0121 0.0075 0.0532 0.0218 0.0026 1.0000
-0.0973 -0.0130 0.0739 0.0080 -0.0211 0.0071 0.0233 1.0000
-0.1336 -0.0138 -0.0603 -0.0272 -0.0323 -0.0150 0.0269 0.4371
0.1453 -0.0002 0.2566 0.1766 0.0861 0.1040 0.1167 0.0956
-0.5877 0.1001 0.2590 -0.2608 -0.0841 -0.2064 0.0467 0.0557
-0.4253 -0.3229 0.2178 0.2090 0.1789 -0.3992 0.0450 0.0408
-0.3436 -0.5384 0.1615 0.2675 -0.1695 -0.2295 0.0537 0.0611
-0.0290 -0.1047 -0.1155 -0.2774 -0.3162 -0.1408 -0.0160 0.0203

1.0000
0.0944 1.0000
0.0613 0.1409 1.0000
0.0156 0.0807 0.2063 1.0000
0.0180 0.1138 0.1182 0.3954 1.0000
0.0279 -0.0700 -0.0580 -0.1227 0.2363 1.0000

**REFERENCES**


[1] **Girichev G.V., Utkin A.N., Revichev Y.F.** Instrum. Exp. Techn. 1984. V. 27. N 2. P. 457−461.

[2] **Girichev G.V., Shlykov S.A., Petrova V.N., Subbotyina N.Y., Lapshina S.B., Danilova T.G.** Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol. 1988. V. 1. N 31. P. 46–49.

[3] **Girichev E.G., Zakharov A.V., Girichev G.V., Bazanov M.I.** Izv. Vyssh. Uchebn. Zaved., Tekhnol. Tekst. Prom. 2000. N 2. P. 142–146.

[4] **Andersen B., Seip H.M., Strand T.G., Stølevik. R.** Acta Chem. Scand. 1969. V. 23. N 9. P. 3224–3234. DOI: 10.3891/acta.chem.scand.23-3224.

[5] **Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Mennucci B., Petersson G.A., Nakatsuji H., Caricato M., Li X., Hratchian H.P., Izmaylov A.F., Bloino J., Zheng G., Sonnenberg J.L., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Montgomery J. A., Jr., Peralta J. E., Ogliaro F., Bearpark M., Heyd J.J., Brothers E., Kudin K.N., Staroverov V.N., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J.C., Iyengar S.S., Tomasi J., Cossi M., Rega N., Millam J.M., Klene M., Knox J.E., Cross J.B., Bakken V., Adamo C., Jaramillo J., Gomperts R., Stratmann R.E., Yazyev O., Austin A.J., Cammi R., Pomelli C., Ochterski J.W., Martin R.L., Morokuma K., Zakrzewski V.G., Voth G.A., Salvador P., Dannenberg J.J., Dapprich S., Daniels A.D., Farkas O., Foresman J.B., Ortiz J.V., Cioslowski J., Fox D.J.** Gaussian 09, Revision D.01. 2009. Gaussian, Inc.: Wallingford, CT.