

## Supplementary Material

All values are dependent on the Si–O–Si angle  $\alpha(\text{Si–O–Si})$  in  $^\circ$ .

If not otherwise specified, average values are given for Si–O bonds and Si atoms in symmetric model compounds.

All charges, populations and volumes (ED and ELI) are cut at an ED iso-value of 0.001 a.u. indicated by the index 001.

Complete reference of the programme GAUSSIAN:

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table 1: Bending-potential energies ( $E_{bend}$ ) in  $\text{kJ mol}^{-1}$  for disiloxane [1], disiloxane···silanol [2], and disiloxane···water [3]; Hydrogen-bond energies ( $E_{HB}$ ) in  $\text{kJ mol}^{-1}$  for [2] and [3]

a(Si–O–Si)	$E_{bend}$ [1]	$E_{bend}$ [2]	$E_{bend}$ [3]	$E_{HB}$ [2]	$E_{HB}$ [3]
50	813.901	—	—	—	—
55	722.932	—	—	—	—
60	604.312	—	—	—	—
65	484.913	—	—	—	—
70	381.008	—	—	—	—
75	292.308	—	—	—	—
80	220.086	—	—	—	—
85	162.971	141.441	143.787	-26.486	-17.980
90	118.921	101.588	103.314	-22.233	-14.298
95	85.598	71.590	73.866	-18.903	-11.321
100	60.799	49.446	51.471	-16.153	-8.064
105	42.582	33.297	35.353	-14.353	-5.785
110	29.298	23.052	23.728	-12.497	-4.151
115	19.716	13.973	15.175	-11.091	-3.250
120	12.817	7.674	9.213	-9.835	-2.309
125	7.993	3.560	5.017	-9.144	-1.662
130	4.685	1.171	2.342	-8.303	-1.068
135	2.585	0.202	0.772	-7.238	-0.572
140	1.258	0.000	0.120	-6.193	-0.351
145	0.584	0.546	0.000	-5.069	-0.180
150	0.236	1.455	0.036	-3.857	-0.058
155	0.000	2.891	0.947	-2.213	0.000
160	0.010	4.130	1.490	-1.027	0.000
165	0.029	5.445	2.007	-0.255	0.000
170	0.257	—	—	—	—
175	0.432	—	—	—	—
180	0.498	—	—	—	—

Table 2: Natural bond orbital delocalization ( $\Delta E_{deloc}$ ) energies in  $\text{kJ mol}^{-1}$  as well as IR red shifts ( $\Delta \text{IR}$ ) of the O–H stretching vibrations in donor molecules in  $\text{cm}^{-1}$  for [1]: disiloxane···silanol and [2]: disiloxane···water; Symm/asymm = symmetric/asymmetric stretching vibrations of the O–H bonds in water

a(Si–O–Si)	$\Delta E_{deloc}[1]$	$\Delta E_{deloc}[2]$	$\Delta \text{IR}[1]$	$\Delta \text{IR}_{symm}[2]$	$\Delta \text{IR}_{asymm}[2]$
85	28.805	12.810	188.10	55.89	33.13
90	29.433	11.221	185.79	53.23	30.01
95	25.958	14.068	179.05	51.81	25.65
100	26.921	11.346	177.78	48.57	28.20
105	27.800	12.728	175.14	50.43	25.02
110	27.507	13.900	172.12	53.47	28.89
115	27.675	12.309	170.91	47.15	26.57
120	27.591	12.770	168.42	48.82	28.51
125	27.214	12.519	164.43	46.57	28.18
130	26.963	12.644	160.67	44.66	27.72
135	25.916	12.602	153.71	42.51	27.12
140	24.283	12.602	143.82	39.86	26.51
145	22.441	12.184	132.50	36.16	25.69
150	20.641	10.634	121.96	29.58	23.54
155	17.710	8.290	106.25	22.26	20.51
160	13.147	5.443	79.82	14.22	15.81
165	8.374	1.507	55.17	5.39	8.25

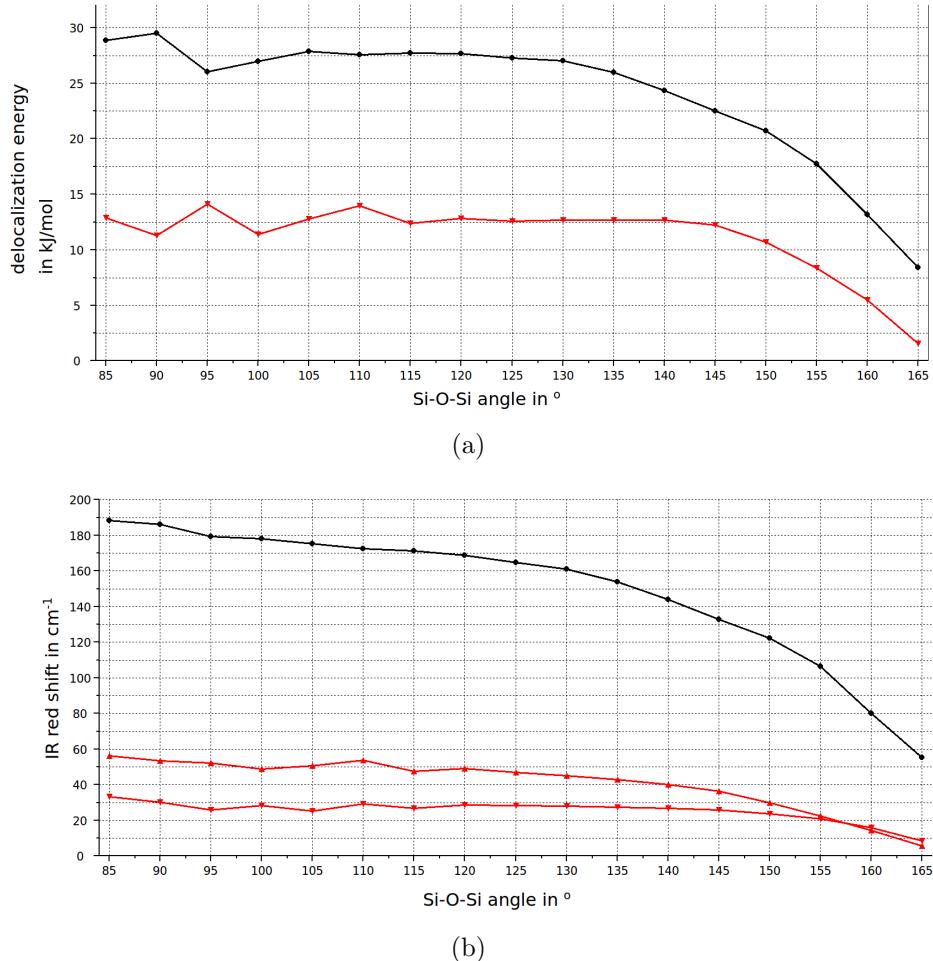


Figure 1: (a) Delocalization energy from natural bond orbital analysis for disiloxane...silanol (black circles) and disiloxane...water (red triangles); (b) IR red shift for the O–H stretching vibration in disiloxane...silanol (black circles), the symmetric O–H stretching vibration in water (red triangles head up), the asymmetric O–H stretching vibration in water (red triangles head down)

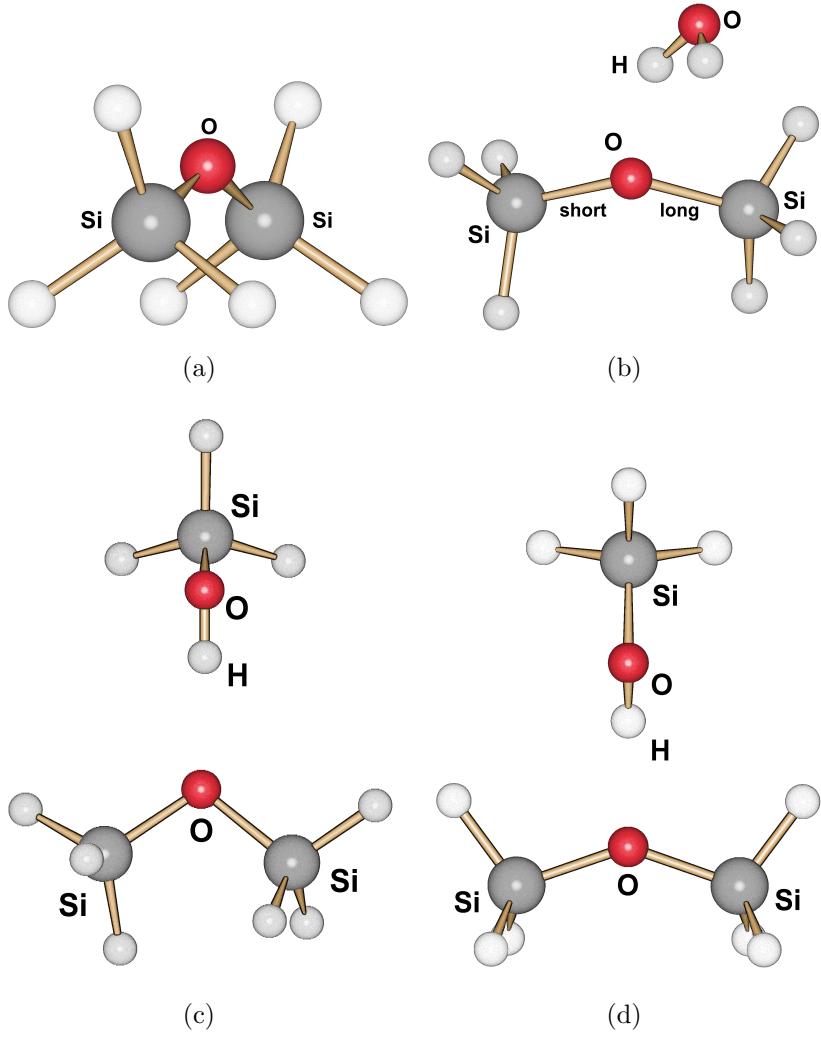


Figure 2: Representative geometries of model compounds. (a) Free disiloxane in its eclipsed conformation at  $\phi=140^\circ$ , (b) Disiloxane···water in its staggered conformation at  $\phi=140^\circ$ , (c) Disiloxane···silanol in its staggered conformation at  $\phi=105^\circ$ , (d) Disiloxane···silanol in its eclipsed conformation at  $\phi=140^\circ$

Table 3: Si–O bond distances (d) and bond-path lengths (bp) in Å, ED ( $\varrho$ ) at the Si–O bcp<sub>s</sub> in eÅ<sup>-3</sup>, Laplacian ( $\nabla^2\varrho$ ) at the Si–O bcp<sub>s</sub> in eÅ<sup>-5</sup>, and Si–O delocalization indices ( $\delta$ ) for free disiloxane H<sub>3</sub>SiOSiH<sub>3</sub>, [1] alternatively critical point between bcp<sub>Si–Si</sub> and O atom

a(Si–O–Si)	d(Si–O)	d(bp)	$\varrho$ (Si–O) or	$\nabla^2\varrho$ (Si–O) or	$\delta$ (Si–O)
			[1] $\varrho$ (bcp <sub>Si–Si</sub> –O)	[1] $\nabla^2\varrho$ (bcp <sub>Si–Si</sub> –O)	
50	2.6479		[1] 0.2057	[1] 1.127	0.3272
55	2.3400		[1] 0.3782	[1] 0.987	0.4960
60	2.1385		[1] 0.4997	[1] 0.054	0.5513
65	2.0081	2.0776	0.5518	0.772	0.5383
70	1.9190	1.9375	0.6059	4.834	0.5056
75	1.8547	1.8627	0.6606	7.742	0.4864
80	1.8077	1.8178	0.7087	10.075	0.4723
85	1.7721	1.7743	0.7500	12.012	0.4618
90	1.7448	1.7461	0.7844	13.623	0.4538
95	1.7237	1.7245	0.8121	14.951	0.4474
100	1.7074	1.7080	0.8340	16.039	0.4425
105	1.6945	1.6950	0.8513	16.944	0.4385
110	1.6846	1.6849	0.8640	17.676	0.4350
115	1.6766	1.6770	0.8734	18.286	0.4320
120	1.6701	1.6705	0.8803	18.811	0.4292
125	1.6645	1.6650	0.8854	19.278	0.4265
130	1.6597	1.6601	0.8891	19.702	0.4240
135	1.6554	1.6559	0.8919	20.095	0.4216
140	1.6515	1.6520	0.8939	20.460	0.4194
145	1.6481	1.6485	0.8956	20.799	0.4174
150	1.6450	1.6454	0.8968	21.109	0.4155
155	1.6423	1.6427	0.8978	21.383	0.4140
160	1.6401	1.6403	0.8986	21.618	0.4127
165	1.6384	1.6385	0.8993	21.808	0.4116
170	1.6371	1.6371	0.8997	21.948	0.4109
175	1.6363	1.6363	0.8999	22.033	0.4105
180	1.6361	1.6361	0.9000	22.060	0.4102

Table 4: Si–Si bond distances ( $d$ ) in Å, ED ( $\varrho$ ) at the Si–Si bcps in eÅ $^{-3}$ , Laplacian ( $\nabla^2\varrho$ ) at the Si–O bcps in eÅ $^{-5}$ , and Si–Si delocalization indices ( $\delta$ ) for free disiloxane H<sub>3</sub>SiOSiH<sub>3</sub>

a(Si–O–Si)	d(Si–Si)	d(bp)	$\varrho$ (Si–Si)	$\nabla^2\varrho$ (Si–Si)	$\delta$ (Si–Si)
50	2.2381	2.2568	0.5989	-3.709	0.4539
55	2.1609	2.1893	0.5876	-3.468	0.3276
60	2.1385	2.1804	0.5581	-2.836	0.2211
65	2.1579				0.1246
70	2.2014				0.0742
75	2.2582				0.0522
80	2.3240				0.0374
85	2.3945				0.0273
90	2.4675				0.0204
95	2.5417				0.0156
100	2.6159				0.0123
105	2.6887				0.0100
110	2.7598				0.0084
115	2.8281				0.0073
120	2.8927				0.0067
125	2.9529				0.0063
130	3.0084				0.0060
135	3.0588				0.0060
140	3.1039				0.0060
145	3.1436				0.0061
150	3.1779				0.0062
155	3.2068				0.0063
160	3.2304				0.0064
165	3.2487				0.0065
170	3.2617				0.0066
175	3.2695				0.0067
180	3.2721				0.0067

Table 5: Si–O bond distances ( $d$ ) in Å, ED ( $\varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-5}$ , and Si–O delocalization indices ( $\delta$ ) for the siloxane group in disiloxane···silanol

a(Si–O–Si)	d(Si–O)	$\varrho$ (Si–O)	$\nabla^2 \varrho$ (Si–O)	$\delta$ (Si–O)
85	1.7717	0.7439	12.154	0.4337
90	1.7472	0.7743	13.587	0.4287
95	1.7278	0.7993	14.827	0.4244
100	1.7163	0.8179	15.591	0.4225
105	1.7026	0.8320	16.333	0.4196
110	1.6963	0.8389	16.866	0.4194
115	1.6886	0.8478	17.431	0.4168
120	1.6823	0.8543	17.913	0.4145
125	1.6769	0.8589	18.339	0.4123
130	1.6724	0.8620	18.717	0.4101
135	1.6682	0.8646	19.086	0.4082
140	1.6643	0.8667	19.431	0.4065
145	1.6606	0.8687	19.774	0.4051
150	1.6573	0.8702	20.093	0.4039
155	1.6543	0.8719	20.385	0.4031
160	1.6507	0.8756	20.723	0.4031
165	1.6474	0.8796	21.044	0.4030

Table 6: Si–O bond distances ( $d$ ) in Å, ED ( $\varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-5}$ , and Si–O delocalization indices ( $\delta$ ) for the shorter Si–O bonds in disiloxane···water

a(Si–O–Si)	d(Si–O)	$\varrho$ (Si–O)	$\nabla^2 \varrho$ (Si–O)	$\delta$ (Si–O)
85	1.7661	0.7643	12.313	0.4498
90	1.7410	0.7859	13.442	0.4403
95	1.7236	0.8077	14.628	0.4339
100	1.7080	0.8296	15.566	0.4329
105	1.6965	0.8446	16.438	0.4296
110	1.6882	0.8546	17.022	0.4273
115	1.6805	0.8639	17.652	0.4253
120	1.6749	0.8689	18.275	0.4219
125	1.6695	0.8738	18.779	0.4201
130	1.6649	0.8773	19.216	0.4182
135	1.6609	0.8797	19.600	0.4163
140	1.6574	0.8811	19.939	0.4145
145	1.6542	0.8824	20.273	0.4130
150	1.6509	0.8842	20.602	0.4120
155	1.6474	0.8873	20.957	0.4115
160	1.6436	0.8919	21.287	0.4124
165	1.6378	0.9018	21.861	0.4151

Table 7: Si–O bond distances ( $d$ ) in Å, ED ( $\varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-5}$ , and Si–O delocalization indices ( $\delta$ ) for the longer Si–O bonds in disiloxane···water

a(Si–O–Si)	d(Si–O)	$\varrho$ (Si–O)	$\nabla^2 \varrho$ (Si–O)	$\delta$ (Si–O)
85	1.7721	0.7538	12.343	0.4400
90	1.7481	0.7753	13.499	0.4305
95	1.7276	0.8018	14.740	0.4272
100	1.7142	0.8191	15.635	0.4228
105	1.7038	0.8318	16.335	0.4195
110	1.6954	0.8414	16.928	0.4165
115	1.6872	0.8512	17.526	0.4146
120	1.6815	0.8566	17.958	0.4112
125	1.6764	0.8606	18.366	0.4098
130	1.6719	0.8635	18.745	0.4076
135	1.6678	0.8656	19.099	0.4057
140	1.6640	0.8673	19.440	0.4040
145	1.6603	0.8690	19.783	0.4026
150	1.6570	0.8706	20.099	0.4014
155	1.6541	0.8719	20.381	0.4004
160	1.6516	0.8733	20.674	0.3995
165	1.6485	0.8761	20.922	0.3993

Table 8: H···O and O···O distances (d) in Å, ED ( $\varrho$ ) at the H···O bcps in eÅ $^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the H···O bcps in eÅ $^{-5}$ , and H···O delocalization indices ( $\delta$ ) in disiloxane···silanol

a(Si–O–Si)	d(H···O)	d(O···O)	$\varrho$ (H···O)	$\nabla^2 \varrho$ (H···O)	$\delta$ (H···O)
85	1.8917	2.8575	0.1812	2.044	0.0744
90	1.8956	2.8597	0.1803	2.036	0.0742
95	1.9038	2.8710	0.1741	2.007	0.0718
100	1.9051	2.8719	0.1750	2.003	0.0727
105	1.9073	2.8743	0.1765	1.993	0.0733
110	1.9149	2.8818	0.1732	1.967	0.0728
115	1.9210	2.8878	0.1718	1.947	0.0728
120	1.9290	2.8956	0.1697	1.921	0.0726
125	1.9396	2.9059	0.1666	1.888	0.0720
130	1.9491	2.9141	0.1645	1.861	0.0718
135	1.9646	2.9285	0.1599	1.816	0.0709
140	1.9867	2.9496	0.1529	1.752	0.0690
145	2.0109	2.9719	0.1458	1.684	0.0671
150	2.0358	2.9947	0.1395	1.614	0.0658
155	2.0762	3.0335	0.1284	1.503	0.0623
160	2.1518	3.0853	0.1082	1.324	0.0590
165	2.2499	3.1484	0.0876	1.105	0.0426

Table 9: H···O and O···O distances ( $d$ ) in Å, ED ( $\varrho$ ) at the H···O bcps in eÅ $^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the H···O bcps in eÅ $^{-5}$ , and H···O delocalization indices ( $\delta$ ) in disiloxane···water

a(Si–O–Si)	$d(\text{H}\cdots\text{O})$	$d(\text{O}\cdots\text{O})$	$\varrho(\text{H}\cdots\text{O})$	$\nabla^2 \varrho(\text{H}\cdots\text{O})$	$\delta(\text{H}\cdots\text{O})$
85	2.0474	2.9181	0.1422	1.818	0.0578
90	2.0572	2.9050	0.1298	1.763	0.0538
95	2.0104	2.9189	0.1403	1.824	0.0598
100	2.0628	2.9117	0.1281	1.737	0.0536
105	2.0448	2.9096	0.1331	1.781	0.0559
110	2.0369	2.9008	0.1368	1.813	0.0575
115	2.0686	2.9189	0.1279	1.713	0.0543
120	2.0610	2.9203	0.1298	1.724	0.0553
125	2.0735	2.9317	0.1270	1.680	0.0547
130	2.0826	2.9467	0.1253	1.640	0.0547
135	2.0925	2.9641	0.1233	1.596	0.0547
140	2.1037	2.9846	0.1212	1.549	0.0549
145	2.1219	3.0102	0.1174	1.484	0.0544
150	2.1590	3.0431	0.1093	1.378	0.0516
155	2.2176	3.0809	0.0974	1.232	0.0460
160	2.3069	3.1254	0.0822	1.035	0.0373
165	2.5327	3.1897	0.0574	0.680	0.0201

Table 10: O–H···O angle (a) in  $^{\circ}$ , O–H distances (d) in Å, ED ( $\varrho$ ) at the O–H bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the O–H bcps in  $e\text{\AA}^{-5}$ , and O–H delocalization indices ( $\delta$ ) in the silanol group of disiloxane···silanol

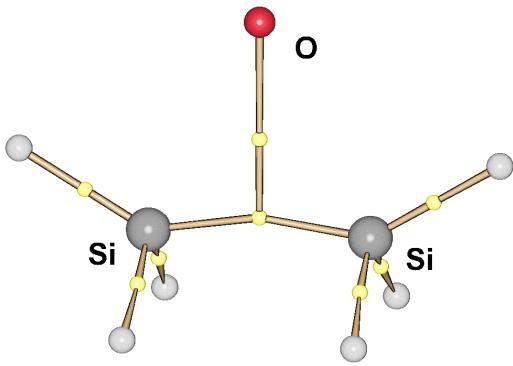
a(Si–O–Si)	a(O–H···O)	d(O–H)	$\varrho$ (O–H)	$\nabla^2 \varrho$ (O–H)	$\delta$ (O–H)
85	175.23	0.9680	2.3961	-62.583	0.5450
90	173.78	0.9678	2.3972	-62.620	0.5455
95	179.71	0.9673	2.4024	-62.853	0.5459
100	177.69	0.9673	2.4020	-62.828	0.5460
105	178.19	0.9673	2.4020	-62.812	0.5460
110	178.85	0.9671	2.4037	-62.833	0.5470
115	178.70	0.9670	2.4047	-62.835	0.5478
120	178.43	0.9668	2.4063	-62.846	0.5496
125	178.00	0.9666	2.4084	-62.865	0.5521
130	176.14	0.9664	2.4106	-62.874	0.5544
135	175.45	0.9660	2.4141	-62.918	0.5578
140	174.93	0.9655	2.4189	-62.986	0.5622
145	173.77	0.9649	2.4243	-63.067	0.5668
150	172.66	0.9643	2.4297	-63.132	0.5724
155	172.10	0.9635	2.4369	-63.237	0.5787
160	163.10	0.9624	2.4471	-63.392	0.5902
165	155.17	0.9613	2.4571	-63.528	0.6025

Table 11: O–H···O angle ( $\alpha$ ) in  $^\circ$ , O–H distances ( $d$ ) in Å, ED ( $\varrho$ ) at the O–H bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the O–H bcps in  $e\text{\AA}^{-5}$ , and O–H delocalization indices ( $\delta$ ) in the water group of disiloxane···water

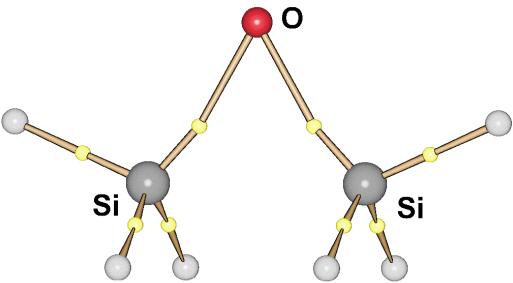
a(Si–O–Si)	a(O–H···O)	d(O–H)	$\varrho$ (O–H)	$\nabla^2 \varrho$ (O–H)	$\delta$ (O–H)
85	148.90	0.9661	2.4696	-63.601	0.6102
90	145.48	0.9658	2.4702	-63.622	0.6149
95	155.95	0.9656	2.4709	-63.682	0.6070
100	145.72	0.9654	2.4728	-63.692	0.6163
105	148.10	0.9655	2.4720	-63.685	0.6131
110	147.91	0.9657	2.4712	-63.645	0.6123
115	145.95	0.9653	2.4743	-63.700	0.6171
120	147.30	0.9654	2.4737	-63.684	0.6150
125	147.18	0.9652	2.4752	-63.700	0.6168
130	148.15	0.9651	2.4765	-63.729	0.6179
135	149.42	0.9649	2.4782	-63.774	0.6191
140	151.05	0.9647	2.4802	-63.823	0.6211
145	152.46	0.9644	2.4831	-63.868	0.6242
150	151.87	0.9639	2.4873	-63.913	0.6298
155	148.58	0.9634	2.4918	-63.940	0.6374
160	142.39	0.9629	2.4969	-63.595	0.6483
165	125.55	0.9621	2.5036	-63.616	0.6609

Table 12: Si–O distances ( $d$ ) in Å, ED ( $\varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-3}$ , Laplacian ( $\nabla^2 \varrho$ ) at the Si–O bcps in  $e\text{\AA}^{-5}$ , and Si–O delocalization indices ( $\delta$ ) in the silanol group of disiloxane···silanol

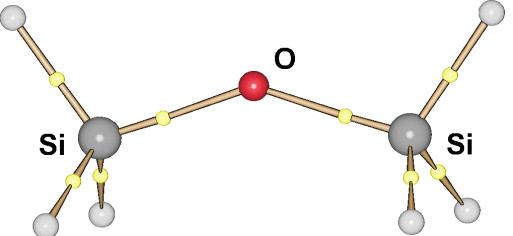
a(Si–O–Si)	d(Si–O)	$\varrho$ (Si–O)	$\nabla^2 \varrho$ (Si–O)	$\delta$ (Si–O)
85	1.6514	0.9269	19.806	0.4504
90	1.6515	0.9265	19.790	0.4501
95	1.6511	0.9278	19.932	0.4501
100	1.6513	0.9273	19.921	0.4498
105	1.6514	0.9268	19.923	0.4494
110	1.6517	0.9261	19.895	0.4490
115	1.6520	0.9255	19.883	0.4487
120	1.6522	0.9247	19.864	0.4482
125	1.6525	0.9238	19.836	0.4477
130	1.6530	0.9225	19.779	0.4470
135	1.6536	0.9211	19.734	0.4463
140	1.6542	0.9197	19.688	0.4455
145	1.6549	0.9179	19.628	0.4445
150	1.6558	0.9156	19.552	0.4434
155	1.6566	0.9136	19.491	0.4423
160	1.6576	0.9112	19.397	0.4413
165	1.6587	0.9086	19.340	0.4401



(a)



(b)



(c)

Figure 3: Representative molecular graphs of free disiloxane, yellow circles represent bond critical points in the electron-density topology. (a)  $\phi=55^\circ$ , T-type shape of molecular graph; (b)  $\phi=70^\circ$ , open form of molecular graph, strained Si–O bond; (c)  $\phi=145^\circ$ , open form of molecular graph, relaxed Si–O bonds.

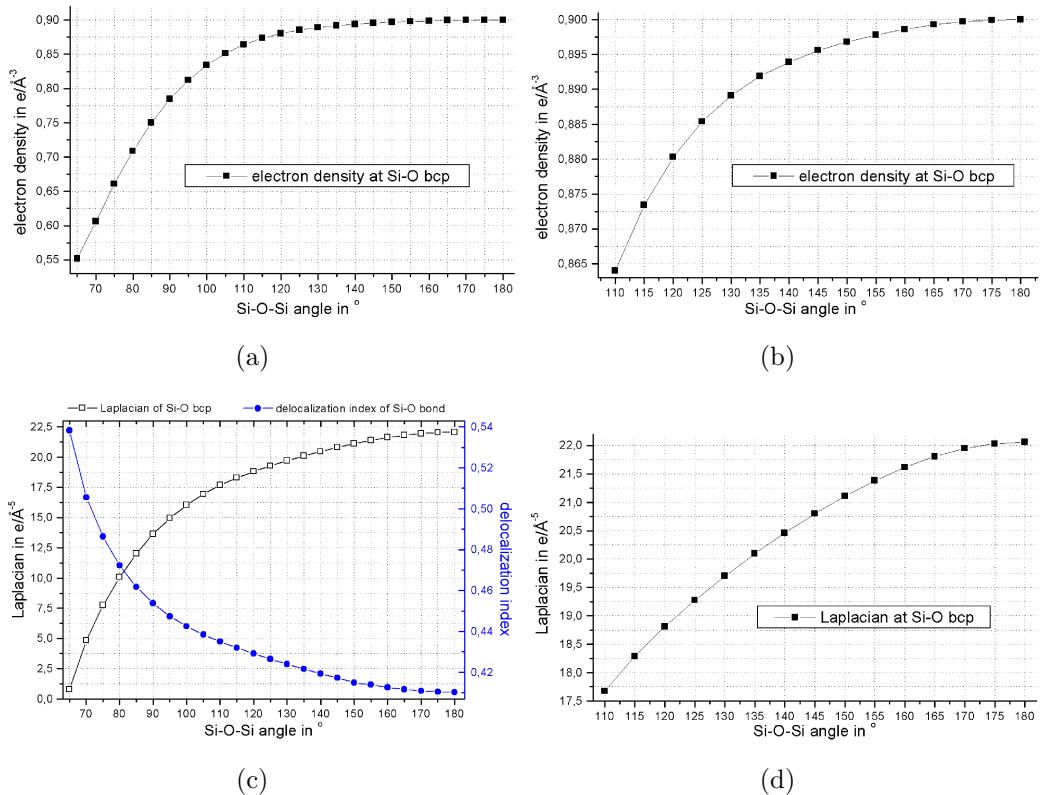


Figure 4: Electron density and Laplacian of the ED at the Si–O bcp of free disiloxane as well as delocalization index of the Si–O bonds

Table 13: Atomic charges ( $Q_{001}$ ) in e and volumes ( $V_{001}$ ) in Å<sup>3</sup> of Si and O atoms in free disiloxane

a(Si–O–Si)	$Q_{001}(\text{Si})$	$V_{001}(\text{Si})$	$Q_{001}(\text{O})$	$V_{001}(\text{O})$
50	2.1573	9.676	-0.4118	22.136
55	2.2501	8.507	-0.6390	21.992
60	2.3824	7.528	-0.9124	21.982
65	2.5600	6.663	-1.2896	22.313
70	2.6678	6.229	-1.4436	21.986
75	2.7243	6.027	-1.5024	21.495
80	2.7650	5.909	-1.5381	21.097
85	2.7949	5.844	-1.5627	20.753
90	2.8165	5.809	-1.5805	20.464
95	2.8327	5.793	-1.5940	20.243
100	2.8466	5.788	-1.6041	20.051
105	2.8546	5.788	-1.6124	19.925
110	2.8618	5.793	-1.6190	19.834
115	2.8679	5.799	-1.6245	19.782
120	2.8730	5.804	-1.6297	19.785
125	2.8773	5.804	-1.6345	19.815
130	2.8814	5.799	-1.6393	19.923
135	2.8849	5.788	-1.6438	19.989
140	2.8883	5.774	-1.6480	20.088
145	2.8912	5.758	-1.6517	20.153
150	2.8937	5.744	-1.6550	20.204
155	2.8958	5.733	-1.6578	20.236
160	2.8977	5.721	-1.6603	20.255
165	2.8993	5.712	-1.6622	20.267
170	2.9003	5.706	-1.6638	20.279
175	2.9009	5.702	-1.6648	20.294
180	2.9013	5.700	-1.6655	20.306

Table 14: Atomic charges ( $Q_{001}$ ) in e and volumes ( $V_{001}$ ) in Å<sup>3</sup> of Si and O atoms in the siloxane group of disiloxane···silanol

a(Si–O–Si)	$Q_{001}(\text{Si})$	$V_{001}(\text{Si})$	$Q_{001}(\text{O})$	$V_{001}(\text{O})$
85	2.8167	5.715	-1.5686	19.669
90	2.8321	5.712	-1.5852	19.404
95	2.8432	5.719	-1.5944	19.257
100	2.8553	5.735	-1.6209	19.149
105	2.8619	5.753	-1.6269	18.990
110	2.8610	5.824	-1.6209	18.858
115	2.8665	5.831	-1.6270	18.772
120	2.8711	5.836	-1.6322	18.726
125	2.8752	5.836	-1.6370	18.720
130	2.8790	5.831	-1.6410	18.762
135	2.8824	5.819	-1.6461	18.838
140	2.8851	5.804	-1.6503	18.909
145	2.8873	5.790	-1.6546	18.983
150	2.8882	5.783	-1.6584	19.036
155	2.8900	5.770	-1.6619	19.122
160	2.8930	5.751	-1.6652	19.272
165	2.8953	5.720	-1.6681	19.430

Table 15: Atomic charges ( $Q_{001}$ ) in e and volumes ( $V_{001}$ ) in Å<sup>3</sup> of Si and O atoms in the siloxane group of disiloxane···water, [1] = longer bond, [2] = shorter bond

a(Si–O–Si)	$Q_{001}(\text{Si})[1]$	$V_{001}(\text{Si})[1]$	$Q_{001}(\text{Si})[2]$	$V_{001}(\text{Si})[2]$	$Q_{001}(\text{O})$	$V_{001}(\text{O})$
85	2.8228	5.601	2.8253	5.662	-1.6002	19.765
90	2.8340	5.640	2.8352	5.671	-1.6069	19.461
95	2.8427	5.738	2.8465	5.697	-1.6119	19.275
100	2.8540	5.665	2.8561	5.693	-1.6274	19.083
105	2.8597	5.693	2.8631	5.718	-1.6317	18.939
110	2.8656	5.696	2.8687	5.733	-1.6383	18.827
115	2.8714	5.720	2.8735	5.741	-1.6425	18.822
120	2.8760	5.756	2.8781	5.752	-1.6417	18.816
125	2.8800	5.750	2.8815	5.769	-1.6444	18.847
130	2.8836	5.743	2.8846	5.785	-1.6480	18.900
135	2.8865	5.735	2.8876	5.793	-1.6517	18.972
140	2.8889	5.728	2.8897	5.791	-1.6553	19.051
145	2.8912	5.718	2.8909	5.781	-1.6587	19.126
150	2.8935	5.702	2.8932	5.771	-1.6622	19.217
155	2.8959	5.680	2.8958	5.755	-1.6659	19.322
160	2.8974	5.665	2.8991	5.725	-1.6699	19.453
165	2.9007	5.639	2.9021	5.704	-1.6747	19.706

Table 16: Atomic charges ( $Q_{001}$ ) in e and volumes ( $V_{001}$ ) in  $\text{\AA}^3$  of Si, O and H atoms in the silanol group of disiloxane···silanol

$a(\text{Si}-\text{O}-\text{Si})$	$Q_{001}(\text{Si})$	$V_{001}(\text{Si})$	$Q_{001}(\text{O})$	$V_{001}(\text{O})$	$Q_{001}(\text{H})$	$V_{001}(\text{H})$
85	2.8889	5.770	-1.4419	21.378	0.6267	2.115
90	2.8888	5.770	-1.4436	21.396	0.6267	2.120
95	2.8885	5.775	-1.4344	21.320	0.6274	2.136
100	2.8887	5.775	-1.4342	21.337	0.6268	2.137
105	2.8887	5.775	-1.4345	21.356	0.6263	2.141
110	2.8886	5.776	-1.4340	21.397	0.6256	2.157
115	2.8881	5.778	-1.4335	21.432	0.6246	2.166
120	2.8882	5.778	-1.4341	21.488	0.6234	2.175
125	2.8876	5.780	-1.4335	21.541	0.6217	2.184
130	2.8875	5.780	-1.4340	21.577	0.6199	2.194
135	2.8877	5.781	-1.4329	21.593	0.6177	2.211
140	2.8873	5.784	-1.4330	21.622	0.6156	2.236
145	2.8870	5.787	-1.4307	21.628	0.6130	2.269
150	2.8867	5.790	-1.4292	21.646	0.6099	2.326
155	2.8865	5.793	-1.4245	21.648	0.6067	2.388
160	2.8866	5.794	-1.4241	21.621	0.6035	2.488
165	2.8860	5.798	-1.4207	21.604	0.6005	2.636

Table 17: Atomic charges ( $Q_{001}$ ) in e and volumes ( $V_{001}$ ) in Å<sup>3</sup> of O and H atoms in the water group of disiloxane···water

a(Si–O–Si)	$Q_{001}(O)$	$V_{001}(O)$	$Q_{001}(H)$	$V_{001}(H)$
85	-1.1115	21.513	0.5957	2.548
90	-1.1121	21.473	0.5952	2.613
95	-1.1080	21.640	0.5959	2.491
100	-1.1116	21.491	0.5944	2.622
105	-1.1113	21.494	0.5948	2.577
110	-1.1116	21.458	0.5943	2.569
115	-1.1108	21.455	0.5933	2.632
120	-1.1080	21.491	0.5936	2.611
125	-1.1067	21.484	0.5927	2.633
130	-1.1060	21.497	0.5916	2.648
135	-1.1042	21.517	0.5902	2.668
140	-1.1032	21.528	0.5879	2.695
145	-1.1015	21.543	0.5853	2.735
150	-1.0995	21.533	0.5825	2.812
155	-1.0972	21.473	0.5799	2.927
160	-1.0946	21.384	0.5765	3.083
165	-1.0900	21.250	0.5747	3.369

Table 18: Number of ELI attractors belonging to oxygen lone-pair basins ( $V_1(O)$ ) and distance from each other in Å, sum of the populations of both oxygen lone-pair basins ( $\Sigma N_{001}(V_1(O))$ ) in e, and sum of the volumes of both oxygen lone-pair basins ( $\Sigma V_{001}(V_1(O))$ ) in Å<sup>3</sup> for the ELI of free disiloxane

a(Si–O–Si)	no(attr)	dist(attr)	$\Sigma N_{001}(V_1(O))$	$\Sigma V_{001}(V_1(O))$
50	4		6.2360	21.586
55	2	1.125	6.3587	21.383
60	2	1.120	6.6366	21.782
65	2	1.113	7.0888	22.403
70	2	1.103	7.3383	22.121
75	2	1.088	7.8240	22.687
80	2	1.068	7.7850	21.960
85	2	1.042	6.2427	19.195
90	2	1.012	5.5275	17.756
95	2	0.976	5.1805	16.874
100	2	0.935	4.9865	16.327
105	2	0.888	4.8410	15.900
110	2	0.835	4.7135	15.549
115	2	0.774	4.6248	15.253
120	2	0.703	4.5586	15.028
125	2	0.621	4.5005	14.826
130	2	0.528	4.4674	14.683
135	2	0.430	4.4337	14.563
140	2	0.343	4.4257	14.490
145	2	0.306	4.4136	14.440
150	2	0.347	4.4277	14.447
155	2	0.447	4.4636	14.489
160	2	0.566	4.5310	14.536
165	2	0.687	4.5680	14.415
170	3	0.799	5.4760	17.546
175	3	0.901	5.7916	18.118
180	3	0.993	5.8631	18.286

Table 19: Sum of the populations in e and volumes in Å<sup>3</sup> of both Si–O bond basins ( $\Sigma N_{001}(V_2(Si,O))$  and  $\Sigma V_{001}(V_2(Si,O))$ ), populations and volumes of the Si–Si bond basins ( $N_{001}(V_2(Si,Si))$  and  $V_{001}(V_2(Si,Si))$ ), distances of the Si–O bond attractors to the oxygen atom (d(att-O)) in Å, and distances of the Si–O bond attractors to the Si–O bond axis (d(att-axis)) in Å for the ELI of free disiloxane

a(Si–O–Si)	$\Sigma N_{001}(V_2(Si,O))$	$\Sigma V_{001}(V_2(Si,O))$	$N_{001}(V_2(Si,Si))$	$V_{001}(V_2(Si,Si))$
50			1.7079	8.410
55			1.6205	6.586
60			1.3412	4.417
65			0.8451	2.417
70			0.5392	1.510
75				
80			d(att-O)	d(att-axis)
85	1.5128	2.170	0.6340	0.238
90	2.2078	3.118	0.6338	0.171
95	2.5444	3.610	0.6333	0.129
100	2.7352	3.859	0.6330	0.096
105	2.8770	4.045	0.6327	0.068
110	2.9989	4.213	0.6312	0.041
115	3.0910	4.374	0.6304	0.014
120	3.1600	4.523	0.6293	0.012
125	3.2174	4.690	0.6279	0.037
130	3.2616	4.872	0.6275	0.061
135	3.2898	5.069	0.6271	0.085
140	3.3004	5.266	0.6265	0.107
145	3.3132	5.436	0.6262	0.128
150	3.3004	5.536	0.6256	0.147
155	3.2706	5.568	0.6251	0.164
160	3.2060	5.570	0.6248	0.177
165	3.1680	5.722	0.6247	0.184
170	2.2589	2.602	0.6237	0.189
175	1.9548	2.047	0.6229	0.192
180	1.8732	1.891	0.6197	

Table 20: ELI values at the Si–O bond and oxygen lone-pair attractors in free disiloxane

$a(\text{Si–O–Si})$	ELI( $V_2(\text{Si}, \text{O})$ )	ELI( $V_1(\text{O})$ )
50		1.7970
55		1.7335
60		1.6868
65		1.6545
70		1.6327
75		1.6179
80		1.6080
85	1.4662	1.6012
90	1.4723	1.5964
95	1.4791	1.5928
100	1.4850	1.5899
105	1.4898	1.5872
110	1.4933	1.5847
115	1.4957	1.5821
120	1.4972	1.5792
125	1.4978	1.5759
130	1.4977	1.5721
135	1.4969	1.5675
140	1.4954	1.5620
145	1.4932	1.5554
150	1.4906	1.5478
155	1.4874	1.5393
160	1.4837	1.5303
165	1.4798	1.5212
170	1.4757	1.5125
175	1.4718	1.5047
180	1.4694	1.4981

Table 21: Number of ELI attractors belonging to oxygen lone-pair basins ( $V_1(O)$ ), individual populations in e and volumes in  $\text{\AA}^3$  of the lone pair involved in the hydrogen bond ( $N_{001}(V_1(O)_{hbond})$  and  $V_{001}(V_1(O)_{hbond})$ ) and not involved in the hydrogen bond ( $N_{001}(V_1(O))$  and  $V_{001}(V_1(O))$ ), sum of the populations and volumes of both oxygen lone-pair basins or of the only oxygen lone-pair basin for  $a(\text{Si}-\text{O}-\text{Si}) \geq 130^\circ$ , respectively, ( $\Sigma N_{001}(V_1(O))$  and  $\Sigma V_{001}(V_1(O))$ ) for the ELI of the siloxane group of disiloxane···silanol

$a(\text{Si}-\text{O}-\text{Si})$	no(attr)	$N_{001}$ ( $V_1(O)_{hbond}$ )	$V_{001}$ ( $V_1(O)_{hbond}$ )	$N_{001}$ ( $V_1(O)$ )	$V_{001}$ ( $V_1(O)$ )	$\Sigma N_{001}$ ( $V_1(O)$ )	$\Sigma V_{001}$ ( $V_1(O)$ )
85	2	2.7527	7.570	2.9551	9.630	5.7078	17.200
90	2	2.6000	7.172	2.7046	9.023	5.3046	16.195
95	2	2.5421	7.446	2.5359	8.285	5.0780	15.731
100	2	2.4791	7.220	2.4340	7.998	4.9131	15.218
105	2	2.4205	7.045	2.3581	7.755	4.7786	14.800
110	2	2.3970	6.955	2.3002	7.553	4.6972	14.508
115	2	2.3536	6.835	2.2659	7.364	4.6195	14.199
120	2	2.3383	6.759	2.2178	7.159	4.5561	13.918
125	2	2.3856	6.813	2.1358	6.918	4.5214	13.731
130	1					4.4736	13.529
135	1					4.4675	13.456
140	1					4.4624	13.447
145	1					4.4712	13.514
150	1					4.5607	13.922
155	1					4.6962	14.432
160	1					4.7756	14.754
165	1					5.0680	15.757

Table 22: Sum of the populations in e and volumes in Å<sup>3</sup> of both Si–O bond basins ( $\Sigma N_{001}(V_2(Si,O))$  and  $\Sigma V_{001}(V_2(Si,O))$ ) for the ELI of the siloxane group of disiloxane···silanol

a(Si–O–Si)	$\Sigma N_{001}(V_2(Si,O))$	$\Sigma V_{001}(V_2(Si,O))$
85	2.0127	2.894
90	2.4176	3.486
95	2.6389	3.756
100	2.8031	3.970
105	2.9332	4.134
110	3.0156	4.257
115	3.0922	4.379
120	3.1561	4.516
125	3.1979	4.656
130	3.2436	4.842
135	3.2628	5.006
140	3.2664	5.129
145	3.2565	5.159
150	3.1662	4.794
155	3.0368	4.389
160	2.9528	4.306
165	2.6613	3.500

Table 23: Number of ELI attractors belonging to oxygen lone-pair basins ( $V_1(O)$ ), individual populations in e and volumes in  $\text{\AA}^3$  of the lone pair involved in the hydrogen bond ( $N_{001}(V_1(O)_{hbond})$  and  $V_{001}(V_1(O)_{hbond})$ ) and not involved in the hydrogen bond ( $N_{001}(V_1(O))$  and  $V_{001}(V_1(O))$ ), sum of the populations and volumes of both oxygen lone-pair basins or of the only oxygen lone-pair basin for  $a(\text{Si}-\text{O}-\text{Si}) \geq 120^\circ$ , respectively, ( $\Sigma N_{001}(V_1(O))$  and  $\Sigma V_{001}(V_1(O))$ ) for the ELI of the siloxane group of disiloxane···water

$a(\text{Si}-\text{O}-\text{Si})$	no(attr)	$N_{001}$ ( $V_1(O)_{hbond}$ )	$V_{001}$ ( $V_1(O)_{hbond}$ )	$N_{001}$ ( $V_1(O)$ )	$V_{001}$ ( $V_1(O)$ )	$\Sigma N_{001}$ ( $V_1(O)$ )	$\Sigma V_{001}$ ( $V_1(O)$ )
85	2	2.8191	7.639	2.9119	9.542	5.7310	17.181
90	2	2.6183	7.187	2.7048	8.978	5.3231	16.165
95	2	2.5110	7.021	2.5797	8.553	5.0907	15.574
100	2	2.4225	6.706	2.4703	8.344	4.8928	15.050
105	2	2.4178	6.738	2.3606	7.948	4.7784	14.686
110	2	2.3605	6.516	2.3084	7.824	4.6689	14.340
115	2	2.3749	6.649	2.2156	7.501	4.5905	14.150
120	1					4.5397	13.963
125	1					4.4901	13.831
130	1					4.4631	13.735
135	1					4.4458	13.674
140	1					4.4474	13.690
145	1					4.4854	13.856
150	1					4.5434	14.091
155	1					4.6426	14.443
160	1					4.7784	14.851
165	1					5.0476	15.723

Table 24: Individual populations in e and volumes in Å<sup>3</sup> of the bond basins belonging to the long ( $N_{001}(V_2(\text{Si},\text{O})_{long})$  and  $V_{001}(V_2(\text{Si},\text{O})_{long})$ ) and the short ( $N_{001}(V_2(\text{Si},\text{O})_{short})$  and  $V_{001}(V_2(\text{Si},\text{O})_{short})$ ) Si–O bonds as well as sums of the populations and volumes of both Si–O bond basins ( $\Sigma N_{001}(V_2(\text{Si},\text{O}))$  and  $\Sigma V_{001}(V_2(\text{Si},\text{O}))$ ) for the ELI of the siloxane group of disiloxane···water

a(Si–O–Si)	$N_{001}$ ( $V_2(\text{Si},\text{O})_{long}$ )	$V_{001}$ ( $V_2(\text{Si},\text{O})_{long}$ )	$N_{001}$ ( $V_2(\text{Si},\text{O})_{short}$ )	$V_{001}$ ( $V_2(\text{Si},\text{O})_{short}$ )	$\Sigma N_{001}$ ( $V_2(\text{Si},\text{O})$ )	$\Sigma V_{001}$ ( $V_2(\text{Si},\text{O})$ )
85	1.0045	1.515	1.0038	1.438	2.0083	2.953
90	1.2007	1.809	1.2001	1.716	2.4008	3.525
95	1.3161	1.928	1.3122	1.866	2.6283	3.794
100	1.4145	2.092	1.4095	1.985	2.8240	4.077
105	1.4718	2.153	1.4683	2.067	2.9401	4.220
110	1.5328	2.237	1.5175	2.143	3.0503	4.380
115	1.5724	2.309	1.5566	2.192	3.1290	4.501
120	1.6110	2.425	1.5746	2.215	3.1856	4.640
125	1.6428	2.500	1.5895	2.270	3.2323	4.770
130	1.6610	2.555	1.6000	2.232	3.2610	4.787
135	1.6726	2.581	1.6076	2.396	3.2802	4.977
140	1.6700	2.560	1.6031	2.382	3.2731	4.942
145	1.6458	2.467	1.5941	2.299	3.2399	4.766
150	1.6150	2.365	1.5723	2.201	3.1873	4.566
155	1.5665	2.219	1.5262	2.094	3.0927	4.313
160	1.4946	2.030	1.4629	1.905	2.9575	3.935
165	1.3569	1.690	1.3385	1.569	2.6954	3.259

Table 25: Population in e and volume in Å<sup>3</sup> of the Si–O bond basin ( $N_{001}(V_2(\text{Si},\text{O}))$  and  $V_{001}(V_2(\text{Si},\text{O}))$ ), sum of populations and volumes of both oxygen lone-pair basins ( $\Sigma N_{001}(V_1(\text{O}))$  and  $\Sigma V_{001}(V_1(\text{O}))$ ), populations and volumes of the O–H bond basin ( $N_{001}(V_1(\text{O},\text{H}))$  and  $V_{001}(V_1(\text{O},\text{H}))$ ) for the ELI of the silanol group of disiloxane···silanol

a(Si–O–Si)	$N_{001}$ ( $V_2(\text{Si},\text{O})$ )	$V_{001}$ ( $V_2(\text{Si},\text{O})$ )	$\Sigma N_{001}$ ( $V_1(\text{O})$ )	$\Sigma V_{001}$ ( $V_1(\text{O})$ )	$N_{001}$ ( $V_1(\text{O},\text{H})$ )	$V_{001}$ ( $V_1(\text{O},\text{H})$ )
85	1.5863	2.407	4.5373	15.751	1.6605	5.098
90	1.5917	2.408	4.5389	15.748	1.6570	5.113
95	1.5882	2.436	4.5356	15.669	1.6615	5.140
100	1.5842	2.429	4.5443	15.699	1.6615	5.139
105	1.5906	2.445	4.5308	15.696	1.6637	5.151
110	1.6019	2.451	4.5300	15.701	1.6612	5.208
115	1.5879	2.430	4.5371	15.746	1.6638	5.231
120	1.5914	2.432	4.5430	15.776	1.6618	5.252
125	1.5922	2.443	4.5384	15.795	1.6613	5.274
130	1.5944	2.431	4.5297	15.841	1.6644	5.283
135	1.6039	2.448	4.5190	15.836	1.6630	5.299
140	1.5934	2.427	4.5310	15.864	1.6675	5.329
145	1.6045	2.433	4.5262	15.848	1.6665	5.364
150	1.6020	2.426	4.5344	15.859	1.6670	5.442
155	1.5993	2.422	4.5320	15.838	1.6615	5.527
160	1.5922	2.385	4.5376	15.819	1.6589	5.619
165	1.5832	2.365	4.5434	15.769	1.6598	5.801

Table 26: Sum of populations in e and volumes in Å<sup>3</sup> of both oxygen lone-pair basins ( $\Sigma N_{001}(V_1(O))$  and  $\Sigma V_{001}(V_1(O))$ ), populations and volumes of the O–H bond basin ( $N_{001}(V_1(O,H))$  and  $V_{001}(V_1(O,H))$ ) for the ELI of the water group of disiloxane···water

a(Si–O–Si)	$\Sigma N_{001}(V_1(O))$	$\Sigma V_{001}(V_1(O))$	$N_{001}(V_1(O,H))$	$V_{001}(V_1(O,H))$
85	4.5112	14.818	1.6643	5.444
90	4.5179	14.976	1.6648	5.437
95	4.5174	15.139	1.6640	5.452
100	4.5093	15.139	1.6649	5.384
105	4.5109	15.108	1.6644	5.368
110	4.5156	15.090	1.6636	5.460
115	4.5156	15.090	1.6636	5.460
120	4.5239	15.147	1.6624	5.424
125	4.5142	15.129	1.6668	5.453
130	4.5176	15.148	1.6644	5.466
135	4.5138	15.177	1.6630	5.482
140	4.5194	15.205	1.6654	5.508
145	4.5215	15.145	1.6621	5.545
150	4.5201	15.175	1.6626	5.637
155	4.5211	15.074	1.6594	5.783
160	4.5184	14.937	1.6582	5.958
165	4.5162	14.636	1.6600	6.366