The gas-phase structure and some reactions of the bulky primary silane (Me$_3$Si)$_3$CSiH$_3$ and the solid-state structure of the bulky dialkyl disilane [(Me$_3$Si)$_3$CSiH$_2$]$_2$[†]

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Electronic Supplementary Information

Electronic supplementary information (ESI) available:

Description of the model parameters for (Me$_3$Si)$_3$CSiH$_3$

Table S1: Geometric parameters (distances in Å, angles in °) for both molecules in the solid-state structure of [(Me$_3$Si)$_3$CSiH$_2$]$_2$.

Table S2: Calculated coordinates for (Me$_3$Si)$_3$CSiH$_3$ at the MP2/6-31(d) level.

Table S3: Interatomic distances (r_a / Å), experimental and theoretical amplitudes of vibration (u_{h1} / Å), and k_{h1} values for the SARACEN GED structure of (Me$_3$Si)$_3$CSiH$_3$.

Table S4: Experimental coordinates determined from the GED analysis of (Me$_3$Si)$_3$CSiH$_3$.

Table S5: Least-squares correlation matrix (× 100) for (Me$_3$Si)$_3$CSiH$_3$.

Table S6: Nozzle-to-film distances (mm), weighting functions (nm^{-1}), correlation parameters, scale factors, electron wavelengths (pm) and sample and nozzle temperatures (K) used in the GED study of (Me$_3$Si)$_3$CSiH$_3$.

Figure S1: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for (Me$_3$Si)$_3$CSiH$_3$

Description of the model parameters for (Me₃Si)₃CSiH₃

The molecular structure of $(Me_3Si)_3CSiH_3$ was described in overall C_1 symmetry, with local C_3 symmetry for the methyl groups, SiH_3 group and $C(SiMe_3)_3$ group. The $SiMe_3$ groups themselves have local C_1 symmetry. Seventeen parameters were used to describe the structure. The Si-H distance (p_1) and average C-H distance (p_2) were used, as were an average and difference to describe the different Si-C distances (p_3 and p_4). p_3 describes the C-SiMe₃ distance, whilst p_3 minus p_4 describes all the other Si-C distances in the molecule.

Eight angle parameters were used including an average and two differences to describe the α C(1)-Si-C angles. p_5 represents the average of C(1)-Si(6)-C(9/13/17), whilst p_6 and p_7 are [C(1)-Si(6)-C(9) minus C(1)-Si(6)-C(13)] and [C(1)-Si(6)-C(9) minus C(1)-Si(6)-C(17)] respectively. Two internal β C-Si-C angles were also used, C(9)-Si(6)-C(13) (p_8) and C(9)-Si(6)-C(17) (p_9). A combination of α and β angles were then used to determine the torsion angles within the $SiMe_3$ groups. ∠Si(2)-C(1)-Si(6) was used to place the $SiMe_3$ groups relative to the SiH_3 group (p_{10}), whilst ∠C(1)-Si(2)-H(3) defined the angles in the SiH_3 group itself (p_{11}). Finally, the average ∠Si-C-H was used for the methyl groups (p_{12}).

Five torsion angles were used to describe motions of the various groups. A torsion for the $SiMe_3$ groups relative to the C(1)-SiMe₃ bond was used [ϕ Si(2)-C(1)-Si(6)-C(9); p_{13}]. Individual torsion angles were used for the methyl groups relative to the Si(6)-CH₃ bonds [ϕ H(10)-C(9)-Si(6)-C(1), ϕ H(14)-C(13)-Si(6)-C(1), ϕ H(18)-C(17)-Si(6)-C(1); $p_{14\text{-}16}$]. Finally a torsion was added to define the twist of the SiH_3 group relative to the C-(SiMe₃)₃ group [ϕ H(3)-Si(2)-C(1)-Si(6); p_{17}].

Table S1 Geometric parameters (distances in Å, angles in °) for both molecules in the solid-state structure of $[(Me_3Si)_3CSiH_2]_2$.[a]

Parameter	Value mol 2
C1-Si1	1.901(3)
C1-Si2	1.904(3)
C1-Si3	1.906(3)
C1-Si4	1.916(3)
Si1-Si1'	2.3738(17)
Si1-H1B	1.43(2)
Si1-H1A	1.40(2)
Si2-C22	1.872(3)
Si2-C23	1.880(3)
Si2-C21	1.883(3)
C21-H21A	0.9700
C21-H21B	0.9700
C21-H21C	0.9700
C22-H22A	0.9700
C22-H22B	0.9700
C22-H22C	0.9700
C23-H23A	0.9700
C23-H23B	0.9700
C23-H23C	0.9700
Si3-C32	1.869(3)
Si3-C31	1.871(3)
Si3-C33	1.872(3)
C31-H31A	0.9700
C31-H31B	0.9700
C31-H31C	0.9700
C32-H32A	0.9700
C32-H32B	0.9700
C32-H32C	0.9700
C33-H33A	0.9700
C33-H33B	0.9700
C33-H33C	0.9700
Si4-C42	1.870(3)

Si4-C41	1.877(3)
Si4-C43	1.877(3)
C41-H41A	0.9700
C41-H41B	0.9700
C41-H41C	0.9700
C42-H42A	0.9700
C42-H42B	0.9700
C42-H42C	0.9700
C43-H43A	0.9700
C43-H43B	0.9700
C43-H43C	0.9700
C2-Si5	1.897(3)
C2-Si7	1.900(3)
C2-Si8	1.906(3)
C2-Si6	1.913(3)
Si5-Si5''	2.3776(17)
Si5-H5B	1.44(3)
Si5-H5A	1.45(3)
Si6-C62	1.870(3)
Si6-C63	1.873(4)
Si6-C61	1.877(3)
C61-H61A	0.9700
C61-H61B	0.9700
C61-H61C	0.9700
C62-H62A	0.9700
C62-H62B	0.9700
C62-H62C	0.9700
C63-H63A	0.9700
C63-H63B	0.9700
C63-H63C	0.9700
Si7-C73	1.875(3)
Si7-C72	1.878(3)
Si7-C71	1.886(3)
C71-H71A	0.9700
C71-H71B	0.9700

C71-H71C	0.9700
C72-H72A	0.9700
C72-H72B	0.9700
C72-H72C	0.9700
C73-H73A	0.9700
C73-H73B	0.9700
C73-H73C	0.9700
Si8-C83	1.871(3)
Si8-C82	1.876(3)
Si8-C81	1.878(3)
C81-H81A	0.9700
C81-H81B	0.9700
C81-H81C	0.9700
C82-H82A	0.9700
C82-H82B	0.9700
C82-H82C	0.9700
C83-H83A	0.9700
C83-H83B	0.9700
C83-H83C	0.9700
Si1-C1-Si2	110.52(13)
Si1-C1-Si3	108.06(13)
Si2-C1-Si3	111.60(13)
Si1-C1-Si4	103.85(13)
Si2-C1-Si4	111.10(13)
Si3-C1-Si4	111.40(13)
C1-Si1-Si1 '	120.05(9)
C1-Si1-H1B	106.6(10)
Si1 ' -Si1-H1B	107.8(10)
C1-Si1-H1A	109.0(10)
Si1 ' -Si1-H1A	107.1(10)
H1B-Si1-H1A	105.4(14)
C22-Si2-C23	106.61(16)
C22-Si2-C21	105.46(15)
C23-Si2-C21	105.70(16)

C22-Si2-C1	112.14(13)
C23-Si2-C1	113.62(13)
C21-Si2-C1	112.70(13)
Si2-C21-H21A	109.5
Si2-C21-H21B	109.5
H21A-C21-H21B	109.5
Si2-C21-H21C	109.5
H21A-C21-H21C	109.5
H21B-C21-H21C	109.5
Si2-C22-H22A	109.5
Si2-C22-H22B	109.5
H22A-C22-H22B	109.5
Si2-C22-H22C	109.5
H22A-C22-H22C	109.5
H22B-C22-H22C	109.5
Si2-C23-H23A	109.5
Si2-C23-H23B	109.5
H23A-C23-H23B	109.5
Si2-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C32-Si3-C31	104.31(15)
C32-Si3-C33	106.43(15)
C31-Si3-C33	107.11(15)
C32-Si3-C1	112.85(14)
C31-Si3-C1	112.60(12)
C33-Si3-C1	112.92(13)
Si3-C31-H31A	109.5
Si3-C31-H31B	109.5
H31A-C31-H31B	109.5
Si3-C31-H31C	109.5
H31A-C31-H31C	109.5
H31B-C31-H31C	109.5
Si3-C32-H32A	109.5
Si3-C32-H32B	109.5

H32A-C32-H32B	109.5
Si3-C32-H32C	109.5
H32A-C32-H32C	109.5
H32B-C32-H32C	109.5
Si3-C33-H33A	109.5
Si3-C33-H33B	109.5
H33A-C33-H33B	109.5
Si3-C33-H33C	109.5
H33A-C33-H33C	109.5
H33B-C33-H33C	109.5
C42-Si4-C41	106.90(15)
C42-Si4-C43	106.99(17)
C41-Si4-C43	105.19(16)
C42-Si4-C1	112.51(14)
C41-Si4-C1	113.19(13)
C43-Si4-C1	111.56(14)
Si4-C41-H41A	109.5
Si4-C41-H41B	109.5
H41A-C41-H41B	109.5
Si4-C41-H41C	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
Si4-C42-H42A	109.5
Si4-C42-H42B	109.5
H42A-C42-H42B	109.5
Si4-C42-H42C	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
Si4-C43-H43A	109.5
Si4-C43-H43B	109.5
H43A-C43-H43B	109.5
Si4-C43-H43C	109.5
H43A-C43-H43C	109.5
H43B-C43-H43C	109.5
Si5-C2-Si7	110.86(13)

Si5-C2-Si8	107.98(13)
Si7-C2-Si8	112.08(13)
Si5-C2-Si6	104.58(13)
Si7-C2-Si6	110.44(13)
Si8-C2-Si6	110.62(13)
C2-Si5-Si5''	119.70(10)
C2-Si5-H5B	109.0(10)
Si5''-Si5-H5B	107.3(10)
C2-Si5-H5A	108.2(11)
Si5''-Si5-H5A	106.4(10)
H5B-Si5-H5A	105.3(15)
C62-Si6-C63	104.39(18)
C62-Si6-C61	107.10(15)
C63-Si6-C61	106.49(17)
C62-Si6-C2	113.26(14)
C63-Si6-C2	112.34(15)
C61-Si6-C2	112.66(13)
Si6-C61-H61A	109.5
Si6-C61-H61B	109.5
H61A-C61-H61B	109.5
Si6-C61-H61C	109.5
H61A-C61-H61C	109.5
H61B-C61-H61C	109.5
Si6-C62-H62A	109.5
Si6-C62-H62B	109.5
H62A-C62-H62B	109.5
Si6-C62-H62C	109.5
H62A-C62-H62C	109.5
H62B-C62-H62C	109.5
Si6-C63-H63A	109.5
Si6-C63-H63B	109.5
H63A-C63-H63B	109.5
Si6-C63-H63C	109.5
H63A-C63-H63C	109.5
H63B-C63-H63C	109.5

C73-Si7-C72	106.26(17)
C73-Si7-C71	106.19(16)
C72-Si7-C71	106.30(16)
C73-Si7-C2	112.02(14)
C72-Si7-C2	112.48(14)
C71-Si7-C2	113.08(13)
Si7-C71-H71A	109.5
Si7-C71-H71B	109.5
H71A-C71-H71B	109.5
Si7-C71-H71C	109.5
H71A-C71-H71C	109.5
H71B-C71-H71C	109.5
Si7-C72-H72A	109.5
Si7-C72-H72B	109.5
H72A-C72-H72B	109.5
Si7-C72-H72C	109.5
H72A-C72-H72C	109.5
H72B-C72-H72C	109.5
Si7-C73-H73A	109.5
Si7-C73-H73B	109.5
H73A-C73-H73B	109.5
Si7-C73-H73C	109.5
H73A-C73-H73C	109.5
H73B-C73-H73C	109.5
C83-Si8-C82	106.31(15)
C83-Si8-C81	106.59(15)
C82-Si8-C81	104.47(17)
C83-Si8-C2	112.90(14)
C82-Si8-C2	112.68(14)
C81-Si8-C2	113.23(13)
Si8-C81-H81A	109.5
Si8-C81-H81B	109.5
H81A-C81-H81B	109.5
Si8-C81-H81C	109.5
H81A-C81-H81C	109.5

H81B-C81-H81C	109.5
Si8-C82-H82A	109.5
Si8-C82-H82B	109.5
H82A-C82-H82B	109.5
Si8-C82-H82C	109.5
H82A-C82-H82C	109.5
H82B-C82-H82C	109.5
Si8-C83-H83A	109.5
Si8-C83-H83B	109.5
H83A-C83-H83B	109.5
Si8-C83-H83C	109.5
H83A-C83-H83C	109.5
H83B-C83-H83C	109.5

[a] Symmetry transformations used to generate equivalent atoms: ' -x+1,-y+1,-z   ' ' -x,-y+1,-z+1

Table S2 Calculated coordinates for $(Me_3Si)_3CSiH_3$ at the MP2/6-31(d) level.

Atom	x	y	z
C(1)	0.0000	0.0000	0.3572
Si(2)	0.0000	0.0000	2.2440
H(3)	-0.3408	-1.3420	2.7937
H(4)	-0.9918	0.9662	2.7937
H(5)	1.3327	0.3758	2.7937
Si(6)	-0.1700	1.8178	-0.2068
Si(7)	-1.4893	-1.0561	-0.2068
Si(8)	1.6593	-0.7617	-0.2068
C(9)	0.8692	2.9860	0.8617
H(10)	0.5132	3.0164	1.8963
H(11)	1.9320	2.7389	0.8787
H(12)	0.7705	4.0013	0.4601
C(13)	0.3398	2.0809	-2.0102
H(14)	0.1654	3.1310	-2.2723
H(15)	1.3984	1.8746	-2.1876
H(16)	-0.2445	1.4679	-2.7011
C(17)	-1.9339	2.4856	-0.0408
H(18)	-1.9233	3.5416	-0.3359
H(19)	-2.6622	1.9784	-0.6780
H(20)	-2.2935	2.4409	0.9913
C(21)	-3.0205	-0.7402	0.8617
H(22)	-3.8505	-1.3334	0.4601
H(23)	-2.8689	-1.0638	1.8963
H(24)	-3.3380	0.3037	0.8787
C(25)	-1.9720	-0.7462	-2.0102
H(26)	-2.3227	0.2738	-2.1876
H(27)	-1.1490	-0.9457	-2.7011
H(28)	-2.7942	-1.4222	-2.2723
C(29)	-1.1856	-2.9176	-0.0408
H(30)	-0.3823	-3.2948	-0.6780
H(31)	-0.9671	-3.2067	0.9913
H(32)	-2.1055	-3.4364	-0.3359
C(33)	2.1513	-2.2457	0.8617

H(34)	2.3557	-1.9526	1.8963
H(35)	1.4060	-3.0426	0.8787
H(36)	3.0800	-2.6679	0.4601
C(37)	3.1196	0.4320	-0.0408
H(38)	3.2606	0.7658	0.9913
H(39)	4.0287	-0.1052	-0.3359
H(40)	3.0445	1.3163	-0.6780
C(41)	1.6322	-1.3348	-2.0102
H(42)	1.3935	-0.5222	-2.7011
H(43)	2.6288	-1.7088	-2.2723
H(44)	0.9243	-2.1484	-2.1876

Table S3 Interatomic distances (r_a / Å), experimental and theoretical amplitudes of vibration (u_{h1} / Å), and k_{h1} values for the SARACEN GED structure of $(Me_3Si)_3CSiH_3$.[a,b]

	Atom pair	r_a	Expt. u_{h1}	k_{h1}	Calc. u_{h1}	Restraint
u_1	C(9)-H(11)	1.089(3)	0.0804(34)	0.0034	0.0744	
u_2	C(21)-H(24)	1.089(3)	0.0804(Tied to u_1)	0.0034	0.0744	
u_3	C(33)-H(35)	1.089(3)	0.0804(Tied to u_1)	0.0034	0.0744	
u_4	C(17)-H(19)	1.089(3)	0.0806(Tied to u_1)	0.0035	0.0746	
u_5	C(29)-H(30)	1.089(3)	0.0806(Tied to u_1)	0.0035	0.0746	
u_6	C(37)-H(40)	1.089(3)	0.0806(Tied to u_1)	0.0035	0.0746	
u_7	C(13)-H(15)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_8	C(25)-H(26)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_9	C(41)-H(44)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{10}	C(13)-H(16)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{11}	C(25)-H(27)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{12}	C(41)-H(42)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{13}	C(17)-H(20)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{14}	C(29)-H(31)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{15}	C(37)-H(38)	1.089(3)	0.0807(Tied to u_1)	0.0035	0.0747	
u_{16}	C(9)-H(10)	1.089(3)	0.0809(Tied to u_1)	0.0035	0.0749	
u_{17}	C(33)-H(34)	1.089(3)	0.0809(Tied to u_1)	0.0035	0.0749	
u_{18}	C(21)-H(23)	1.089(3)	0.0809(Tied to u_1)	0.0035	0.0749	
u_{19}	C(13)-H(14)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{20}	C(25)-H(28)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{21}	C(41)-H(43)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{22}	C(9)-H(12)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{23}	C(17)-H(18)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{24}	C(21)-H(22)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{25}	C(29)-H(32)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{26}	C(33)-H(36)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{27}	C(37)-H(39)	1.089(3)	0.0812(Tied to u_1)	0.0035	0.0751	
u_{28}	Si(2)-H(3)	1.492(5)	0.0792(85)	0.0036	0.0857	0.0857(90)
u_{29}	Si(2)-H(4)	1.492(5)	0.0792(Tied to u_{28})	0.0036	0.0857	
u_{30}	Si(2)-H(5)	1.492(5)	0.0792(Tied to u_{28})	0.0036	0.0857	
u_{31}	H(10)...H(12)	1.746(9)	0.1211(fixed)	0.0022	0.1211	
u_{32}	H(22)...H(23)	1.746(9)	0.1211(fixed)	0.0023	0.1211	

u_{33}	H(34)...H(36)	1.746(9)	0.1211(fixed)	0.0022	0.1211
u_{34}	H(14)...H(15)	1.746(9)	0.1209(fixed)	0.0021	0.1209
u_{35}	H(18)...H(19)	1.746(9)	0.1208(fixed)	0.0022	0.1208
u_{36}	H(26)...H(28)	1.746(9)	0.1209(fixed)	0.0021	0.1209
u_{37}	H(30)...H(32)	1.746(9)	0.1208(fixed)	0.0022	0.1208
u_{38}	H(39)...H(40)	1.746(9)	0.1208(fixed)	0.0023	0.1208
u_{39}	H(43)...H(44)	1.745(9)	0.1209(fixed)	0.002	0.1209
u_{40}	H(18)...H(20)	1.746(9)	0.1210(fixed)	0.0023	0.1210
u_{41}	H(31)...H(32)	1.746(9)	0.1210(fixed)	0.0023	0.1210
u_{42}	H(38)...H(39)	1.746(9)	0.1210(fixed)	0.0023	0.1210
u_{43}	H(11)...H(12)	1.745(9)	0.1208(fixed)	0.0019	0.1208
u_{44}	H(14)...H(16)	1.746(9)	0.1210(fixed)	0.0022	0.1210
u_{45}	H(22)...H(24)	1.745(9)	0.1208(fixed)	0.002	0.1208
u_{46}	H(27)...H(28)	1.746(9)	0.1210(fixed)	0.0022	0.1210
u_{47}	H(35)...H(36)	1.745(9)	0.1208(fixed)	0.002	0.1208
u_{48}	H(42)...H(43)	1.746(9)	0.1210(fixed)	0.0022	0.1210
u_{49}	H(10)...H(11)	1.746(9)	0.1207(fixed)	0.0028	0.1207
u_{50}	H(23)...H(24)	1.746(9)	0.1206(fixed)	0.0028	0.1206
u_{51}	H(34)...H(35)	1.746(9)	0.1206(fixed)	0.0028	0.1206
u_{52}	H(15)...H(16)	1.746(9)	0.1206(fixed)	0.0027	0.1206
u_{53}	H(26)...H(27)	1.746(9)	0.1206(fixed)	0.0027	0.1206
u_{54}	H(42)...H(44)	1.746(9)	0.1206(fixed)	0.0026	0.1206
u_{55}	H(19)...H(20)	1.746(9)	0.1206(fixed)	0.003	0.1206
u_{56}	H(30)...H(31)	1.746(9)	0.1206(fixed)	0.003	0.1206
u_{57}	H(38)...H(40)	1.746(9)	0.1206(fixed)	0.003	0.1206
u_{58}	Si(6)-C(13)	1.891(1)	0.0621(100)	0.0028	0.0548
u_{59}	Si(7)-C(25)	1.891(1)	0.0621(Tied to u_{58})	0.0028	0.0548
u_{60}	Si(8)-C(41)	1.891(1)	0.0621(Tied to u_{58})	0.0028	0.0548
u_{61}	Si(6)-C(17)	1.891(1)	0.0621(Tied to u_{58})	0.0028	0.0548
u_{62}	Si(7)-C(29)	1.891(1)	0.0621(Tied to u_{58})	0.0028	0.0548
u_{63}	Si(8)-C(37)	1.891(1)	0.0621(Tied to u_{58})	0.0028	0.0548
u_{64}	C(1)-Si(2)	1.891(1)	0.0643(Tied to u_{58})	0.0027	0.0568
u_{65}	Si(6)-C(9)	1.891(1)	0.0622(Tied to u_{58})	0.0028	0.0549
u_{66}	Si(7)-C(21)	1.891(1)	0.0622(Tied to u_{58})	0.0028	0.0549
u_{67}	Si(8)-C(33)	1.891(1)	0.0622(Tied to u_{58})	0.0028	0.0549

u_{68}	C(1)-Si(6)	1.904(2)	0.0672(Tied to u_{58})	0.002	0.0593
u_{69}	C(1)-Si(7)	1.904(2)	0.0672(Tied to u_{58})	0.002	0.0593
u_{70}	C(1)-Si(8)	1.904(2)	0.0672(Tied to u_{58})	0.002	0.0593
u_{71}	H(15)...H(40)	2.207(33)	0.3487(fixed)	0.1445	0.3487
u_{72}	H(30)...H(44)	2.207(33)	0.3459(fixed)	0.1438	0.3459
u_{73}	H(19)...H(26)	2.207(33)	0.3480(fixed)	0.1442	0.3480
u_{74}	H(3)...H(4)	2.402(11)	0.1445(fixed)	0.0035	0.1445
u_{75}	H(3)...H(5)	2.402(11)	0.1445(fixed)	0.0035	0.1445
u_{76}	H(4)...H(5)	2.402(11)	0.1445(fixed)	0.0035	0.1445
u_{77}	H(31)...H(35)	2.321(40)	0.3994(fixed)	0.149	0.3994
u_{78}	H(11)...H(38)	2.321(40)	0.3985(fixed)	0.1489	0.3985
u_{79}	H(20)...H(24)	2.321(40)	0.4003(fixed)	0.1492	0.4003
u_{80}	H(30)...H(35)	2.689(59)	0.4003(fixed)	0.1323	0.4003
u_{81}	H(11)...H(40)	2.689(59)	0.3996(fixed)	0.1322	0.3996
u_{82}	H(19)...H(24)	2.689(59)	0.4011(fixed)	0.1326	0.4011
u_{83}	Si(6)...H(18)	2.500(5)	0.1234(fixed)	-0.0059	0.1234
u_{84}	Si(8)...H(39)	2.500(5)	0.1234(Tied to u_{83})	-0.0059	0.1234
u_{85}	Si(7)...H(32)	2.500(5)	0.1234(Tied to u_{83})	-0.0059	0.1234
u_{86}	Si(6)...H(12)	2.500(5)	0.1243(Tied to u_{83})	-0.0058	0.1243
u_{87}	Si(7)...H(22)	2.500(5)	0.1243(Tied to u_{83})	-0.0059	0.1243
u_{88}	Si(8)...H(36)	2.500(5)	0.1243(Tied to u_{83})	-0.0059	0.1243
u_{89}	Si(6)...H(14)	2.500(5)	0.1235(Tied to u_{83})	-0.0059	0.1235
u_{90}	Si(7)...H(28)	2.500(5)	0.1235(Tied to u_{83})	-0.0059	0.1235
u_{91}	Si(8)...H(43)	2.500(5)	0.1235(Tied to u_{83})	-0.0058	0.1235
u_{92}	Si(7)...H(31)	2.500(5)	0.1213(Tied to u_{83})	-0.0067	0.1213
u_{93}	Si(6)...H(20)	2.500(5)	0.1213(Tied to u_{83})	-0.0067	0.1213
u_{94}	Si(8)...H(38)	2.500(5)	0.1213(Tied to u_{83})	-0.0067	0.1213
u_{95}	Si(6)...H(10)	2.500(5)	0.1234(Tied to u_{83})	-0.0066	0.1234
u_{96}	Si(7)...H(23)	2.499(5)	0.1234(Tied to u_{83})	-0.0067	0.1234
u_{97}	Si(8)...H(34)	2.500(5)	0.1234(Tied to u_{83})	-0.0066	0.1234
u_{98}	Si(6)...H(16)	2.500(5)	0.1218(Tied to u_{83})	-0.0067	0.1218
u_{99}	Si(8)...H(42)	2.500(5)	0.1218(Tied to u_{83})	-0.0066	0.1218
u_{100}	Si(7)...H(27)	2.500(5)	0.1218(Tied to u_{83})	-0.0066	0.1218
u_{101}	Si(6)...H(15)	2.499(5)	0.1216(Tied to u_{83})	-0.0069	0.1216
u_{102}	Si(7)...H(26)	2.500(5)	0.1216(Tied to u_{83})	-0.0068	0.1216

u_{103}	Si(8)...H(44)	2.500(5)	0.1216(Tied to u_{83})	-0.0068	0.1216
u_{104}	H(27)...H(44)	2.534(58)	0.4259(fixed)	0.1135	0.4259
u_{105}	H(16)...H(26)	2.534(58)	0.4266(fixed)	0.1138	0.4266
u_{106}	H(15)...H(42)	2.534(58)	0.4256(fixed)	0.1132	0.4256
u_{107}	Si(6)...H(11)	2.500(5)	0.1209(Tied to u_{83})	-0.0067	0.1209
u_{108}	Si(7)...H(24)	2.500(5)	0.1209(Tied to u_{83})	-0.0068	0.1209
u_{109}	Si(8)...H(35)	2.500(5)	0.1209(Tied to u_{83})	-0.0068	0.1209
u_{110}	Si(7)...H(30)	2.499(5)	0.1202(Tied to u_{83})	-0.007	0.1202
u_{111}	Si(8)...H(40)	2.499(5)	0.1202(Tied to u_{83})	-0.007	0.1202
u_{112}	Si(6)...H(19)	2.499(5)	0.1202(Tied to u_{83})	-0.007	0.1202
u_{113}	H(16)...H(42)	2.689(56)	0.4895(fixed)	0.1063	0.4895
u_{114}	H(27)...H(42)	2.689(56)	0.4902(fixed)	0.1065	0.4902
u_{115}	H(16)...H(27)	2.689(56)	0.4911(fixed)	0.1067	0.4911
u_{116}	H(3)...H(31)	2.829(31)	0.3494(fixed)	0.0712	0.3494
u_{117}	H(4)...H(20)	2.829(31)	0.3496(fixed)	0.0713	0.3496
u_{118}	H(5)...H(38)	2.829(31)	0.3498(fixed)	0.0713	0.3498
u_{119}	H(3)...H(23)	2.695(50)	0.3785(fixed)	0.0991	0.3785
u_{120}	H(4)...H(10)	2.695(50)	0.3771(fixed)	0.0987	0.3771
u_{121}	H(5)...H(34)	2.695(50)	0.3780(fixed)	0.0989	0.3780
u_{122}	C(1)...H(3)	2.793(9)	0.1273(fixed)	-0.0046	0.1273
u_{123}	C(1)...H(4)	2.793(9)	0.1273(fixed)	-0.0046	0.1273
u_{124}	C(1)...H(5)	2.793(9)	0.1273(fixed)	-0.0046	0.1273
u_{125}	C(29)...H(35)	2.901(24)	0.2855(fixed)	0.1185	0.2855
u_{126}	H(11)...C(37)	2.901(24)	0.2841(fixed)	0.1183	0.2841
u_{127}	C(17)...H(24)	2.901(24)	0.2865(fixed)	0.1187	0.2865
u_{128}	H(22)...H(32)	3.040(32)	0.3568(fixed)	0.0602	0.3568
u_{129}	H(12)...H(18)	3.040(32)	0.3565(fixed)	0.0601	0.3565
u_{130}	H(36)...H(39)	3.040(32)	0.3569(fixed)	0.0602	0.3569
u_{131}	H(14)...H(18)	2.903(39)	0.3331(fixed)	0.0535	0.3331
u_{132}	H(39)...H(43)	2.903(39)	0.3327(fixed)	0.0533	0.3327
u_{133}	H(28)...H(32)	2.903(39)	0.3329(fixed)	0.0534	0.3329
u_{134}	H(4)...H(23)	2.885(60)	0.4495(fixed)	0.0539	0.4495
u_{135}	H(3)...H(34)	2.885(60)	0.4493(fixed)	0.0538	0.4493
u_{136}	H(5)...H(10)	2.885(60)	0.4492(fixed)	0.0537	0.4492
u_{137}	H(22)...H(28)	3.045(30)	0.3550(fixed)	0.0745	0.3550

u_{138}	H(36)...H(43)	3.045(30)	0.3546(fixed)	0.0743	0.3546	
u_{139}	H(12)...H(14)	3.045(30)	0.3543(fixed)	0.0744	0.3543	
u_{140}	H(27)...C(41)	3.030(25)	0.3041(fixed)	0.0826	0.3041	
u_{141}	C(13)...H(42)	3.030(24)	0.3028(fixed)	0.0822	0.3028	
u_{142}	H(16)...C(25)	3.030(25)	0.3048(fixed)	0.0827	0.3048	
u_{143}	C(9)...C(17)	3.023(16)	0.1159(91)	0.0007	0.1058	0.1058(110)
u_{144}	C(21)...C(29)	3.023(16)	0.1159(Tied to u_{143})	0.0007	0.1058	
u_{145}	C(33)...C(37)	3.023(16)	0.1159(Tied to u_{143})	0.0007	0.1058	
u_{146}	H(10)...H(20)	3.143(45)	0.3867(fixed)	0.0479	0.3867	
u_{147}	H(23)...H(31)	3.143(45)	0.3871(fixed)	0.048	0.3871	
u_{148}	H(34)...H(38)	3.143(45)	0.3870(fixed)	0.048	0.3870	
u_{149}	C(13)...C(17)	2.923(21)	0.1191(Tied to u_{143})	0.0004	0.1088	
u_{150}	C(25)...C(29)	2.923(21)	0.1191(Tied to u_{143})	0.0004	0.1088	
u_{151}	C(37)...C(41)	2.923(21)	0.1191(Tied to u_{143})	0.0004	0.1088	
u_{152}	C(9)...C(13)	3.064(9)	0.1209(Tied to u_{143})	0.0005	0.1104	
u_{153}	C(21)...C(25)	3.064(9)	0.1209(Tied to u_{143})	0.0005	0.1104	
u_{154}	C(33)...C(41)	3.064(9)	0.1209(Tied to u_{143})	0.0005	0.1104	
u_{155}	C(9)...H(18)	3.164(22)	0.2270(fixed)	0.0042	0.2270	
u_{156}	C(21)...H(32)	3.164(22)	0.2269(fixed)	0.0042	0.2269	
u_{157}	C(33)...H(39)	3.164(22)	0.2270(fixed)	0.0042	0.2270	
u_{158}	Si(2)...Si(6)	3.030(5)	0.0977(36)	0.0001	0.0926	0.0926(90)
u_{159}	Si(2)...Si(7)	3.030(5)	0.0977(Tied to u_{158})	0.0001	0.0926	
u_{160}	Si(2)...Si(8)	3.030(5)	0.0977(Tied to u_{158})	0.0001	0.0926	
u_{161}	H(5)...H(11)	2.877(50)	0.5409(fixed)	0.0292	0.5409	
u_{162}	H(3)...H(35)	2.877(50)	0.5409(fixed)	0.0292	0.5409	
u_{163}	H(4)...H(24)	2.877(50)	0.5412(fixed)	0.0292	0.5412	
u_{164}	H(14)...C(17)	3.068(30)	0.2371(fixed)	0.0098	0.2371	
u_{165}	C(37)...H(43)	3.068(30)	0.2370(fixed)	0.0097	0.2370	
u_{166}	Si(2)...H(23)	3.091(27)	0.3061(fixed)	0.0565	0.3061	
u_{167}	Si(2)...H(34)	3.091(27)	0.3058(fixed)	0.0564	0.3058	
u_{168}	H(28)...C(29)	3.068(30)	0.2371(fixed)	0.0097	0.2371	
u_{169}	Si(2)...H(10)	3.091(27)	0.3054(fixed)	0.0562	0.3054	
u_{170}	H(22)...C(29)	3.238(22)	0.2688(fixed)	0.0092	0.2688	
u_{171}	H(12)...C(17)	3.238(22)	0.2687(fixed)	0.0091	0.2687	
u_{172}	H(36)...C(37)	3.238(22)	0.2687(fixed)	0.0091	0.2687	

u_{173}	H(12)...C(13)	3.189(19)	0.2439(fixed)	0.0163	0.2439
u_{174}	H(36)...C(41)	3.189(19)	0.2440(fixed)	0.0163	0.2440
u_{175}	H(22)...C(25)	3.189(19)	0.2441(fixed)	0.0163	0.2441
u_{176}	H(15)...C(37)	3.035(24)	0.2984(fixed)	0.071	0.2984
u_{177}	C(29)...H(44)	3.035(24)	0.2966(fixed)	0.0706	0.2966
u_{178}	C(13)...H(40)	3.000(23)	0.2940(fixed)	0.0522	0.2940
u_{179}	H(30)...C(41)	3.000(23)	0.2936(fixed)	0.052	0.2936
u_{180}	C(17)...H(26)	3.035(24)	0.2980(fixed)	0.0709	0.2980
u_{181}	H(19)...C(25)	3.000(23)	0.2940(fixed)	0.0521	0.2940
u_{182}	H(39)...C(41)	3.117(27)	0.2325(fixed)	0.0022	0.2325
u_{183}	C(25)...H(32)	3.117(27)	0.2324(fixed)	0.0022	0.2324
u_{184}	C(13)...H(18)	3.117(27)	0.2325(fixed)	0.0022	0.2325
u_{185}	H(10)...C(17)	3.210(29)	0.2904(fixed)	0.0052	0.2904
u_{186}	H(23)...C(29)	3.210(29)	0.2906(fixed)	0.0051	0.2906
u_{187}	H(34)...C(37)	3.210(29)	0.2905(fixed)	0.0051	0.2905
u_{188}	C(1)...C(9)	3.147(5)	0.1370(106)	0.0003	0.0981
u_{189}	C(1)...C(33)	3.147(5)	0.1370(Tied to u_{188})	0.0003	0.0981
u_{190}	C(1)...C(21)	3.147(5)	0.1370(Tied to u_{188})	0.0003	0.0981
u_{191}	C(1)...C(13)	3.163(7)	0.1377(Tied to u_{188})	0.0002	0.0986
u_{192}	C(1)...C(25)	3.163(7)	0.1377(Tied to u_{188})	0.0002	0.0986
u_{193}	C(1)...C(41)	3.163(7)	0.1377(Tied to u_{188})	0.0002	0.0986
u_{194}	Si(7)...Si(8)	3.167(3)	0.0883(fixed)	-0.0001	0.0883
u_{195}	C(1)...C(29)	3.178(6)	0.1379(Tied to u_{188})	0.0002	0.0987
u_{196}	Si(6)...Si(8)	3.167(3)	0.0883(fixed)	-0.0001	0.0883
u_{197}	C(1)...C(37)	3.178(6)	0.1379(Tied to u_{188})	0.0002	0.0987
u_{198}	Si(6)...Si(7)	3.167(3)	0.0883(fixed)	-0.0001	0.0883
u_{199}	C(1)...C(17)	3.178(6)	0.1379(Tied to u_{188})	0.0002	0.0987
u_{200}	H(27)...H(30)	2.944(56)	0.3720(fixed)	0.0311	0.3720
u_{201}	H(40)...H(42)	2.943(56)	0.3720(fixed)	0.031	0.3720
u_{202}	H(16)...H(19)	2.943(56)	0.3722(fixed)	0.0311	0.3722
u_{203}	C(21)...H(28)	3.251(19)	0.2500(fixed)	0.0057	0.2500
u_{204}	C(33)...H(43)	3.251(19)	0.2499(fixed)	0.0056	0.2499
u_{205}	C(9)...H(14)	3.251(19)	0.2500(fixed)	0.0056	0.2500
u_{206}	H(30)...C(33)	3.298(46)	0.3299(fixed)	0.0292	0.3299
u_{207}	C(9)...H(40)	3.298(46)	0.3303(fixed)	0.0293	0.3303

u_{208}	H(19)...C(21)	3.298(46)	0.3303(fixed)	0.0293	0.3303
u_{209}	C(21)...H(31)	3.292(30)	0.2366(fixed)	-0.0013	0.2366
u_{210}	C(9)...H(20)	3.292(30)	0.2367(fixed)	-0.0013	0.2367
u_{211}	C(33)...H(38)	3.292(30)	0.2366(fixed)	-0.0013	0.2366
u_{212}	H(11)...H(15)	3.287(36)	0.4179(fixed)	0.0454	0.4179
u_{213}	H(35)...H(44)	3.287(36)	0.4179(fixed)	0.0452	0.4179
u_{214}	H(24)...H(26)	3.287(36)	0.4181(fixed)	0.0454	0.4181
u_{215}	H(3)...Si(7)	3.186(21)	0.2044(fixed)	0.0009	0.2044
u_{216}	H(4)...Si(6)	3.186(21)	0.2044(fixed)	0.0009	0.2044
u_{217}	H(5)...Si(8)	3.186(21)	0.2044(fixed)	0.0009	0.2044
u_{218}	H(3)...C(33)	3.210(40)	0.2912(fixed)	0.0092	0.2912
u_{219}	H(5)...C(9)	3.210(40)	0.2912(fixed)	0.0092	0.2912
u_{220}	H(4)...C(21)	3.210(40)	0.2913(fixed)	0.0092	0.2913
u_{221}	H(40)...C(41)	3.090(38)	0.2358(fixed)	-0.0021	0.2358
u_{222}	C(13)...H(19)	3.089(38)	0.2358(fixed)	-0.0022	0.2358
u_{223}	C(25)...H(30)	3.090(38)	0.2357(fixed)	-0.0021	0.2357
u_{224}	C(9)...H(15)	3.299(21)	0.2590(fixed)	0.0011	0.2590
u_{225}	C(33)...H(44)	3.300(21)	0.2589(fixed)	0.0011	0.2589
u_{226}	C(21)...H(26)	3.299(21)	0.2591(fixed)	0.0011	0.2591
u_{227}	H(31)...C(33)	3.169(38)	0.3469(fixed)	0.0245	0.3469
u_{228}	C(9)...H(38)	3.169(38)	0.3470(fixed)	0.0246	0.3470
u_{229}	H(20)...C(21)	3.169(38)	0.3472(fixed)	0.0246	0.3472
u_{230}	C(25)...H(44)	3.259(43)	0.3721(fixed)	0.0392	0.3721
u_{231}	C(13)...H(26)	3.259(43)	0.3725(fixed)	0.0394	0.3725
u_{232}	H(15)...C(41)	3.259(43)	0.3728(fixed)	0.0394	0.3728
u_{233}	H(27)...C(29)	3.143(36)	0.2640(fixed)	-0.0017	0.2640
u_{234}	C(37)...H(42)	3.143(36)	0.2639(fixed)	-0.0017	0.2639
u_{235}	H(16)...C(17)	3.143(36)	0.2640(fixed)	-0.0018	0.2640
u_{236}	H(10)...H(18)	3.359(42)	0.4342(fixed)	-0.015	0.4342
u_{237}	H(34)...H(39)	3.359(42)	0.4342(fixed)	-0.0151	0.4342
u_{238}	H(23)...H(32)	3.359(42)	0.4342(fixed)	-0.0151	0.4342
u_{239}	Si(8)...H(30)	3.269(27)	0.2751(fixed)	0.0255	0.2751
u_{240}	Si(6)...H(40)	3.269(27)	0.2753(fixed)	0.0256	0.2753
u_{241}	Si(7)...H(19)	3.269(27)	0.2753(fixed)	0.0255	0.2753
u_{242}	H(24)...C(25)	3.375(23)	0.2915(fixed)	-0.0012	0.2915

u_{243}	H(35)...C(41)	3.375(23)	0.2914(fixed)	-0.0012	0.2914
u_{244}	H(11)...C(13)	3.375(23)	0.2914(fixed)	-0.0012	0.2914
u_{245}	Si(7)...H(44)	3.331(26)	0.2947(fixed)	0.0375	0.2947
u_{246}	Si(6)...H(26)	3.331(26)	0.2953(fixed)	0.0378	0.2953
u_{247}	Si(8)...H(15)	3.331(26)	0.2955(fixed)	0.0378	0.2955
u_{248}	H(3)...C(29)	3.441(26)	0.2710(fixed)	0.0137	0.2710
u_{249}	H(4)...C(17)	3.441(26)	0.2710(fixed)	0.0137	0.2710
u_{250}	H(5)...C(37)	3.441(26)	0.2710(fixed)	0.0137	0.2710
u_{251}	H(4)...C(9)	3.281(42)	0.2924(fixed)	0.0039	0.2924
u_{252}	H(5)...C(33)	3.281(42)	0.2924(fixed)	0.0039	0.2924
u_{253}	H(3)...C(21)	3.281(42)	0.2924(fixed)	0.0039	0.2924
u_{254}	H(14)...H(19)	3.272(50)	0.3819(fixed)	-0.0096	0.3819
u_{255}	H(40)...H(43)	3.272(50)	0.3817(fixed)	-0.0097	0.3817
u_{256}	H(28)...H(30)	3.272(50)	0.3817(fixed)	-0.0097	0.3817
u_{257}	C(1)...H(11)	3.328(16)	0.2438(fixed)	0.0084	0.2438
u_{258}	C(1)...H(35)	3.328(16)	0.2439(fixed)	0.0084	0.2439
u_{259}	C(1)...H(24)	3.328(16)	0.2440(fixed)	0.0084	0.2440
u_{260}	C(1)...H(16)	3.381(17)	0.2290(fixed)	0.0038	0.2290
u_{261}	C(1)...H(42)	3.381(17)	0.2289(fixed)	0.0038	0.2289
u_{262}	C(1)...H(27)	3.381(17)	0.2290(fixed)	0.0038	0.2290
u_{263}	C(1)...H(31)	3.389(17)	0.2135(fixed)	-0.0001	0.2135
u_{264}	C(1)...H(20)	3.389(17)	0.2136(fixed)	-0.0001	0.2136
u_{265}	C(1)...H(38)	3.389(17)	0.2135(fixed)	-0.0001	0.2135
u_{266}	Si(2)...C(9)	3.356(9)	0.1857(149)	0.0024	0.1664	0.1664(170)
u_{267}	Si(2)...C(33)	3.356(9)	0.1857(Tied to u_{266})	0.0023	0.1664
u_{268}	Si(2)...C(21)	3.356(9)	0.1857(Tied to u_{266})	0.0023	0.1664
u_{269}	H(12)...H(15)	3.428(37)	0.4182(fixed)	-0.0071	0.4182
u_{270}	H(36)...H(44)	3.428(37)	0.4181(fixed)	-0.007	0.4181
u_{271}	H(22)...H(26)	3.428(37)	0.4183(fixed)	-0.0071	0.4183
u_{272}	C(1)...H(23)	3.437(19)	0.2245(fixed)	0.0078	0.2245
u_{273}	C(1)...H(34)	3.437(19)	0.2244(fixed)	0.0078	0.2244
u_{274}	C(1)...H(10)	3.437(19)	0.2244(fixed)	0.0077	0.2244
u_{275}	H(22)...H(31)	3.588(40)	0.4075(fixed)	-0.0179	0.4075
u_{276}	H(36)...H(38)	3.588(40)	0.4075(fixed)	-0.0179	0.4075
u_{277}	H(12)...H(20)	3.588(40)	0.4076(fixed)	-0.0179	0.4076

u_{278}	C(1)...H(26)	3.417(19)	0.2184(fixed)	0.0029	0.2184	
u_{279}	C(1)...H(44)	3.417(19)	0.2182(fixed)	0.0029	0.2182	
u_{280}	C(1)...H(15)	3.417(19)	0.2184(fixed)	0.0029	0.2184	
u_{281}	C(1)...H(30)	3.442(18)	0.2033(fixed)	-0.0012	0.2033	
u_{282}	C(1)...H(40)	3.442(18)	0.2034(fixed)	-0.0011	0.2034	
u_{283}	C(1)...H(19)	3.442(18)	0.2034(fixed)	-0.0012	0.2034	
u_{284}	H(16)...C(41)	3.496(40)	0.4344(fixed)	0.02	0.4344	
u_{285}	C(25)...H(42)	3.496(40)	0.4342(fixed)	0.0199	0.4342	
u_{286}	C(13)...H(27)	3.496(40)	0.4347(fixed)	0.0199	0.4347	
u_{287}	H(27)...H(32)	3.421(44)	0.3905(fixed)	-0.0205	0.3905	
u_{288}	C(29)...C(33)	3.584(18)	0.1880(fixed)	0.0095	0.1880	
u_{289}	H(39)...H(42)	3.421(44)	0.3903(fixed)	-0.0205	0.3903	
u_{290}	C(9)...C(37)	3.584(18)	0.1881(fixed)	0.0095	0.1881	
u_{291}	H(16)...H(18)	3.421(44)	0.3904(fixed)	-0.0207	0.3904	
u_{292}	C(17)...C(21)	3.584(18)	0.1881(fixed)	0.0095	0.1881	
u_{293}	Si(2)...H(31)	3.667(21)	0.2761(fixed)	0.0227	0.2761	
u_{294}	Si(2)...H(20)	3.667(21)	0.2762(fixed)	0.0228	0.2762	
u_{295}	Si(2)...H(38)	3.667(21)	0.2763(fixed)	0.0228	0.2763	
u_{296}	Si(8)...C(29)	3.546(10)	0.1802(92)	0.0027	0.1447	0.1447(150)
u_{297}	Si(6)...C(37)	3.546(10)	0.1802(Tied to u_{296})	0.0027	0.1447	
u_{298}	Si(7)...C(17)	3.546(10)	0.1802(Tied to u_{296})	0.0027	0.1447	
u_{299}	H(24)...H(28)	3.636(35)	0.4397(fixed)	-0.0249	0.4397	
u_{300}	H(35)...H(43)	3.636(35)	0.4395(fixed)	-0.0249	0.4395	
u_{301}	H(11)...H(14)	3.636(35)	0.4394(fixed)	-0.0248	0.4394	
u_{302}	H(3)...Si(8)	3.597(26)	0.1998(fixed)	-0.0069	0.1998	
u_{303}	H(5)...Si(6)	3.597(26)	0.1998(fixed)	-0.0069	0.1998	
u_{304}	H(4)...Si(7)	3.597(26)	0.1998(fixed)	-0.0069	0.1998	
u_{305}	Si(2)...H(11)	3.439(32)	0.4175(fixed)	-0.0062	0.4175	
u_{306}	Si(2)...H(35)	3.439(32)	0.4175(fixed)	-0.0062	0.4175	
u_{307}	Si(2)...H(24)	3.439(32)	0.4176(fixed)	-0.0063	0.4176	
u_{308}	Si(7)...C(41)	3.646(13)	0.1936(Tied to u_{296})	0.0017	0.1555	
u_{309}	Si(8)...C(13)	3.646(13)	0.1936(Tied to u_{296})	0.0017	0.1555	
u_{310}	Si(6)...C(25)	3.646(13)	0.1936(Tied to u_{296})	0.0017	0.1555	
u_{311}	H(20)...H(23)	3.613(49)	0.5579(fixed)	0.006	0.5579	
u_{312}	H(31)...H(34)	3.613(49)	0.5576(fixed)	0.006	0.5576	

u_{313}	H(10)...H(38)	3.613(49)	0.5574(fixed)	0.0062	0.5574
u_{314}	C(25)...C(41)	3.725(20)	0.2195(fixed)	0.0064	0.2195
u_{315}	C(13)...C(41)	3.725(20)	0.2196(fixed)	0.0064	0.2196
u_{316}	C(13)...C(25)	3.725(20)	0.2196(fixed)	0.0064	0.2196
u_{317}	Si(7)...H(35)	3.688(17)	0.2641(fixed)	0.0542	0.2641
u_{318}	Si(8)...H(11)	3.688(17)	0.2635(fixed)	0.054	0.2635
u_{319}	Si(6)...H(24)	3.688(17)	0.2646(fixed)	0.0542	0.2646
u_{320}	H(30)...H(36)	3.725(49)	0.4790(fixed)	0.0056	0.4790
u_{321}	H(12)...H(40)	3.725(49)	0.4792(fixed)	0.0058	0.4792
u_{322}	H(19)...H(22)	3.725(49)	0.4791(fixed)	0.0056	0.4791
u_{323}	H(32)...H(35)	3.836(25)	0.3061(fixed)	0.0936	0.3061
u_{324}	H(11)...H(39)	3.836(25)	0.3050(fixed)	0.0932	0.3050
u_{325}	H(18)...H(24)	3.836(25)	0.3072(fixed)	0.0937	0.3072
u_{326}	Si(8)...H(31)	3.639(35)	0.2877(fixed)	-0.0021	0.2877
u_{327}	Si(6)...H(38)	3.639(35)	0.2877(fixed)	-0.0021	0.2877
u_{328}	Si(7)...H(20)	3.639(35)	0.2878(fixed)	-0.0021	0.2878
u_{329}	Si(6)...H(42)	3.814(17)	0.2660(fixed)	0.0343	0.2660
u_{330}	Si(7)...H(16)	3.814(17)	0.2669(fixed)	0.0346	0.2669
u_{331}	Si(8)...H(27)	3.814(17)	0.2667(fixed)	0.0345	0.2667
u_{332}	H(30)...H(43)	3.622(29)	0.4008(fixed)	0.0272	0.4008
u_{333}	H(14)...H(40)	3.622(29)	0.4015(fixed)	0.027	0.4015
u_{334}	H(19)...H(28)	3.622(29)	0.4015(fixed)	0.0271	0.4015
u_{335}	C(13)...C(37)	3.701(17)	0.2132(fixed)	0.0049	0.2132
u_{336}	C(29)...C(41)	3.701(17)	0.2133(fixed)	0.0049	0.2133
u_{337}	C(17)...C(25)	3.701(17)	0.2134(fixed)	0.0049	0.2134
u_{338}	H(32)...H(44)	3.732(29)	0.3815(fixed)	0.0538	0.3815
u_{339}	H(15)...H(39)	3.732(29)	0.3831(fixed)	0.0542	0.3831
u_{340}	H(18)...H(26)	3.732(29)	0.3827(fixed)	0.0541	0.3827
u_{341}	H(14)...H(26)	3.824(23)	0.4768(fixed)	0.0253	0.4768
u_{342}	H(28)...H(44)	3.824(23)	0.4759(fixed)	0.025	0.4759
u_{343}	H(15)...H(43)	3.824(23)	0.4768(fixed)	0.0255	0.4768
u_{344}	H(15)...H(38)	3.622(45)	0.3481(fixed)	0.0318	0.3481
u_{345}	H(31)...H(44)	3.622(45)	0.3468(fixed)	0.0315	0.3468
u_{346}	H(20)...H(26)	3.622(45)	0.3479(fixed)	0.0317	0.3479
u_{347}	Si(8)...H(16)	3.850(33)	0.3403(fixed)	-0.0055	0.3403

u_{348}	Si(7)...H(42)	3.850(33)	0.3401(fixed)	-0.0055	0.3401
u_{349}	Si(6)...H(27)	3.850(33)	0.3403(fixed)	-0.0055	0.3403
u_{350}	H(16)...H(40)	3.653(40)	0.3703(fixed)	0.0062	0.3703
u_{351}	H(30)...H(42)	3.654(40)	0.3693(fixed)	0.0064	0.3693
u_{352}	H(19)...H(27)	3.653(40)	0.3700(fixed)	0.0062	0.3700
u_{353}	H(26)...H(42)	3.830(25)	0.5439(fixed)	0.0148	0.5439
u_{354}	H(16)...H(44)	3.830(25)	0.5440(fixed)	0.0152	0.5440
u_{355}	H(15)...H(27)	3.830(25)	0.5443(fixed)	0.0149	0.5443
u_{356}	Si(2)...C(29)	3.948(15)	0.2022(57)	-0.002	0.1632
u_{357}	Si(2)...C(17)	3.948(15)	0.2022(Tied to u_{356})	-0.002	0.1632
u_{358}	Si(2)...C(37)	3.948(15)	0.2023(Tied to u_{356})	-0.0021	0.1633
u_{359}	H(27)...H(43)	3.956(26)	0.3284(fixed)	0.041	0.3284
u_{360}	H(14)...H(42)	3.955(26)	0.3272(fixed)	0.0401	0.3272
u_{361}	H(16)...H(28)	3.955(26)	0.3301(fixed)	0.0408	0.3301
u_{362}	H(4)...H(11)	3.703(54)	0.4623(fixed)	-0.0378	0.4623
u_{363}	H(5)...H(35)	3.703(54)	0.4624(fixed)	-0.0379	0.4624
u_{364}	H(3)...H(24)	3.702(54)	0.4625(fixed)	-0.038	0.4625
u_{365}	C(9)...H(19)	3.964(12)	0.1233(fixed)	-0.0283	0.1233
u_{366}	C(21)...H(30)	3.965(12)	0.1232(fixed)	-0.0282	0.1232
u_{367}	C(33)...H(40)	3.964(12)	0.1234(fixed)	-0.0283	0.1234
u_{368}	H(11)...C(17)	3.951(13)	0.1275(fixed)	-0.0452	0.1275
u_{369}	H(24)...C(29)	3.951(13)	0.1284(fixed)	-0.0455	0.1284
u_{370}	H(35)...C(37)	3.951(13)	0.1281(fixed)	-0.0453	0.1281
u_{371}	C(13)...H(20)	3.887(19)	0.1238(fixed)	-0.0287	0.1238
u_{372}	C(25)...H(31)	3.887(19)	0.1237(fixed)	-0.0286	0.1237
u_{373}	H(38)...C(41)	3.887(19)	0.1239(fixed)	-0.0287	0.1239
u_{374}	H(15)...C(17)	3.877(18)	0.1279(fixed)	-0.0362	0.1279
u_{375}	H(26)...C(29)	3.877(18)	0.1277(fixed)	-0.0361	0.1277
u_{376}	C(37)...H(44)	3.878(18)	0.1271(fixed)	-0.0359	0.1271
u_{377}	H(3)...H(30)	4.076(41)	0.3469(fixed)	-0.0109	0.3469
u_{378}	H(4)...H(19)	4.076(41)	0.3470(fixed)	-0.011	0.3470
u_{379}	H(5)...H(40)	4.076(41)	0.3470(fixed)	-0.011	0.3470
u_{380}	Si(7)...C(33)	3.992(10)	0.1704(Tied to u_{356})	-0.0008	0.1375
u_{381}	Si(8)...C(9)	3.992(10)	0.1705(Tied to u_{356})	-0.0008	0.1376
u_{382}	Si(6)...C(21)	3.992(10)	0.1705(Tied to u_{356})	-0.0008	0.1376

u_{383}	H(10)...C(13)	3.974(8)	0.1328(fixed)	-0.044	0.1328
u_{384}	H(23)...C(25)	3.974(8)	0.1336(fixed)	-0.0443	0.1336
u_{385}	H(34)...C(41)	3.974(8)	0.1333(fixed)	-0.0441	0.1333
u_{386}	C(9)...H(16)	3.993(7)	0.1264(fixed)	-0.0365	0.1264
u_{387}	C(33)...H(42)	3.993(7)	0.1255(fixed)	-0.0361	0.1255
u_{388}	C(21)...H(27)	3.993(7)	0.1262(fixed)	-0.0363	0.1262
u_{389}	H(30)...H(34)	4.123(55)	0.4005(fixed)	-0.035	0.4005
u_{390}	H(19)...H(23)	4.123(55)	0.4010(fixed)	-0.0351	0.4010
u_{391}	H(10)...H(40)	4.123(55)	0.4003(fixed)	-0.0348	0.4003
u_{392}	C(1)...H(12)	4.054(5)	0.1256(fixed)	-0.0415	0.1256
u_{393}	C(1)...H(36)	4.054(5)	0.1260(fixed)	-0.0416	0.1260
u_{394}	C(1)...H(22)	4.054(5)	0.1263(fixed)	-0.0417	0.1263
u_{395}	H(11)...H(18)	4.143(20)	0.2414(fixed)	-0.0521	0.2414
u_{396}	H(24)...H(32)	4.143(20)	0.2423(fixed)	-0.0525	0.2423
u_{397}	H(35)...H(39)	4.143(20)	0.2421(fixed)	-0.0523	0.2421
u_{398}	Si(8)...C(25)	4.078(10)	0.1820(Tied to u_{356})	-0.0018	0.1469
u_{399}	Si(6)...C(41)	4.078(10)	0.1820(Tied to u_{356})	-0.0018	0.1469
u_{400}	Si(7)...C(13)	4.078(10)	0.1820(Tied to u_{356})	-0.0018	0.1469
u_{401}	C(1)...H(32)	4.095(6)	0.1218(fixed)	-0.0271	0.1218
u_{402}	C(1)...H(18)	4.095(6)	0.1219(fixed)	-0.0272	0.1219
u_{403}	C(1)...H(39)	4.095(6)	0.1220(fixed)	-0.0272	0.1220
u_{404}	C(1)...H(43)	4.078(6)	0.1226(fixed)	-0.0338	0.1226
u_{405}	C(1)...H(14)	4.077(6)	0.1233(fixed)	-0.0341	0.1233
u_{406}	C(1)...H(28)	4.077(6)	0.1231(fixed)	-0.034	0.1231
u_{407}	H(26)...H(44)	4.000(67)	0.4241(fixed)	-0.0148	0.4241
u_{408}	H(15)...H(26)	4.000(67)	0.4245(fixed)	-0.0148	0.4245
u_{409}	H(15)...H(44)	4.000(67)	0.4244(fixed)	-0.0145	0.4244
u_{410}	H(22)...H(30)	4.193(21)	0.2657(fixed)	-0.0226	0.2657
u_{411}	H(12)...H(19)	4.192(21)	0.2658(fixed)	-0.0228	0.2658
u_{412}	H(36)...H(40)	4.192(21)	0.2658(fixed)	-0.0228	0.2658
u_{413}	H(14)...H(20)	4.076(27)	0.2385(fixed)	-0.0259	0.2385
u_{414}	H(38)...H(43)	4.076(27)	0.2385(fixed)	-0.026	0.2385
u_{415}	H(28)...H(31)	4.076(27)	0.2385(fixed)	-0.0258	0.2385
u_{416}	H(15)...H(18)	4.083(26)	0.2474(fixed)	-0.0398	0.2474
u_{417}	H(39)...H(44)	4.083(26)	0.2468(fixed)	-0.0394	0.2468

u_{418}	H(26)...H(32)	4.083(26)	0.2472(fixed)	-0.0397	0.2472
u_{419}	H(12)...H(38)	3.860(45)	0.3836(fixed)	-0.0365	0.3836
u_{420}	H(31)...H(36)	3.860(45)	0.3838(fixed)	-0.0367	0.3838
u_{421}	H(20)...H(22)	3.860(45)	0.3842(fixed)	-0.0368	0.3842
u_{422}	H(12)...H(16)	4.169(18)	0.2464(fixed)	-0.0298	0.2464
u_{423}	H(22)...H(27)	4.169(18)	0.2465(fixed)	-0.0296	0.2465
u_{424}	H(36)...H(42)	4.169(18)	0.2458(fixed)	-0.0294	0.2458
u_{425}	H(23)...H(28)	4.161(20)	0.2652(fixed)	-0.0463	0.2652
u_{426}	H(34)...H(43)	4.161(20)	0.2649(fixed)	-0.0461	0.2649
u_{427}	H(10)...H(14)	4.161(20)	0.2647(fixed)	-0.0459	0.2647
u_{428}	H(3)...H(32)	4.184(32)	0.3389(fixed)	-0.0148	0.3389
u_{429}	H(4)...H(18)	4.184(32)	0.3390(fixed)	-0.0148	0.3390
u_{430}	H(5)...H(39)	4.184(32)	0.3391(fixed)	-0.0149	0.3391
u_{431}	C(29)...H(34)	4.205(37)	0.3864(fixed)	-0.0323	0.3864
u_{432}	C(17)...H(23)	4.205(37)	0.3867(fixed)	-0.0324	0.3867
u_{433}	H(10)...C(37)	4.206(37)	0.3861(fixed)	-0.0322	0.3861
u_{434}	H(10)...H(19)	4.222(27)	0.2812(fixed)	-0.0321	0.2812
u_{435}	H(23)...H(30)	4.222(27)	0.2812(fixed)	-0.0321	0.2812
u_{436}	H(34)...H(40)	4.222(27)	0.2812(fixed)	-0.0321	0.2812
u_{437}	H(11)...H(20)	4.238(28)	0.2521(fixed)	-0.0559	0.2521
u_{438}	H(24)...H(31)	4.237(28)	0.2528(fixed)	-0.0563	0.2528
u_{439}	H(35)...H(38)	4.238(28)	0.2525(fixed)	-0.0561	0.2525
u_{440}	H(3)...H(22)	4.125(45)	0.3551(fixed)	-0.044	0.3551
u_{441}	H(5)...H(36)	4.125(45)	0.3549(fixed)	-0.0439	0.3549
u_{442}	H(4)...H(12)	4.126(45)	0.3545(fixed)	-0.0437	0.3545
u_{443}	H(40)...H(44)	4.093(36)	0.2368(fixed)	-0.0483	0.2368
u_{444}	H(26)...H(30)	4.093(36)	0.2373(fixed)	-0.0485	0.2373
u_{445}	H(15)...H(19)	4.093(36)	0.2375(fixed)	-0.0487	0.2375
u_{446}	H(10)...H(15)	4.285(19)	0.2577(fixed)	-0.0569	0.2577
u_{447}	H(34)...H(44)	4.285(19)	0.2580(fixed)	-0.057	0.2580
u_{448}	H(23)...H(26)	4.285(19)	0.2584(fixed)	-0.0572	0.2584
u_{449}	H(5)...H(12)	4.198(42)	0.3160(fixed)	-0.0578	0.3160
u_{450}	H(3)...H(36)	4.198(42)	0.3166(fixed)	-0.058	0.3166
u_{451}	H(4)...H(22)	4.198(42)	0.3170(fixed)	-0.0582	0.3170
u_{452}	H(27)...H(31)	4.129(36)	0.2550(fixed)	-0.0373	0.2550

u_{453}	H(38)...H(42)	4.129(36)	0.2551(fixed)	-0.0374	0.2551
u_{454}	H(16)...H(20)	4.129(36)	0.2551(fixed)	-0.0374	0.2551
u_{455}	H(26)...C(41)	4.268(39)	0.3447(fixed)	-0.0243	0.3447
u_{456}	C(13)...H(44)	4.268(39)	0.3443(fixed)	-0.0241	0.3443
u_{457}	H(15)...C(25)	4.268(39)	0.3446(fixed)	-0.0244	0.3446
u_{458}	C(29)...H(36)	4.230(26)	0.3184(fixed)	-0.0397	0.3184
u_{459}	H(12)...C(37)	4.230(26)	0.3182(fixed)	-0.0396	0.3182
u_{460}	C(17)...H(22)	4.229(26)	0.3185(fixed)	-0.0399	0.3185
u_{461}	H(16)...H(43)	4.308(58)	0.4813(fixed)	-0.0294	0.4813
u_{462}	H(28)...H(42)	4.308(58)	0.4814(fixed)	-0.0296	0.4814
u_{463}	H(14)...H(27)	4.307(58)	0.4821(fixed)	-0.0298	0.4821
u_{464}	H(11)...H(16)	4.338(21)	0.2795(fixed)	-0.0467	0.2795
u_{465}	H(35)...H(42)	4.338(21)	0.2789(fixed)	-0.0463	0.2789
u_{466}	H(24)...H(27)	4.338(21)	0.2794(fixed)	-0.0466	0.2794
u_{467}	H(3)...Si(6)	4.324(10)	0.1276(fixed)	-0.0162	0.1276
u_{468}	H(4)...Si(8)	4.324(10)	0.1276(fixed)	-0.0162	0.1276
u_{469}	H(5)...Si(7)	4.324(10)	0.1276(fixed)	-0.0162	0.1276
u_{470}	C(13)...H(38)	4.161(40)	0.2963(fixed)	-0.0184	0.2963
u_{471}	H(31)...C(41)	4.161(40)	0.2961(fixed)	-0.0184	0.2961
u_{472}	H(20)...C(25)	4.161(40)	0.2964(fixed)	-0.0184	0.2964
u_{473}	H(16)...C(37)	4.267(37)	0.3345(fixed)	-0.027	0.3345
u_{474}	C(29)...H(42)	4.267(37)	0.3340(fixed)	-0.0268	0.3340
u_{475}	C(17)...H(27)	4.267(37)	0.3344(fixed)	-0.027	0.3344
u_{476}	Si(2)...H(30)	4.463(29)	0.2572(fixed)	-0.0173	0.2572
u_{477}	Si(2)...H(19)	4.463(29)	0.2573(fixed)	-0.0173	0.2573
u_{478}	Si(2)...H(40)	4.463(29)	0.2573(fixed)	-0.0173	0.2573
u_{479}	Si(2)...H(12)	4.363(11)	0.1929(fixed)	-0.0559	0.1929
u_{480}	Si(2)...H(22)	4.362(11)	0.1941(fixed)	-0.0562	0.1941
u_{481}	Si(2)...H(36)	4.363(11)	0.1937(fixed)	-0.056	0.1937
u_{482}	C(13)...H(43)	4.471(27)	0.3302(fixed)	-0.0319	0.3302
u_{483}	H(28)...C(41)	4.471(27)	0.3305(fixed)	-0.0321	0.3305
u_{484}	H(14)...C(25)	4.471(27)	0.3308(fixed)	-0.0322	0.3308
u_{485}	Si(6)...H(23)	4.470(29)	0.3101(fixed)	-0.0212	0.3101
u_{486}	Si(7)...H(34)	4.470(29)	0.3100(fixed)	-0.0211	0.3100
u_{487}	Si(8)...H(10)	4.470(29)	0.3099(fixed)	-0.0211	0.3099

u_{488}	H(4)...H(31)	4.652(37)	0.3265(fixed)	0.0036	0.3265
u_{489}	H(5)...H(20)	4.652(37)	0.3266(fixed)	0.0036	0.3266
u_{490}	H(3)...H(38)	4.652(37)	0.3267(fixed)	0.0036	0.3267
u_{491}	H(5)...H(23)	4.528(28)	0.3235(fixed)	0.0374	0.3235
u_{492}	H(4)...H(34)	4.528(28)	0.3233(fixed)	0.0372	0.3233
u_{493}	H(3)...H(10)	4.528(28)	0.3229(fixed)	0.0371	0.3229
u_{494}	H(32)...C(33)	4.587(20)	0.2153(fixed)	-0.025	0.2153
u_{495}	C(9)...H(39)	4.587(20)	0.2158(fixed)	-0.0252	0.2158
u_{496}	H(18)...C(21)	4.587(20)	0.2156(fixed)	-0.0251	0.2156
u_{497}	Si(8)...H(26)	4.533(27)	0.2748(fixed)	-0.0188	0.2748
u_{498}	Si(6)...H(44)	4.533(27)	0.2745(fixed)	-0.0187	0.2745
u_{499}	Si(7)...H(15)	4.533(27)	0.2747(fixed)	-0.0188	0.2747
u_{500}	C(29)...H(43)	4.450(23)	0.3148(fixed)	-0.031	0.3148
u_{501}	H(14)...C(37)	4.450(23)	0.3152(fixed)	-0.0313	0.3152
u_{502}	C(17)...H(28)	4.450(23)	0.3153(fixed)	-0.0312	0.3153
u_{503}	Si(8)...H(32)	4.580(12)	0.1718(fixed)	-0.0315	0.1718
u_{504}	Si(6)...H(39)	4.580(12)	0.1721(fixed)	-0.0316	0.1721
u_{505}	Si(7)...H(18)	4.580(12)	0.1720(fixed)	-0.0316	0.1720
u_{506}	H(32)...C(41)	4.531(23)	0.2955(fixed)	-0.0229	0.2955
u_{507}	C(13)...H(39)	4.531(23)	0.2956(fixed)	-0.023	0.2956
u_{508}	H(18)...C(25)	4.531(23)	0.2957(fixed)	-0.023	0.2957
u_{509}	H(5)...H(31)	4.675(39)	0.3387(fixed)	0.01	0.3387
u_{510}	H(3)...H(20)	4.675(39)	0.3388(fixed)	0.01	0.3388
u_{511}	H(4)...H(38)	4.675(39)	0.3389(fixed)	0.01	0.3389
u_{512}	Si(7)...H(43)	4.640(14)	0.1858(fixed)	-0.0428	0.1858
u_{513}	Si(8)...H(14)	4.640(14)	0.1869(fixed)	-0.0432	0.1869
u_{514}	Si(6)...H(28)	4.640(14)	0.1866(fixed)	-0.0431	0.1866
u_{515}	C(25)...H(43)	4.714(22)	0.2469(fixed)	-0.0424	0.2469
u_{516}	H(14)...C(41)	4.713(22)	0.2482(fixed)	-0.0429	0.2482
u_{517}	C(13)...H(28)	4.713(22)	0.2478(fixed)	-0.0427	0.2478
u_{518}	Si(2)...C(13)	4.724(6)	0.1255(30)	-0.0059	0.1036
u_{519}	Si(2)...C(41)	4.724(6)	0.1255(Tied to u_{518})	-0.0059	0.1036
u_{520}	Si(2)...C(25)	4.724(6)	0.1255(Tied to u_{518})	-0.0059	0.1036
u_{521}	H(4)...C(29)	4.847(32)	0.2400(fixed)	-0.0174	0.2400
u_{522}	H(5)...C(17)	4.847(32)	0.2400(fixed)	-0.0174	0.2400

u_{523}	H(3)...C(37)	4.847(32)	0.2400(fixed)	-0.0175	0.2400
u_{524}	Si(2)...H(18)	4.807(17)	0.2143(fixed)	-0.0325	0.2143
u_{525}	Si(2)...H(32)	4.807(17)	0.2142(fixed)	-0.0323	0.2142
u_{526}	Si(2)...H(39)	4.807(17)	0.2144(fixed)	-0.0325	0.2144
u_{527}	Si(6)...C(33)	4.782(4)	0.1273(Tied to u_{518})	-0.0061	0.1051
u_{528}	Si(8)...C(21)	4.782(4)	0.1273(Tied to u_{518})	-0.0061	0.1051
u_{529}	Si(7)...C(9)	4.782(4)	0.1273(Tied to u_{518})	-0.0061	0.1051
u_{530}	H(11)...H(34)	4.733(35)	0.4555(fixed)	0.0858	0.4555
u_{531}	H(23)...H(35)	4.733(35)	0.4557(fixed)	0.0859	0.4557
u_{532}	H(10)...H(24)	4.733(35)	0.4557(fixed)	0.0859	0.4557
u_{533}	Si(7)...C(37)	4.834(5)	0.1225(Tied to u_{518})	-0.0059	0.1012
u_{534}	Si(6)...C(29)	4.834(5)	0.1225(Tied to u_{518})	-0.0059	0.1012
u_{535}	Si(8)...C(17)	4.834(5)	0.1225(Tied to u_{518})	-0.0059	0.1012
u_{536}	H(15)...H(20)	4.774(15)	0.1530(fixed)	-0.0611	0.1530
u_{537}	H(26)...H(31)	4.774(15)	0.1528(fixed)	-0.061	0.1528
u_{538}	H(38)...H(44)	4.774(15)	0.1527(fixed)	-0.0608	0.1527
u_{539}	H(3)...C(9)	4.830(10)	0.1852(fixed)	-0.0177	0.1852
u_{540}	H(4)...C(33)	4.830(10)	0.1852(fixed)	-0.0178	0.1852
u_{541}	H(5)...C(21)	4.830(10)	0.1852(fixed)	-0.0178	0.1852
u_{542}	H(11)...H(19)	4.816(9)	0.1508(fixed)	-0.0703	0.1508
u_{543}	H(24)...H(30)	4.816(9)	0.1513(fixed)	-0.0704	0.1513
u_{544}	H(35)...H(40)	4.816(9)	0.1512(fixed)	-0.0704	0.1512
u_{545}	H(10)...H(16)	4.822(9)	0.1608(fixed)	-0.0744	0.1608
u_{546}	H(23)...H(27)	4.822(9)	0.1606(fixed)	-0.0745	0.1606
u_{547}	H(34)...H(42)	4.823(9)	0.1603(fixed)	-0.0742	0.1603
u_{548}	Si(7)...H(36)	4.846(15)	0.2168(fixed)	-0.0498	0.2168
u_{549}	Si(8)...H(12)	4.846(15)	0.2165(fixed)	-0.0496	0.2165
u_{550}	Si(6)...H(22)	4.845(15)	0.2169(fixed)	-0.0499	0.2169
u_{551}	H(27)...H(35)	4.943(35)	0.3628(fixed)	0.0532	0.3628
u_{552}	H(11)...H(42)	4.943(35)	0.3622(fixed)	0.0529	0.3622
u_{553}	H(16)...H(24)	4.943(35)	0.3632(fixed)	0.0533	0.3632
u_{554}	Si(6)...H(43)	4.958(14)	0.2138(fixed)	-0.0406	0.2138
u_{555}	Si(7)...H(14)	4.957(14)	0.2145(fixed)	-0.0409	0.2145
u_{556}	Si(8)...H(28)	4.957(14)	0.2142(fixed)	-0.0408	0.2142
u_{557}	H(11)...C(33)	4.926(22)	0.3435(fixed)	0.0481	0.3435

u_{558}	C(21)...H(35)	4.926(22)	0.3439(fixed)	0.0482	0.3439
u_{559}	C(9)...H(24)	4.926(22)	0.3444(fixed)	0.0483	0.3444
u_{560}	Si(6)...H(34)	4.981(14)	0.2061(fixed)	0.0057	0.2061
u_{561}	Si(8)...H(23)	4.981(14)	0.2061(fixed)	0.0057	0.2061
u_{562}	Si(7)...H(10)	4.981(14)	0.2060(fixed)	0.0057	0.2060
u_{563}	Si(2)...H(26)	4.967(13)	0.2000(fixed)	-0.0025	0.2000
u_{564}	Si(2)...H(44)	4.967(13)	0.1999(fixed)	-0.0025	0.1999
u_{565}	Si(2)...H(15)	4.967(13)	0.2001(fixed)	-0.0025	0.2001
u_{566}	C(25)...H(35)	5.048(22)	0.2700(fixed)	0.0381	0.2700
u_{567}	H(11)...C(41)	5.048(22)	0.2694(fixed)	0.038	0.2694
u_{568}	C(13)...H(24)	5.048(22)	0.2702(fixed)	0.0383	0.2702
u_{569}	H(3)...H(11)	4.863(34)	0.4388(fixed)	-0.0222	0.4388
u_{570}	H(4)...H(35)	4.863(34)	0.4389(fixed)	-0.0222	0.4389
u_{571}	H(5)...H(24)	4.863(34)	0.4390(fixed)	-0.0222	0.4390
u_{572}	H(5)...C(29)	5.065(28)	0.2178(fixed)	-0.0174	0.2178
u_{573}	H(3)...C(17)	5.065(28)	0.2178(fixed)	-0.0174	0.2178
u_{574}	H(4)...C(37)	5.065(28)	0.2178(fixed)	-0.0174	0.2178
u_{575}	H(27)...C(33)	5.090(23)	0.2729(fixed)	0.0207	0.2729
u_{576}	C(9)...H(42)	5.090(23)	0.2724(fixed)	0.0205	0.2724
u_{577}	H(16)...C(21)	5.090(23)	0.2731(fixed)	0.0208	0.2731
u_{578}	H(31)...H(43)	4.797(47)	0.4017(fixed)	-0.0474	0.4017
u_{579}	H(20)...H(28)	4.797(47)	0.4022(fixed)	-0.0475	0.4022
u_{580}	H(14)...H(38)	4.797(47)	0.4020(fixed)	-0.0477	0.4020
u_{581}	H(3)...C(25)	5.061(20)	0.2039(fixed)	-0.0116	0.2039
u_{582}	H(4)...C(13)	5.061(20)	0.2039(fixed)	-0.0116	0.2039
u_{583}	H(5)...C(41)	5.061(20)	0.2039(fixed)	-0.0116	0.2039
u_{584}	H(16)...H(38)	4.879(45)	0.3507(fixed)	-0.0585	0.3507
u_{585}	H(31)...H(42)	4.880(45)	0.3501(fixed)	-0.058	0.3501
u_{586}	H(20)...H(27)	4.880(45)	0.3505(fixed)	-0.0584	0.3505
u_{587}	H(16)...H(39)	5.012(44)	0.4213(fixed)	-0.0506	0.4213
u_{588}	H(32)...H(42)	5.012(44)	0.4208(fixed)	-0.0503	0.4208
u_{589}	H(18)...H(27)	5.012(44)	0.4212(fixed)	-0.0505	0.4212
u_{590}	Si(6)...H(30)	5.062(14)	0.1948(fixed)	-0.0081	0.1948
u_{591}	Si(7)...H(40)	5.062(14)	0.1949(fixed)	-0.008	0.1949
u_{592}	Si(8)...H(19)	5.062(14)	0.1949(fixed)	-0.008	0.1949

u_{593}	Si(2)...H(16)	5.125(13)	0.1996(fixed)	-0.0154	0.1996
u_{594}	Si(2)...H(42)	5.125(13)	0.1995(fixed)	-0.0154	0.1995
u_{595}	Si(2)...H(27)	5.125(13)	0.1996(fixed)	-0.0154	0.1996
u_{596}	H(5)...C(13)	5.141(22)	0.2149(fixed)	-0.0121	0.2149
u_{597}	H(3)...C(41)	5.141(22)	0.2149(fixed)	-0.0121	0.2149
u_{598}	H(4)...C(25)	5.141(22)	0.2149(fixed)	-0.0121	0.2149
u_{599}	H(30)...C(37)	5.112(26)	0.2849(fixed)	0.0163	0.2849
u_{600}	C(17)...H(40)	5.112(26)	0.2851(fixed)	0.0164	0.2851
u_{601}	H(19)...C(29)	5.112(26)	0.2851(fixed)	0.0163	0.2851
u_{602}	H(3)...H(44)	5.151(23)	0.2885(fixed)	0.0094	0.2885
u_{603}	H(5)...H(15)	5.151(23)	0.2888(fixed)	0.0096	0.2888
u_{604}	H(4)...H(26)	5.151(23)	0.2887(fixed)	0.0095	0.2887
u_{605}	H(32)...H(34)	5.189(39)	0.4235(fixed)	-0.0738	0.4235
u_{606}	H(18)...H(23)	5.189(39)	0.4240(fixed)	-0.074	0.4240
u_{607}	H(10)...H(39)	5.189(39)	0.4234(fixed)	-0.0739	0.4234
u_{608}	C(21)...H(44)	5.199(25)	0.2999(fixed)	0.0279	0.2999
u_{609}	C(9)...H(26)	5.199(25)	0.3004(fixed)	0.0281	0.3004
u_{610}	H(15)...C(33)	5.199(25)	0.3006(fixed)	0.0282	0.3006
u_{611}	H(16)...H(30)	5.059(38)	0.4019(fixed)	0.0421	0.4019
u_{612}	H(19)...H(42)	5.059(38)	0.4014(fixed)	0.0419	0.4014
u_{613}	H(27)...H(40)	5.059(38)	0.4020(fixed)	0.0421	0.4020
u_{614}	Si(6)...H(31)	5.205(14)	0.1951(fixed)	-0.0143	0.1951
u_{615}	Si(8)...H(20)	5.205(14)	0.1951(fixed)	-0.0143	0.1951
u_{616}	Si(7)...H(38)	5.205(14)	0.1951(fixed)	-0.0143	0.1951
u_{617}	Si(6)...H(35)	5.143(14)	0.2185(fixed)	-0.0168	0.2185
u_{618}	Si(7)...H(11)	5.143(14)	0.2185(fixed)	-0.0168	0.2185
u_{619}	Si(8)...H(24)	5.143(14)	0.2185(fixed)	-0.0169	0.2185
u_{620}	H(16)...C(29)	5.188(26)	0.3198(fixed)	0.029	0.3198
u_{621}	C(17)...H(42)	5.187(26)	0.3191(fixed)	0.0287	0.3191
u_{622}	H(27)...C(37)	5.187(26)	0.3197(fixed)	0.0289	0.3197
u_{623}	C(25)...C(33)	5.278(16)	0.1745(fixed)	-0.0082	0.1745
u_{624}	C(9)...C(41)	5.278(16)	0.1745(fixed)	-0.0082	0.1745
u_{625}	C(13)...C(21)	5.278(16)	0.1745(fixed)	-0.0082	0.1745
u_{626}	C(9)...H(34)	5.233(17)	0.2833(fixed)	0.0312	0.2833
u_{627}	H(23)...C(33)	5.233(17)	0.2835(fixed)	0.0313	0.2835

u_{628}	H(10)...C(21)	5.233(17)	0.2831(fixed)	0.0311	0.2831
u_{629}	H(32)...H(36)	5.168(31)	0.3657(fixed)	-0.0755	0.3657
u_{630}	H(12)...H(39)	5.168(31)	0.3657(fixed)	-0.0755	0.3657
u_{631}	H(18)...H(22)	5.168(31)	0.3659(fixed)	-0.0757	0.3659
u_{632}	H(10)...H(23)	5.296(46)	0.4673(fixed)	0.0532	0.4673
u_{633}	H(23)...H(34)	5.296(46)	0.4676(fixed)	0.0534	0.4676
u_{634}	H(10)...H(34)	5.296(46)	0.4674(fixed)	0.0533	0.4674
u_{635}	H(26)...H(43)	5.263(38)	0.3753(fixed)	-0.0789	0.3753
u_{636}	H(14)...H(44)	5.263(38)	0.3754(fixed)	-0.0792	0.3754
u_{637}	H(15)...H(28)	5.263(38)	0.3750(fixed)	-0.0793	0.3750
u_{638}	H(5)...H(30)	5.379(44)	0.3313(fixed)	-0.0242	0.3313
u_{639}	H(4)...H(40)	5.379(44)	0.3314(fixed)	-0.0242	0.3314
u_{640}	H(3)...H(19)	5.379(44)	0.3314(fixed)	-0.0242	0.3314
u_{641}	C(9)...C(33)	5.354(10)	0.1791(fixed)	-0.006	0.1791
u_{642}	C(21)...C(33)	5.354(10)	0.1791(fixed)	-0.006	0.1791
u_{643}	C(9)...C(21)	5.354(10)	0.1791(fixed)	-0.006	0.1791
u_{644}	H(32)...H(43)	5.254(30)	0.3880(fixed)	-0.063	0.3880
u_{645}	H(14)...H(39)	5.253(30)	0.3885(fixed)	-0.0635	0.3885
u_{646}	H(18)...H(28)	5.253(30)	0.3885(fixed)	-0.0633	0.3885
u_{647}	H(5)...H(18)	5.526(38)	0.3116(fixed)	-0.0409	0.3116
u_{648}	H(4)...H(32)	5.526(38)	0.3115(fixed)	-0.0408	0.3115
u_{649}	H(3)...H(39)	5.526(38)	0.3116(fixed)	-0.0409	0.3116
u_{650}	H(14)...H(28)	5.392(26)	0.3774(fixed)	-0.082	0.3774
u_{651}	H(28)...H(43)	5.393(26)	0.3772(fixed)	-0.0816	0.3772
u_{652}	H(14)...H(43)	5.392(26)	0.3774(fixed)	-0.0819	0.3774
u_{653}	C(29)...C(37)	5.430(11)	0.1493(fixed)	-0.0063	0.1493
u_{654}	C(17)...C(37)	5.430(11)	0.1492(fixed)	-0.0063	0.1492
u_{655}	C(17)...C(29)	5.430(11)	0.1492(fixed)	-0.0063	0.1492
u_{656}	H(30)...H(39)	5.478(31)	0.3322(fixed)	0.0179	0.3322
u_{657}	H(18)...H(40)	5.478(31)	0.3324(fixed)	0.018	0.3324
u_{658}	H(19)...H(32)	5.478(31)	0.3324(fixed)	0.0179	0.3324
u_{659}	Si(2)...H(28)	5.475(6)	0.1498(fixed)	-0.0343	0.1498
u_{660}	Si(2)...H(43)	5.476(6)	0.1495(fixed)	-0.0342	0.1495
u_{661}	Si(2)...H(14)	5.475(6)	0.1499(fixed)	-0.0344	0.1499
u_{662}	H(4)...H(30)	5.528(32)	0.2706(fixed)	-0.0424	0.2706

u_{663}	H(3)...H(40)	5.528(32)	0.2707(fixed)	-0.0425	0.2707
u_{664}	H(5)...H(19)	5.528(32)	0.2707(fixed)	-0.0425	0.2707
u_{665}	H(11)...H(43)	5.580(27)	0.3546(fixed)	0.0328	0.3546
u_{666}	H(14)...H(24)	5.580(27)	0.3554(fixed)	0.0331	0.3554
u_{667}	H(28)...H(35)	5.580(27)	0.3553(fixed)	0.0329	0.3553
u_{668}	C(21)...C(41)	5.521(13)	0.1578(fixed)	-0.0076	0.1578
u_{669}	C(13)...C(33)	5.521(13)	0.1578(fixed)	-0.0076	0.1578
u_{670}	C(9)...C(25)	5.521(13)	0.1578(fixed)	-0.0076	0.1578
u_{671}	H(22)...H(44)	5.617(28)	0.3482(fixed)	0.0374	0.3482
u_{672}	H(12)...H(26)	5.617(28)	0.3487(fixed)	0.0376	0.3487
u_{673}	H(15)...H(36)	5.617(28)	0.3491(fixed)	0.0377	0.3491
u_{674}	H(22)...H(35)	5.559(14)	0.3931(fixed)	0.0376	0.3931
u_{675}	H(11)...H(36)	5.559(14)	0.3923(fixed)	0.0374	0.3923
u_{676}	H(12)...H(24)	5.559(14)	0.3933(fixed)	0.0378	0.3933
u_{677}	H(3)...H(27)	5.504(17)	0.2422(fixed)	-0.0234	0.2422
u_{678}	H(4)...H(16)	5.504(17)	0.2423(fixed)	-0.0234	0.2423
u_{679}	H(5)...H(42)	5.504(17)	0.2422(fixed)	-0.0234	0.2422
u_{680}	H(31)...C(37)	5.477(32)	0.3029(fixed)	-0.0074	0.3029
u_{681}	C(17)...H(38)	5.477(32)	0.3030(fixed)	-0.0074	0.3030
u_{682}	H(20)...C(29)	5.477(32)	0.3031(fixed)	-0.0074	0.3031
u_{683}	H(27)...H(36)	5.606(31)	0.3650(fixed)	0.0097	0.3650
u_{684}	H(12)...H(42)	5.606(31)	0.3643(fixed)	0.0095	0.3643
u_{685}	H(16)...H(22)	5.606(31)	0.3652(fixed)	0.0098	0.3652
u_{686}	Si(8)...H(22)	5.576(6)	0.1498(fixed)	-0.04	0.1498
u_{687}	Si(6)...H(36)	5.576(6)	0.1497(fixed)	-0.0399	0.1497
u_{688}	Si(7)...H(12)	5.576(6)	0.1495(fixed)	-0.0399	0.1495
u_{689}	Si(7)...H(39)	5.611(7)	0.1437(fixed)	-0.0308	0.1437
u_{690}	Si(8)...H(18)	5.611(7)	0.1437(fixed)	-0.0307	0.1437
u_{691}	Si(6)...H(32)	5.611(7)	0.1436(fixed)	-0.0307	0.1436
u_{692}	H(3)...H(26)	5.527(24)	0.2433(fixed)	-0.0258	0.2433
u_{693}	H(4)...H(15)	5.527(24)	0.2433(fixed)	-0.0258	0.2433
u_{694}	H(5)...H(44)	5.527(24)	0.2433(fixed)	-0.0258	0.2433
u_{695}	C(25)...C(37)	5.552(13)	0.1715(fixed)	-0.0069	0.1715
u_{696}	C(17)...C(41)	5.552(13)	0.1715(fixed)	-0.0069	0.1715
u_{697}	C(13)...C(29)	5.552(13)	0.1715(fixed)	-0.0069	0.1715

u_{698}	C(25)...H(40)	5.478(22)	0.2582(fixed)	0.0047	0.2582
u_{699}	C(13)...H(30)	5.478(22)	0.2581(fixed)	0.0046	0.2581
u_{700}	H(19)...C(41)	5.478(22)	0.2581(fixed)	0.0046	0.2581
u_{701}	C(9)...H(23)	5.569(34)	0.3856(fixed)	-0.0089	0.3856
u_{702}	C(21)...H(34)	5.569(34)	0.3855(fixed)	-0.0089	0.3855
u_{703}	H(10)...C(33)	5.569(34)	0.3855(fixed)	-0.0089	0.3855
u_{704}	H(3)...H(28)	5.608(24)	0.2561(fixed)	-0.0248	0.2561
u_{705}	H(4)...H(14)	5.608(24)	0.2561(fixed)	-0.0248	0.2561
u_{706}	H(5)...H(43)	5.608(24)	0.2560(fixed)	-0.0248	0.2560
u_{707}	H(16)...C(33)	5.690(32)	0.3488(fixed)	-0.0121	0.3488
u_{708}	C(21)...H(42)	5.690(32)	0.3487(fixed)	-0.0122	0.3487
u_{709}	C(9)...H(27)	5.690(32)	0.3489(fixed)	-0.0122	0.3489
u_{710}	H(23)...H(44)	5.657(26)	0.3212(fixed)	0.0131	0.3212
u_{711}	H(10)...H(26)	5.658(26)	0.3217(fixed)	0.0134	0.3217
u_{712}	H(15)...H(34)	5.658(26)	0.3219(fixed)	0.0135	0.3219
u_{713}	H(26)...H(40)	5.525(41)	0.4017(fixed)	0.0162	0.4017
u_{714}	H(19)...H(44)	5.525(41)	0.4014(fixed)	0.0161	0.4014
u_{715}	H(15)...H(30)	5.525(41)	0.4015(fixed)	0.0161	0.4015
u_{716}	H(30)...H(38)	5.729(32)	0.3182(fixed)	-0.0073	0.3182
u_{717}	H(20)...H(40)	5.729(32)	0.3184(fixed)	-0.0072	0.3184
u_{718}	H(19)...H(31)	5.729(32)	0.3184(fixed)	-0.0072	0.3184
u_{719}	H(30)...H(40)	5.568(30)	0.3047(fixed)	-0.0003	0.3047
u_{720}	H(19)...H(40)	5.568(30)	0.3050(fixed)	-0.0002	0.3050
u_{721}	H(19)...H(30)	5.568(30)	0.3048(fixed)	-0.0002	0.3048
u_{722}	H(27)...H(39)	5.785(32)	0.3634(fixed)	0.0197	0.3634
u_{723}	H(16)...H(32)	5.785(32)	0.3635(fixed)	0.0199	0.3635
u_{724}	H(18)...H(42)	5.785(32)	0.3627(fixed)	0.0194	0.3627
u_{725}	H(5)...H(16)	5.740(23)	0.2593(fixed)	-0.039	0.2593
u_{726}	H(3)...H(42)	5.741(23)	0.2592(fixed)	-0.0389	0.2592
u_{727}	H(4)...H(27)	5.740(23)	0.2592(fixed)	-0.039	0.2592
u_{728}	H(20)...H(31)	5.817(29)	0.3540(fixed)	-0.0023	0.3540
u_{729}	H(31)...H(38)	5.817(29)	0.3540(fixed)	-0.0023	0.3540
u_{730}	H(20)...H(38)	5.817(29)	0.3540(fixed)	-0.0023	0.3540
u_{731}	H(11)...H(35)	5.629(38)	0.3924(fixed)	-0.0104	0.3924
u_{732}	H(24)...H(35)	5.629(38)	0.3927(fixed)	-0.0105	0.3927

u_{733}	H(11)...H(24)	5.629(38)	0.3932(fixed)	-0.0102	0.3932
u_{734}	H(11)...H(26)	5.765(29)	0.3366(fixed)	-0.0063	0.3366
u_{735}	H(24)...H(44)	5.765(29)	0.3362(fixed)	-0.0066	0.3362
u_{736}	H(15)...H(35)	5.765(29)	0.3367(fixed)	-0.0064	0.3367
u_{737}	H(3)...H(43)	5.824(29)	0.2772(fixed)	-0.0386	0.2772
u_{738}	H(4)...H(28)	5.824(29)	0.2774(fixed)	-0.0387	0.2774
u_{739}	H(5)...H(14)	5.824(29)	0.2774(fixed)	-0.0388	0.2774
u_{740}	H(26)...H(35)	5.822(26)	0.2899(fixed)	-0.0083	0.2899
u_{741}	H(11)...H(44)	5.822(26)	0.2893(fixed)	-0.0082	0.2893
u_{742}	H(15)...H(24)	5.822(26)	0.2901(fixed)	-0.0083	0.2901
u_{743}	C(29)...H(38)	5.902(14)	0.2101(fixed)	-0.0165	0.2101
u_{744}	C(17)...H(31)	5.902(14)	0.2101(fixed)	-0.0165	0.2101
u_{745}	H(20)...C(37)	5.902(14)	0.2101(fixed)	-0.0165	0.2101
u_{746}	H(27)...H(34)	5.875(25)	0.3110(fixed)	-0.0322	0.3110
u_{747}	H(16)...H(23)	5.875(25)	0.3111(fixed)	-0.0323	0.3111
u_{748}	H(10)...H(42)	5.875(25)	0.3105(fixed)	-0.0322	0.3105
u_{749}	H(26)...C(37)	5.761(33)	0.3274(fixed)	-0.0114	0.3274
u_{750}	C(17)...H(44)	5.761(33)	0.3272(fixed)	-0.0114	0.3272
u_{751}	H(15)...C(29)	5.761(33)	0.3274(fixed)	-0.0114	0.3274
u_{752}	H(3)...H(12)	5.829(12)	0.2117(fixed)	-0.0818	0.2117
u_{753}	H(4)...H(36)	5.829(12)	0.2125(fixed)	-0.082	0.2125
u_{754}	H(5)...H(22)	5.829(12)	0.2128(fixed)	-0.0821	0.2128
u_{755}	H(14)...C(21)	5.952(20)	0.2668(fixed)	-0.0361	0.2668
u_{756}	C(9)...H(43)	5.953(20)	0.2665(fixed)	-0.0359	0.2665
u_{757}	H(28)...C(33)	5.953(20)	0.2666(fixed)	-0.036	0.2666
u_{758}	H(3)...C(13)	5.905(10)	0.1433(fixed)	-0.0236	0.1433
u_{759}	H(4)...C(41)	5.905(10)	0.1433(fixed)	-0.0236	0.1433
u_{760}	H(5)...C(25)	5.905(10)	0.1433(fixed)	-0.0236	0.1433
u_{761}	C(29)...H(39)	5.939(12)	0.2077(fixed)	-0.0196	0.2077
u_{762}	H(18)...C(37)	5.939(12)	0.2076(fixed)	-0.0196	0.2076
u_{763}	C(17)...H(32)	5.939(12)	0.2076(fixed)	-0.0196	0.2076
u_{764}	C(25)...H(36)	5.939(22)	0.2778(fixed)	-0.0418	0.2778
u_{765}	H(12)...C(41)	5.939(22)	0.2777(fixed)	-0.0417	0.2777
u_{766}	C(13)...H(22)	5.939(22)	0.2778(fixed)	-0.0418	0.2778
u_{767}	C(13)...H(23)	5.949(25)	0.2716(fixed)	-0.044	0.2716

u_{768}	C(25)...H(34)	5.949(25)	0.2714(fixed)	-0.0439	0.2714
u_{769}	H(10)...C(41)	5.949(25)	0.2713(fixed)	-0.0438	0.2713
u_{770}	C(13)...H(34)	5.951(15)	0.2085(fixed)	-0.0188	0.2085
u_{771}	H(23)...C(41)	5.951(15)	0.2085(fixed)	-0.0189	0.2085
u_{772}	H(10)...C(25)	5.951(15)	0.2086(fixed)	-0.0188	0.2086
u_{773}	H(26)...C(33)	5.940(24)	0.2408(fixed)	-0.0367	0.2408
u_{774}	C(9)...H(44)	5.940(24)	0.2406(fixed)	-0.0366	0.2406
u_{775}	H(15)...C(21)	5.940(24)	0.2408(fixed)	-0.0368	0.2408
u_{776}	H(24)...C(41)	5.964(13)	0.2082(fixed)	-0.0224	0.2082
u_{777}	C(13)...H(35)	5.964(13)	0.2082(fixed)	-0.0224	0.2082
u_{778}	H(11)...C(25)	5.964(13)	0.2083(fixed)	-0.0224	0.2083
u_{779}	H(5)...H(32)	6.006(28)	0.2468(fixed)	-0.0552	0.2468
u_{780}	H(3)...H(18)	6.006(28)	0.2469(fixed)	-0.0553	0.2469
u_{781}	H(4)...H(39)	6.006(28)	0.2470(fixed)	-0.0554	0.2470
u_{782}	H(31)...H(39)	5.938(42)	0.3500(fixed)	-0.021	0.3500
u_{783}	H(18)...H(38)	5.938(42)	0.3500(fixed)	-0.021	0.3500
u_{784}	H(20)...H(32)	5.938(42)	0.3501(fixed)	-0.021	0.3501
u_{785}	H(16)...H(35)	5.999(31)	0.3864(fixed)	-0.0043	0.3864
u_{786}	H(24)...H(42)	5.999(31)	0.3863(fixed)	-0.0044	0.3863
u_{787}	H(11)...H(27)	5.999(31)	0.3864(fixed)	-0.0043	0.3864
u_{788}	H(16)...H(31)	5.922(29)	0.3326(fixed)	-0.0081	0.3326
u_{789}	H(20)...H(42)	5.922(29)	0.3322(fixed)	-0.0085	0.3322
u_{790}	H(27)...H(38)	5.922(29)	0.3326(fixed)	-0.0083	0.3326
u_{791}	H(22)...C(41)	6.081(14)	0.2173(fixed)	-0.0205	0.2173
u_{792}	C(13)...H(36)	6.081(14)	0.2173(fixed)	-0.0205	0.2173
u_{793}	H(12)...C(25)	6.081(14)	0.2173(fixed)	-0.0205	0.2173
u_{794}	C(29)...H(40)	5.891(20)	0.1972(fixed)	-0.0217	0.1972
u_{795}	H(19)...C(37)	5.891(20)	0.1972(fixed)	-0.0217	0.1972
u_{796}	C(17)...H(30)	5.891(20)	0.1972(fixed)	-0.0217	0.1972
u_{797}	C(9)...H(35)	5.921(20)	0.2790(fixed)	-0.0409	0.2790
u_{798}	H(11)...C(21)	5.922(20)	0.2791(fixed)	-0.0408	0.2791
u_{799}	H(24)...C(33)	5.921(20)	0.2791(fixed)	-0.041	0.2791
u_{800}	H(22)...C(33)	6.089(17)	0.2516(fixed)	-0.0382	0.2516
u_{801}	C(9)...H(36)	6.089(17)	0.2516(fixed)	-0.0382	0.2516
u_{802}	H(12)...C(21)	6.089(17)	0.2515(fixed)	-0.0381	0.2515

u_{803}	H(5)...H(26)	6.118(20)	0.2442(fixed)	-0.0204	0.2442
u_{804}	H(4)...H(44)	6.117(20)	0.2440(fixed)	-0.0205	0.2440
u_{805}	H(3)...H(16)	6.134(19)	0.2554(fixed)	-0.0228	0.2554
u_{806}	H(3)...H(15)	6.118(20)	0.2442(fixed)	-0.0204	0.2442
u_{807}	H(4)...H(42)	6.134(19)	0.2553(fixed)	-0.0228	0.2553
u_{808}	H(5)...H(27)	6.134(19)	0.2554(fixed)	-0.0228	0.2554
u_{809}	H(16)...H(36)	6.221(36)	0.4015(fixed)	-0.0261	0.4015
u_{810}	H(22)...H(42)	6.221(36)	0.4014(fixed)	-0.0261	0.4014
u_{811}	H(12)...H(27)	6.221(36)	0.4016(fixed)	-0.0261	0.4016
u_{812}	H(11)...H(23)	6.061(18)	0.4611(fixed)	-0.0348	0.4611
u_{813}	H(10)...H(35)	6.061(18)	0.4610(fixed)	-0.0349	0.4610
u_{814}	H(24)...H(34)	6.061(18)	0.4611(fixed)	-0.035	0.4611
u_{815}	H(20)...C(41)	6.145(19)	0.2180(fixed)	-0.0282	0.2180
u_{816}	C(25)...H(38)	6.145(19)	0.2180(fixed)	-0.0282	0.2180
u_{817}	C(13)...H(31)	6.145(19)	0.2180(fixed)	-0.0282	0.2180
u_{818}	H(31)...H(40)	6.096(33)	0.3074(fixed)	-0.0342	0.3074
u_{819}	H(20)...H(30)	6.096(33)	0.3075(fixed)	-0.0341	0.3075
u_{820}	H(19)...H(38)	6.096(33)	0.3075(fixed)	-0.0342	0.3075
u_{821}	C(25)...H(39)	6.264(20)	0.2341(fixed)	-0.0304	0.2341
u_{822}	H(18)...C(41)	6.264(20)	0.2341(fixed)	-0.0305	0.2341
u_{823}	C(13)...H(32)	6.264(20)	0.2341(fixed)	-0.0305	0.2341
u_{824}	H(16)...H(34)	6.259(31)	0.3435(fixed)	-0.0422	0.3435
u_{825}	H(23)...H(42)	6.259(31)	0.3434(fixed)	-0.0422	0.3434
u_{826}	H(10)...H(27)	6.259(31)	0.3435(fixed)	-0.0421	0.3435
u_{827}	C(9)...C(29)	6.312(7)	0.1265(fixed)	-0.0123	0.1265
u_{828}	C(17)...C(33)	6.312(7)	0.1266(fixed)	-0.0123	0.1266
u_{829}	C(21)...C(37)	6.312(7)	0.1265(fixed)	-0.0123	0.1265
u_{830}	H(12)...H(34)	6.201(19)	0.3182(fixed)	-0.0414	0.3182
u_{831}	H(23)...H(36)	6.200(19)	0.3192(fixed)	-0.0415	0.3192
u_{832}	H(10)...H(22)	6.200(19)	0.3186(fixed)	-0.0418	0.3186
u_{833}	H(22)...H(34)	6.375(48)	0.4319(fixed)	-0.0598	0.4319
u_{834}	H(12)...H(23)	6.375(48)	0.4318(fixed)	-0.0597	0.4318
u_{835}	H(10)...H(36)	6.375(48)	0.4318(fixed)	-0.0598	0.4318
u_{836}	H(12)...C(33)	6.298(15)	0.2298(fixed)	-0.0688	0.2298
u_{837}	C(21)...H(36)	6.298(15)	0.2304(fixed)	-0.0689	0.2304

u_{838}	C(9)...H(22)	6.298(15)	0.2305(fixed)	-0.069	0.2305
u_{839}	H(26)...H(38)	6.297(37)	0.3556(fixed)	-0.0272	0.3556
u_{840}	H(20)...H(44)	6.297(37)	0.3554(fixed)	-0.0273	0.3554
u_{841}	H(15)...H(31)	6.297(37)	0.3555(fixed)	-0.0272	0.3555
u_{842}	C(9)...H(31)	6.451(18)	0.2461(fixed)	-0.0107	0.2461
u_{843}	H(20)...C(33)	6.451(18)	0.2462(fixed)	-0.0107	0.2462
u_{844}	C(21)...H(38)	6.451(18)	0.2461(fixed)	-0.0107	0.2461
u_{845}	H(10)...H(31)	6.515(31)	0.3474(fixed)	0.0192	0.3474
u_{846}	H(20)...H(34)	6.515(31)	0.3474(fixed)	0.0193	0.3474
u_{847}	H(23)...H(38)	6.516(31)	0.3475(fixed)	0.0194	0.3475
u_{848}	H(23)...C(37)	6.493(21)	0.2490(fixed)	-0.0001	0.2490
u_{849}	H(10)...C(29)	6.493(21)	0.2489(fixed)	-0.0001	0.2489
u_{850}	C(17)...H(34)	6.493(21)	0.2489(fixed)	-0.0001	0.2489
u_{851}	H(32)...C(37)	6.454(12)	0.1740(fixed)	-0.045	0.1740
u_{852}	C(17)...H(39)	6.454(12)	0.1743(fixed)	-0.0452	0.1743
u_{853}	H(18)...C(29)	6.454(12)	0.1742(fixed)	-0.0451	0.1742
u_{854}	C(21)...H(43)	6.500(14)	0.1887(fixed)	-0.0569	0.1887
u_{855}	C(9)...H(28)	6.500(14)	0.1896(fixed)	-0.0571	0.1896
u_{856}	H(14)...C(33)	6.500(14)	0.1898(fixed)	-0.0572	0.1898
u_{857}	H(11)...C(29)	6.458(17)	0.2707(fixed)	-0.0091	0.2707
u_{858}	C(17)...H(35)	6.458(17)	0.2709(fixed)	-0.0091	0.2709
u_{859}	H(24)...C(37)	6.458(17)	0.2709(fixed)	-0.0091	0.2709
u_{860}	H(12)...H(43)	6.578(29)	0.3786(fixed)	-0.0736	0.3786
u_{861}	H(28)...H(36)	6.578(29)	0.3788(fixed)	-0.0739	0.3788
u_{862}	H(14)...H(22)	6.578(29)	0.3789(fixed)	-0.074	0.3789
u_{863}	H(14)...C(29)	6.517(16)	0.2183(fixed)	-0.0558	0.2183
u_{864}	C(17)...H(43)	6.517(16)	0.2174(fixed)	-0.0554	0.2174
u_{865}	H(28)...C(37)	6.517(16)	0.2180(fixed)	-0.0557	0.2180
u_{866}	H(26)...H(34)	6.539(29)	0.3046(fixed)	-0.0601	0.3046
u_{867}	H(15)...H(23)	6.539(29)	0.3047(fixed)	-0.0602	0.3047
u_{868}	H(10)...H(44)	6.540(29)	0.3044(fixed)	-0.0599	0.3044
u_{869}	C(9)...H(30)	6.541(19)	0.2246(fixed)	-0.0154	0.2246
u_{870}	C(21)...H(40)	6.541(19)	0.2246(fixed)	-0.0153	0.2246
u_{871}	H(19)...C(33)	6.541(19)	0.2247(fixed)	-0.0154	0.2247
u_{872}	H(11)...H(31)	6.510(29)	0.3892(fixed)	-0.0047	0.3892

u_{873}	H(20)...H(35)	6.510(29)	0.3893(fixed)	-0.0046	0.3893
u_{874}	H(24)...H(38)	6.510(29)	0.3892(fixed)	-0.0046	0.3892
u_{875}	H(14)...H(23)	6.647(29)	0.3469(fixed)	-0.0778	0.3469
u_{876}	H(28)...H(34)	6.647(29)	0.3466(fixed)	-0.0777	0.3466
u_{877}	H(10)...H(43)	6.647(29)	0.3464(fixed)	-0.0775	0.3464
u_{878}	H(26)...H(39)	6.553(38)	0.3678(fixed)	-0.0461	0.3678
u_{879}	H(18)...H(44)	6.553(38)	0.3675(fixed)	-0.0461	0.3675
u_{880}	H(15)...H(32)	6.553(38)	0.3677(fixed)	-0.0461	0.3677
u_{881}	H(28)...H(40)	6.479(23)	0.2868(fixed)	-0.0509	0.2868
u_{882}	H(14)...H(30)	6.479(23)	0.2870(fixed)	-0.0511	0.2870
u_{883}	H(19)...H(43)	6.480(23)	0.2862(fixed)	-0.0506	0.2862
u_{884}	H(11)...H(30)	6.574(28)	0.3324(fixed)	0.006	0.3324
u_{885}	H(19)...H(35)	6.575(28)	0.3326(fixed)	0.0061	0.3326
u_{886}	H(24)...H(40)	6.575(28)	0.3326(fixed)	0.0062	0.3326
u_{887}	H(26)...H(36)	6.636(30)	0.3187(fixed)	-0.0745	0.3187
u_{888}	H(12)...H(44)	6.637(30)	0.3183(fixed)	-0.0742	0.3183
u_{889}	H(15)...H(22)	6.636(30)	0.3187(fixed)	-0.0746	0.3187
u_{890}	H(4)...H(43)	6.734(10)	0.1670(fixed)	-0.0609	0.1670
u_{891}	H(3)...H(14)	6.734(10)	0.1675(fixed)	-0.0611	0.1675
u_{892}	H(5)...H(28)	6.734(10)	0.1673(fixed)	-0.061	0.1673
u_{893}	H(23)...H(40)	6.852(29)	0.3144(fixed)	-0.0212	0.3144
u_{894}	H(10)...H(30)	6.852(29)	0.3144(fixed)	-0.0213	0.3144
u_{895}	H(19)...H(34)	6.852(29)	0.3144(fixed)	-0.0212	0.3144
u_{896}	H(23)...H(43)	6.869(17)	0.2516(fixed)	-0.061	0.2516
u_{897}	H(10)...H(28)	6.869(17)	0.2523(fixed)	-0.0612	0.2523
u_{898}	H(14)...H(34)	6.869(17)	0.2523(fixed)	-0.0613	0.2523
u_{899}	H(32)...H(38)	6.940(14)	0.2204(fixed)	-0.0587	0.2204
u_{900}	H(18)...H(31)	6.940(14)	0.2205(fixed)	-0.0588	0.2205
u_{901}	H(20)...H(39)	6.940(14)	0.2207(fixed)	-0.0589	0.2207
u_{902}	H(32)...H(39)	6.953(15)	0.2378(fixed)	-0.0598	0.2378
u_{903}	H(18)...H(39)	6.953(15)	0.2379(fixed)	-0.0599	0.2379
u_{904}	H(18)...H(32)	6.953(15)	0.2378(fixed)	-0.0599	0.2378
u_{905}	H(32)...H(40)	6.866(22)	0.2285(fixed)	-0.058	0.2285
u_{906}	H(19)...H(39)	6.866(22)	0.2287(fixed)	-0.0581	0.2287
u_{907}	H(18)...H(30)	6.866(22)	0.2286(fixed)	-0.0581	0.2286

u_{908}	H(22)...H(43)	7.050(17)	0.2553(fixed)	-0.0722	0.2553
u_{909}	H(12)...H(28)	7.050(17)	0.2559(fixed)	-0.0724	0.2559
u_{910}	H(14)...H(36)	7.049(17)	0.2562(fixed)	-0.0726	0.2562
u_{911}	H(22)...H(36)	6.980(9)	0.3160(fixed)	-0.097	0.3160
u_{912}	H(12)...H(36)	6.981(9)	0.3157(fixed)	-0.0968	0.3157
u_{913}	H(12)...H(22)	6.980(9)	0.3160(fixed)	-0.097	0.3160
u_{914}	H(24)...H(43)	6.969(13)	0.2203(fixed)	-0.0781	0.2203
u_{915}	H(11)...H(28)	6.969(13)	0.2210(fixed)	-0.0783	0.2210
u_{916}	H(14)...H(35)	6.969(13)	0.2213(fixed)	-0.0784	0.2213
u_{917}	H(12)...H(35)	6.894(26)	0.2876(fixed)	-0.1048	0.2876
u_{918}	H(11)...H(22)	6.894(26)	0.2882(fixed)	-0.105	0.2882
u_{919}	H(24)...H(36)	6.894(26)	0.2879(fixed)	-0.1051	0.2879
u_{920}	C(9)...H(32)	7.171(6)	0.1518(fixed)	-0.0443	0.1518
u_{921}	H(18)...C(33)	7.171(6)	0.1520(fixed)	-0.0444	0.1520
u_{922}	C(21)...H(39)	7.171(6)	0.1521(fixed)	-0.0444	0.1521
u_{923}	H(12)...C(29)	7.183(6)	0.1502(fixed)	-0.058	0.1502
u_{924}	C(17)...H(36)	7.183(6)	0.1506(fixed)	-0.0581	0.1506
u_{925}	H(22)...C(37)	7.183(6)	0.1507(fixed)	-0.0582	0.1507
u_{926}	H(14)...H(31)	7.122(19)	0.2381(fixed)	-0.0768	0.2381
u_{927}	H(20)...H(43)	7.122(19)	0.2374(fixed)	-0.0765	0.2374
u_{928}	H(28)...H(38)	7.122(19)	0.2379(fixed)	-0.0768	0.2379
u_{929}	H(28)...H(39)	7.182(24)	0.2930(fixed)	-0.0774	0.2930
u_{930}	H(14)...H(32)	7.182(24)	0.2933(fixed)	-0.0775	0.2933
u_{931}	H(18)...H(43)	7.182(24)	0.2926(fixed)	-0.0772	0.2926
u_{932}	H(23)...H(39)	7.323(20)	0.2606(fixed)	-0.0303	0.2606
u_{933}	H(18)...H(34)	7.323(20)	0.2605(fixed)	-0.0303	0.2605
u_{934}	H(10)...H(32)	7.323(20)	0.2604(fixed)	-0.0303	0.2604
u_{935}	H(12)...H(31)	7.392(17)	0.2491(fixed)	-0.0684	0.2491
u_{936}	H(20)...H(36)	7.392(17)	0.2496(fixed)	-0.0684	0.2496
u_{937}	H(22)...H(38)	7.392(17)	0.2496(fixed)	-0.0685	0.2496
u_{938}	H(11)...H(32)	7.395(17)	0.2693(fixed)	-0.0531	0.2693
u_{939}	H(18)...H(35)	7.395(17)	0.2696(fixed)	-0.0532	0.2696
u_{940}	H(24)...H(39)	7.395(17)	0.2696(fixed)	-0.0533	0.2696
u_{941}	H(12)...H(30)	7.386(19)	0.2388(fixed)	-0.0609	0.2388
u_{942}	H(22)...H(40)	7.386(19)	0.2392(fixed)	-0.0611	0.2392

u_{943}	H(19)...H(36)	7.386(19)	0.2391(fixed)	-0.061	0.2391
u_{944}	H(22)...H(39)	8.007(9)	0.1824(fixed)	-0.0851	0.1824
u_{945}	H(18)...H(36)	8.007(9)	0.1824(fixed)	-0.0851	0.1824
u_{946}	H(12)...H(32)	8.007(9)	0.1820(fixed)	-0.0849	0.1820

[a] Estimated standard deviations, obtained in the least squares refinement, are given in parentheses.

[b] Amplitudes not refined were fixed at the values obtained using the HF/6-31G(d) force field.

Table S4 Experimental coordinates (Å) determined from the GED analysis of $(Me_3Si)_3CSiH_3$

Atom	x	y	z
C(1)	0.0000	0.0000	0.0000
Si(2)	-1.8903	0.0000	0.0000
H(3)	-2.4345	-1.3152	-0.4484
H(4)	-2.4345	1.0459	-0.9148
H(5)	-2.4345	0.2693	1.3632
Si(6)	0.5282	1.8297	0.0000
Si(7)	0.5282	-0.9149	-1.5846
Si(8)	0.5282	-0.9149	1.5846
C(9)	-0.5807	2.8975	1.0970
H(10)	-1.5971	2.9678	0.7065
H(11)	-0.6591	2.5000	2.1101
H(12)	-0.2064	3.9184	1.1871
C(13)	2.3244	2.0881	0.5295
H(14)	2.6173	3.1382	0.4849
H(15)	2.5013	1.7547	1.5533
H(16)	3.0214	1.5392	-0.1056
C(17)	0.5209	2.6349	-1.7103
H(18)	0.7705	3.6961	-1.6642
H(19)	1.2422	2.1705	-2.3844
H(20)	-0.4547	2.5612	-2.1932
C(21)	-0.5807	-0.4987	-3.0578
H(22)	-0.2064	-0.9311	-3.9870
H(23)	-1.5971	-0.8720	-2.9234
H(24)	-0.6591	0.5774	-3.2201
C(25)	2.3244	-0.5855	-2.0731
H(26)	2.5013	0.4678	-2.2963
H(27)	3.0214	-0.8611	-1.2802
H(28)	2.6173	-1.1491	-2.9602
C(29)	0.5209	-2.7986	-1.4268
H(30)	1.2422	-3.1502	-0.6875
H(31)	-0.4547	-3.1800	-1.1215
H(32)	0.7705	-3.2892	-2.3688
C(33)	-0.5807	-2.3988	1.9608

H(34)	-1.5971	-2.0957	2.2169
H(35)	-0.6591	-3.0774	1.1100
H(36)	-0.2064	-2.9872	2.7999
C(37)	0.5209	0.1637	3.1370
H(38)	-0.4547	0.6187	3.3147
H(39)	0.7705	-0.4068	4.0330
H(40)	1.2422	0.9797	3.0719
C(41)	2.3244	-1.5026	1.5436
H(42)	3.0214	-0.6782	1.3858
H(43)	2.6173	-1.9891	2.4753
H(44)	2.5013	-2.2225	0.7430

Table S5 Least-squares correlation matrix ($\times$ 100) for $(Me_3Si)_3CSiH_3$.[a]

	p_4	p_{10}	p_{13}	u_{188}	k_2
p_3	97	59		54	
p_4		59			
p_9			61		
p_{10}				65	
u_{58}					75

[a] k_2 is a scale factor.

Table S6 Nozzle-to-film distances (mm), weighting functions (nm^{-1}), correlation parameters, scale factors, electron wavelengths (pm) and sample and nozzle temperatures (K) used in the GED study of $(Me_3Si)_3CSiH_3$.

Nozzle-film distance[a]	259.04	96.23
Δs	1.0	2.0
s_{min}	20.0	80.0
sw_1	40.0	100.0
sw_2	120.0	276.0
s_{max}	140.0	320.0
Correlation Parameter	0.4981	0.4887
Scale Factor[b]	0.810(7)	0.825(11)
Electron Wavelength	6.13	6.13
Sample Temperature	415	426
Nozzle Temperature	416	448

[a] Determined by reference to the scattering pattern of benzene vapour.

[b] Values in parentheses are the estimated standard deviation.

Fig*u*re S1 Experimental and final weighted difference (experimental minus theoretical) molecular-scattering intensities for $(Me_3Si)_3CSiH_3$