Electronic Supplementary Information for Dalton Transactions

The gas-phase structure of the decasilsesquioxane $Si_{10}O_{15}H_{10}$

Derek A. Wann, Franck Rataboul, Anthony M. Reilly, Heather E. Robertson, Paul D. Lickiss and David W. H. Rankin

Supplementary Information

Table S1 Experimental parameters for the GED analysis of $Si_{10}O_{15}H_{10}$.[a]

Nozzle-to-film distance	253.55	93.83
T_{nozzle}	423	453
T_{sample}	413	433
Δs	1	2
s_{min}	3.0	10.2
sw_1	4.0	12.0
sw_2	12.0	36.2
s_{max}	13.0	38.0
Correlation parameter	0.497	0.491
Scale factor, k	0.808(4)	0.808(10)

[a] Distances in mm, s values in nm^{-1} and temperatures, T, in K. Values in parentheses are estimated standard deviations of the last digits.

Table S2 Calculated [MP2/6-311++G(3df,3pd)] coordinates (Å) for $Si_{10}O_{15}H_{10}$.

	x	*y*	*Z*
Si(1)	–2.5540	0.8298	1.5843
Si(2)	0.0000	2.6854	1.5843
Si(3)	2.5540	0.8298	1.5843
Si(4)	1.5785	–2.1726	1.5843
Si(5)	–1.5785	–2.1726	1.5843
Si(6)	–2.5540	0.8298	–1.5843
Si(7)	–1.5785	–2.1726	–1.5843
Si(8)	1.5785	–2.1726	–1.5843
Si(9)	2.5540	0.8298	–1.5843
Si(10)	0.0000	2.6854	–1.5843
O(11)	0.0000	–2.2571	1.9581
O(12)	1.3267	1.8260	1.9581
O(13)	–1.3267	1.8260	–1.9581
O(14)	–2.1466	–0.6975	–1.9581
O(15)	0.0000	–2.2571	–1.9581
O(16)	2.1466	–0.6975	–1.9581
O(17)	1.3267	1.8260	–1.9581
H(18)	2.3029	–3.1696	2.3574
H(19)	3.7261	1.2107	2.3574
H(20)	3.7261	1.2107	–2.3574
H(21)	2.3029	–3.1696	–2.3574
H(22)	–2.3029	–3.1696	–2.3574
H(23)	–3.7261	1.2107	–2.3574
O(24)	0.0000	3.0566	0.0000
O(25)	–2.9070	0.9445	0.0000
O(26)	–1.7966	–2.4728	0.0000
O(27)	1.7966	–2.4728	0.0000
O(28)	2.9070	0.9445	0.0000
H(29)	0.0000	3.9179	–2.3574
O(30)	2.1466	–0.6975	1.9581
O(31)	–1.3267	1.8260	1.9581
H(32)	0.0000	3.9179	2.3574
O(33)	–2.1466	–0.6975	1.9581
H(34)	–3.7261	1.2107	2.3574
H(35)	–2.3029	–3.1696	2.3574

Energy (not zero-point corrected) = –4025.01654 Hartrees.

Table S3 Refined and calculated RMS amplitudes of vibration (u), associated r_a distances and corresponding distance correction values (r_a–r_e) for $Si_{10}O_{15}H_{10}$.[a]

	Atom pair	r_a	$u_{(GED)}$	r_a–r_e	$u_{MD(calc.)}$
u_1	Si(1)–H(34)	146.6(7)	7.7(7)	0.8	7.5
u_2	Si(1)–O(31)	162.5(2)	4.7(1)	0.9	5.0
u_3	Si(1)–O(25)	163.1(3)	4.7(tied to u_2)	0.9	5.0
u_5	H(18)···O(27)	251.0(17)	10.6(tied to u_7)	1.0	9.5
u_4	O(11)···H(18)	253.6(10)	10.9(tied to u_7)	1.4	9.9
u_7	O(11)···O(26)	263.9(2)	9.4(2)	0.3	8.4
u_6	O(11)···O(30)	265.2(4)	9.5(tied to u_7)	0.6	8.6
u_9	Si(1)···Si(2)	310.7(3)	9.0(1)	–4.7	8.6
u_8	Si(1)···Si(6)	312.8(5)	8.7(tied to u_9)	–3.1	8.4
u_{10}	O(24)···O(25)	359.2(14)	35.7(tied to u_{11})	0.7	35.8
u_{12}	O(11)···O(15)	369.9(16)	34.3(tied to u_{11})	–14.3	34.5
u_{11}	Si(1)···O(24)	372.4(7)	19.6(2)	–1.0	19.6
u_{13}	Si(1)···O(13)	375.4(8)	19.6(tied to u_{11})	–8.7	19.7
u_{14}	Si(1)···O(11)	395.2(4)	24.1(tied to u_{11})	–6.2	24.1
u_{15}	Si(1)···H(32)	402.3(9)	17.0(tied to u_{11})	–6.2	17.1
u_{16}	Si(1)···H(23)	409.5(6)	10.9(tied to u_{11})	–1.8	10.9
u_{17}	O(11)···O(12)	414.7(6)	52.1(tied to u_{11})	–13.4	52.3
u_{18}	Si(1)···Si(7)	440.6(2)	12.3(2)	–5.9	10.8
u_{20}	O(11)···O(14)	458.9(13)	43.0(tied to u_{21})	–7.6	31.0
u_{21}	O(11)···O(25)	463.4(6)	40.3(27)	–8.8	29.0
u_{22}	H(18)···H(21)	471.5(41)	22.3(fixed)	3.3	22.3
u_{19}	H(18)···H(19)	467.6(8)	22.3(fixed)	3.3	22.3
u_{23}	H(18)···O(26)	473.7(8)	26.3(tied to u_{28})	–3.7	24.3
u_{25}	Si(1)···O(30)	483.3(5)	47.0(tied to u_{28})	–11.3	44.2
u_{24}	O(11)···H(21)	486.8(16)	20.8(tied to u_{28})	–6.7	19.3
u_{26}	O(11)···H(19)	501.7(13)	20.7(tied to u_{28})	–9.4	19.2
u_{27}	Si(1)···Si(3)	503.9(5)	22.1(tied to u_{28})	–6.4	20.5
u_{28}	Si(1)···O(15)	520.1(5)	29.4(9)	–11.4	27.2
u_{29}	Si(1)···H(22)	554.9(10)	18.4(tied to u_{31})	–6.1	17.0
u_{30}	O(11)···O(24)	556.3(9)	48.0(tied to u_{31})	–7.4	44.4
u_{32}	O(11)···O(13)	557.4(11)	44.2(tied to u_{31})	–17.8	40.9
u_{31}	Si(1)···O(27)	565.8(11)	26.0(6)	–2.0	24.0
u_{33}	O(24)···O(26)	584.0(22)	28.2(tied to u_{31})	3.9	26.1
u_{35}	Si(1)···O(16)	591.5(5)	38.2(tied to u_{31})	–13.4	35.3
u_{34}	Si(1)···Si(8)	592.4(2)	18.2(tied to u_{31})	–7.9	16.8
u_{36}	O(11)···H(32)	603.6(14)	50.8(tied to u_{31})	–15.5	46.9
u_{37}	Si(1)···H(18)	623.1(13)	25.2(tied to u_{31})	–11.2	23.3
u_{38}	H(18)···H(20)	652.4(20)	24.3(fixed)	–5.1	24.3
u_{39}	O(11)···H(20)	652.0(10)	28.0(fixed)	–12.1	28.0
u_{40}	H(18)···O(24)	698.3(14)	25.7(fixed)	–5.7	25.7
u_{41}	Si(1)···H(20)	731.6(8)	18.5(fixed)	–10.2	18.5
u_{42}	H(18)···H(32)	729.9(28)	24.9(fixed)	–16.9	24.9
u_{43}	O(11)···H(29)	735.1(9)	36.0(fixed)	–15.3	36.1

u_{44}	H(18)···H(23)	868.8(15)	20.8(fixed)	–12.6	20.8

[a] Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 1 for atom numbering.

Table S4 GED-determined coordinates (Å) for $Si_{10}O_{15}H_{10}$.

	x	*y*	*z*
Si(1)	-2.1708	1.5772	1.5797
Si(2)	0.8292	2.5520	1.5797
Si(3)	2.6833	0.0000	1.5797
Si(4)	0.8292	-2.5520	1.5797
Si(5)	-2.1708	-1.5772	1.5797
Si(6)	-2.1708	1.5772	-1.5797
Si(7)	-2.1708	-1.5772	-1.5797
Si(8)	0.8292	-2.5520	-1.5797
Si(9)	2.6833	0.0000	-1.5797
Si(10)	0.8292	2.5520	-1.5797
O(11)	-0.6954	-2.1404	1.9209
O(12)	1.8207	1.3228	1.9209
O(13)	-0.6954	2.1404	-1.9209
O(14)	-2.2505	0.0000	-1.9209
O(15)	-0.6954	-2.1404	-1.9209
O(16)	1.8207	-1.3228	-1.9209
O(17)	1.8207	1.3228	-1.9209
H(18)	1.2132	-3.7338	2.3412
H(19)	3.9260	0.0000	2.3412
H(20)	3.9260	0.0000	-2.3412
H(21)	1.2132	-3.7338	-2.3412
H(22)	-3.1762	-2.3076	-2.3412
H(23)	-3.1762	2.3076	-2.3412
O(24)	0.9424	2.9003	0.0000
O(25)	-2.4672	1.7925	0.0000
O(26)	-2.4672	-1.7925	0.0000
O(27)	0.9424	-2.9003	0.0000
O(28)	3.0496	0.0000	0.0000
H(29)	1.2132	3.7338	-2.3412
O(30)	1.8207	-1.3228	1.9209
O(31)	-0.6954	2.1404	1.9209
H(32)	1.2132	3.7338	2.3412
O(33)	-2.2505	0.0000	1.9209
H(34)	-3.1762	2.3076	2.3412
H(35)	-3.1762	-2.3076	2.3412

Table S5 Least-squares correlation matrix (×100) for the GED refinement of $Si_{10}O_{15}H_{10}$.[a]

	p_5	u_{21}	u_{28}	u_{32}	k_2
p_4	–87	68	63		
p_4		–65	–67		
u_2					75
u_{21}			64		
u_{28}				62	

[a] Only absolute values ≥ 50 are shown. k_2 is a scale factor.

Figure S1 Molecular-intensity scattering and difference (experimental minus theoretical) curves for $Si_{10}O_{15}H_{10}$.

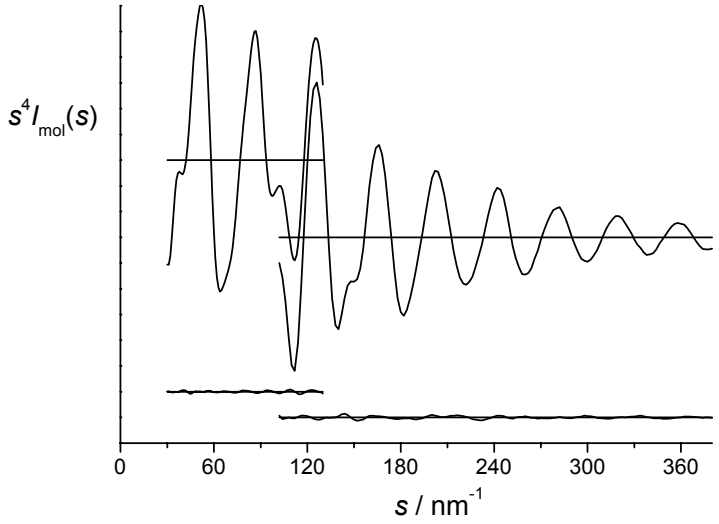

Figure S2 Eigenvector diagram [RHF/6-31G(d)] showing the vibrational motions associated with the 17 cm^{-1} mode.

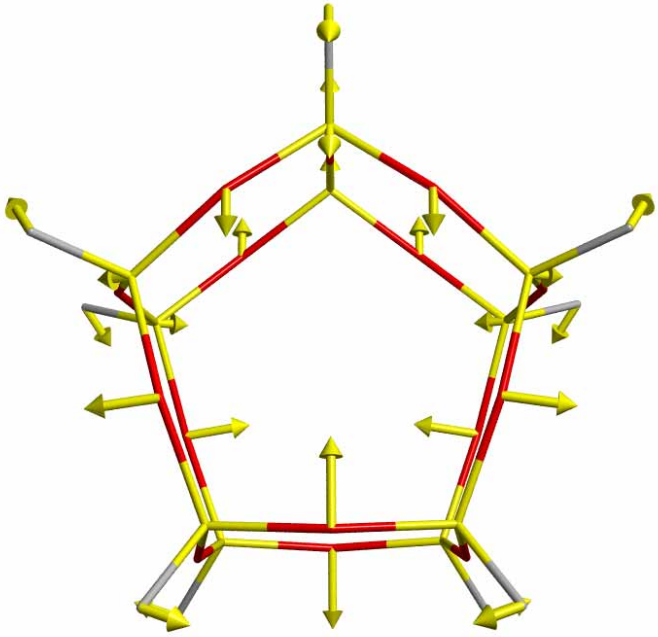

Figure S3 Eigenvector diagram [RHF/6-31G(d)] showing the vibrational motions associated with the 22 cm^{-1} mode.