Supplementary Information for PCCP Article

Chemically-bound Xenon in Fibrous Silica

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High-level quantum chemical calculations reported here predict the existence and remarkable stability, of chemically-bound xenon atoms in fibrous silica. The results may support the suggestion of Sanloup and coworkers that chemically-bound xenon and silica account for the problem of missing xenon (by a factor of 20!) from the atmospheres of Earth and Mars. So far, the host silica was assumed to be quartz, which is in contradiction with theory. The xenon-fibrous silica molecule is computed to be stable well beyond room temperature. The calculated Raman spectra of the species agree well with the main features of the experiments by Sanloup et al. The results predict computationally the existence of a new family of noble-gas containing materials. The fibrous silica species are finite molecules, their laboratory preparation should be feasible, and potential applications are possible.

Methods

Single point energy multi-reference MCQDPT calculations were performed using active space constructed from 12 electrons in 12 orbitals. It was the largest active space we were able to use considering the system size. Orbitals included in the active space are shown in the Figure 1.

Table 1 MCQDPT energies for the minimum energy Structure 1,and for Transition State Structures 2 and 6,first TS's on the main the decomposition paths.

	E [hartree]
Structure 1	-2387,7247
Structure 2	-2387,6596
Structure 6	-2387,6580

Geometry of Stationary points

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Table 2 Geometry parameters for structure 1. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(1-4)	2.174	R(6-16)	1.684	A(5-1-6)	179.6	A(2-18-16)	91.1	A(4-16-20)	117.5
R(1-5)	2.174	R(7-17)	1.684	A(5-1-7)	71.7	A(2-20-16)	91.1	A(5-17-7)	98.2
R(1-6)	2.171	R(8-12)	0.948	A(1-5-17)	95.1	A(9-3-11)	108.0	A(5-17-19)	117.5
R(1-7)	2.171	R(9-13)	0.948	A(6-1-7)	108.0	A(9-3-19)	113.8	A(5-17-21)	117.5
R(2-8)	1.649	R(10-14)	0.929	A(1-6-16)	95.1	A(9-3-21)	113.8	A(6-16-18)	117.9
R(2-10)	1.657	R(11-15)	0.929	A(1-7-17)	95.1	A(3-9-13)	115.5	A(6-16-20)	117.9
R(2-18)	1.713	R(16-18)	1.695	A(8-2-10)	108.0	A(11-3-19)	116.1	A(7-17-19)	117.9
R(2-20)	1.713	R(16-20)	1.695	A(8-2-18)	113.8	A(11-3-21)	116.1	A(7-17-21)	117.9
R(3-9)	1.649	R(17-19)	1.695	A(8-2-20)	113.8	A(3-11-15)	115.9	A(18-16-20)	89.5
R(3-11)	1.657	R(17-21)	1.695	A(2-8-12)	115.5	A(19-3-21)	88.3	A(19-17-21)	89.5
R(3-19)	1.713	A(4-1-5)	108.7	A(10-2-18)	116.1	A(3-19-17)	91.1		
R(3-21)	1.713	A(4-1-6)	71.7	A(10-2-20)	116.1	A(3-21-17)	91.1		
R(4-16)	1.682	A(4-1-7)	179.6	A(2-10-14)	115.9	A(4-16-6)	98.2		
R(5-17)	1.682	A(1-4-16)	95.1	A(18-2-20)	88.3	A(4-16-18)	117.5		

Table 3 Geometry parameters for structure 2. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(1-2)	2.120	R(10-12)	1.704	A(1-4-6)	92.0	A(4-6-10)	101.1	A(9-17-19)	113.4
R(1-4)	2.117	R(11-17)	1.707	A(1-5-7)	100.7	A(5-7-9)	109.5	A(10-12-13)	111.9
R(1-5)	2.038	R(12-13)	1.653	A(2-6-3)	88.5	A(5-7-11)	106.9	A(10-12-14)	118.3
R(2-6)	1.723	R(12-14)	1.661	A(2-6-4)	91.9	A(8-6-10)	88.0	A(11-17-18)	111.4
R(3-6)	2.354	R(13-15)	0.966	A(2-6-8)	119.7	A(6-8-12)	92.1	A(11-17-19)	118.7
R(3-7)	1.618	R(14-16)	0.968	A(2-6-10)	114.2	A(6-10-12)	91.5	A(13-12-14)	107.1
R(4-6)	1.745	R(17-18)	1.652	A(6-3-7)	129.0	A(9-7-11)	89.3	A(12-13-15)	114.6
R(5-7)	1.787	R(17-19)	1.658	A(3-6-4)	75.9	A(7-9-17)	90.9	A(12-14-16)	114.6
R(6-8)	1.700	R(18-20)	0.967	A(3-6-8)	81.1	A(7-11-17)	90.9	A(18-17-19)	107.6
R(6-10)	1.718	R(19-21)	0.969	A(3-6-10)	157.3	A(8-12-10)	88.2	A(17-18-20)	114.9
R(7-9)	1.700	A(2-1-4)	72.1	A(3-7-5)	102.4	A(8-12-13)	115.2	A(17-19-21)	114.7
R(7-11)	1.706	A(2-1-5)	143.9	A(3-7-9)	124.4	A(8-12-14)	115.6		
R(8-12)	1.707	A(1-2-6)	92.5	A(3-7-11)	123.3	A(9-17-11)	88.9		
R(9-17)	1.713	A(4-1-5)	84.9	A(4-6-8)	140.1	A(9-17-18)	116.4		

Table 4 Geometry parameters for structure 3. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(1-2)	2.121	R(10-12)	1.701	A(1-4-6)	92.0	A(4-6-10)	86.8	A(9-17-19)	113.4
R(1-4)	2.040	R(11-17)	1.697	A(1-5-7)	105.0	A(5-7-9)	112.3	A(10-12-13)	111.6
R(1-5)	2.165	R(12-13)	1.655	A(2-6-3)	109.0	A(5-7-11)	109.4	A(10-12-14)	118.0
R(2-6)	1.803	R(12-14)	1.664	A(2-6-4)	82.7	A(8-6-10)	87.2	A(11-17-18)	112.3
R(3-6)	1.722	R(13-15)	0.967	A(2-6-8)	92.3	A(6-8-12)	91.6	A(11-17-19)	118.8
R(3-7)	1.663	R(14-16)	0.968	A(2-6-10)	128.3	A(6-10-12)	92.3	A(13-12-14)	106.9
R(4-6)	1.891	R(17-18)	1.651	A(6-3-7)	135.4	A(9-7-11)	90.5	A(12-13-15)	114.0
R(5-7)	1.716	R(17-19)	1.659	A(3-6-4)	89.4	A(7-9-17)	89.7	A(12-14-16)	113.5
R(6-8)	1.737	R(18-20)	0.967	A(3-6-8)	103.2	A(7-11-17)	90.2	A(18-17-19)	107.1
R(6-10)	1.714	R(19-21)	0.968	A(3-6-10)	121.4	A(8-12-10)	88.9	A(17-18-20)	114.6
R(7-9)	1.690	A(2-1-4)	71.8	A(3-7-5)	112.4	A(8-12-13)	117.4	A(17-19-21)	114.6
R(7-11)	1.711	A(2-1-5)	130.2	A(3-7-9)	119.1	A(8-12-14)	113.7		
R(8-12)	1.697	A(1-2-6)	92.0	A(3-7-11)	110.9	A(9-17-11)	89.6		
R(9-17)	1.730	A(4-1-5)	80.4	A(4-6-8)	167.4	A(9-17-18)	115.2		

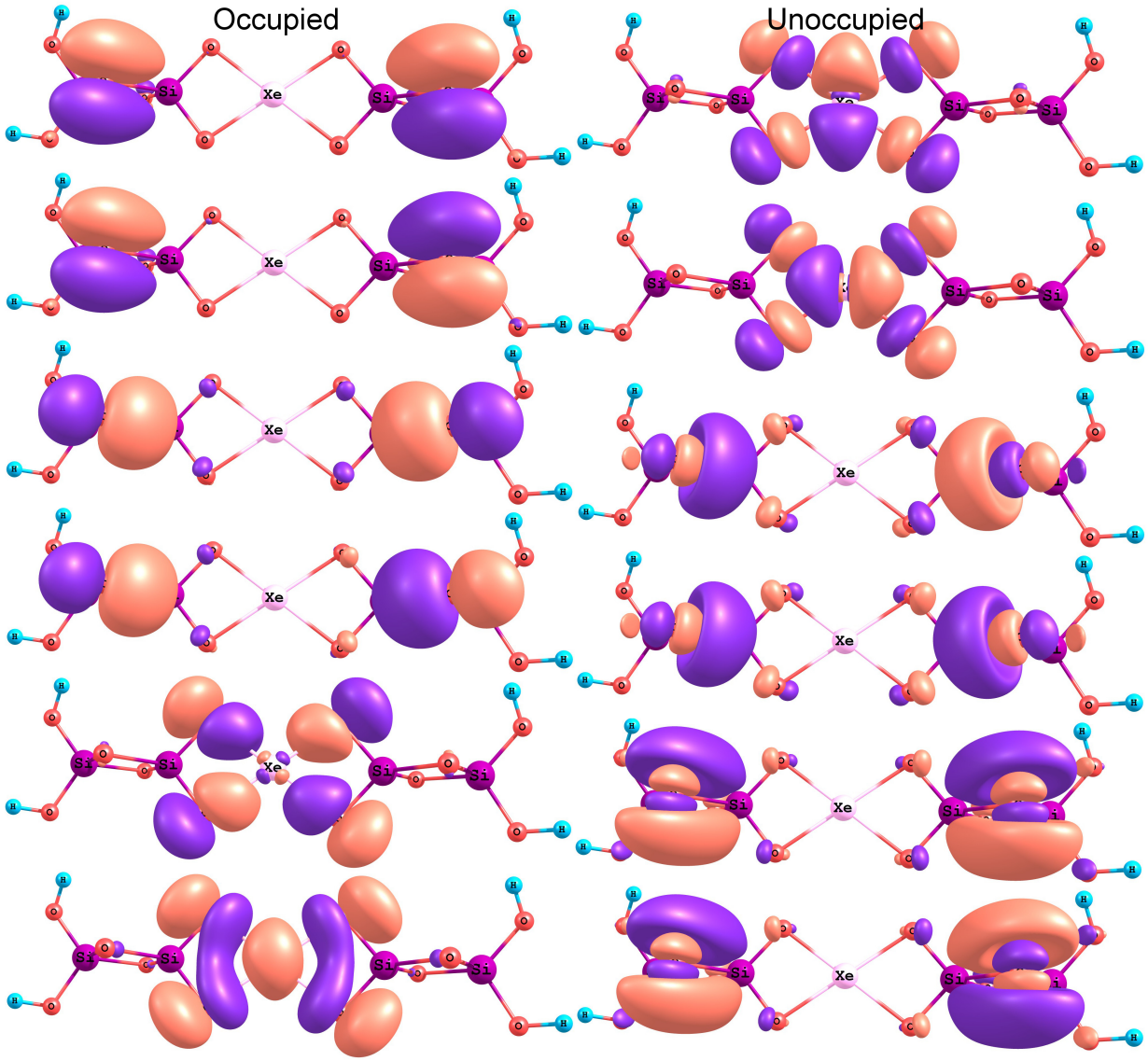

Figure 1 Orbitals included in the active space for MCQDPT calculations presented for the minimum structure of the $Si_2H_2O_6{-}Xe{-}Si_2H_2O_6$ molecule.

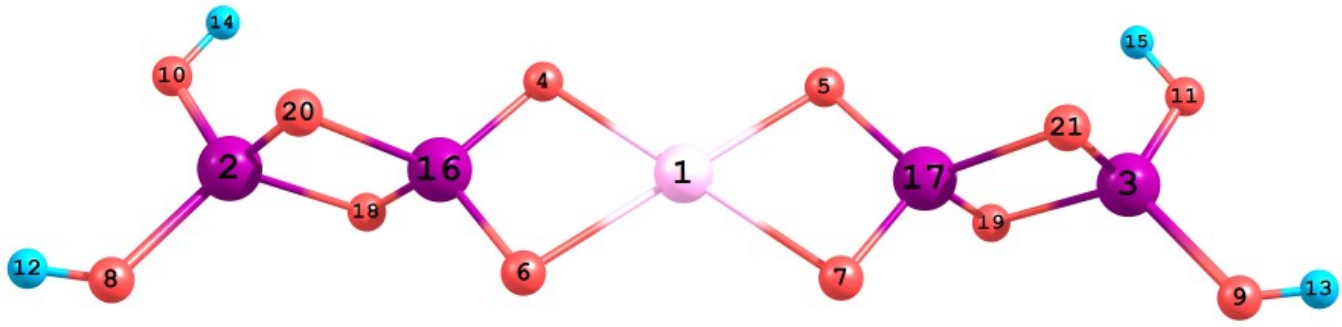

Figure 2 View of the geometry of structure 1.

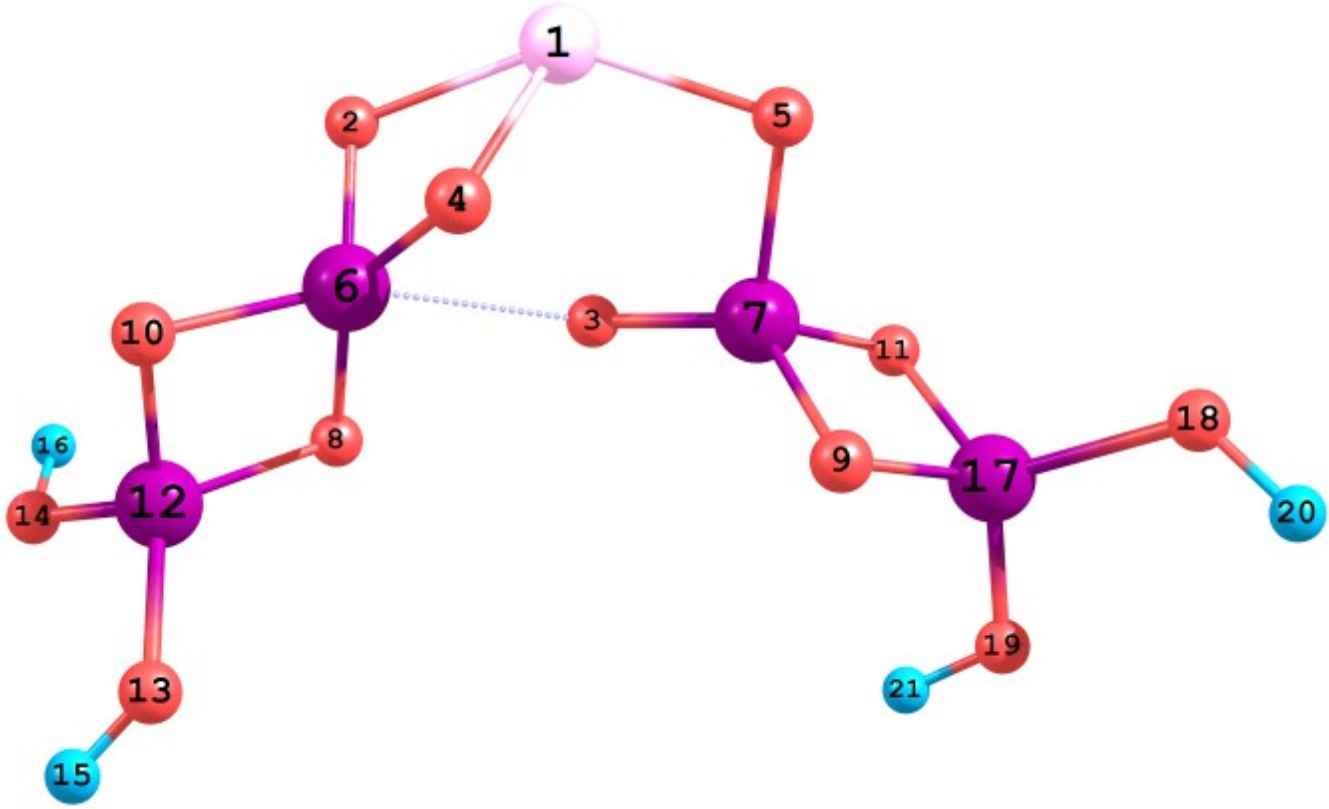

Figure 3 View of the geometry of structure 2.

Table 5 Geometry parameters for structure 4. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(1-2)	2.186	R(10-12)	1.709	A(4-1-5)	84.5	A(8-6-10)	89.4	A(10-12-14)	117.8
R(1-4)	1.939	R(11-17)	1.716	A(1-5-7)	101.4	A(6-8-12)	90.5	A(11-17-18)	114.5
R(1-5)	2.148	R(12-13)	1.654	A(2-6-3)	111.7	A(6-10-12)	90.9	A(11-17-19)	115.2
R(2-6)	1.709	R(12-14)	1.661	A(2-6-8)	107.3	A(9-7-11)	91.1	A(13-12-14)	106.8
R(3-6)	1.700	R(13-15)	0.967	A(2-6-10)	120.4	A(7-9-17)	89.6	A(12-13-15)	113.9
R(3-7)	1.676	R(14-16)	0.968	A(6-3-7)	145.5	A(7-11-17)	89.4	A(12-14-16)	114.4
R(5-7)	1.716	R(17-18)	1.650	A(3-6-8)	108.8	A(8-12-10)	89.1	A(18-17-19)	107.1
R(6-8)	1.709	R(17-19)	1.658	A(3-6-10)	115.8	A(8-12-13)	115.5	A(17-18-20)	115.1
R(6-10)	1.697	R(18-20)	0.968	A(3-7-5)	111.0	A(8-12-14)	115.0	A(17-19-21)	115.9
R(7-9)	1.695	R(19-21)	0.968	A(3-7-9)	116.3	A(9-17-11)	89.9		
R(7-11)	1.700	A(2-1-4)	79.0	A(3-7-11)	113.0	A(9-17-18)	112.9		
R(8-12)	1.709	A(2-1-5)	133.8	A(5-7-9)	115.1	A(9-17-19)	116.9		
R(9-17)	1.715	A(1-2-6)	96.9	A(5-7-11)	108.7	A(10-12-13)	112.4		

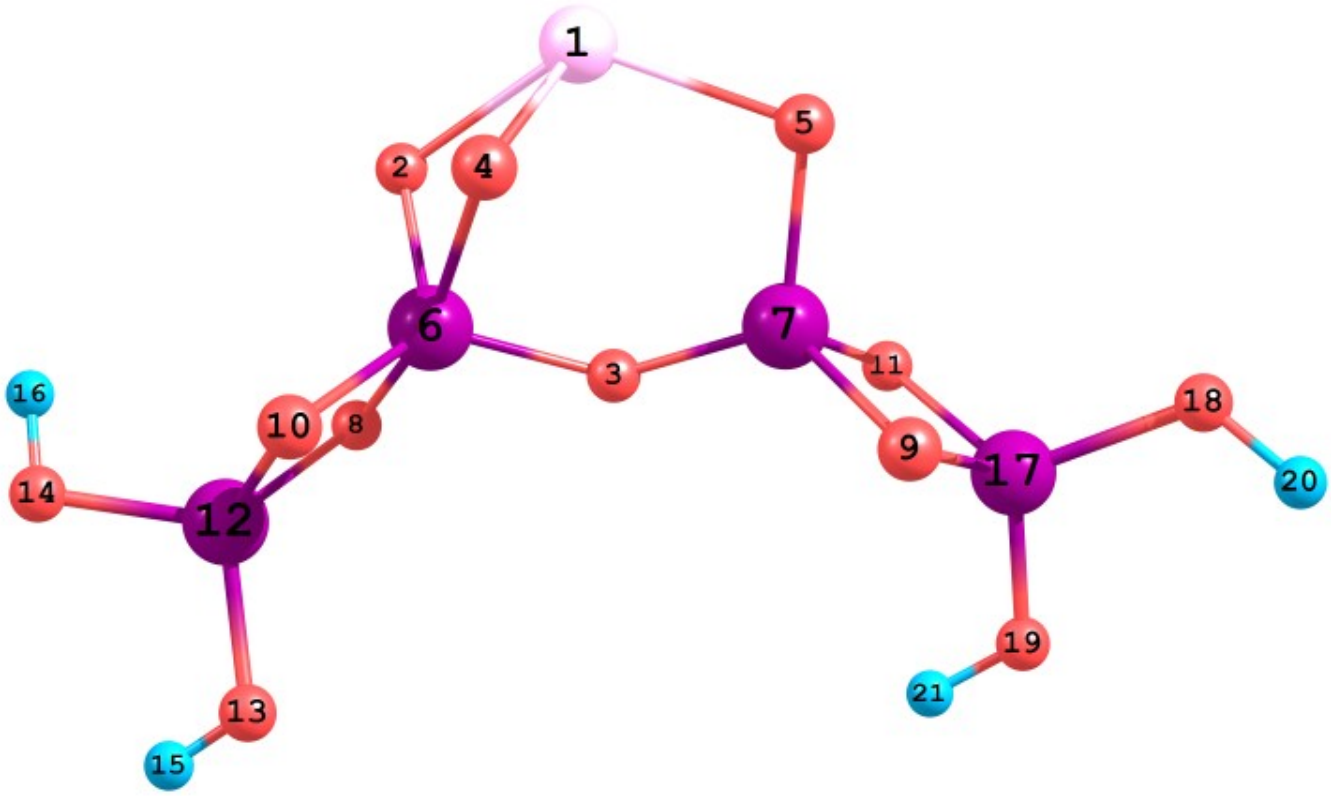

Figure 4 View of the geometry of structure 3.

Table 6 Geometry parameters for structure 5. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(1-5)	1.695	R(11-12)	1.648	A(2-5-3)	89.7	A(7-11-9)	99.0	A(16-17-19)	115.4
R(1-7)	1.482	R(11-13)	1.658	A(2-5-9)	114.2	A(7-11-12)	105.8	A(16-18-20)	115.4
R(2-5)	1.701	R(12-14)	0.967	A(2-6-3)	89.7	A(7-11-13)	116.1		
R(2-6)	1.704	R(13-15)	0.968	A(2-6-4)	120.2	A(8-16-10)	98.5		
R(3-5)	1.702	R(16-17)	1.649	A(2-6-8)	114.4	A(8-16-17)	108.5		
R(3-6)	1.700	R(16-18)	1.655	A(5-3-6)	90.1	A(8-16-18)	117.4		
R(4-6)	1.697	R(17-19)	0.967	A(3-5-9)	114.1	A(9-11-12)	114.6		
R(4-10)	1.476	R(18-20)	0.969	A(3-6-4)	114.8	A(9-11-13)	113.5		
R(5-9)	1.667	A(5-1-7)	107.7	A(3-6-8)	117.3	A(10-16-17)	117.3		
R(6-8)	1.666	A(1-5-2)	122.1	A(6-4-10)	108.8	A(10-16-18)	106.9		
R(7-11)	1.732	A(1-5-3)	116.1	A(4-6-8)	101.4	A(12-11-13)	107.6		
R(8-16)	1.683	A(1-5-9)	101.4	A(4-10-16)	110.5	A(11-12-14)	114.5		
R(9-11)	1.678	A(1-7-11)	110.1	A(5-9-11)	111.4	A(11-13-15)	115.7		
R(10-16)	1.725	A(5-2-6)	90.0	A(6-8-16)	111.8	A(17-16-18)	108.4		

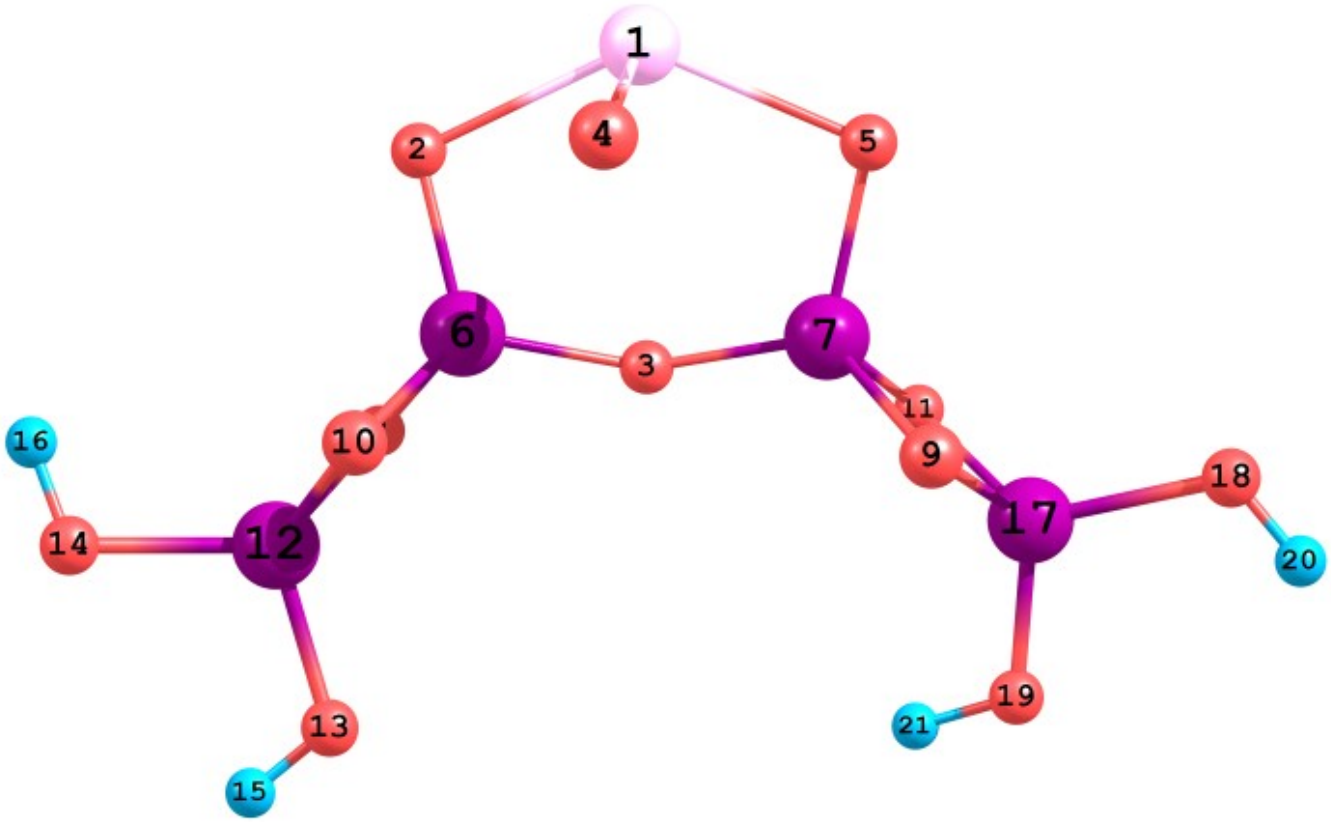

Figure 5 View of the geometry of structure 4.

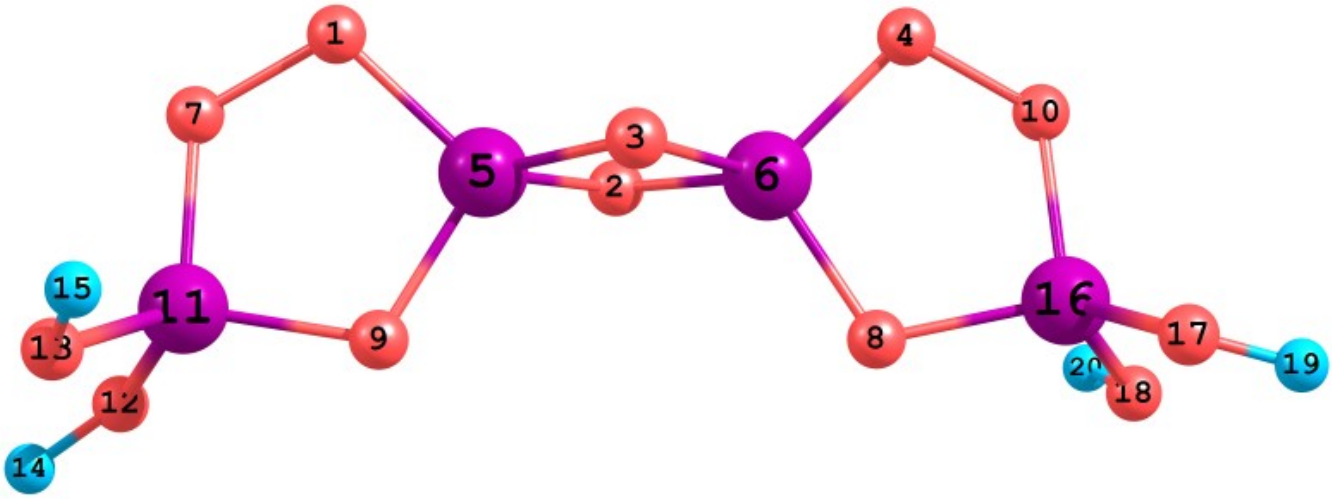

Figure 6 View of the geometry of structure 5.

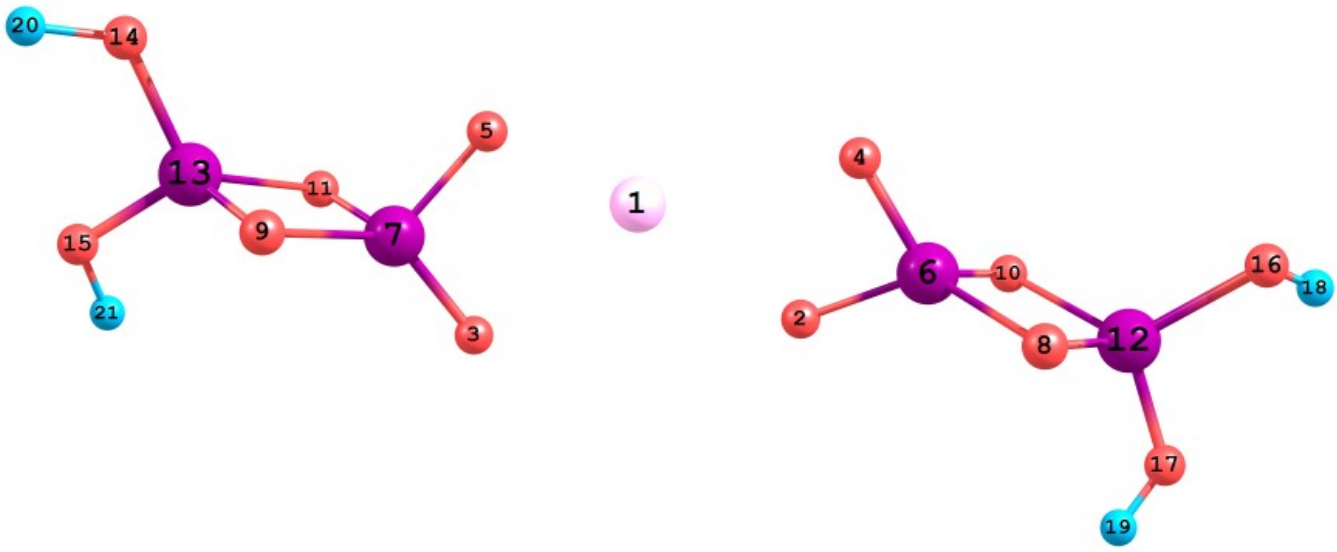

Figure 7 View of the geometry of structure 6.

Table 7 Geometry parameters for structure 6. 'R' stands for interatomic distance in angstroms and 'A' stands for angle in degrees.

R(2-6)	1.660	R(11-13)	1.720	A(2-6-10)	122.6	A(9-7-11)	89.1	A(11-13-14)	117.2
R(3-7)	1.616	R(12-16)	1.648	A(3-7-5)	102.7	A(7-9-13)	91.2	A(11-13-15)	114.7
R(4-6)	1.655	R(12-17)	1.647	A(3-7-9)	123.2	A(7-11-13)	91.1	A(16-12-17)	106.3
R(5-7)	1.757	R(13-14)	1.653	A(3-7-11)	125.7	A(8-12-10)	88.0	A(12-16-18)	114.6
R(6-8)	1.691	R(13-15)	1.652	A(4-6-8)	122.1	A(8-12-16)	118.5	A(12-17-19)	115.3
R(6-10)	1.691	R(14-20)	0.968	A(4-6-10)	122.2	A(8-12-17)	112.6	A(14-13-15)	104.0
R(7-9)	1.709	R(15-21)	0.968	A(5-7-9)	107.8	A(9-13-11)	88.5	A(13-14-20)	114.3
R(7-11)	1.704	R(16-18)	0.968	A(5-7-11)	106.9	A(9-13-14)	114.6	A(13-15-21)	114.3
R(8-12)	1.724	R(17-19)	0.967	A(8-6-10)	90.2	A(9-13-15)	118.2		
R(9-13)	1.713	A(2-6-4)	82.8	A(6-8-12)	91.0	A(10-12-16)	112.5		
R(10-12)	1.728	A(2-6-8)	120.9	A(6-10-12)	90.8	A(10-12-17)	118.8		