SUPPORTING INFORMATION

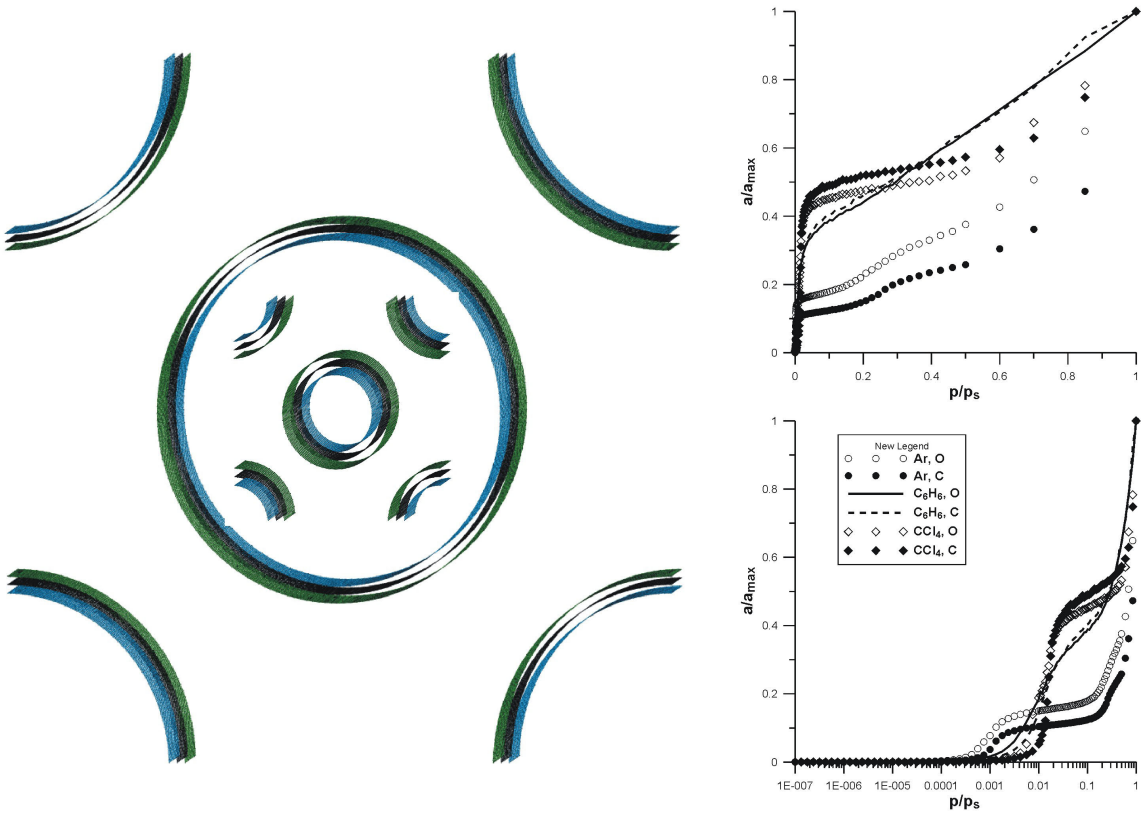

Fig. S1. Simulation box for the reference system (l_{box} = 26.0 nm) using for α_s construction (in order to compare the dimensions of the studied systems with the reference one in the internal tube of the reference system the largest studied bundle (i.e., l_{box} = 8.0 nm) is shown). Additionally, adsorption isotherms of Ar, C_6H_6, and CCl_4 on the reference bundles of closed and opened multiwalled carbon nanotubes are presented.

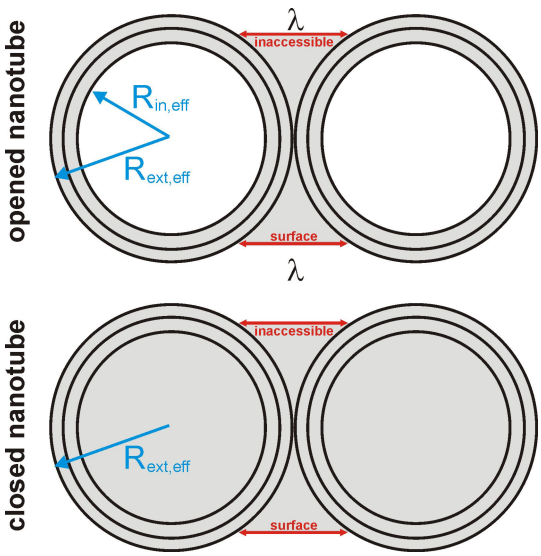

Fig. S2. The procedure of calculation of the absolute geometric surface area.

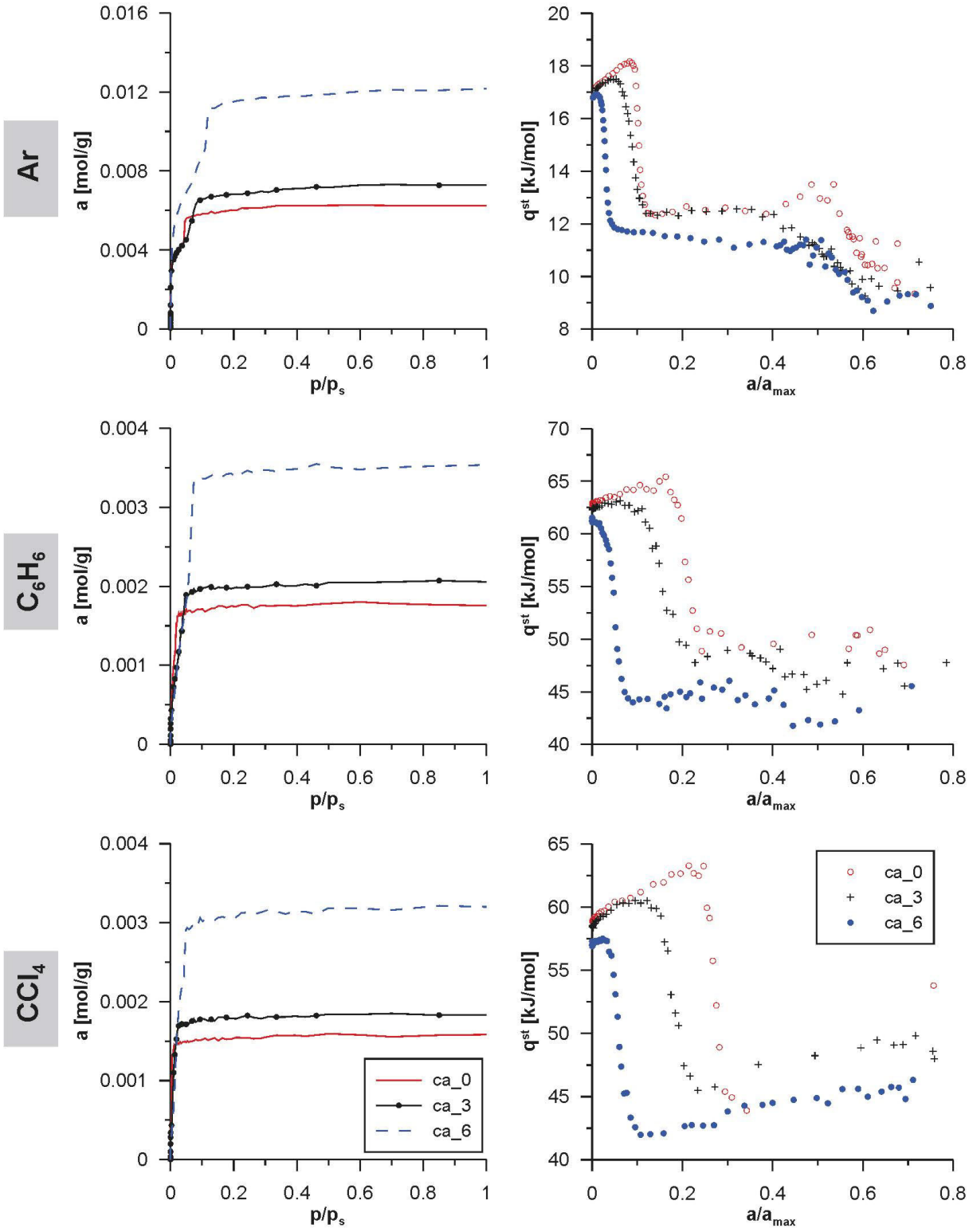

Fig. S3. Simulated isotherms and isosteric adsorption enthalpy plots for C_62 structures. Ar was simulated for the T = 87 K, C_6H_6 and CCl_4 for 298 K.

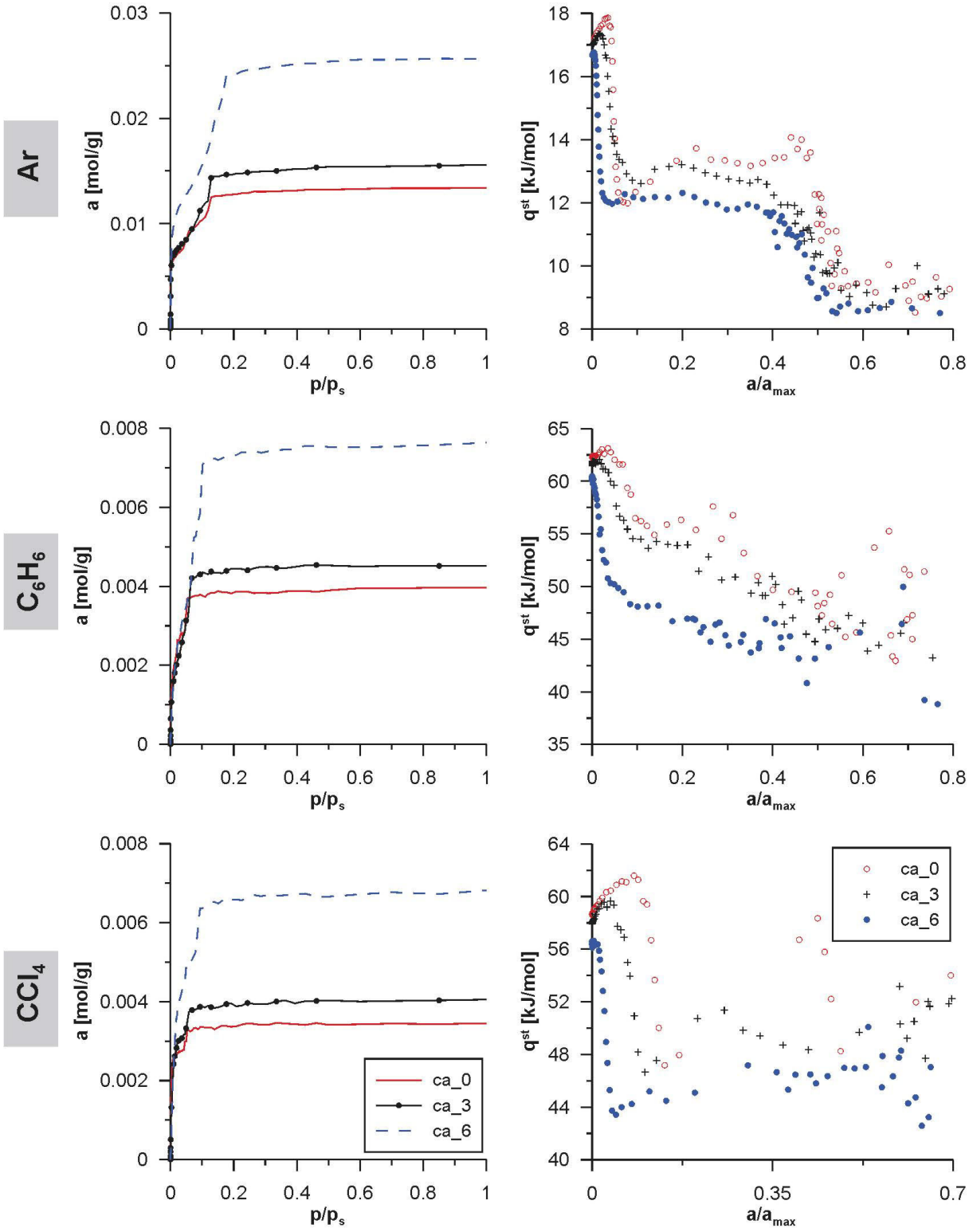

Fig. S4. Simulated isotherms and isosteric adsorption enthalpy plots for O_62 structures.

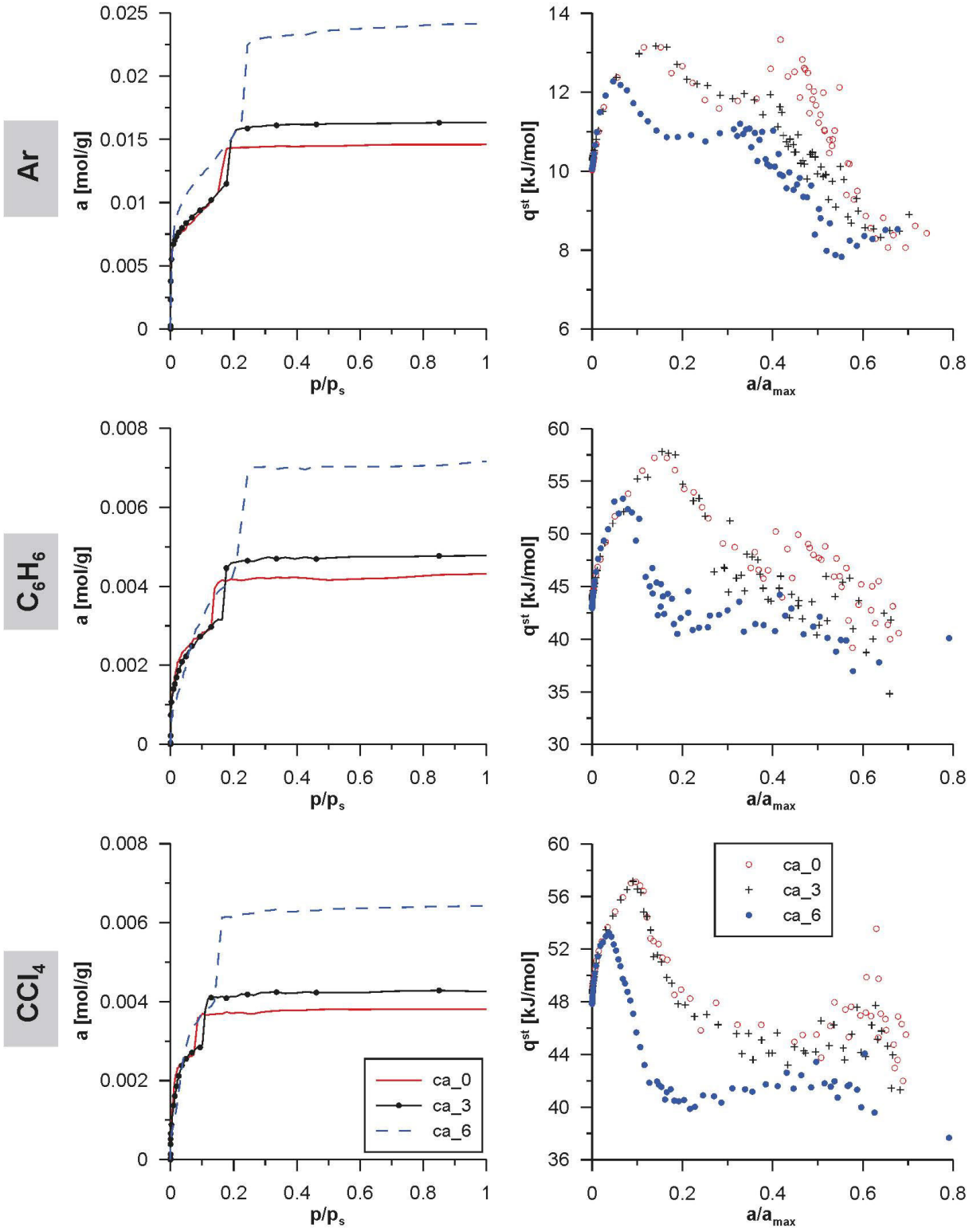

Fig. S5. Simulated isotherms and isosteric adsorption enthalpy plots for C_70 structures.

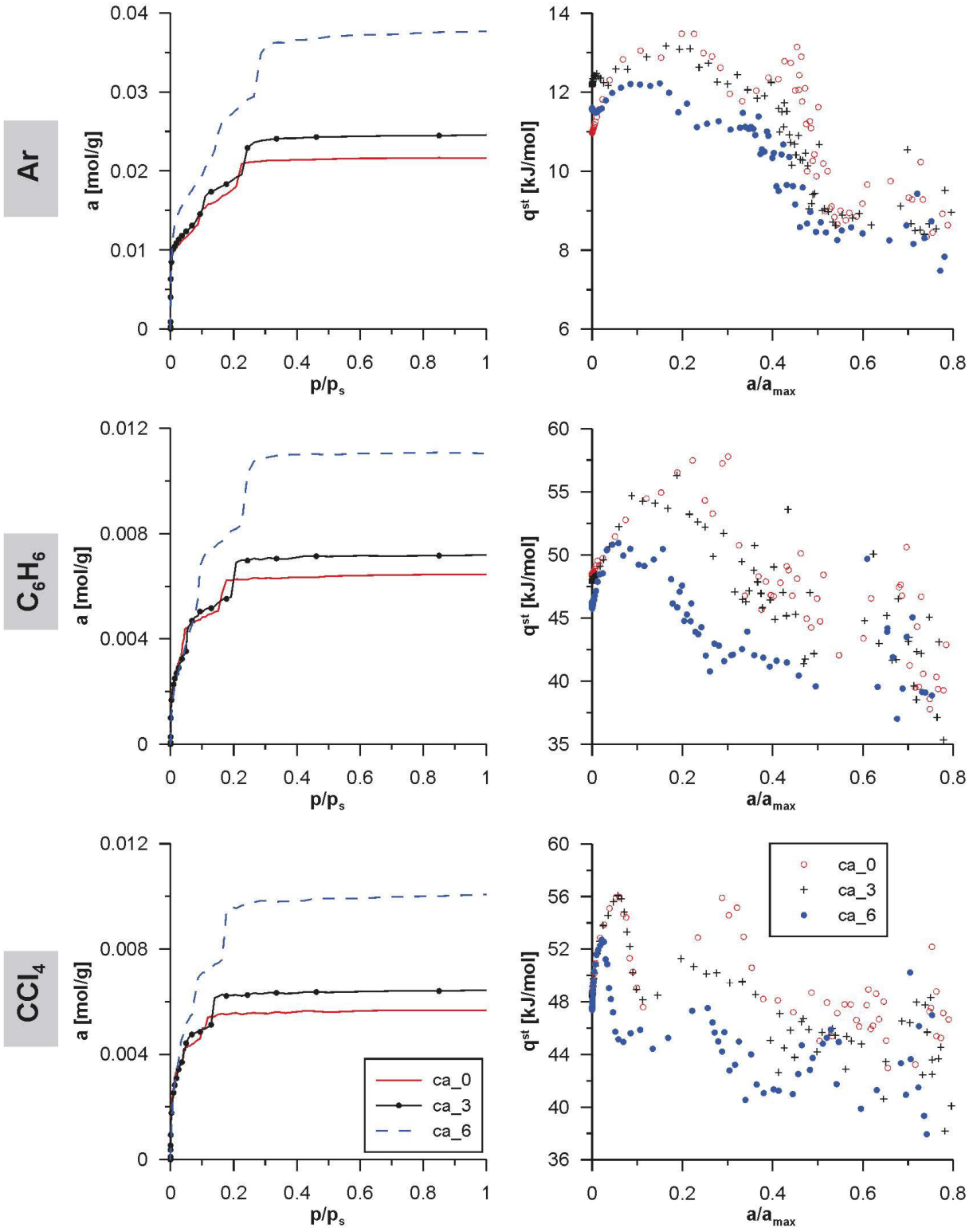

Fig. S6. Simulated isotherms and isosteric adsorption enthalpy plots for O_70 structures.

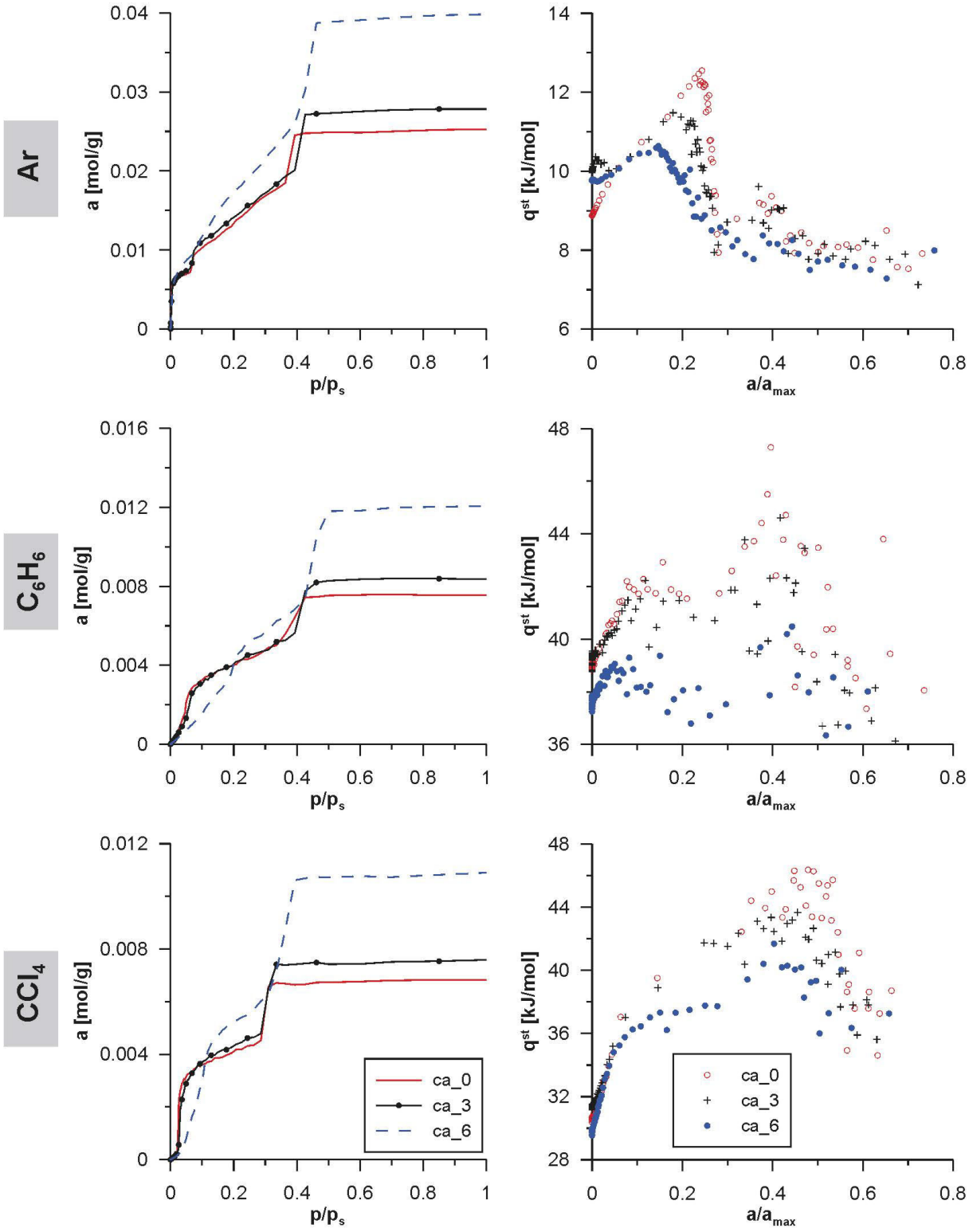

Fig. S7. Simulated isotherms and isosteric adsorption enthalpy plots for C_80 structures.

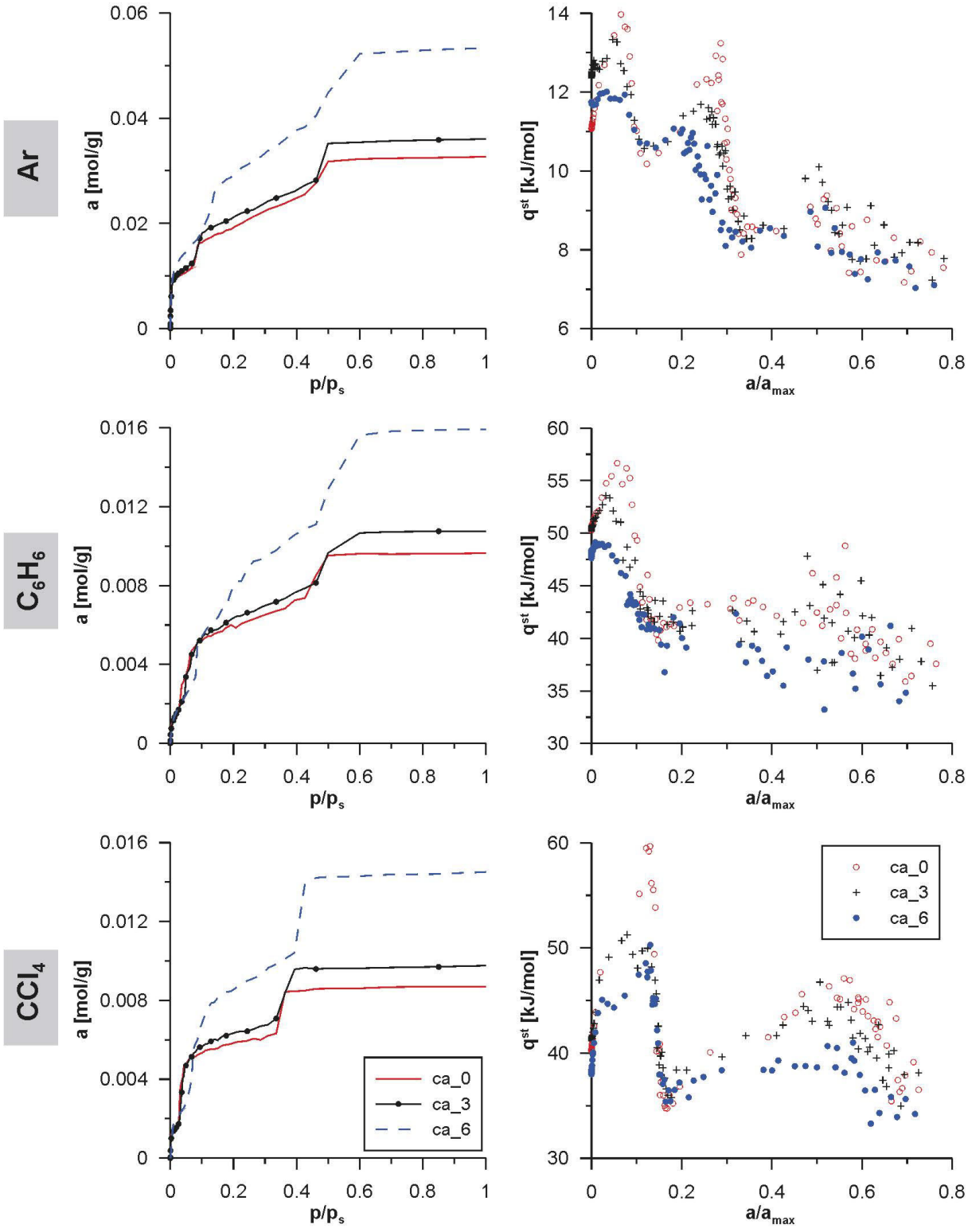

Fig. S8. Simulated isotherms and isosteric adsorption enthalpy plots for O_80 structures.

Table S1. The values of the parameters applied in simulations.

Molecule	*Centre*	σ [nm]	ε/k_B [K]	*Reference*
Ar	***Ar***	0.3405	119.8	36
CCl_4	***C***	0.46	39.0	37
	Cl	0.35	105.0	
Benzene	***ua***[*)]	0.3246	89.4	38
Carbon structures	***C***	0.34	28.0	40, 41 and the references therein

*) – united atom

Tables S2. The values of the α_s for swings on simulated isotherms for the structure 62.

C_62_ca_0

	Ar	C_6H_6	CCl_4
a	0.00278	0.00734	0.00522
b	0.0539	0.179	0.572
c	0.501	0.492	

C_62_ca_3

	Ar	C_6H_6	CCl_4
a	0.00278	0.0101	0.00169
b	0.0539	0.253	0.143
c	0.522	0.616	0.748

C_62_ca_6

	Ar	C_6H_6	CCl_4
a	0.00206	0.0242	0.00169
b	0.0539	0.379	0.143
c	0.540	0.683	0.836

O_62_ca_0

	Ar	C_6H_6	CCl_4
a	0.00293	0.00272	0.00256
b	0.118	0.0396	0.0162
c	0.505	0.494	0.0527
d	0.570	0.609	0.857

O_62_ca_3

	Ar	C_6H_6	CCl_4
a	0.00293	0.0396	0.00256
b	0.0661	0.632	0.0229
c	0.536		0.466
d	0.570		0.857

O_62_ca_6

	Ar	C_6H_6	CCl_4
a	0.00398	0.0113	0.00624
b	0.235	0.678	0.0330
c	0.640		0.559
d			0.897

Tables S3. The values of the α_s for swings on simulated isotherms for the structure 70.

C_70_ca_0

	Ar	C_6H_6	CCl_4
a	0.0357	0.0467	0.00306
b	0.603	0.757	0.0952
c			0.884

C_70_ca_3

	Ar	C_6H_6	CCl_4
a	0.0357	0.0467	0.00228
b	0.510	0.670	0.0952
c	0.650	0.802	0.897

C_70_ca_6

	Ar	C_6H_6	CCl_4
a	0.0357	0.0467	0.0139
b	0.493	0.683	0.927
c	0.727	0.868	

O_70_ca_0

	Ar	C_6H_6	CCl_4
a	0.0661	0.0537	0.00189
b	0.551	0.587	0.0330
c	0.737	0.750	0.521
d			0.901

O_70_ca_3

	Ar	C_6H_6	CCl_4
a	0.118	0.0537	0.00256
b	0.562	0.632	0.0527
c	0.770	0.750	0.521
d			0.857
e			0.921

O_70_ca_6

	Ar	C_6H_6	CCl_4
a	0.118	0.0775	0.00344
b	0.617	0.680	0.0527
c	0.855	0.848	0.441
d			0.820
e			0.901
f			0.954

Tables S4. The values of the α_s for swings on simulated isotherms for the structure 80.

C_80_ca_0

	Ar	C_6H_6	CCl_4
a	0.390	0.179	0.114
b	0.603	0.720	0.748
c	1.00	1.05	0.982

C_80_ca_3

	Ar	C_6H_6	CCl_4
a	0.0539	0.757	0.220
b	0.434	1.05	0.836
c	1.03		0.982

C_80_ca_6

	Ar	C_6H_6	CCl_4
a	0.0539	0.746	0.897
b	0.584	0.851	1.01
c	1.07	1.13	

O_80_ca_0

	Ar	C_6H_6	CCl_4
a	0.0277	0.0396	0.0162
b	0.424	0.574	0.844
c	0.551	0.708	0.995
d	1.14	1.12	

O_80_ca_3

	Ar	C_6H_6	CCl_4
a	0.0417	0.0396	0.0330
b	0.460	0.597	0.869
c	0.551	0.714	1.00
d	0.737	1.12	
e	1.14		

O_80_ca_6

	Ar	C_6H_6	CCl_4
a	0.0661	0.0537	0.104
b	0.617	0.678	0.441
c	0.737	0.818	0.921
d	1.00	1.25	1.03
e	1.14		

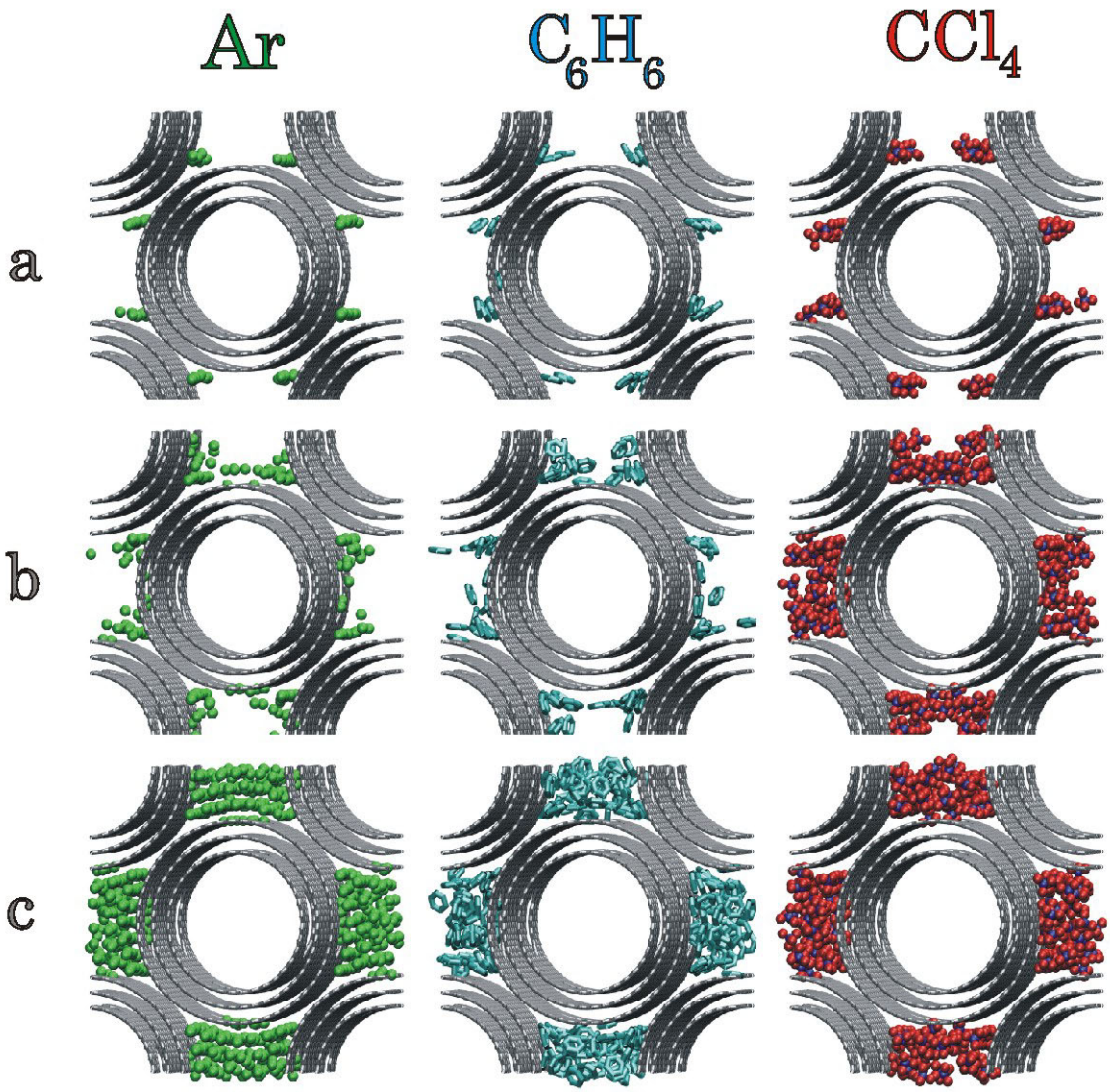

Fig. S9. Snapshots for C_62_ca_3 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S2).

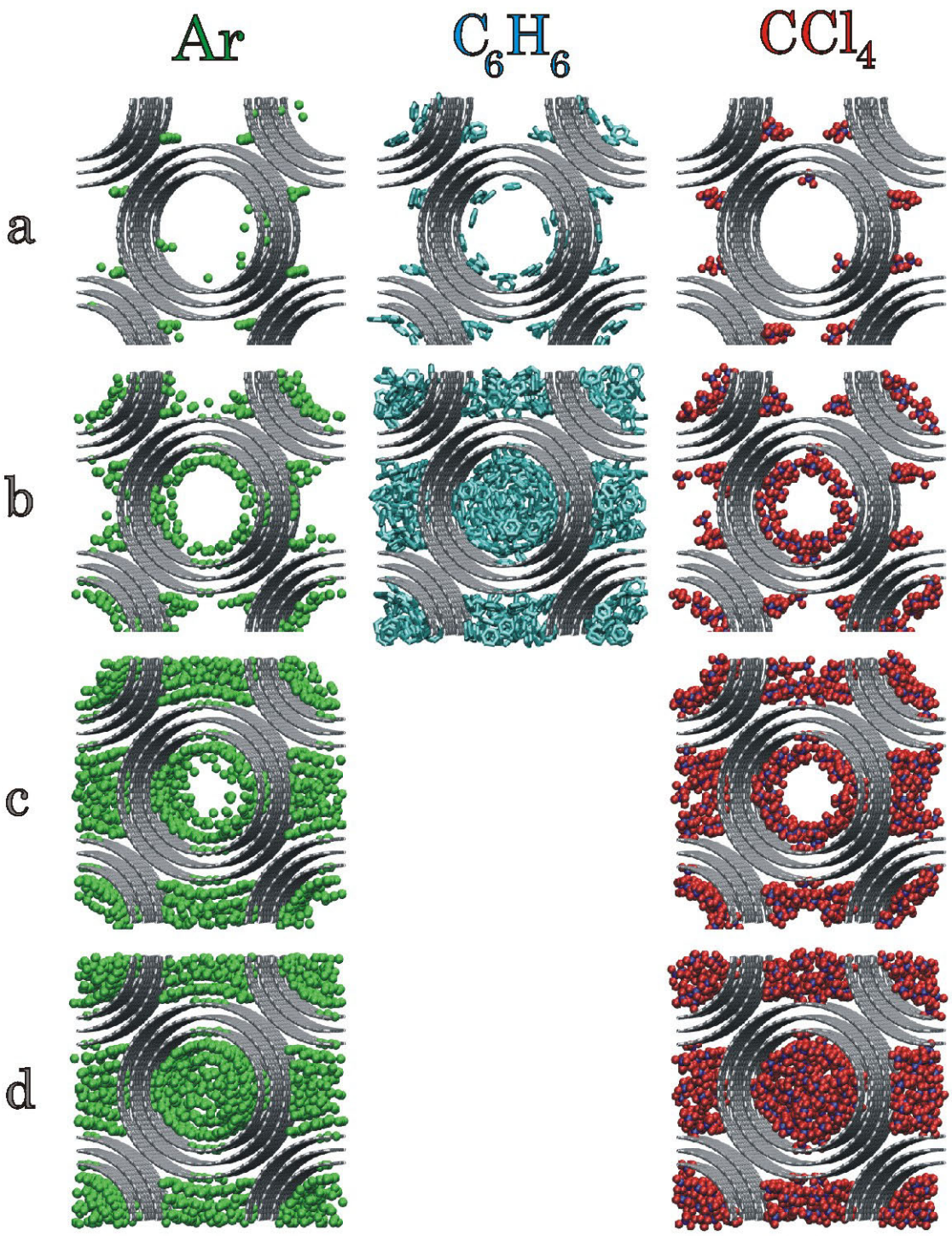

Fig. S10. Snapshots for O_62_ca_3 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – d swings* are tabulated in tables S2).

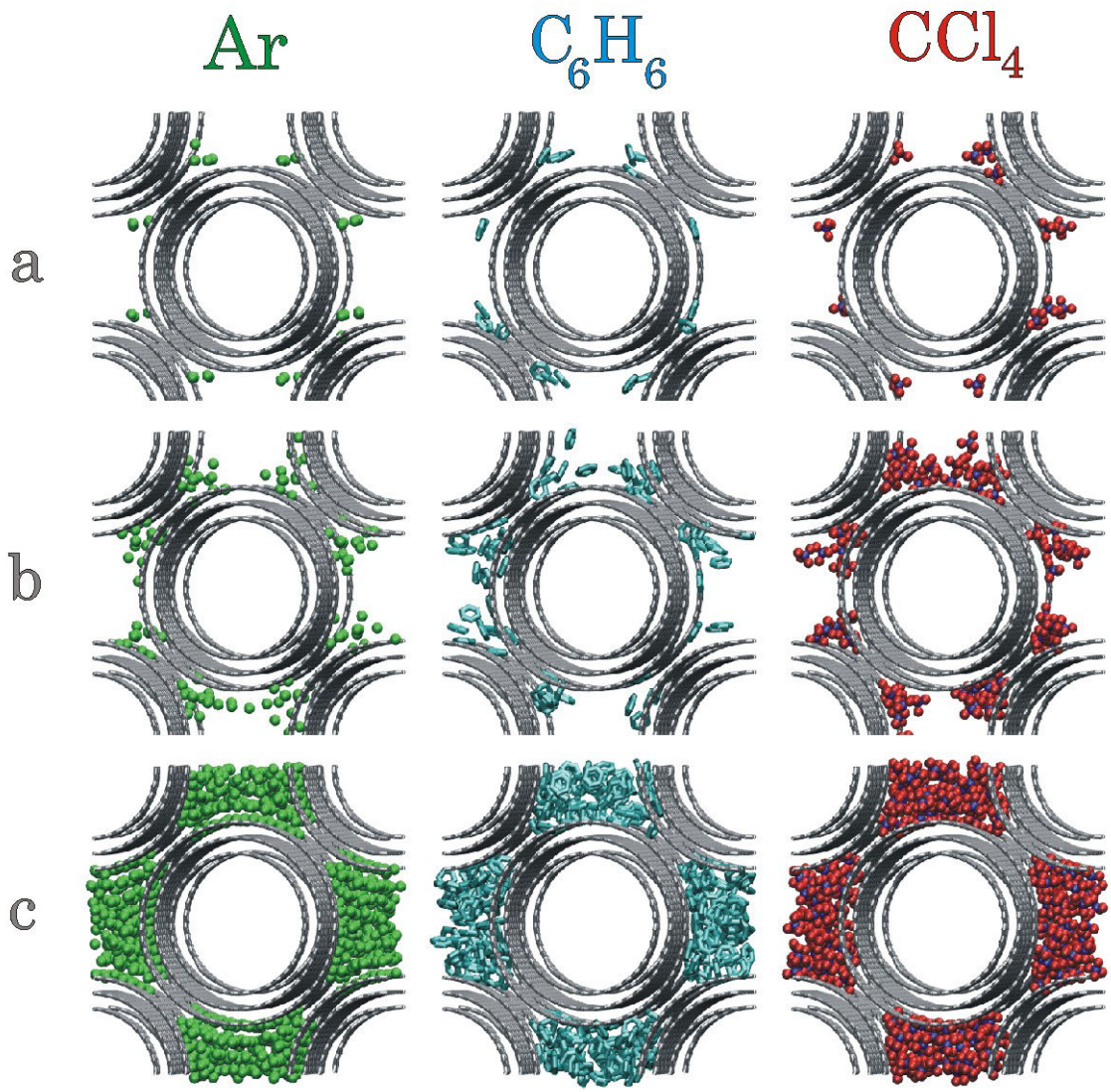

Fig. S11. Snapshots for C_62_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S2).

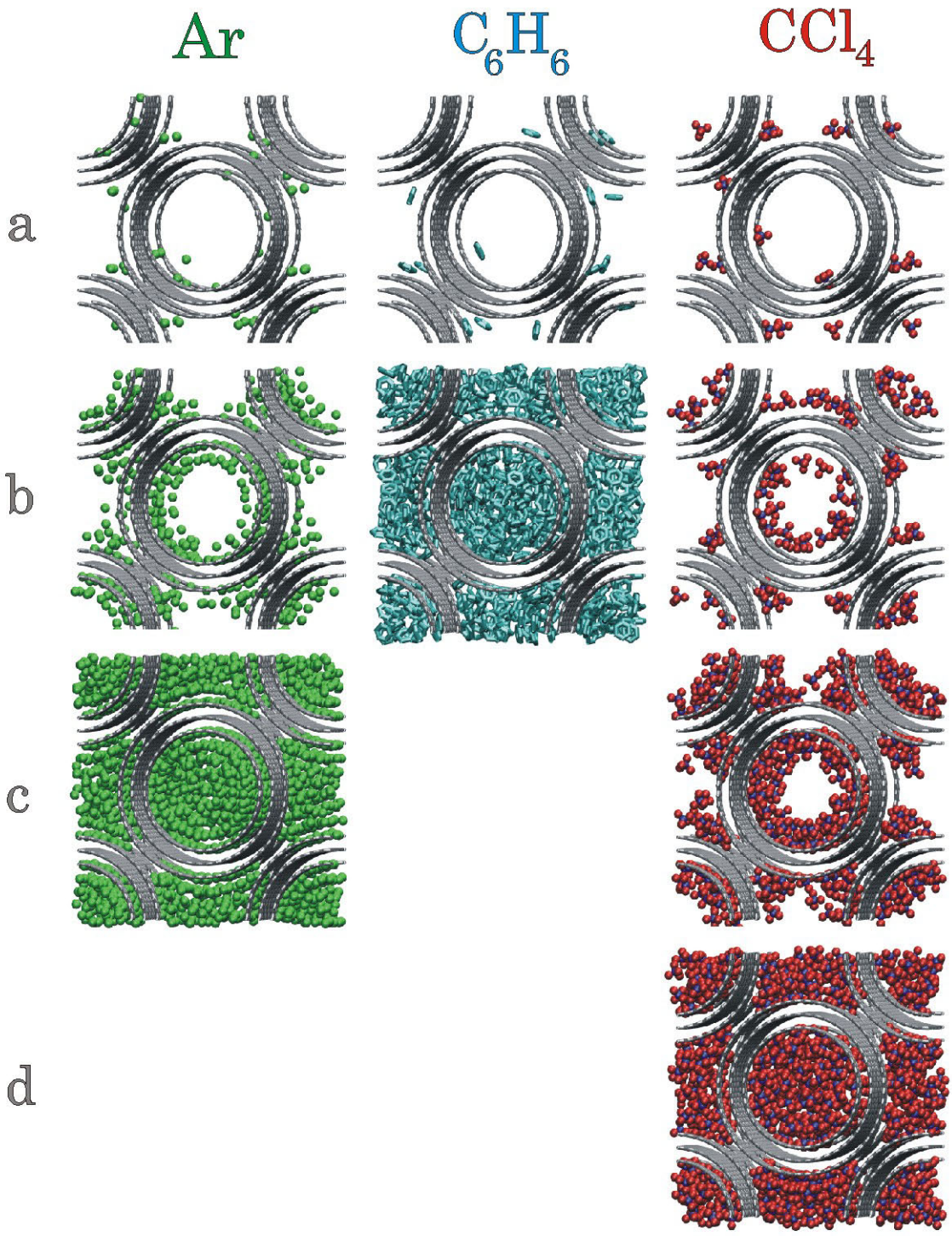

Fig. S12. Snapshots for O_62_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – d swings* are tabulated in tables S2).

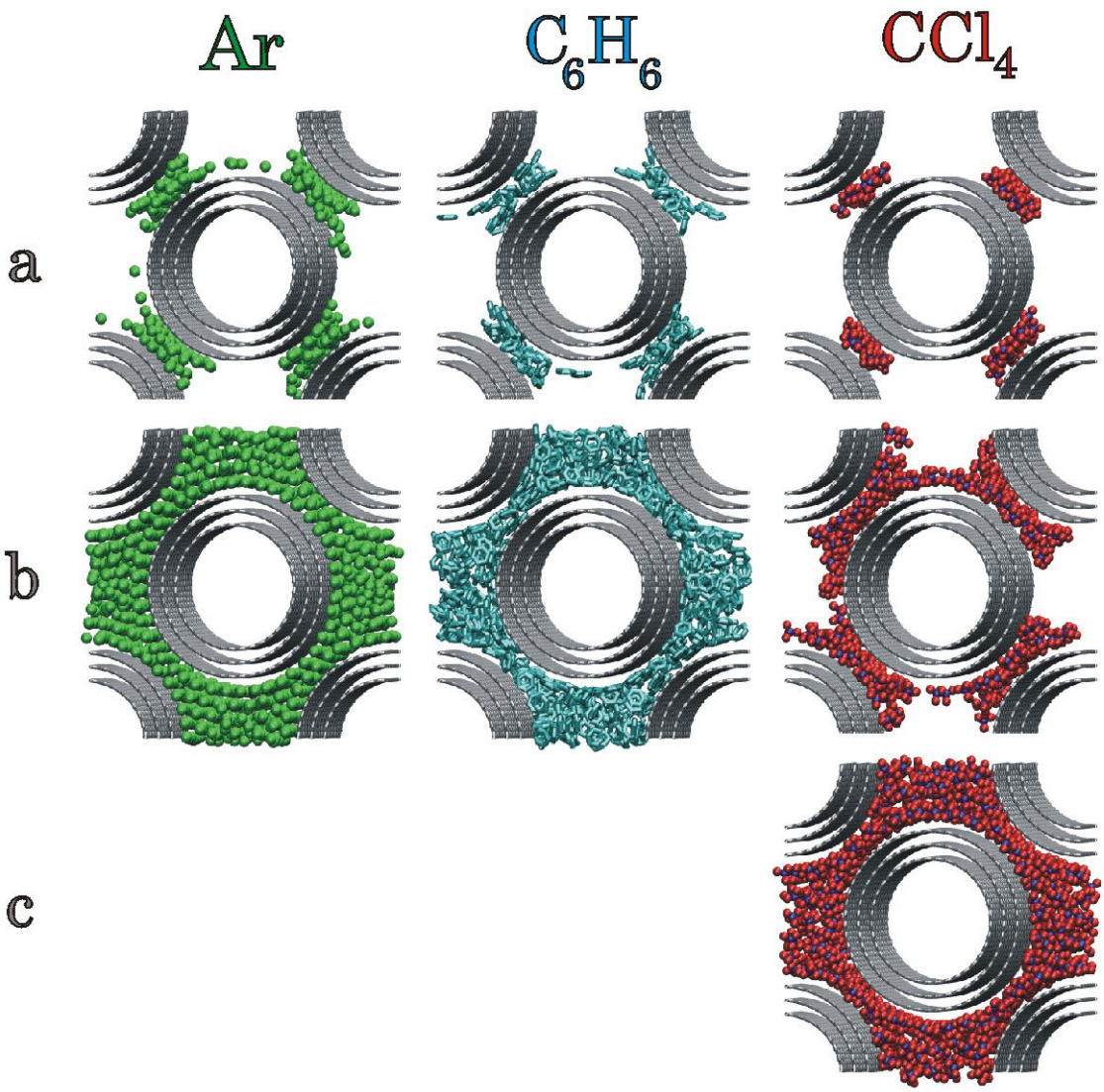

Fig. S13. Snapshots for C_70_ca_0 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S3).

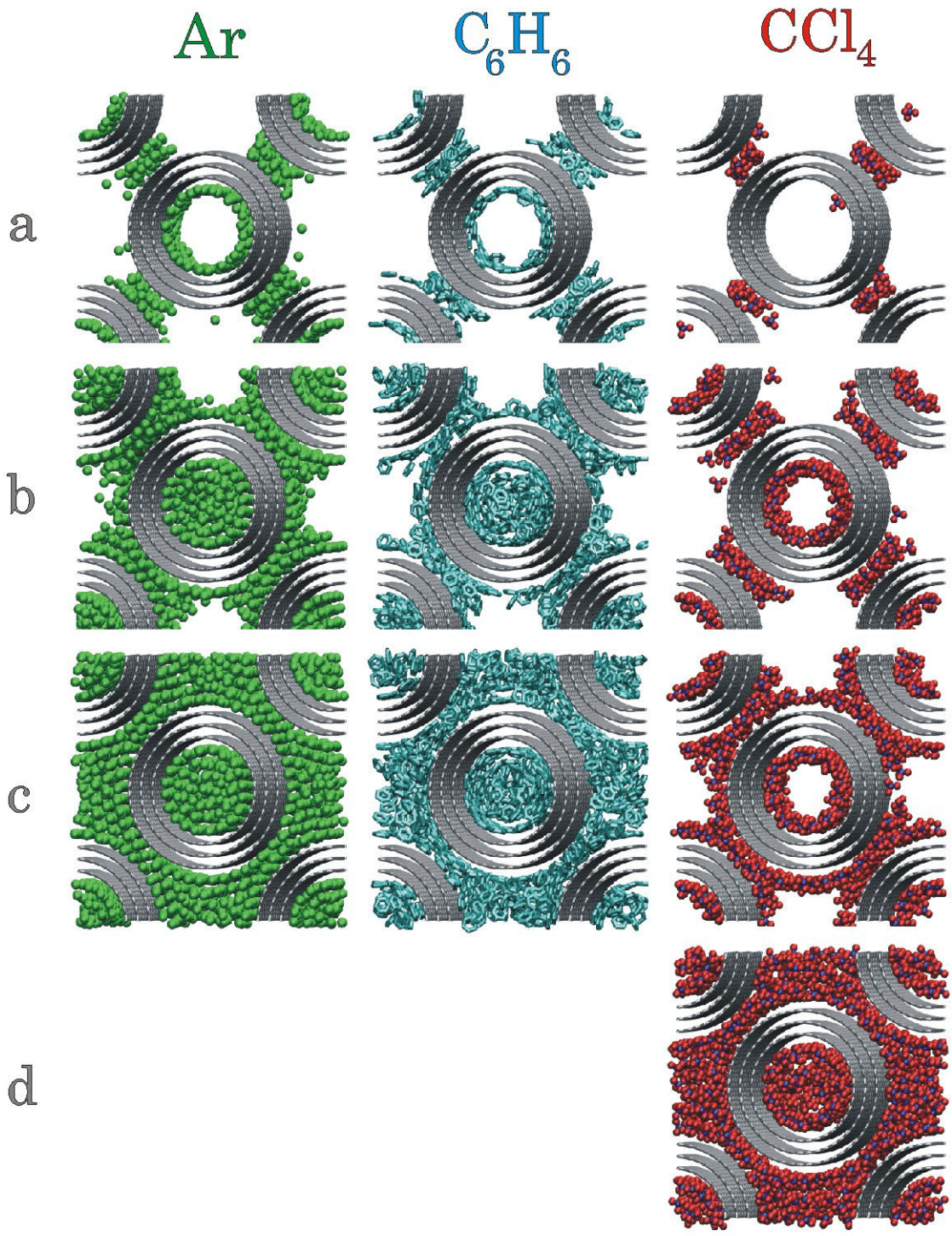

Fig. S14. Snapshots for O_70_ca_0 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – d swings* are tabulated in tables S3).

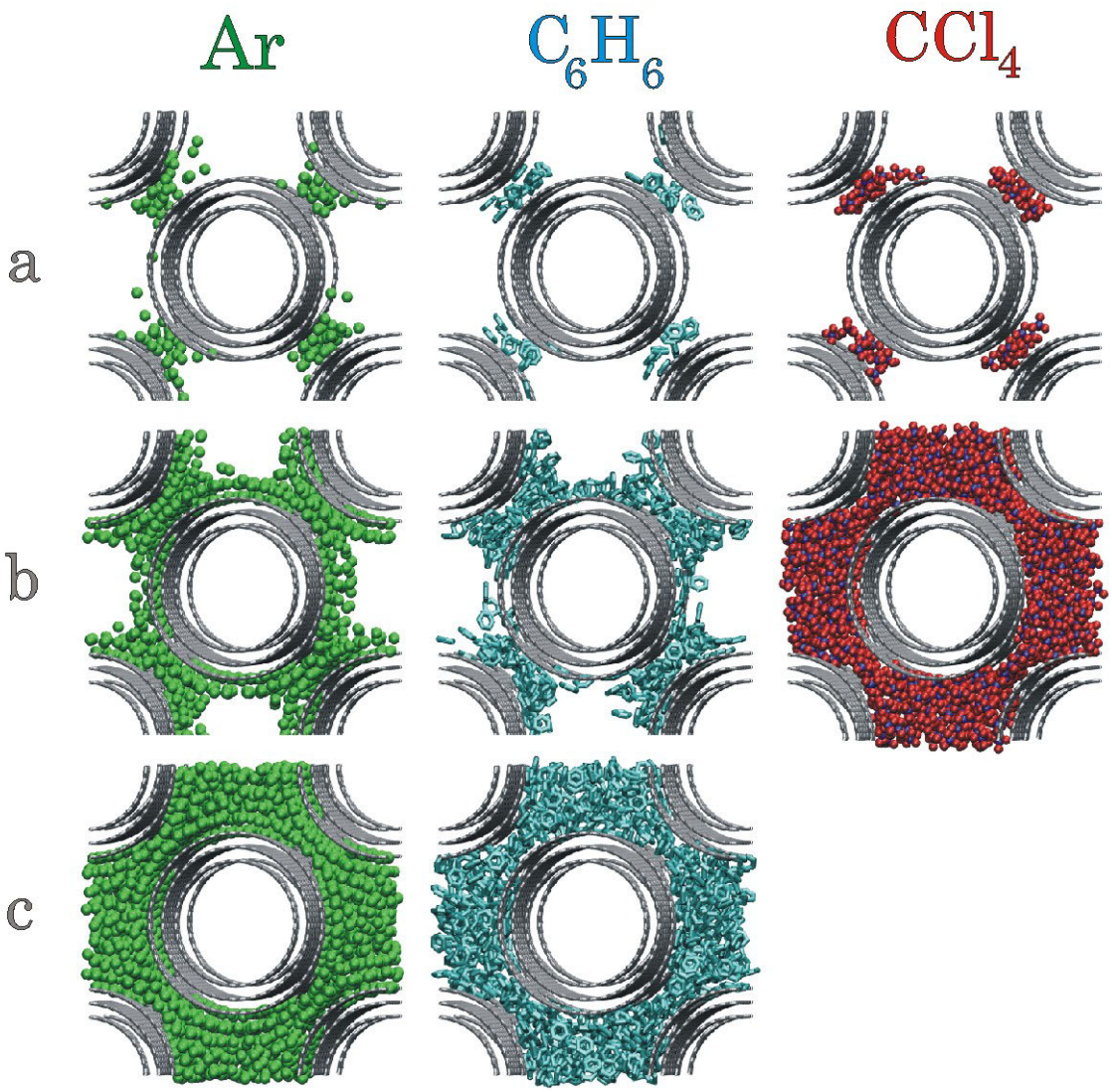

Fig. S15. Snapshots for C_70_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S3).

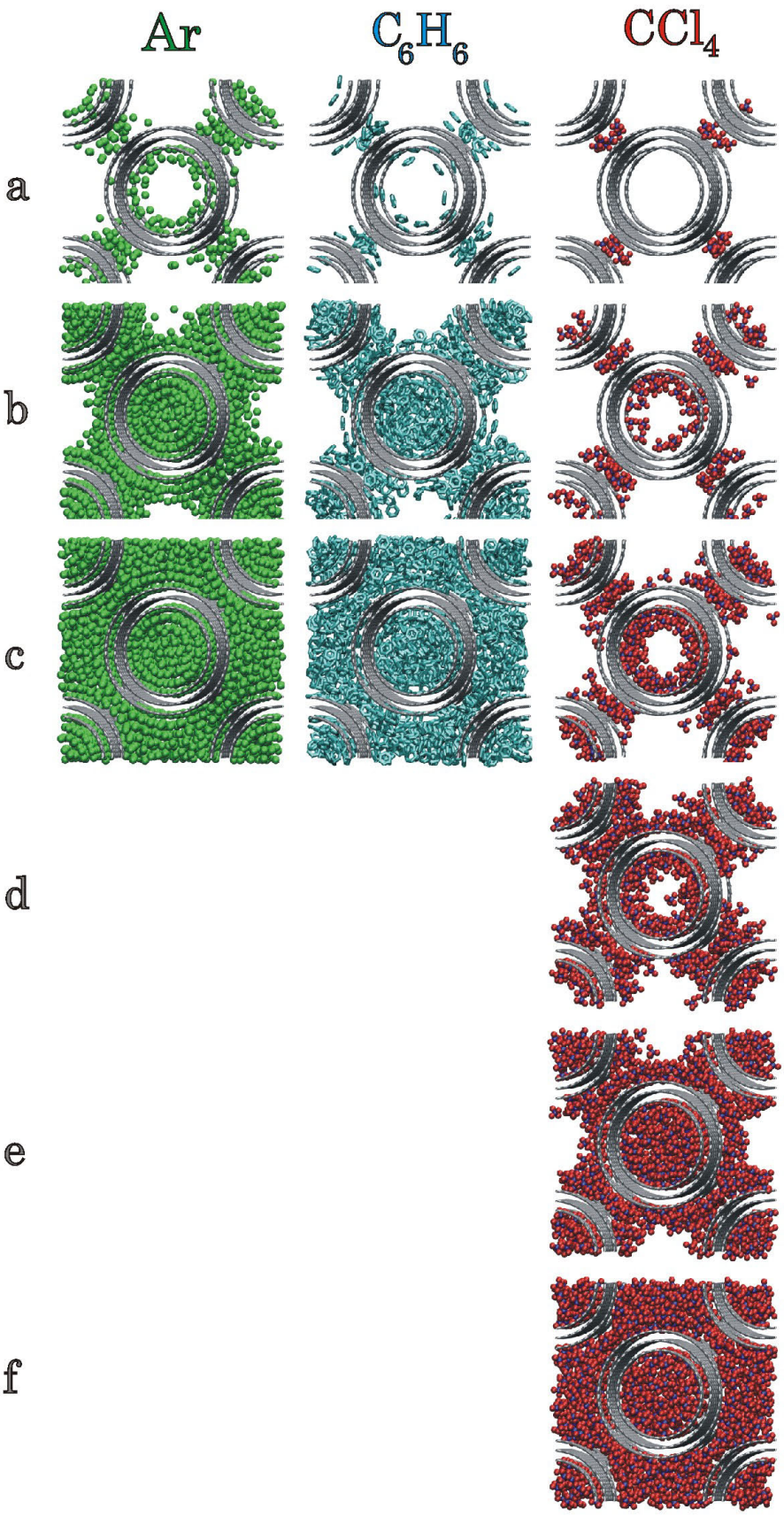

Fig. S16. Snapshots for O_70_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – f swings* are tabulated in tables S3).

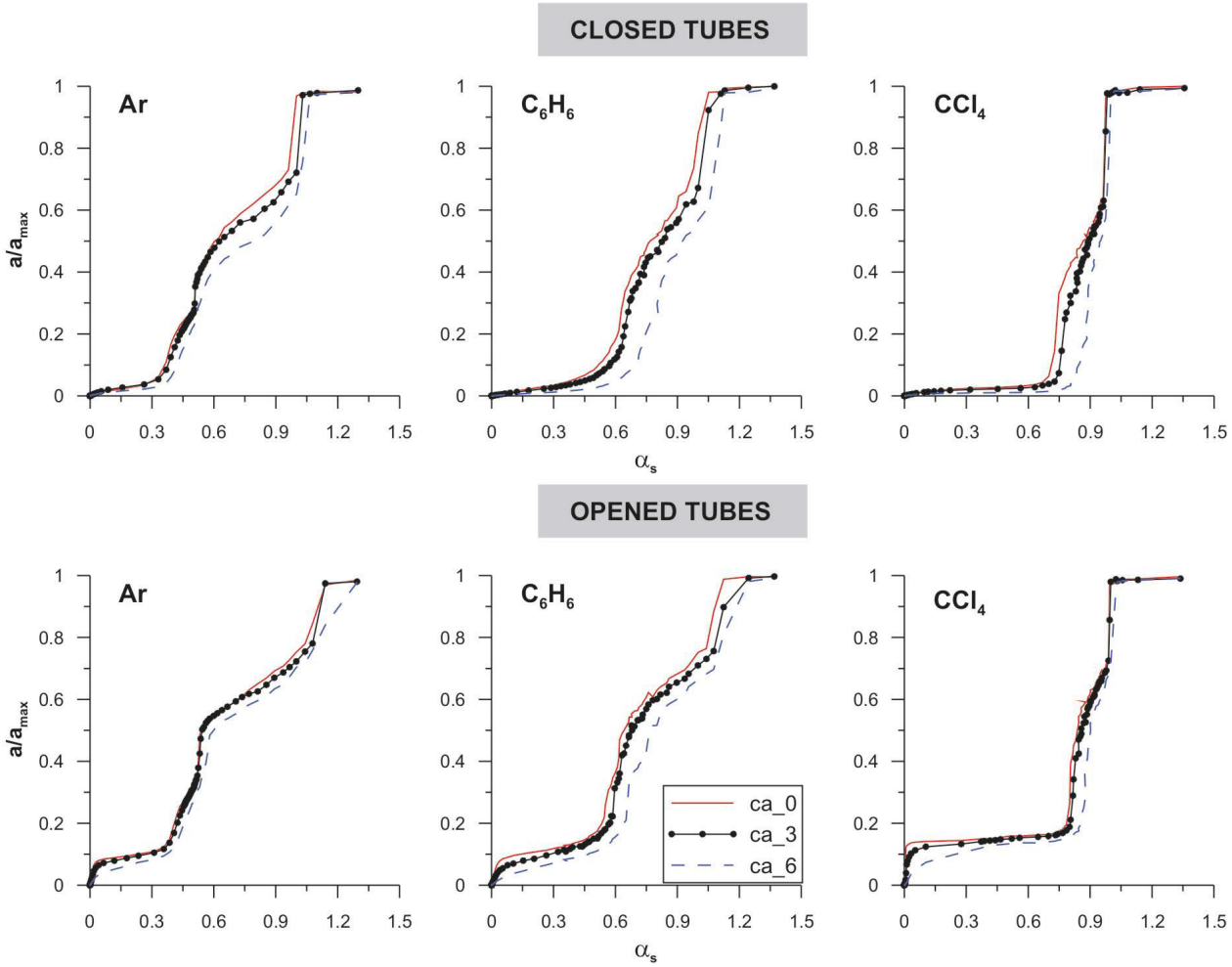

Fig. S17. High resolution α_s-plots for adsorption in the structures 80

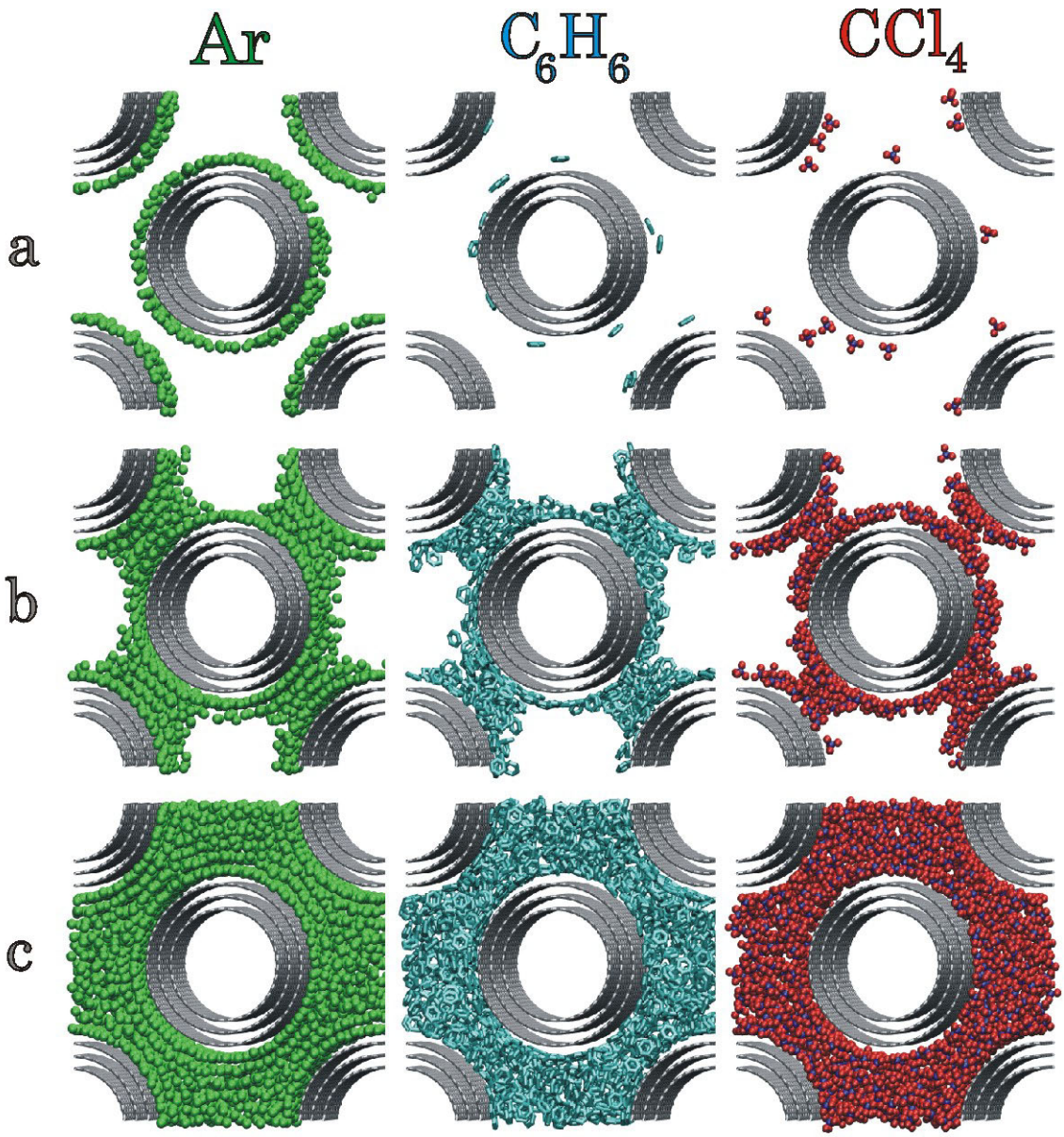

Fig. S18. Snapshots for C_80_ca_0 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S4).

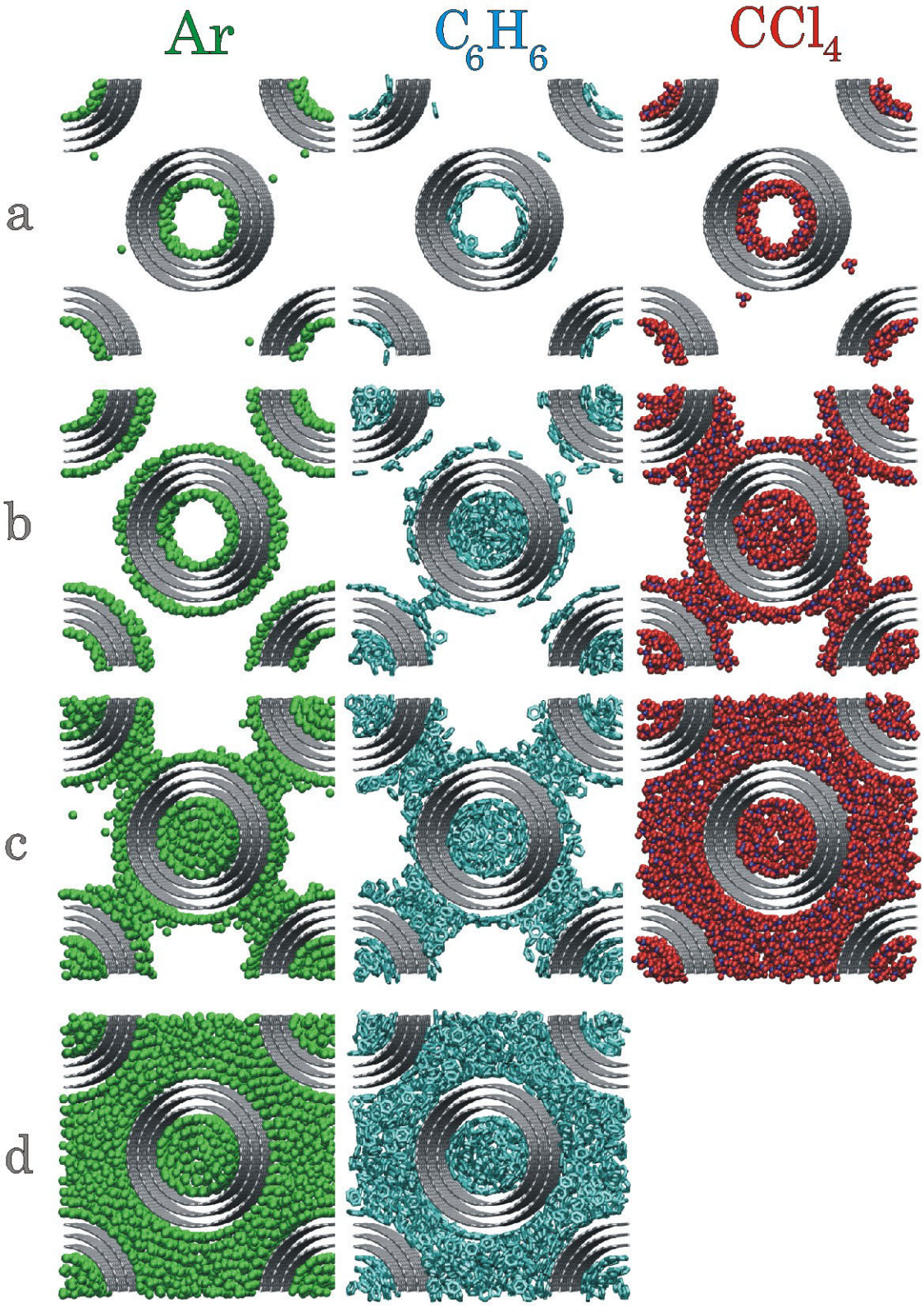

Fig. S19. Snapshots for O_80_ca_0 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – d swings* are tabulated in tables S4).

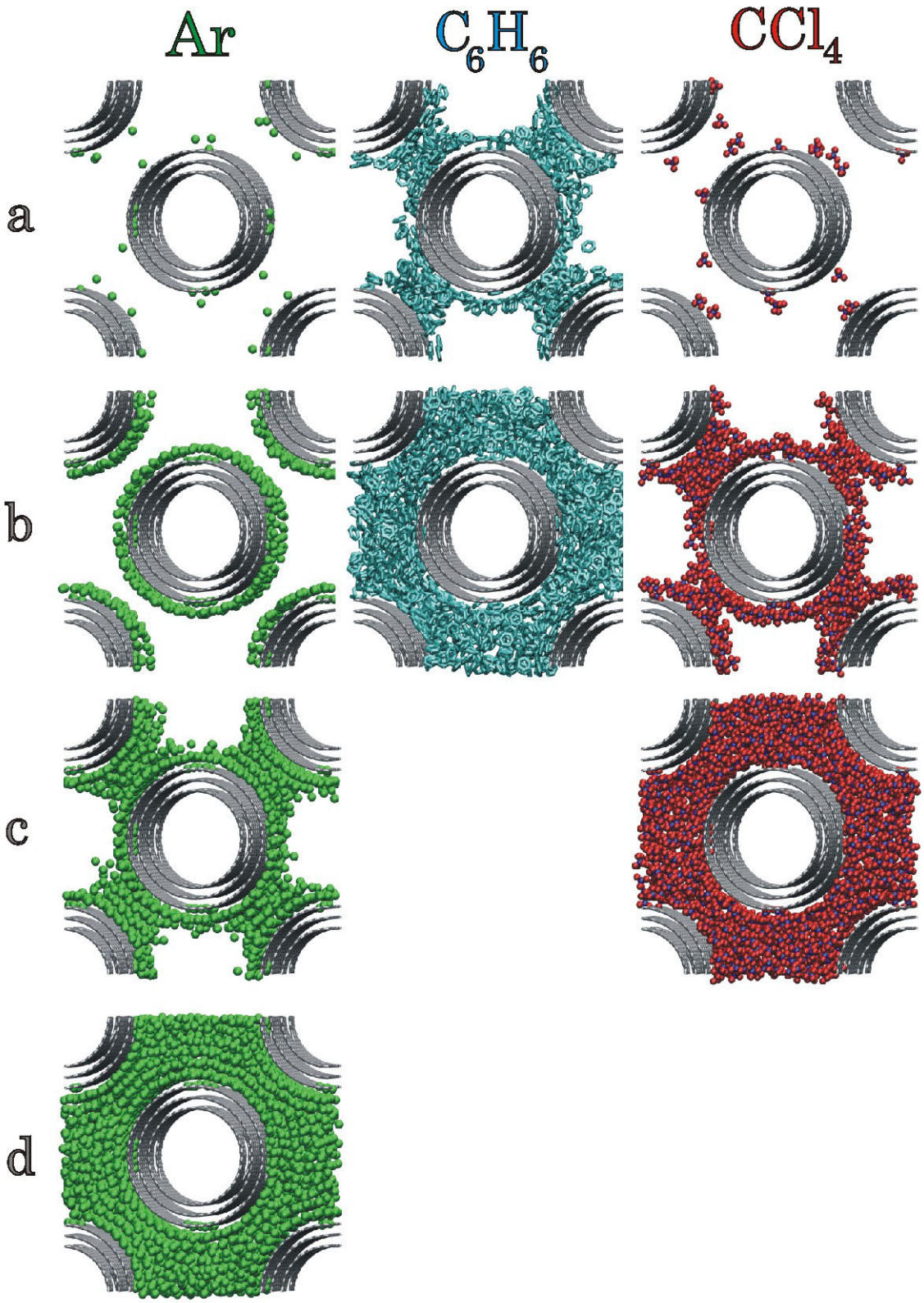

Fig. S20. Snapshots for C_80_ca_3 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – d swings* are tabulated in tables S4).

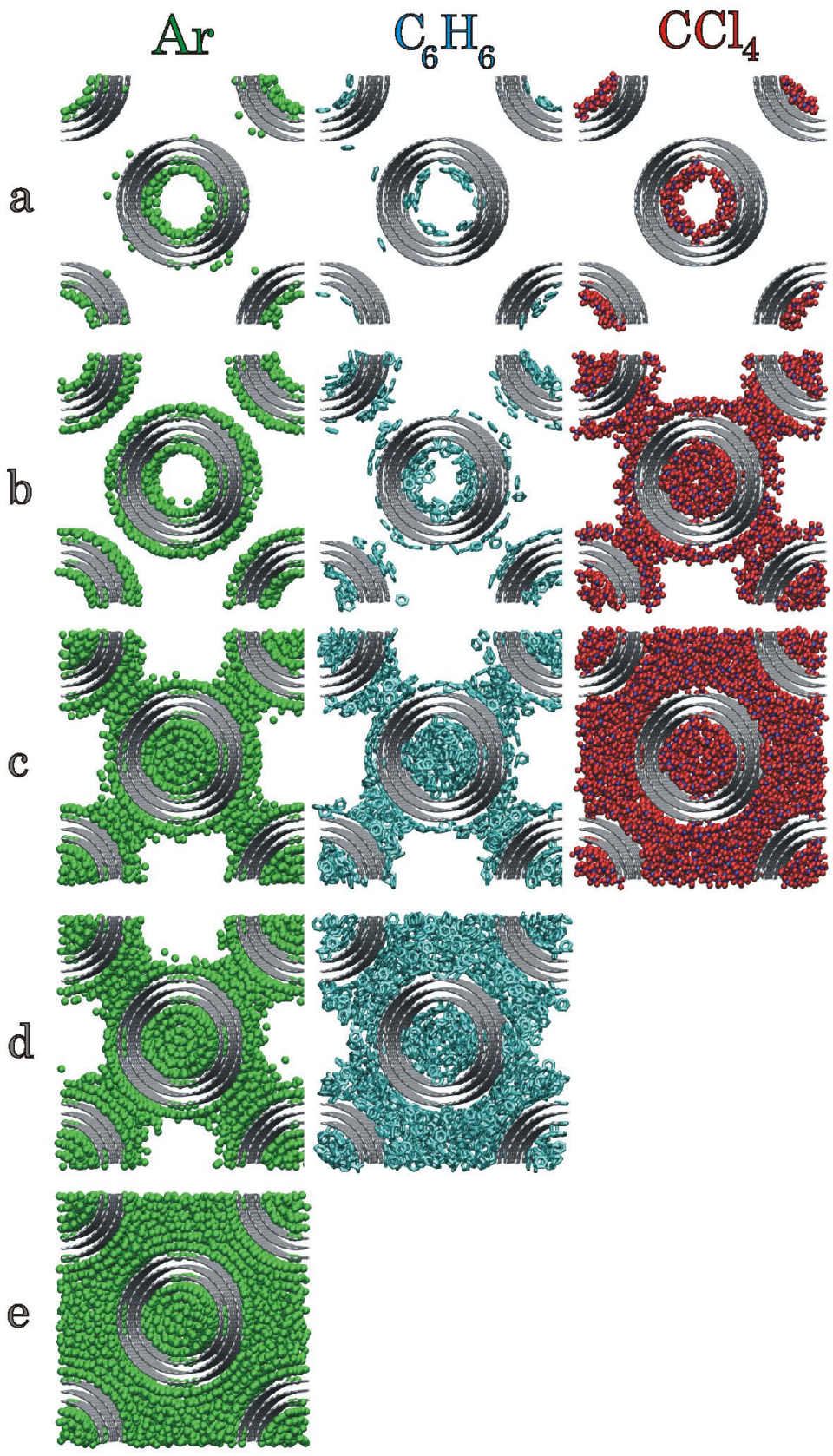

Fig. S21. Snapshots for O_80_ca_3 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – e swings* are tabulated in tables S4).

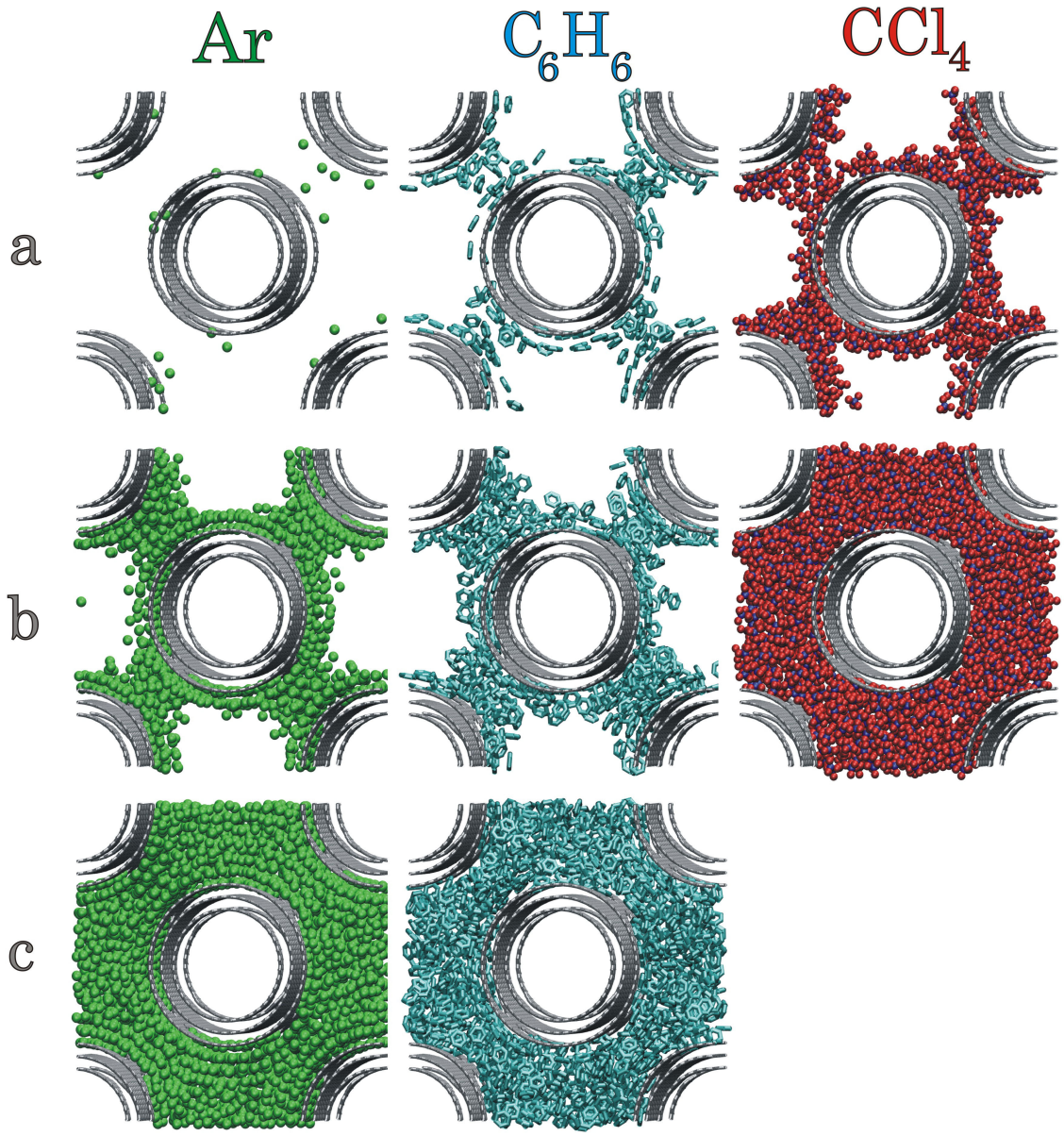

Fig. S22. Snapshots for C_80_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – c swings* are tabulated in tables S4).

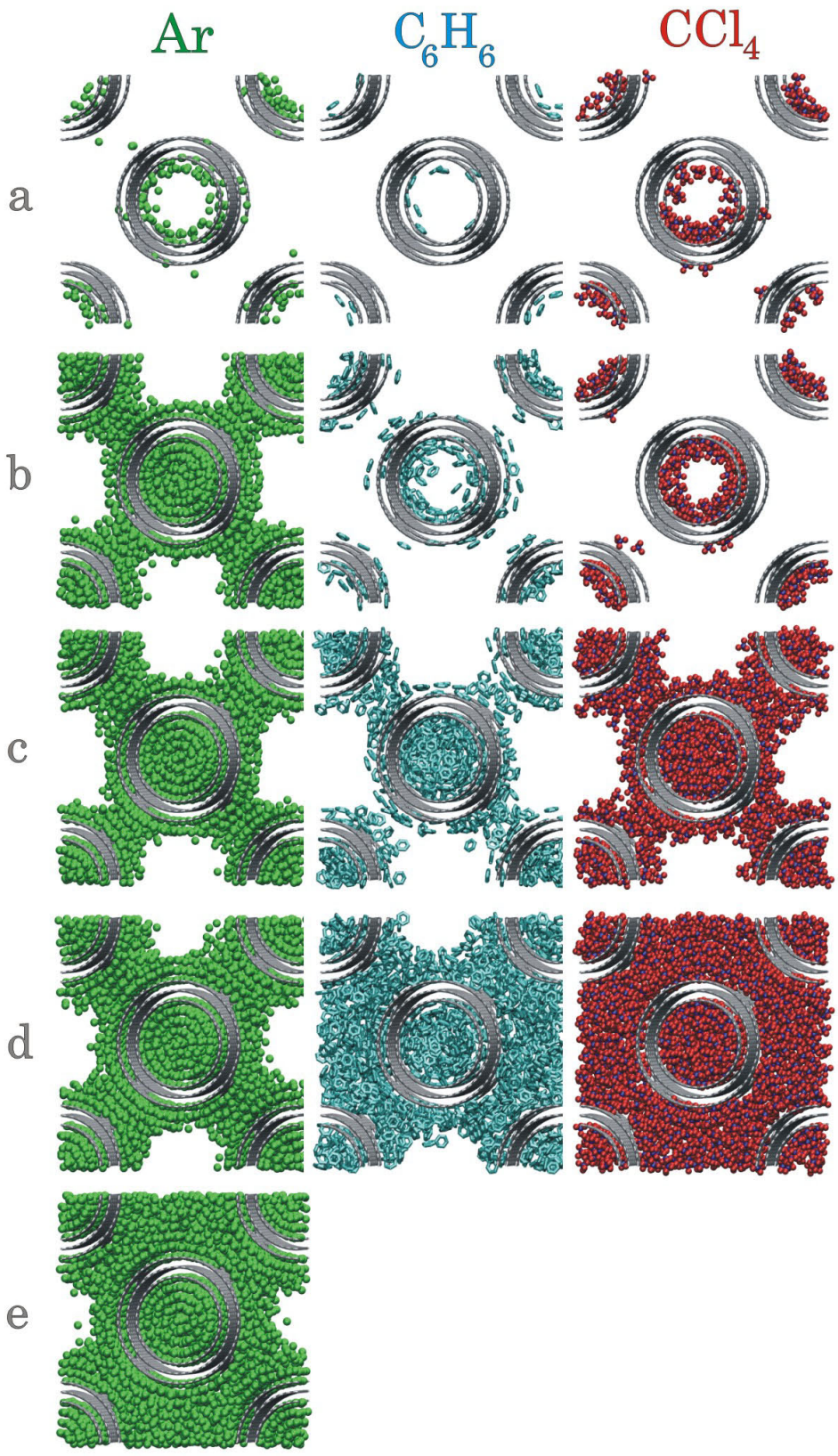

Fig. S23. Snapshots for O_80_ca_6 structure in relation to the swings appearing on the α_s-plots (the α_s values for *a – e swings* are tabulated in tables S4).

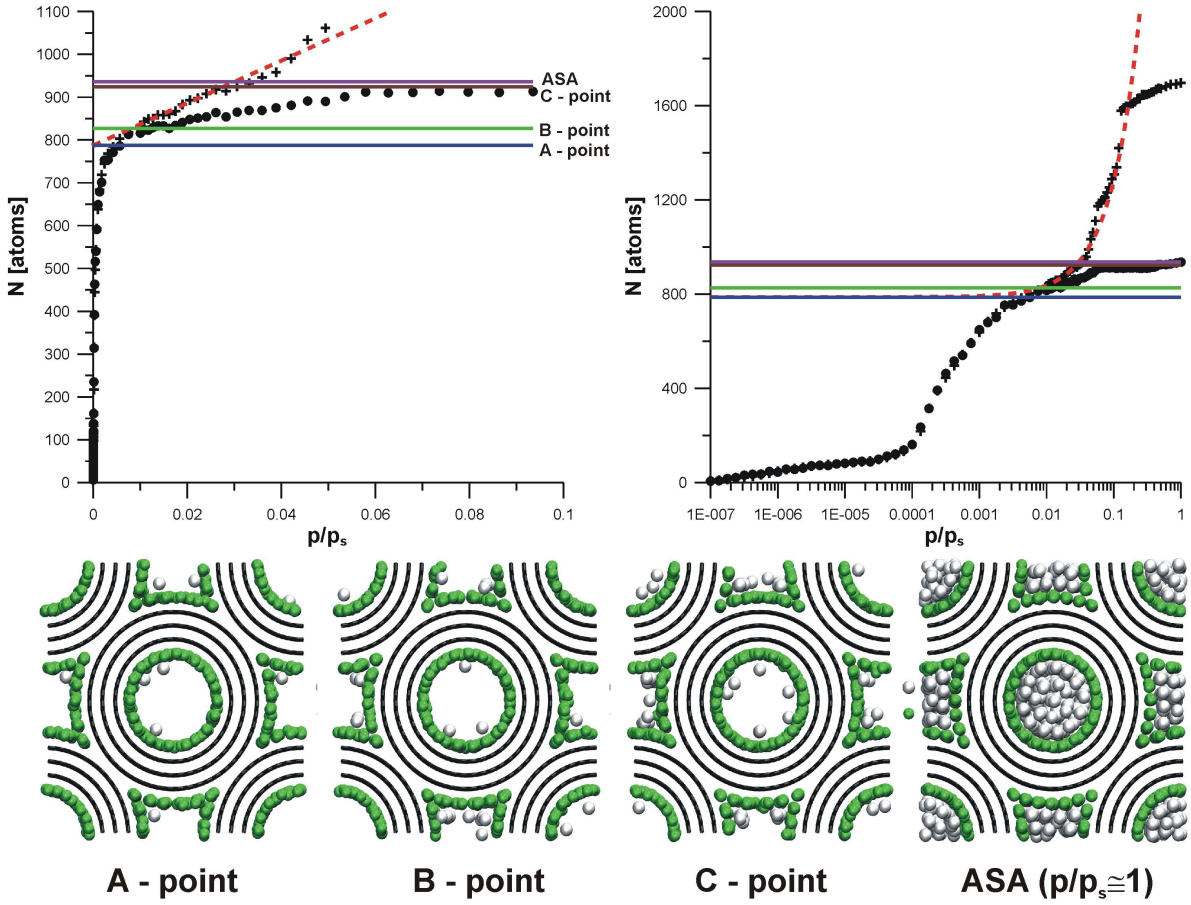

Fig. S24. Upper panel – Ar adsorption isotherm for 62_ca0 structure with marked monolayer adsorption values for A, B, and C-points and ASA method. Bottom panel – the situation in the simulation box with separated molecules adsorbed in monolayer.

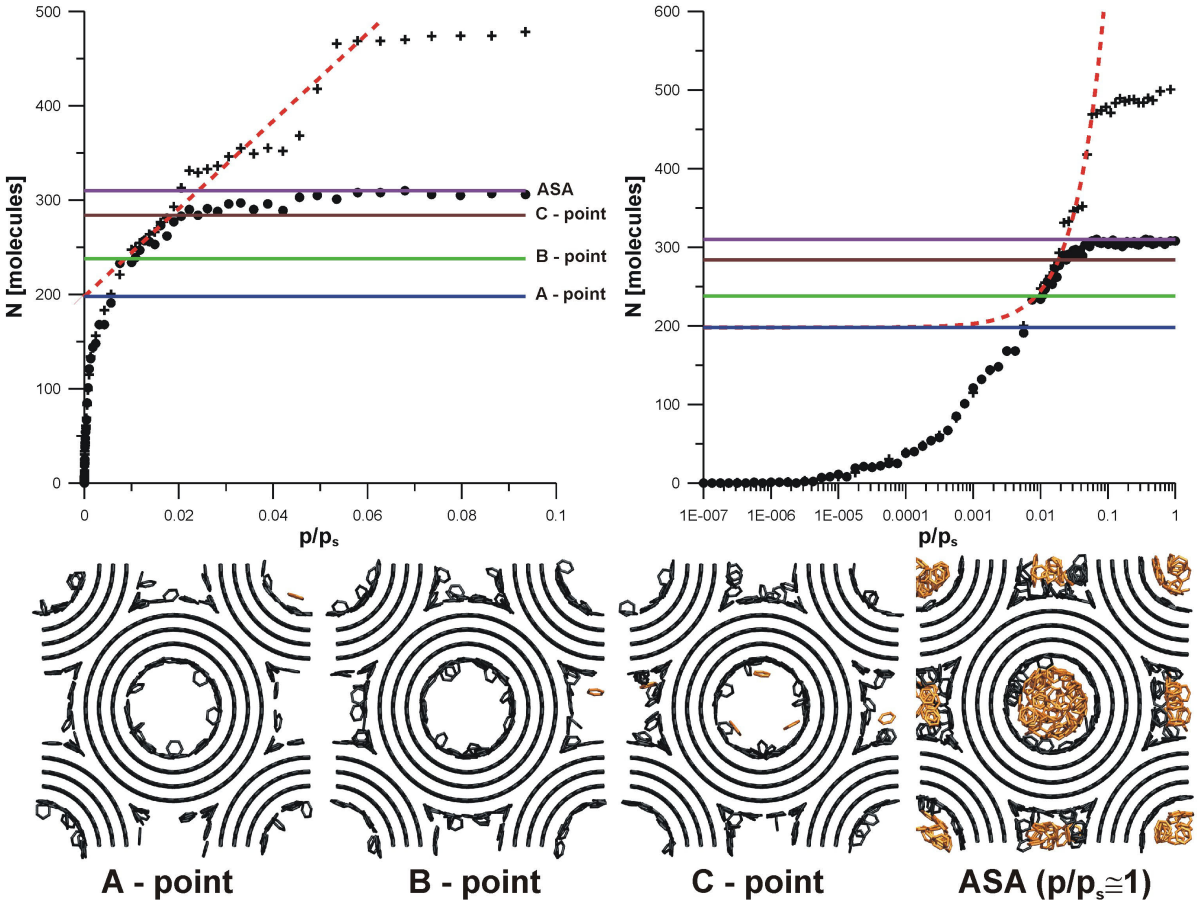

Fig. S25. The same as in Fig. S24 but for C_6H_6 adsorption.

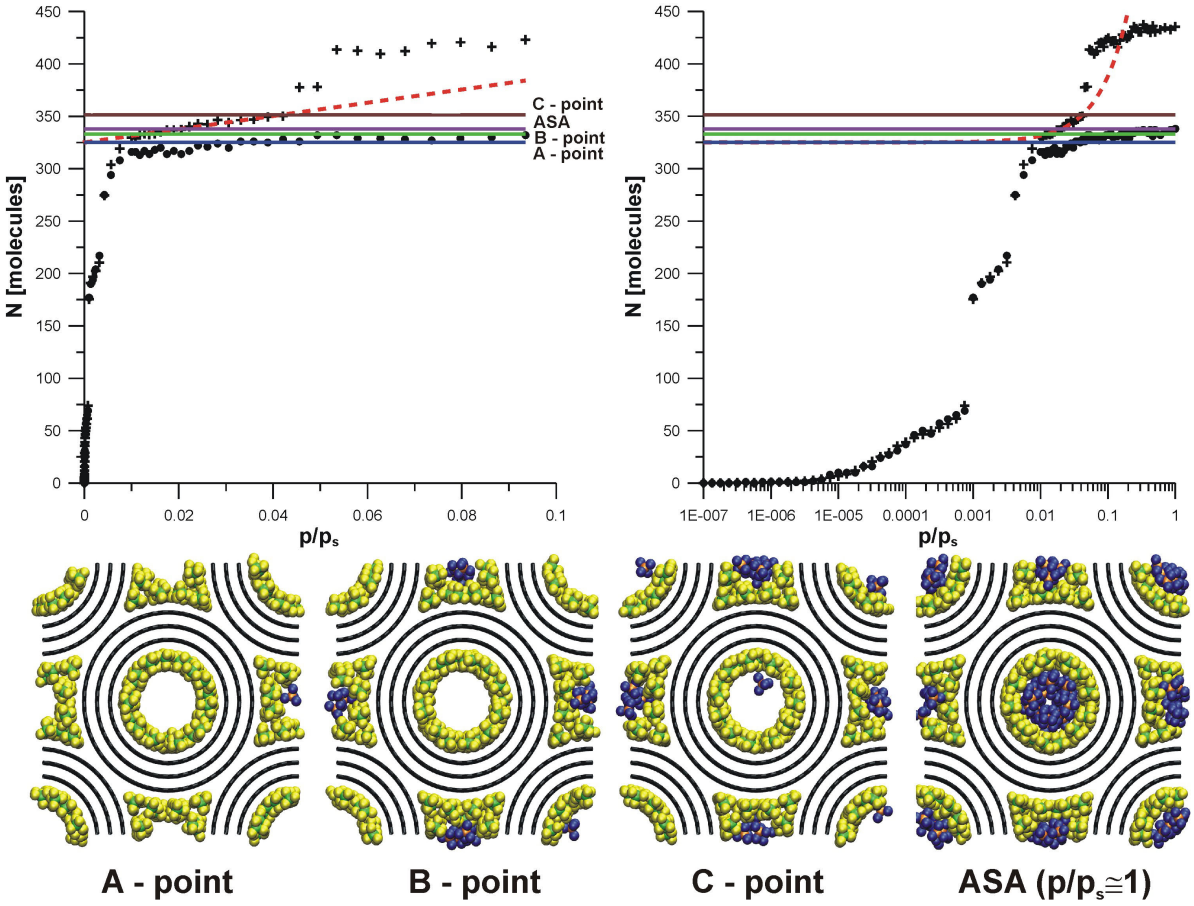

Fig. S26. The same as in Fig. S24 but for CCl_4 adsorption.