Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Structures and IR/UV spectra of neutral and ionic phenol-Ar_n cluster isomers (n≤4): competition between hydrogen bonding and stacking **

Matthias Schmies,[1] Alexander Patzer,[1] Masaaki Fujii,[2] and Otto Dopfer[1]*

[1] Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623 Berlin, Germany

[2] Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama 226-8503, Japan

* E-mail: dopfer@physik.tu-berlin.de

** dedicated to Bernhard Brutschy on the occasion of this 65th birthday

Table T1. O-H stretch frequencies (ν_{OH} in cm^{-1}) of selected PhOH-Ar_n isomers calculated at the M06-2X level compared to available experimental values.

n	Exp[a]	M06-2X	isomer
0	3658	3658	PhOH
1		3648	(H00)
	3656	3656	(10)
2		3647	(H10)
		3651	$(11)^H$
	3656	3654	(11)
		3655	(20)
3		3649	(H11)
	3654	3652	(30)
		3652	(21)
		3653	(H20)
		3651	$(21)^H$
4		3650	(H30)
		3650	(H21)
		3655	(22)
		3653	(40)
		3648	(40) T
	3653	3648	(31)

[a] S. Ishiuchi et al., *Phys. Chem. Chem. Phys.*, 2011, **13**, 2409.

Table T2. Frequencies of intermolecular modes of (10) and (11) in the S_0 and S_1 states evaluated at the RI-CC2/aug-cc-pVDZ level. Harmonic frequencies are scaled by 0.752. Available experimental values in the S_1 state are given for comparison.

(01)	S_0	S_1	S_1 (exp)[a]	(11)	S_0	S_1	S_1 (exp)[b]
b_x	20	20	20	b_{xs}	13	13	14
b_y	35	37		b_{ys}	18	20	20
s_z	41	45	45	b_{xa}	25	25	
				s_{zs}	36	39	36
				s_{za}	45	49	
				b_{ya}	50	49	

[a] M. Mons et al., *J. Chem. Phys.*,1990, **92**, 2155.

[b] S. Ishiuchi et al., *J. Phys. Chem. A*, 2007, **111**, 7569.

Figure Captions

Figure F1. Structures and relative energies (in cm^{-1}) of various (20) isomers of PhOH-Ar_2 in the S_0 state calculated at the M06-2X/aug-cc-pVTZ level. The relative energies are derived from D_e (D_0) values.

Figure F2. (a) Experimental ΔS_1 shifts of various isomers of PhOH-Ar_n (n≤4) with respect to the S_1 origin of bare PhOH (n=0) at 36350 cm^{-1}. (b) ΔS_1 shifts calculated for various isomers of PhOH-Ar_n (n≤4) with respect to the S_1 origin of bare PhOH (n=0) at 36349 cm^{-1} using adiabatic transition energies without ZPE.

Figure F3. Structures and relative energies (in cm^{-1}) of various (20) isomers of PhOH-Ar_2 in the D_0 state calculated at the M06-2X/aug-cc-pVTZ level. The relative energies are derived from D_e (D_0) values.

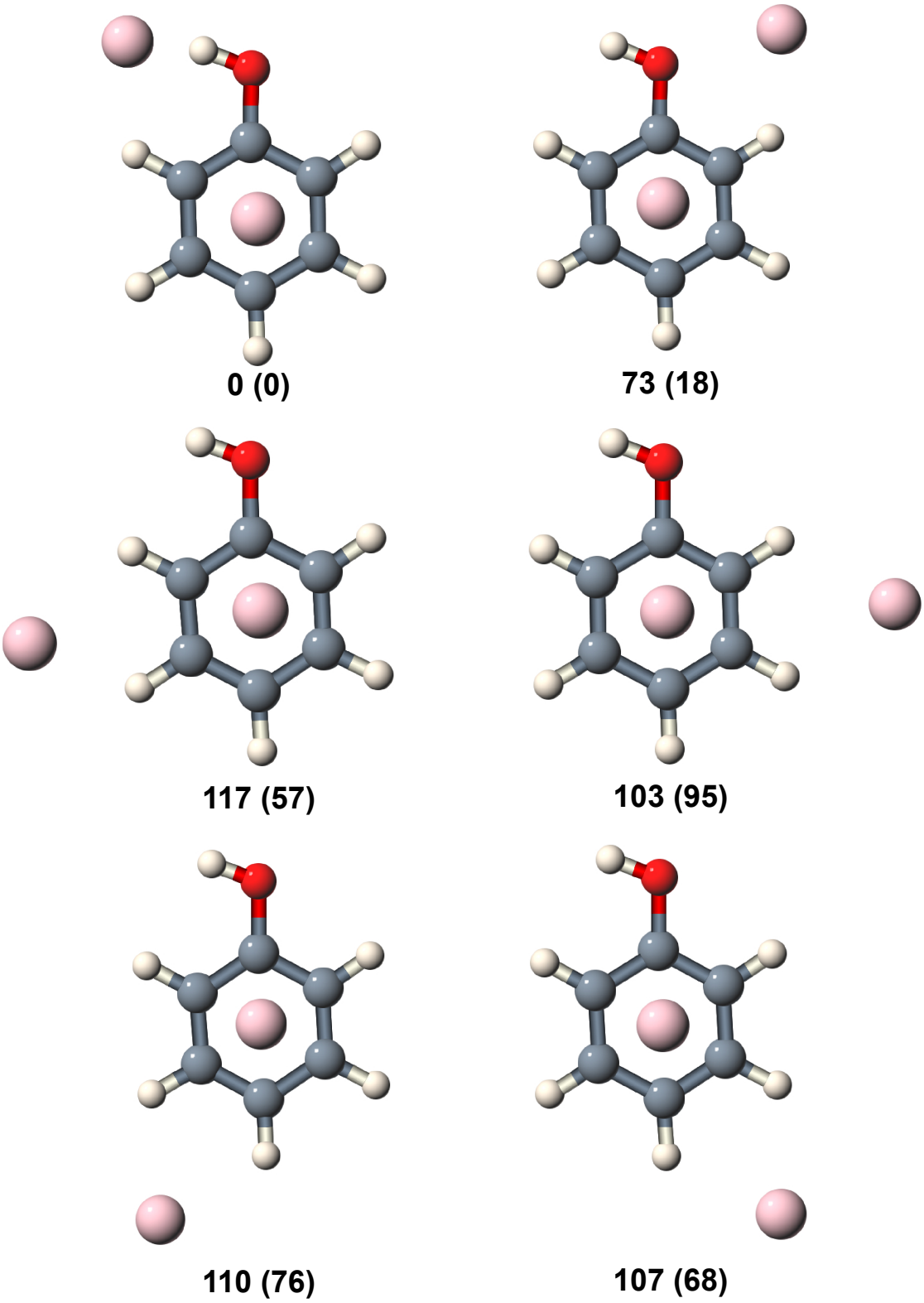

Figure F1

.

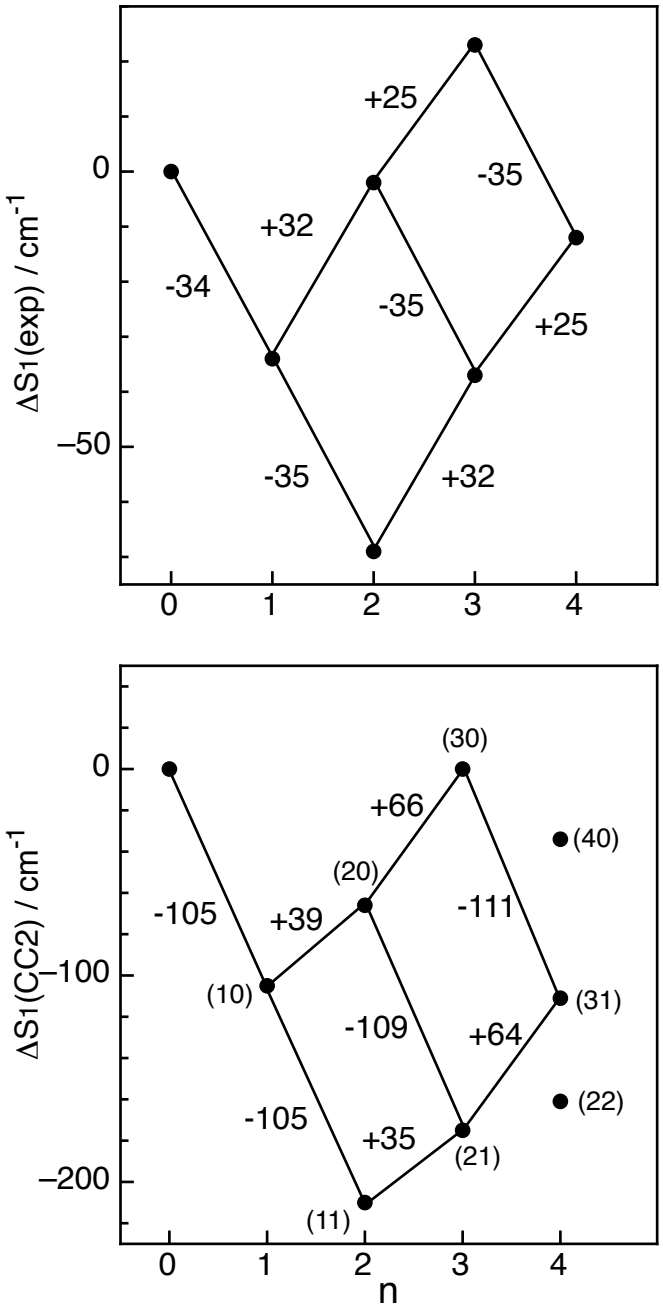
ΔS1(exp) / cm-1
0
–50
+25
-35
+32
-34
-35
+25
-35
+32
0
1
2
3
4
ΔS1(CC2) / cm-1
0
–100
–200
(30)
+66
(40)
(20)
-105
+39
-111
(10)
(31)
-109
+64
(22)
-105
+35
(21)
(11)
0
1
2
3
4
n

Figure F2

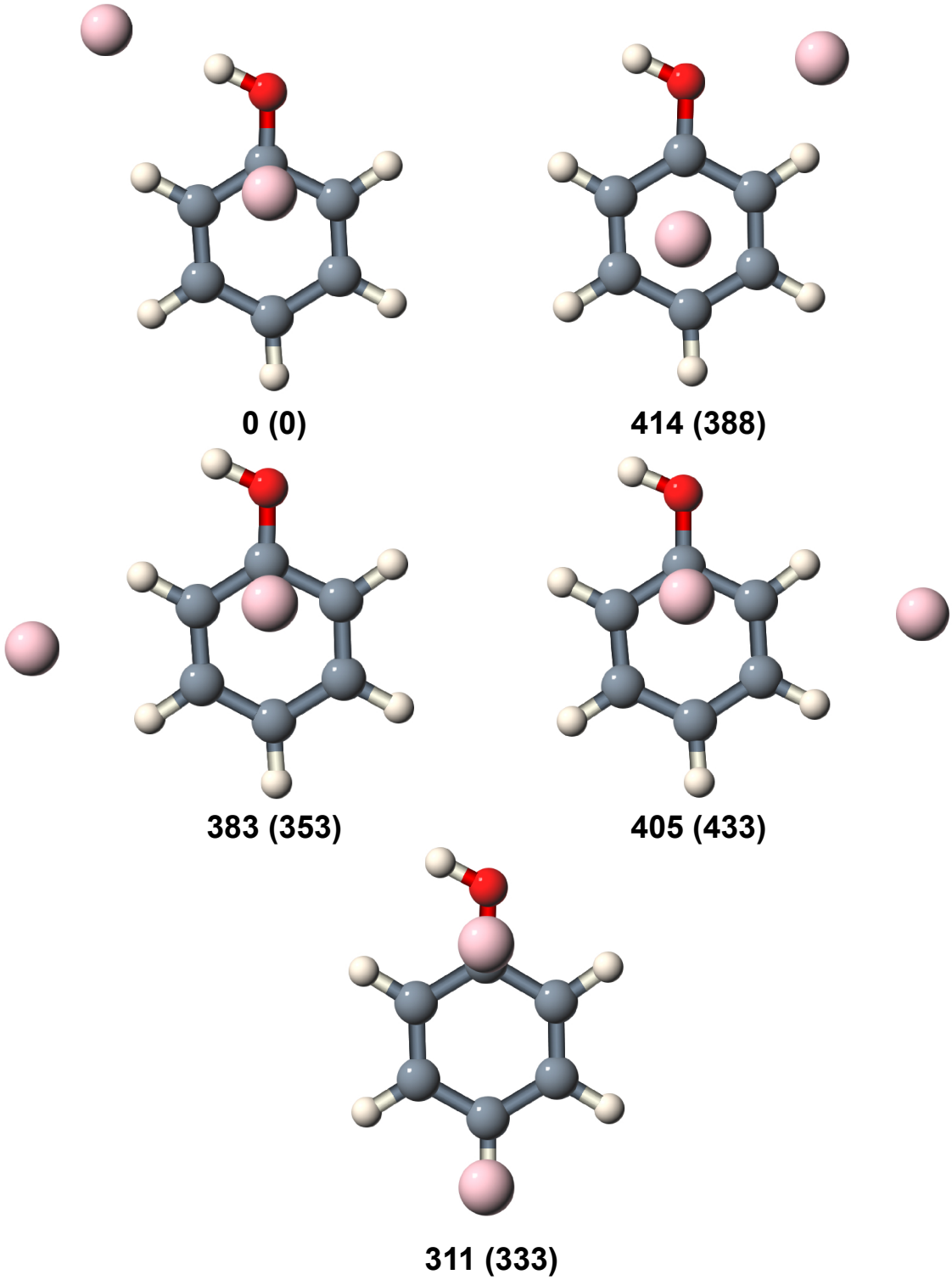

Figure F3