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Global and Local Minima of Protonated Acetonitrile Clusters

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SUPPORTING INFORMATION:

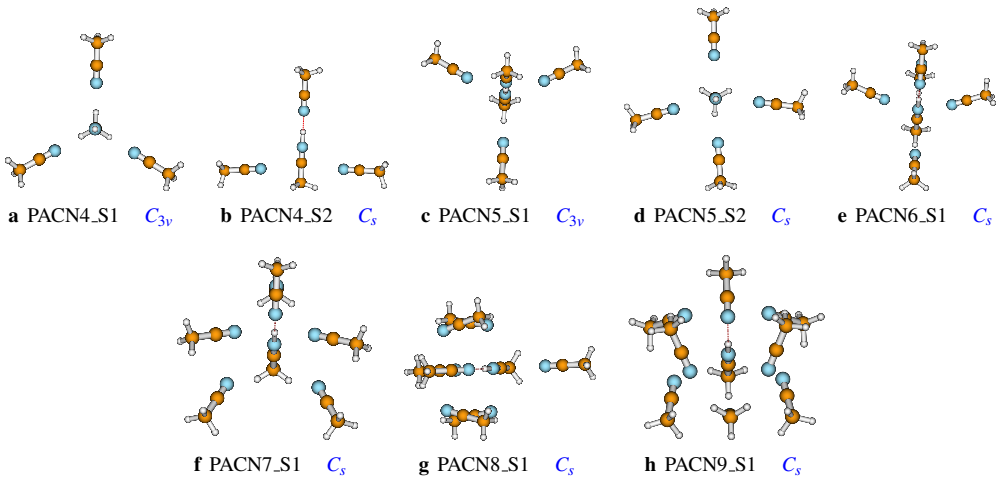

Fig. S 1 Symmetric structures of the protonated acetonitrile clusters which are found to be transition states.

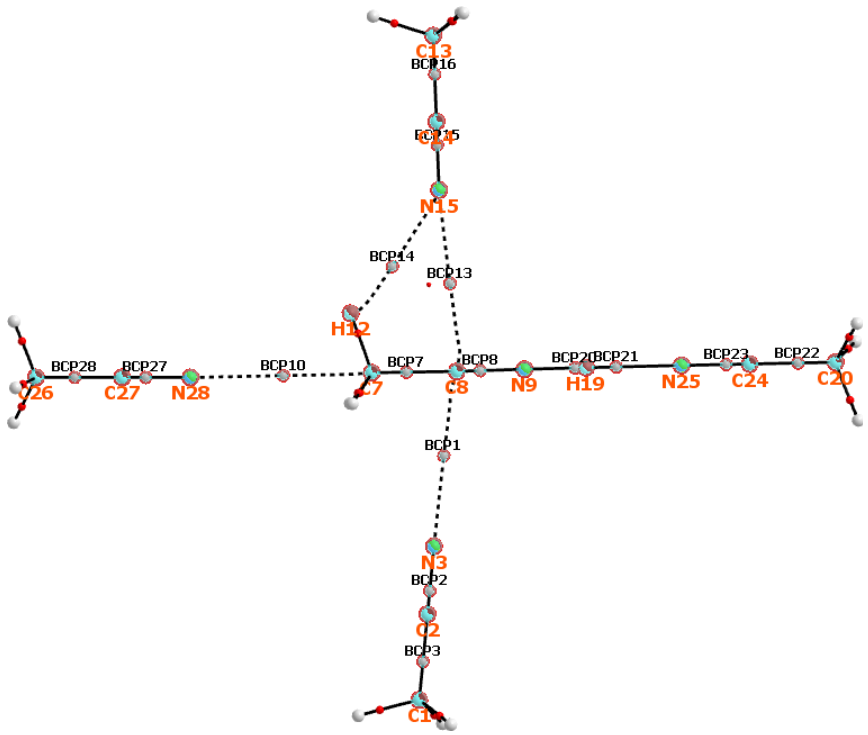

Fig. S 2 PACN5_5 showing selected ACP and BCP numbering shown.

Table S 1 Topological parameters of the QTAIM calculated bond paths in PACN5_5. The numbers of the Bond critical points (CP) are shown in Fig. S2.

BCP #	Name	Atoms	(ρ/ea_0^{-3})	$(\nabla^2\rho/ea_0^{-5})$	DI(A,B)
13	BCP13	C8 - N15	0.0072	0.0256	0.02
10	BCP10	C7 - N28	0.0076	0.0287	0.04
1	BCP1	N3 - C8	0.0086	0.0315	0.03
14	BCP14	H12 - N15	0.0088	0.0302	0.04
21	BCP21	H19 - N25	0.0615	0.1169	0.16
20	BCP20	N9 - H19	0.2630	-1.3453	0.43
3	BCP3	C1 - C2	0.2631	-0.6854	1.04
16	BCP16	C13 - C14	0.2631	-0.6854	1.04
28	BCP28	C26 - C27	0.2631	-0.6843	1.04
22	BCP22	C20 - C24	0.2632	-0.6905	1.04
7	BCP7	C7 - C8	0.2652	-0.7219	1.03
11	BCP11	C7 - H11	0.2770	-0.9947	0.90
9	BCP9	C7 - H10	0.2770	-0.9947	0.90
30	BCP30	C26 - H30	0.2772	-0.9681	0.94
31	BCP31	C26 - H31	0.2772	-0.9681	0.94
29	BCP29	C26 - H29	0.2772	-0.9683	0.94
18	BCP18	C13 - H17	0.2772	-0.9694	0.94
19	BCP19	C13 - H18	0.2772	-0.9694	0.94
5	BCP5	C1 - H5	0.2773	-0.9696	0.94
6	BCP6	C1 - H6	0.2773	-0.9697	0.94
17	BCP17	C13 - H16	0.2773	-0.9700	0.94
4	BCP4	C1 - H4	0.2773	-0.9701	0.94

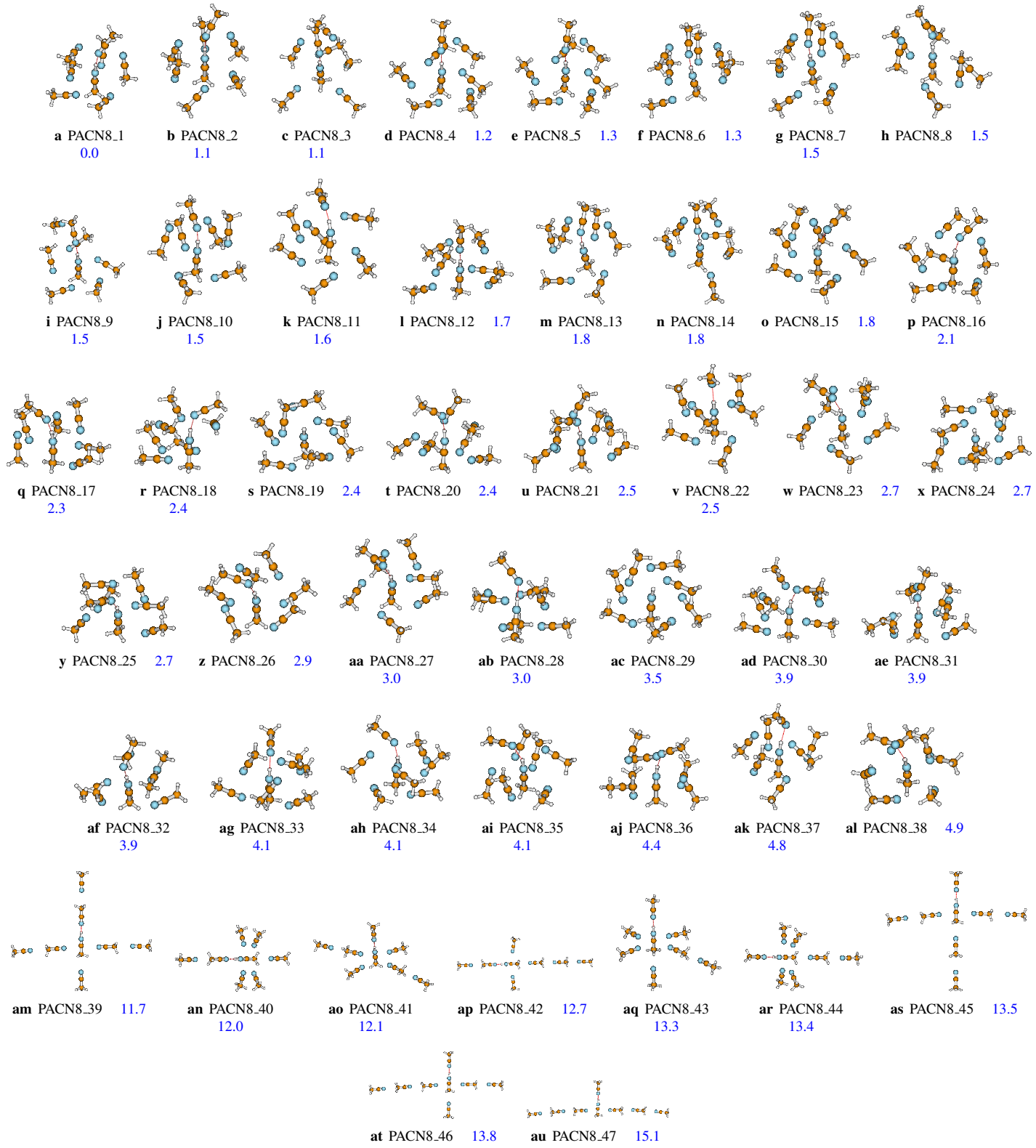

Fig. S 3 Structures and relatives electronic energies of the protonated acetonitrile octamer, $H^+(MeCN)_8$ as optimized at the MN15/6-31++G(d,p) level of theory. The relative electronic energies are zero point energy (ZPE) corrected. Each sub-caption indicates the name of the structure followed by its relative energy.

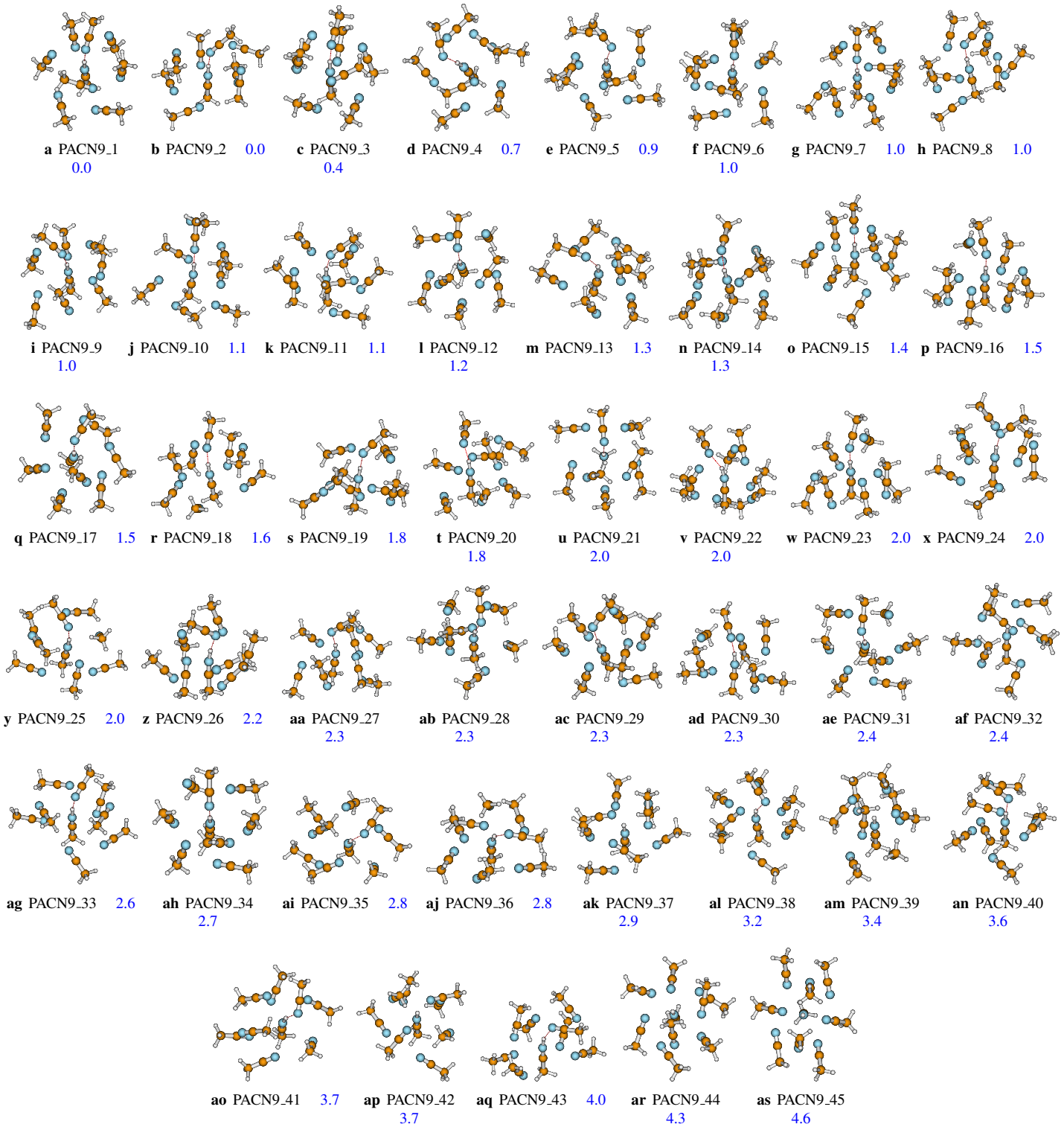

Fig. S 4 Structures and relatives electronic energies of the protonated acetonitrile nonamer, $H^+(MeCN)_9$ as optimized at the MN15/6-31++G(d,p) level of theory. The relative electronic energies are zero point energy (ZPE) corrected. Each sub-caption indicates the name of the structure followed by its relative energy.

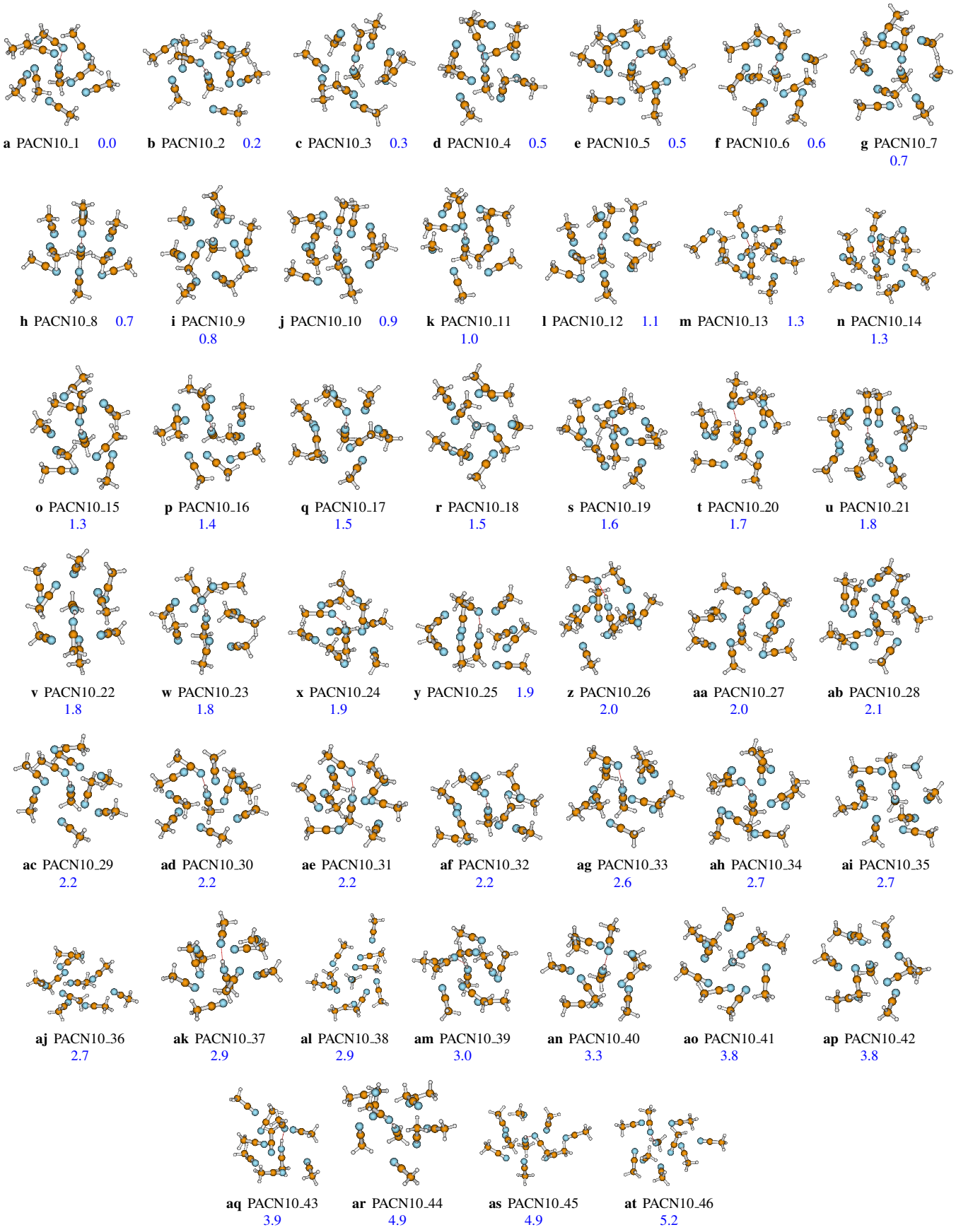

Fig. S 5 Structures and relatives electronic energies of the protonated acetonitrile decamer, $H^+(MeCN)_{10}$ as optimized at the MN15/6-31++G(d,p) level of theory. The relative electronic energies are zero point energy (ZPE) corrected. Each sub-caption indicates the name of the structure followed by its relative energy.