

# LIST OF THE DATA FILES For

Role of black carbon in the formation of primary organic aerosols: Insights from molecular dynamics simulations

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**Table.** List of files that contain optimized atomistic configurations of organic molecules adsorbed on onion-like nanoparticles.

Molecule	Number	Nanoparticle(nm)	Filename	Molecule	Number	Nanoparticle (nm)	Filename
C <sub>2</sub> H <sub>4</sub>	30	3.64	1.xyz	C <sub>2</sub> H <sub>4</sub>	30	none	43.xyz
C <sub>2</sub> H <sub>4</sub>	60	3.64	2.xyz	C <sub>2</sub> H <sub>4</sub>	60	none	44.xyz
C <sub>2</sub> H <sub>4</sub>	90	3.64	3.xyz	C <sub>2</sub> H <sub>4</sub>	90	none	45.xyz
C <sub>2</sub> H <sub>4</sub>	120	3.64	4.xyz	C <sub>2</sub> H <sub>4</sub>	120	none	46.xyz
C <sub>2</sub> H <sub>4</sub>	150	3.64	5.xyz	C <sub>2</sub> H <sub>4</sub>	150	none	47.xyz
C <sub>2</sub> H <sub>4</sub>	180	3.64	6.xyz	C <sub>2</sub> H <sub>4</sub>	180	none	48.xyz
C <sub>2</sub> H <sub>4</sub>	210	3.64	7.xyz	C <sub>2</sub> H <sub>4</sub>	210	none	49.xyz
C <sub>3</sub> H <sub>6</sub>	30	3.64	8.xyz	C <sub>3</sub> H <sub>6</sub>	30	none	50.xyz
C <sub>3</sub> H <sub>6</sub>	60	3.64	9.xyz	C <sub>3</sub> H <sub>6</sub>	60	none	51.xyz
C <sub>3</sub> H <sub>6</sub>	90	3.64	10.xyz	C <sub>3</sub> H <sub>6</sub>	90	none	52.xyz
C <sub>3</sub> H <sub>6</sub>	120	3.64	11.xyz	C <sub>3</sub> H <sub>6</sub>	120	none	53.xyz
C <sub>3</sub> H <sub>6</sub>	150	3.64	12.xyz	C <sub>3</sub> H <sub>6</sub>	150	none	54.xyz
C <sub>3</sub> H <sub>6</sub>	180	3.64	13.xyz	C <sub>3</sub> H <sub>6</sub>	180	none	55.xyz
C <sub>3</sub> H <sub>6</sub>	210	3.64	14.xyz	C <sub>3</sub> H <sub>6</sub>	210	none	56.xyz
C <sub>7</sub> H <sub>8</sub>	30	3.64	15.xyz	C <sub>7</sub> H <sub>8</sub>	30	none	57.xyz
C <sub>7</sub> H <sub>8</sub>	60	3.64	16.xyz	C <sub>7</sub> H <sub>8</sub>	60	none	58.xyz
C <sub>7</sub> H <sub>8</sub>	90	3.64	17.xyz	C <sub>7</sub> H <sub>8</sub>	90	none	59.xyz
C <sub>7</sub> H <sub>8</sub>	120	3.64	18.xyz	C <sub>7</sub> H <sub>8</sub>	120	none	60.xyz
C <sub>7</sub> H <sub>8</sub>	150	3.64	19.xyz	C <sub>7</sub> H <sub>8</sub>	150	none	61.xyz
C <sub>7</sub> H <sub>8</sub>	180	3.64	20.xyz	C <sub>7</sub> H <sub>8</sub>	180	none	62.xyz
C <sub>7</sub> H <sub>8</sub>	210	3.64	21.xyz	C <sub>7</sub> H <sub>8</sub>	210	none	63.xyz
C <sub>8</sub> H <sub>8</sub>	30	3.64	22.xyz	C <sub>8</sub> H <sub>8</sub>	30	none	64.xyz
C <sub>8</sub> H <sub>8</sub>	60	3.64	23.xyz	C <sub>8</sub> H <sub>8</sub>	60	none	65.xyz
C <sub>8</sub> H <sub>8</sub>	90	3.64	24.xyz	C <sub>8</sub> H <sub>8</sub>	90	none	66.xyz
C <sub>8</sub> H <sub>8</sub>	120	3.64	25.xyz	C <sub>8</sub> H <sub>8</sub>	120	none	67.xyz
C <sub>8</sub> H <sub>8</sub>	150	3.64	26.xyz	C <sub>8</sub> H <sub>8</sub>	150	none	68.xyz
C <sub>8</sub> H <sub>8</sub>	180	3.64	27.xyz	C <sub>8</sub> H <sub>8</sub>	180	none	69.xyz
C <sub>8</sub> H <sub>8</sub>	210	3.64	28.xyz	C <sub>8</sub> H <sub>8</sub>	210	none	70.xyz
C <sub>8</sub> H <sub>10</sub>	30	3.64	29.xyz	C <sub>8</sub> H <sub>10</sub>	30	none	71.xyz
C <sub>8</sub> H <sub>10</sub>	60	3.64	30.xyz	C <sub>8</sub> H <sub>10</sub>	60	none	72.xyz
C <sub>8</sub> H <sub>10</sub>	90	3.64	31.xyz	C <sub>8</sub> H <sub>10</sub>	90	none	73.xyz
C <sub>8</sub> H <sub>10</sub>	120	3.64	32.xyz	C <sub>8</sub> H <sub>10</sub>	120	none	74.xyz

C <sub>8</sub> H <sub>10</sub>	150	3.64	33.xyz	C <sub>8</sub> H <sub>10</sub>	150	none	75.xyz
C <sub>8</sub> H <sub>10</sub>	180	3.64	34.xyz	C <sub>8</sub> H <sub>10</sub>	180	none	76.xyz
C <sub>8</sub> H <sub>10</sub>	210	3.64	35.xyz	C <sub>8</sub> H <sub>10</sub>	210	none	77.xyz
C <sub>8</sub> H <sub>10</sub>	30	3.64	36.xyz	C <sub>8</sub> H <sub>10</sub>	30	none	78.xyz
C <sub>8</sub> H <sub>10</sub>	60	3.64	37.xyz	C <sub>8</sub> H <sub>10</sub>	60	none	79.xyz
C <sub>8</sub> H <sub>10</sub>	90	3.64	38.xyz	C <sub>8</sub> H <sub>10</sub>	90	none	80.xyz
C <sub>8</sub> H <sub>10</sub>	120	3.64	39.xyz	C <sub>8</sub> H <sub>10</sub>	120	none	81.xyz
C <sub>8</sub> H <sub>10</sub>	150	3.64	40.xyz	C <sub>8</sub> H <sub>10</sub>	150	none	82.xyz
C <sub>8</sub> H <sub>10</sub>	180	3.64	41.xyz	C <sub>8</sub> H <sub>10</sub>	180	none	83.xyz
C <sub>8</sub> H <sub>10</sub>	210	3.64	42.xyz	C <sub>8</sub> H <sub>10</sub>	210	none	84.xyz

Note: These .xyz files provide the atomistic configurations of the adsorbed organic molecules and nanoparticles by giving the total number of atoms that will be read on the first line, the number of atoms in the nanoparticle, the number of molecules, and the number of atoms in each molecule on the second, and the atom type and three atomic Cartesian coordinates in the following lines. These files can be directly visualized by the VMD (Visual Molecular Dynamics), an open-source software developed at University of Illinois at Urbana-Champaign.