Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Noble Gas Encapsulation: Clathrate Hydrates and their HF Doped Analogues

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Supporting Information

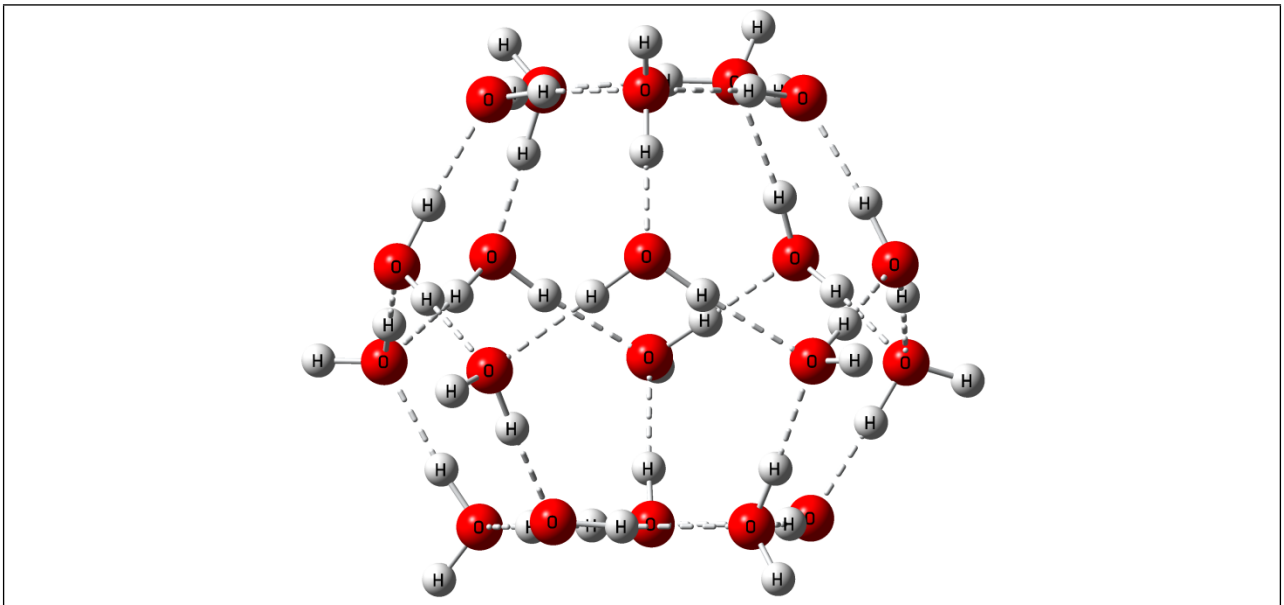
Table S1. Hardness (η, eV) and electrophilicity (ω, eV) values calculated at ωB97X-D/6-311+G(d,p) level of theory for the nNg@512 and nNg@HF512 systems.

Systems	η	ω	Systems	η	ω
5^{12}	12.020	0.759	$HF5^{12}$	12.067	0.798
$1He@5^{12}$	12.173	0.724	$1He@HF5^{12}$	12.220	0.761
$2He@5^{12}$	12.242	0.717	$2He@HF5^{12}$	12.303	0.746
$3He@5^{12}$	12.323	0.694	$3He@HF5^{12}$	12.371	0.729
$4He@5^{12}$	12.361	0.693	$4He@HF5^{12}$	12.407	0.729
$5He@5^{12}$	12.374	0.697	$5He@HF5^{12}$	12.436	0.723
$1Ne@5^{12}$	12.113	0.738	$1Ne@HF5^{12}$	12.160	0.776
$2Ne@5^{12}$	12.163	0.745	$2Ne@HF5^{12}$	12.234	0.772
$3Ne@5^{12}$	12.227	0.725	$3Ne@HF5^{12}$	12.279	0.761
$1Ar@5^{12}$	12.107	0.743	$1Ar@HF5^{12}$	12.160	0.778
$2Ar@5^{12}$	12.242	0.753	$2Ar@HF5^{12}$	12.245	0.786

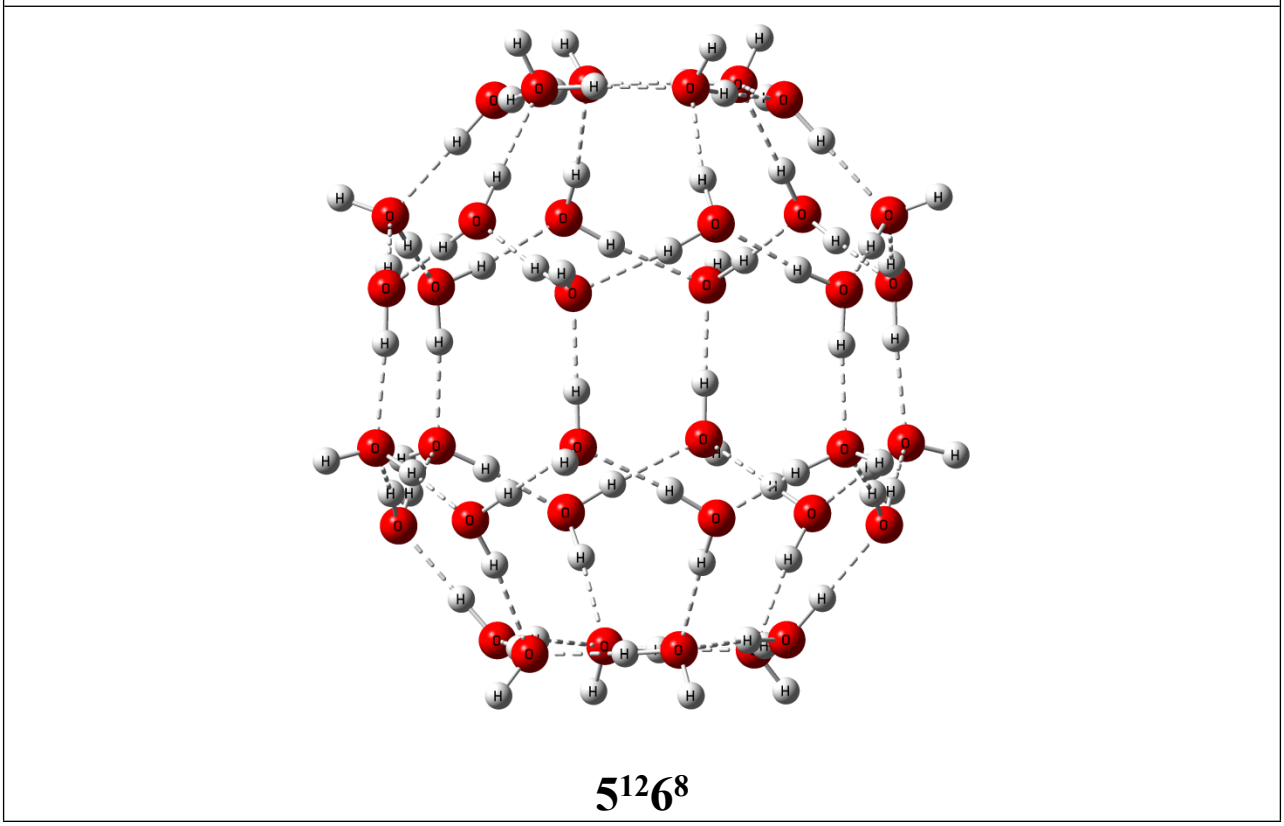
Table S2. Hardness (η, eV) and electrophilicity (ω, eV) values calculated at *ω*B97X-D/6-311+G(d,p) level of theory for the nNg@51268 and nNg@HF51268 systems.

Systems	η	ω	Systems	η	ω
$5^{12}6^{8}$	11.872	0.733	$HF5^{12}6^{8}$	11.887	0.747
$1He@5^{12}6^{8}$	11.890	0.728	$1He@HF5^{12}6^{8}$	11.903	0.744
$2He@5^{12}6^{8}$	11.929	0.720	$2He@HF5^{12}6^{8}$	11.944	0.734
$3He@5^{12}6^{8}$	11.922	0.721	$3He@HF5^{12}6^{8}$	11.936	0.736
$4He@5^{12}6^{8}$	11.974	0.710	$4He@HF5^{12}6^{8}$	11.981	0.726
$5He@5^{12}6^{8}$	11.990	0.707	$5He@HF5^{12}6^{8}$	12.007	0.721
$6He@5^{12}6^{8}$	12.006	0.703	$6He@HF5^{12}6^{8}$	12.022	0.716
$7He@5^{12}6^{8}$	12.026	0.702	$7He@HF5^{12}6^{8}$	12.067	0.707
$8He@5^{12}6^{8}$	12.042	0.702	$8He@HF5^{12}6^{8}$	12.061	0.716
$9He@5^{12}6^{8}$	12.084	0.696	$9He@HF5^{12}6^{8}$	12.108	0.708
$10He@5^{12}6^{8}$	-	-	$10He@HF5^{12}6^{8}$	12.132	0.698
$1Ne@5^{12}6^{8}$	11.853	0.737	$1Ne@HF5^{12}6^{8}$	11.877	0.750
$2Ne@5^{12}6^{8}$	11.855	0.738	$2Ne@HF5^{12}6^{8}$	11.867	0.753
$3Ne@5^{12}6^{8}$	11.852	0.737	$3Ne@HF5^{12}6^{8}$	11.871	0.754
$4Ne@5^{12}6^{8}$	11.888	0.733	$4Ne@HF5^{12}6^{8}$	11.893	0.749
$5Ne@5^{12}6^{8}$	11.900	0.732	$5Ne@HF5^{12}6^{8}$	11.916	0.745
$6Ne@5^{12}6^{8}$	11.920	0.724	$6Ne@HF5^{12}6^{8}$	11.933	0.738
$1Ar@5^{12}6^{8}$	11.744	0.763	$1Ar@HF5^{12}6^{8}$	11.792	0.771
$2Ar@5^{12}6^{8}$	11.798	0.749	$2Ar@HF5^{12}6^{8}$	11.822	0.765
$3Ar@5^{12}6^{8}$	11.840	0.737	$3Ar@HF5^{12}6^{8}$	11.851	0.752
$4Ar@5^{12}6^{8}$	11.887	0.738	$4Ar@HF5^{12}6^{8}$	11.901	0.755
$5Ar@5^{12}6^{8}$	11.924	0.741	$5Ar@HF5^{12}6^{8}$	11.938	0.754
$6Ar@5^{12}6^{8}$	11.938	0.736	$6Ar@HF5^{12}6^{8}$	11.953	0.750

Figure S1. Minimum energy structures of 5^{12} and $5^{12}6^{8}$ at ωB97X-D/6-311+G(d,p) level of theory.

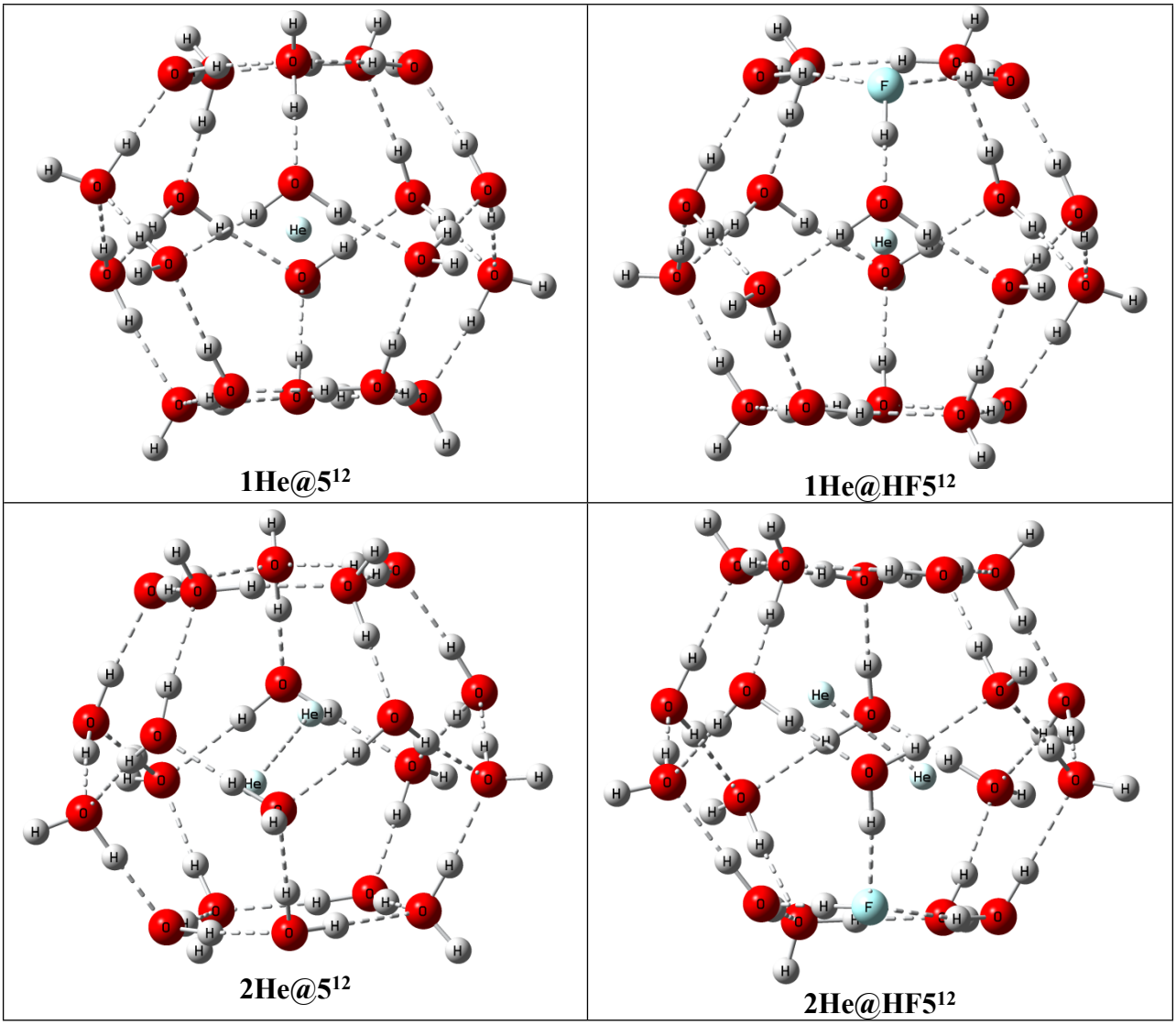


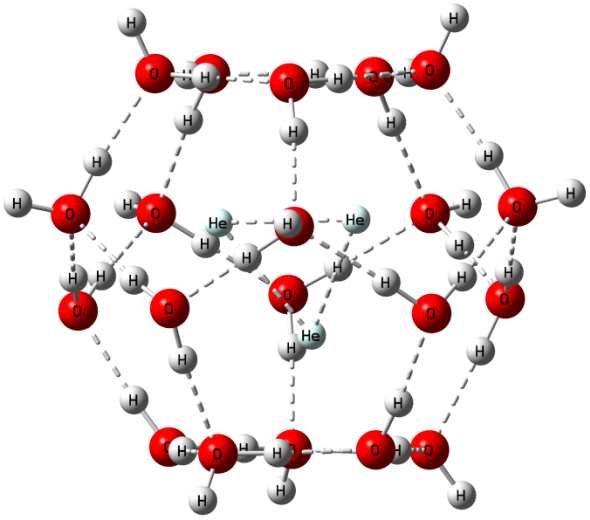
5^{12}



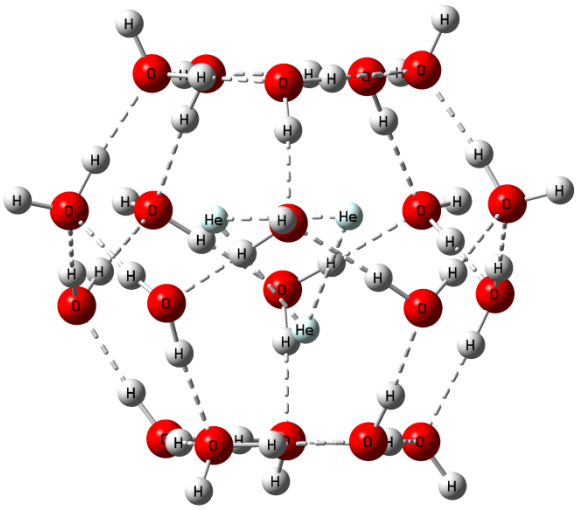
$5^{12}6^{8}$

Figure S2. Minimum energy structures of nNg@5^{12}, nNg@HF5^{12} {Ng = He (n = 1 - 5), Ne (n = 1 - 3), Ar (n = 1 - 2)} and nNg@$5^{12}6^8$, nNg@HF$5^{12}6^8$ {Ng = He (n = 1 – 9/10), Ne and Ar (n = 1 - 6)} at ωB97X-D/6-311+G(d,p) level of theory.





3He@5^{12}



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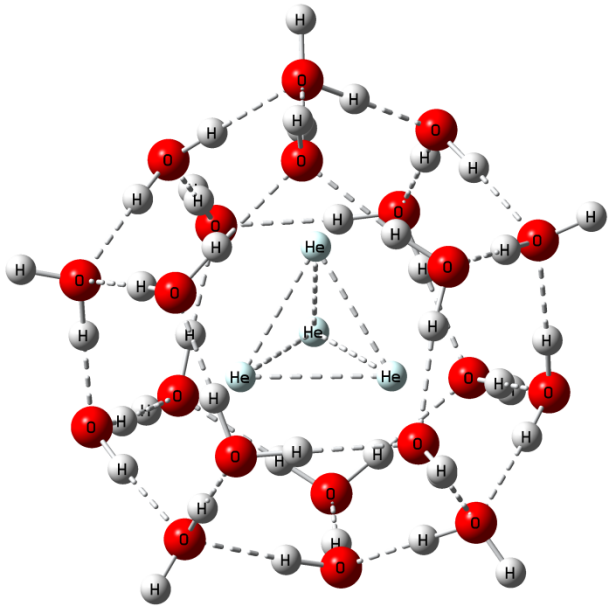
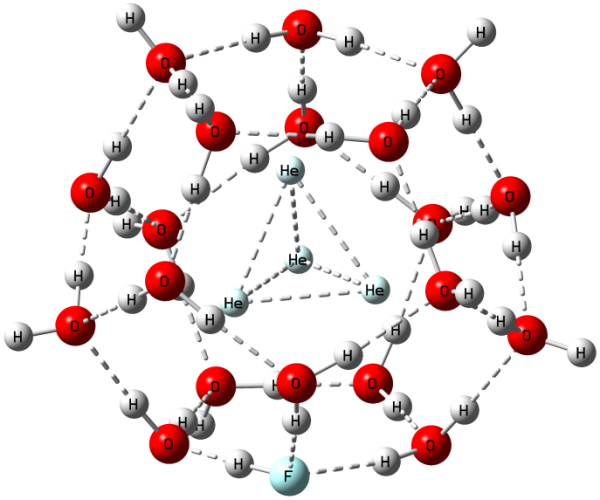
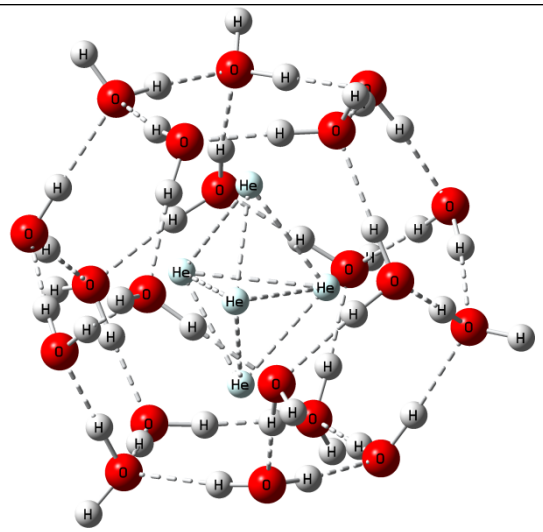
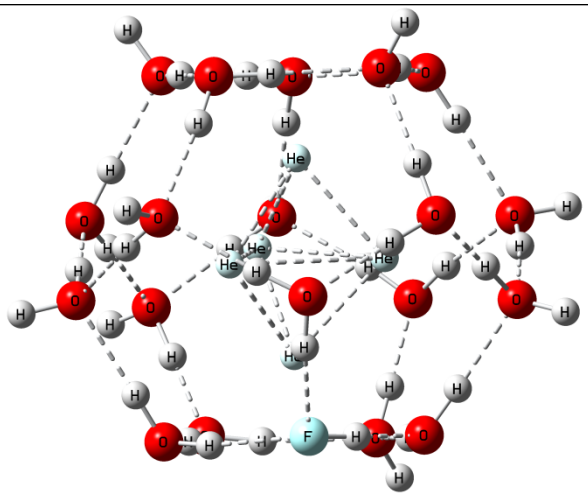
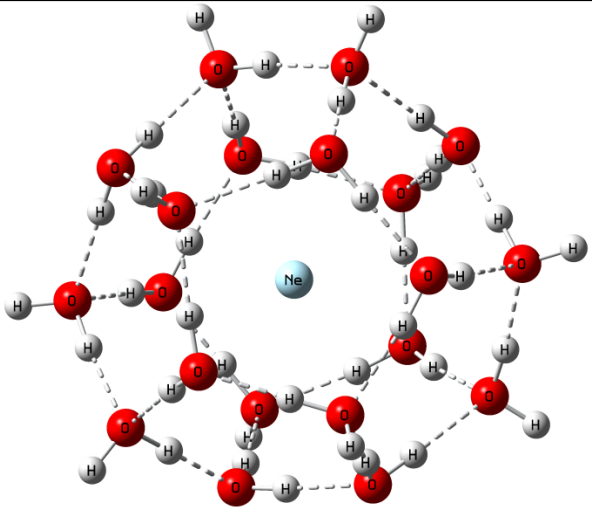
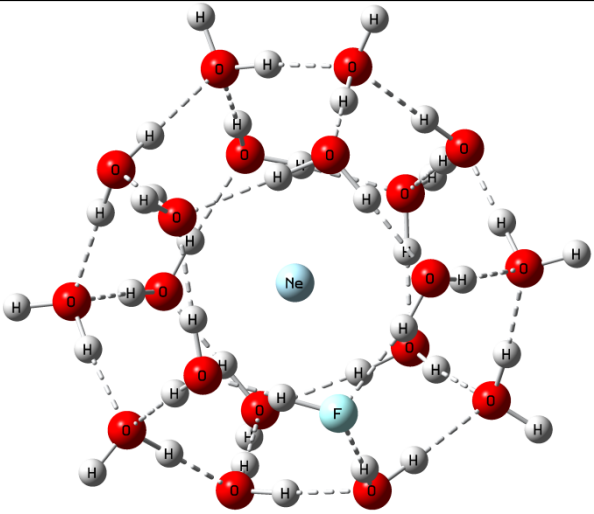
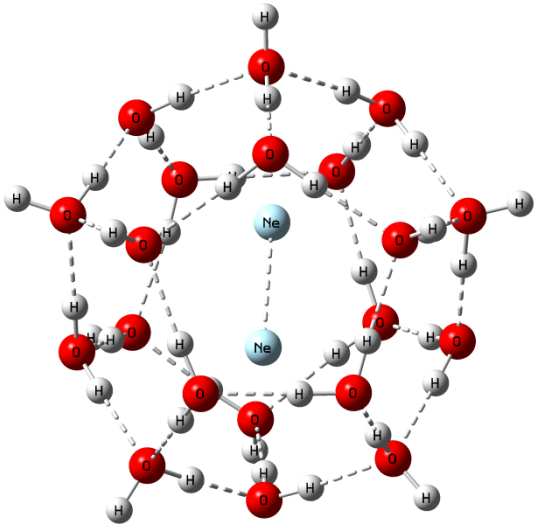
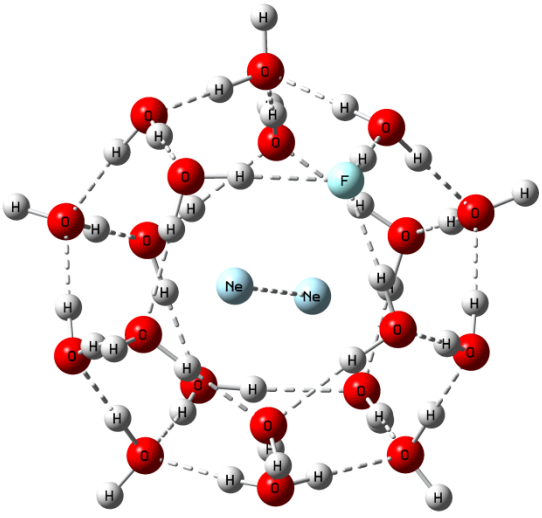
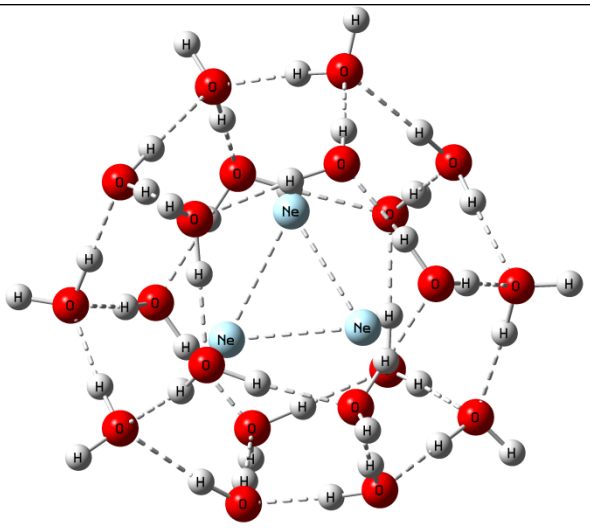


4He@5^{12}

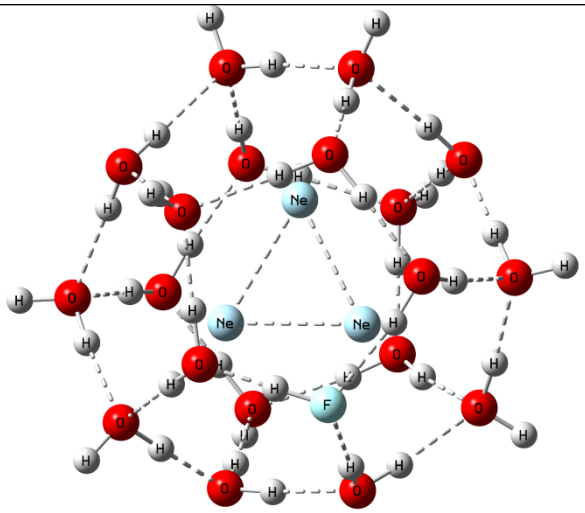


4He@HF5^{12}

 **5He@5^{12}**	 **5He@HF5^{12}**
 **1Ne@5^{12}**	 **1Ne@HF5^{12}**
 **2Ne@5^{12}**	 **2Ne@HF5^{12}**



3Ne@5^{12}



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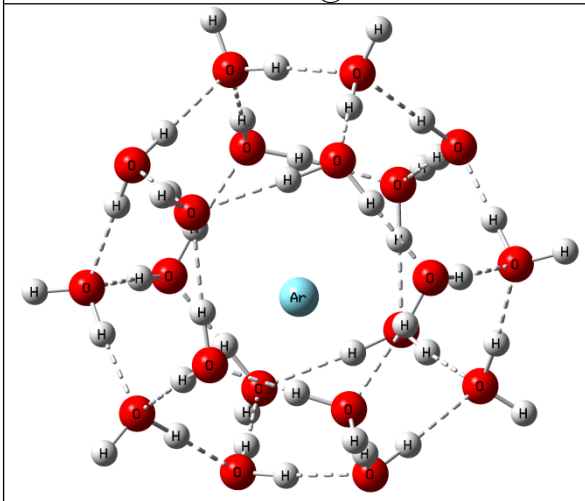

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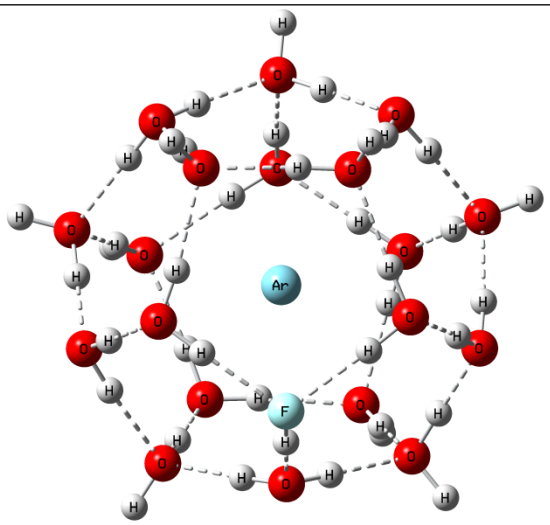

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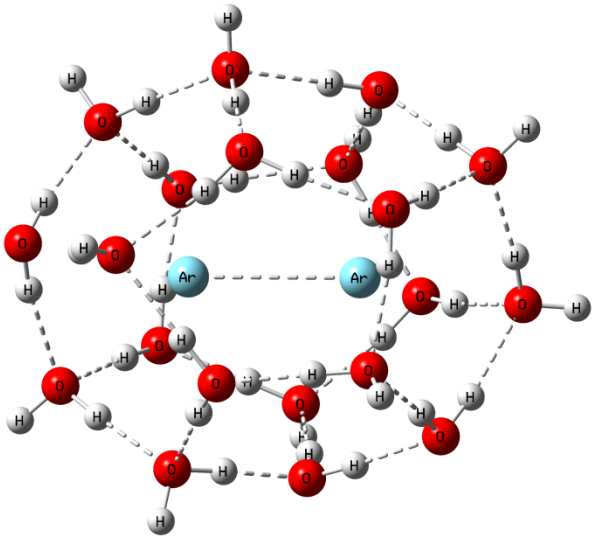

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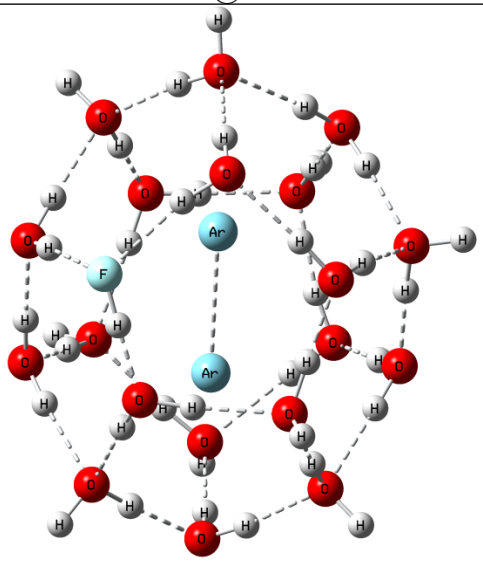

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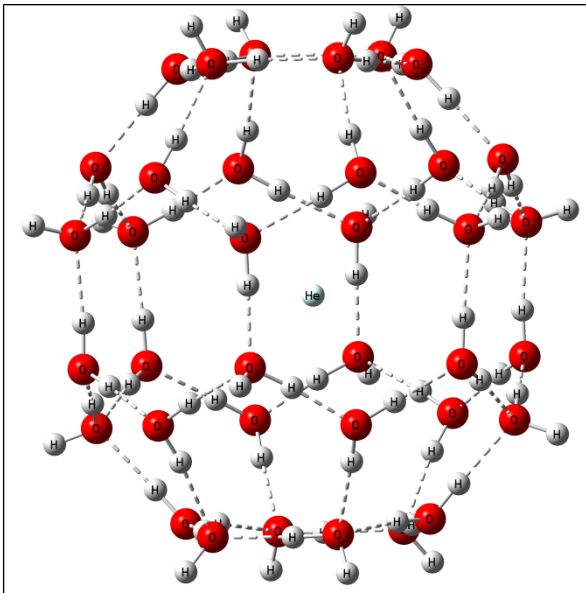
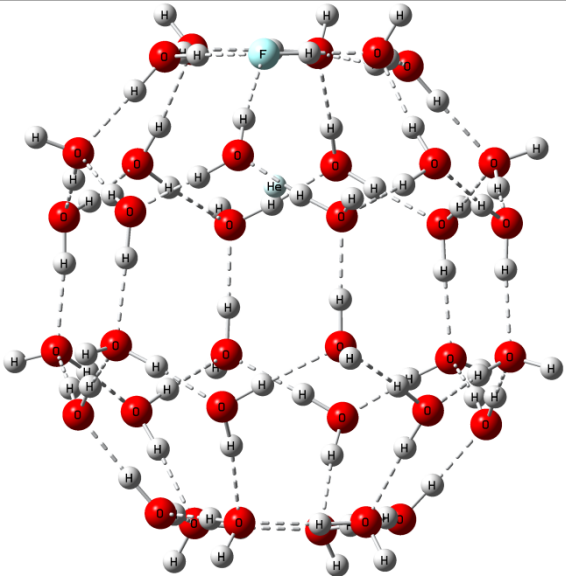
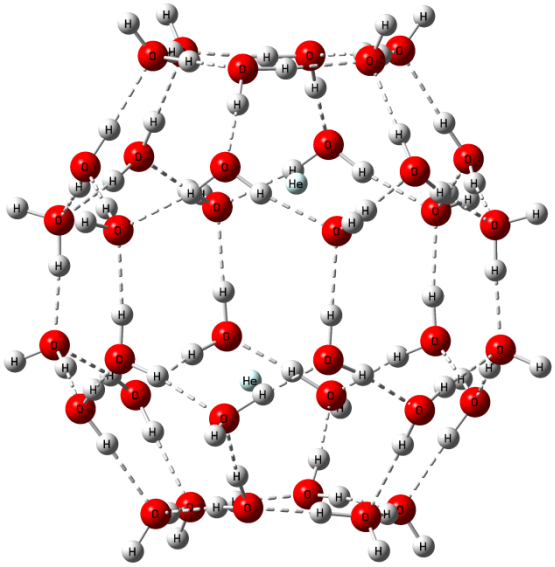
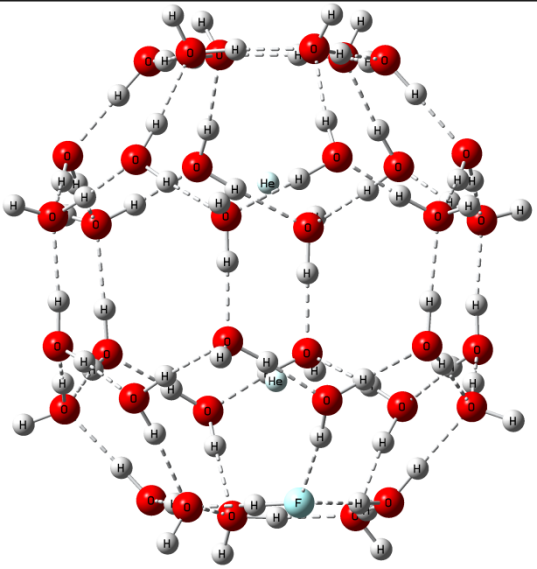
	
1He@$5^{12}6^{8}$	**1He@HF$5^{12}6^{8}$**
	
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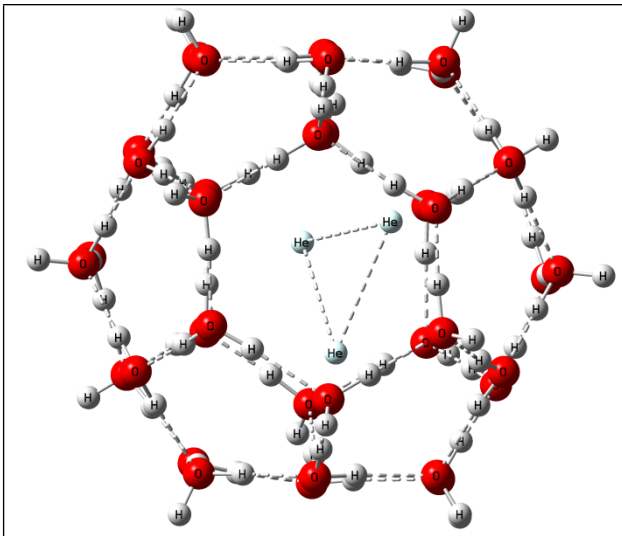

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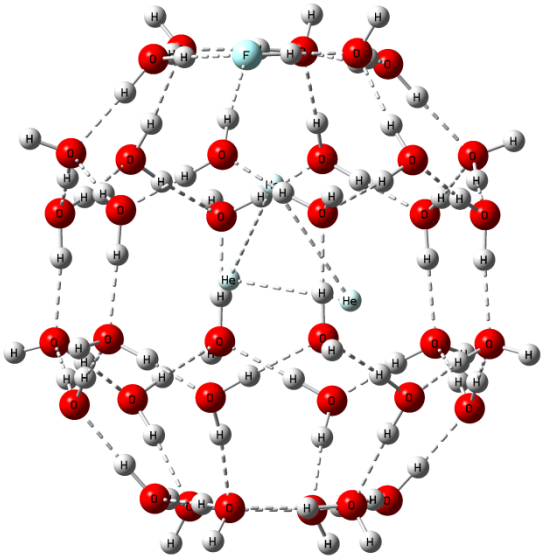
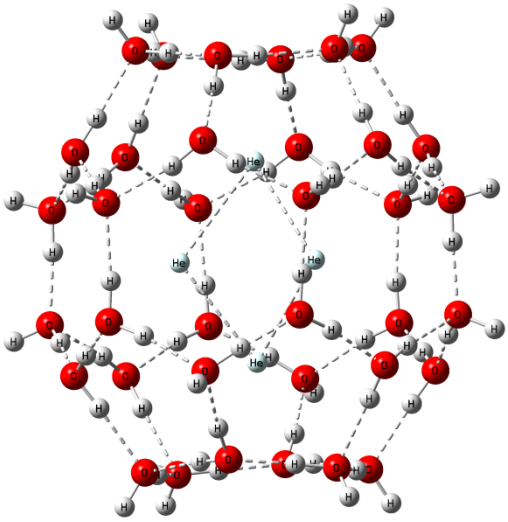


3He@HF$5^{12}6^8$



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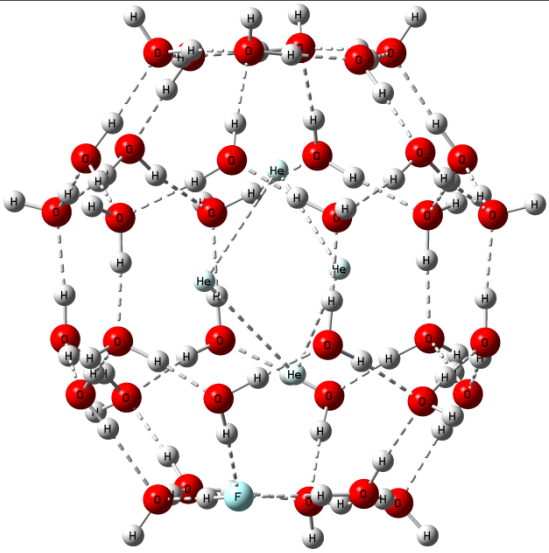
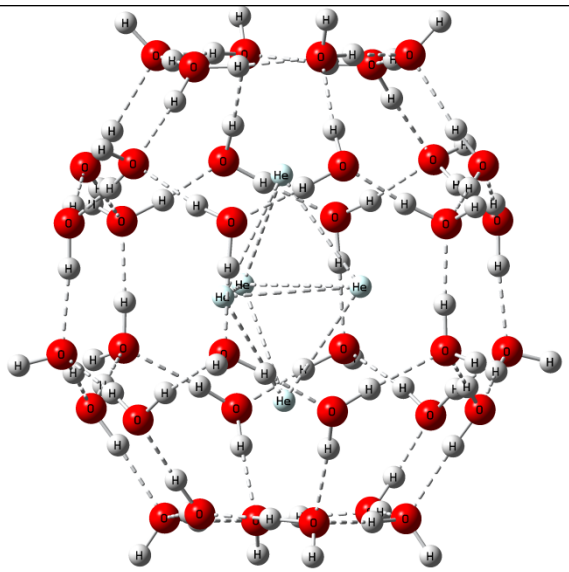
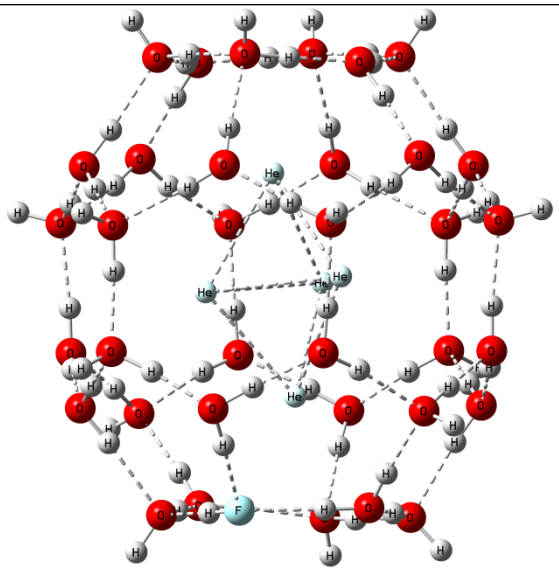


4He@$5^{12}6^8$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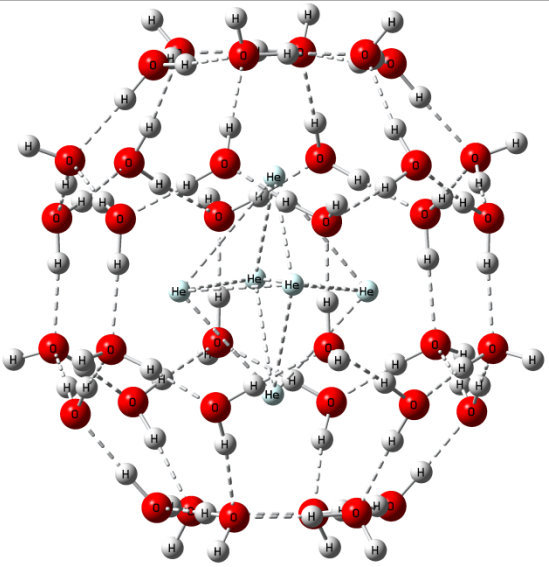	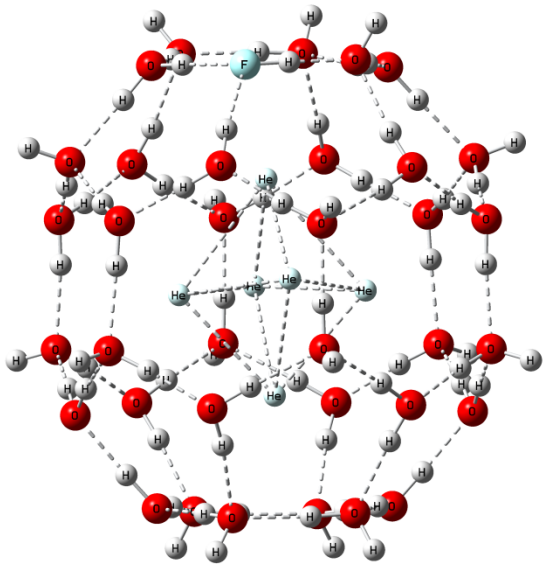
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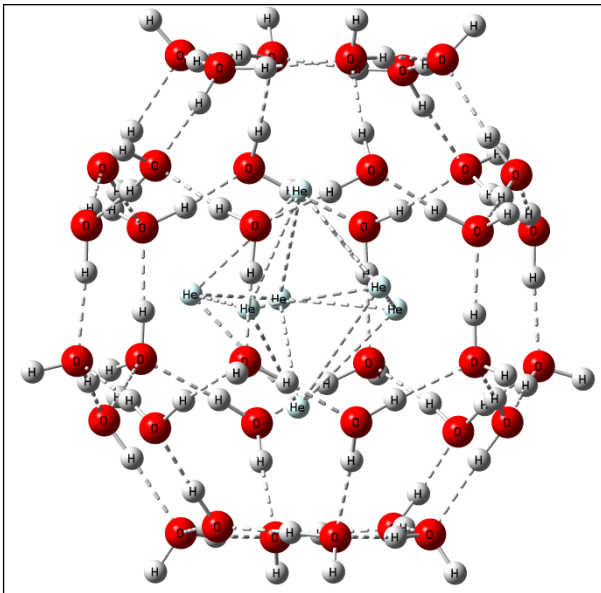

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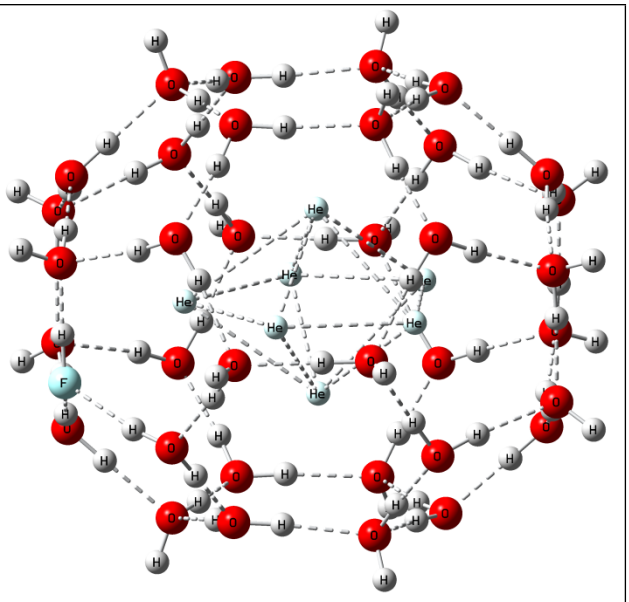

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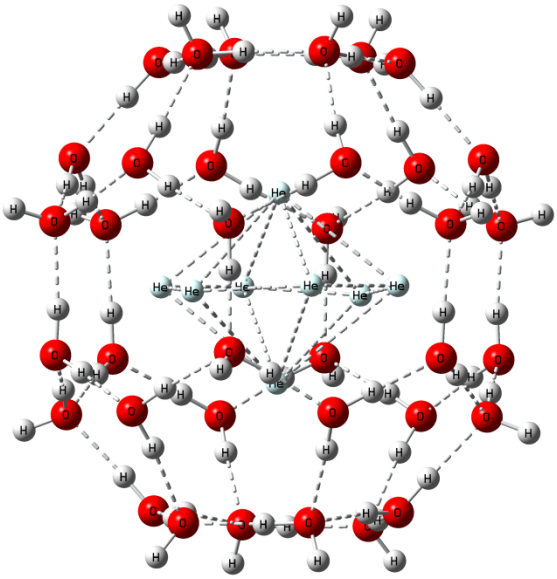

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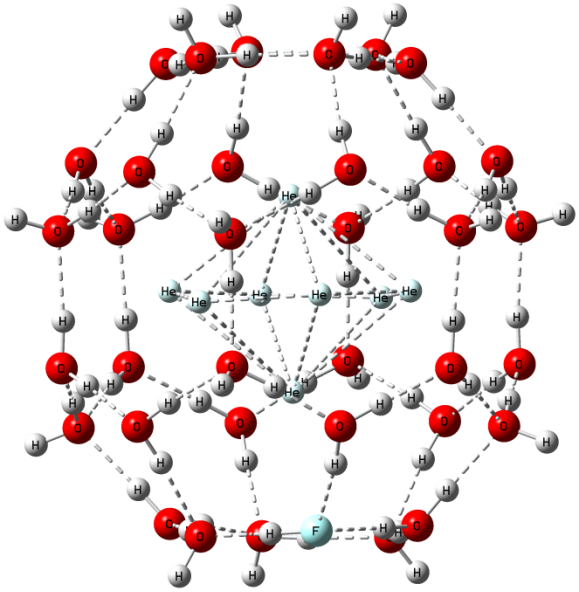
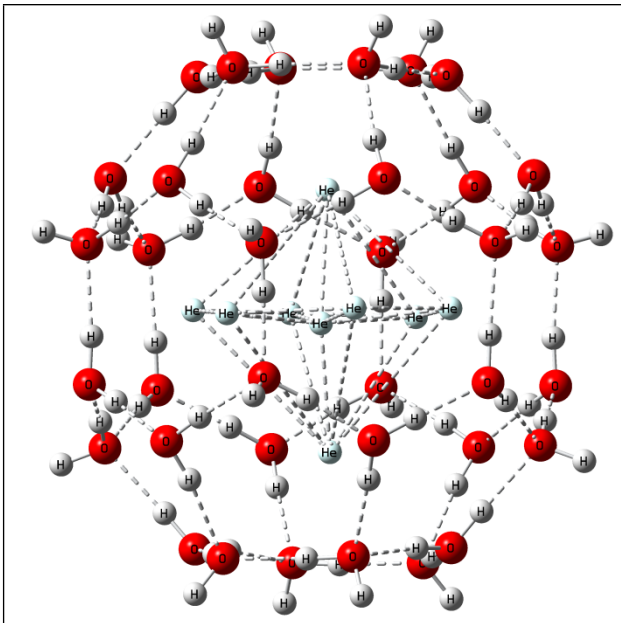


8He@HF$5^{12}6^8$



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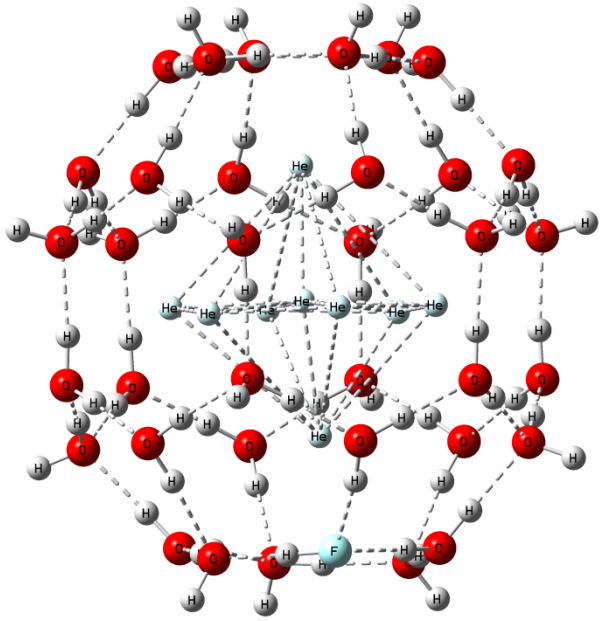

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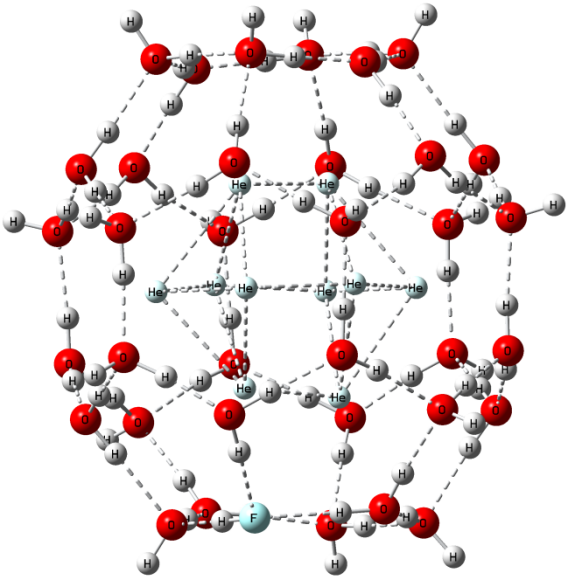

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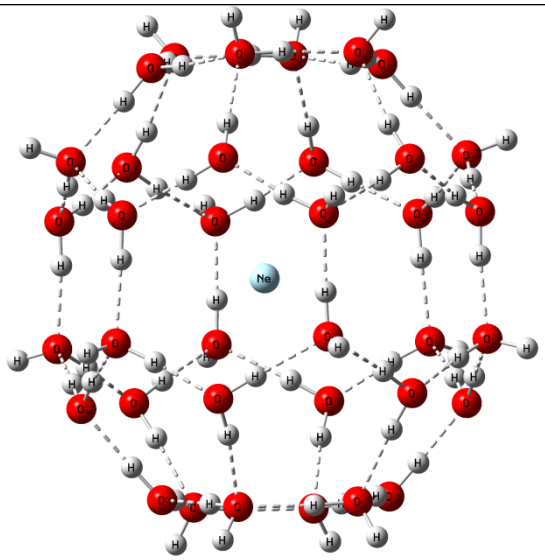
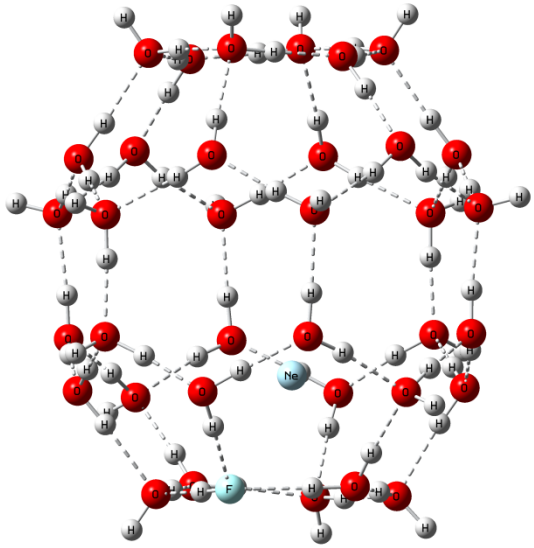
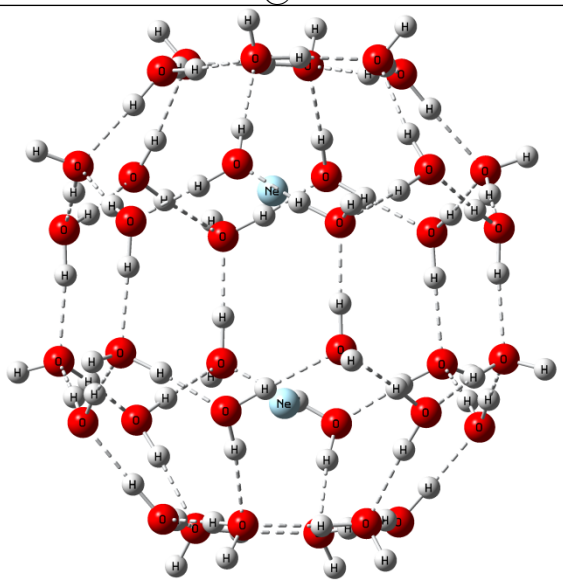
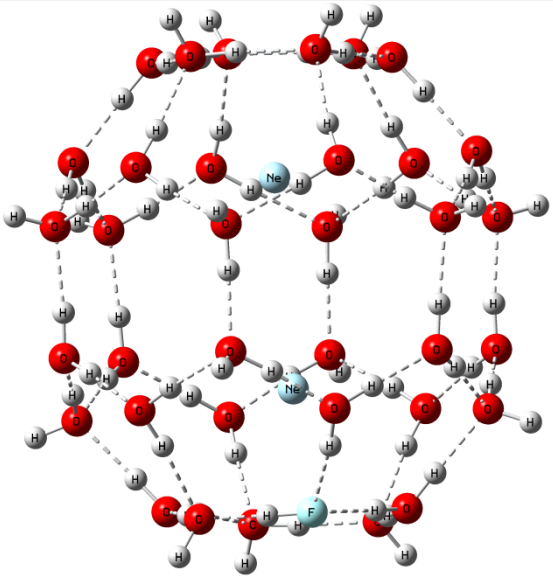
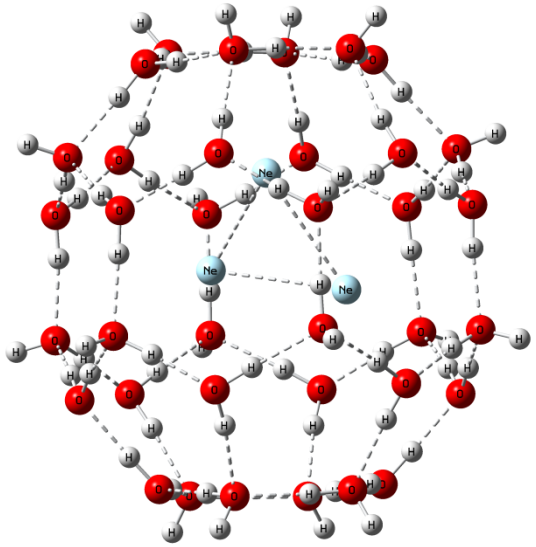
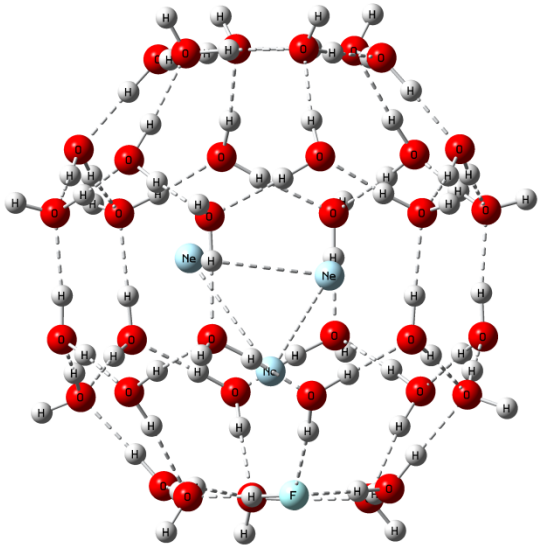
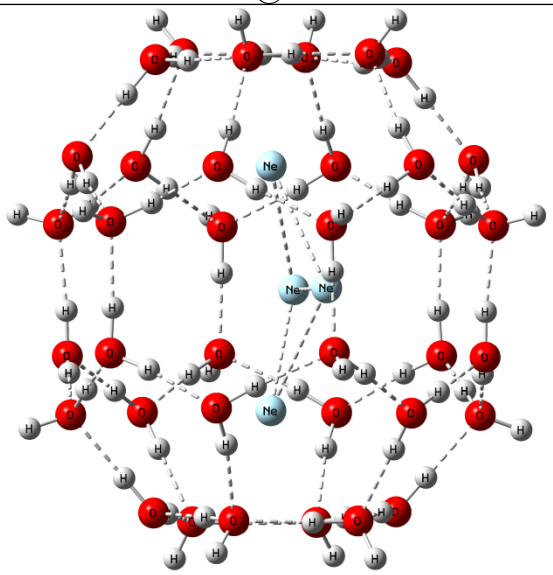
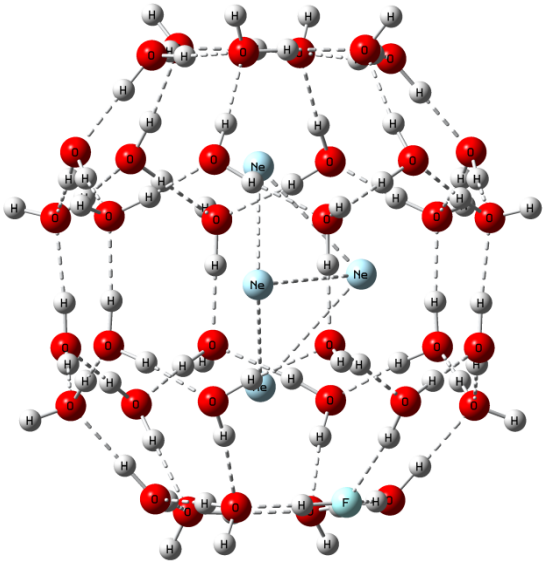
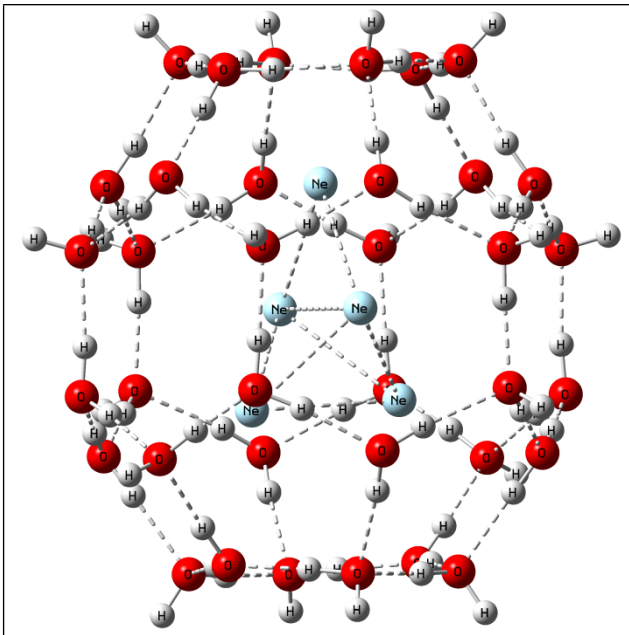
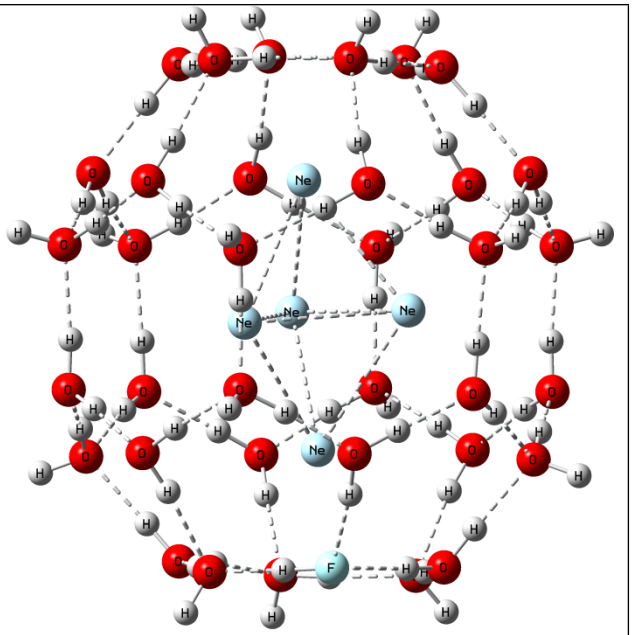
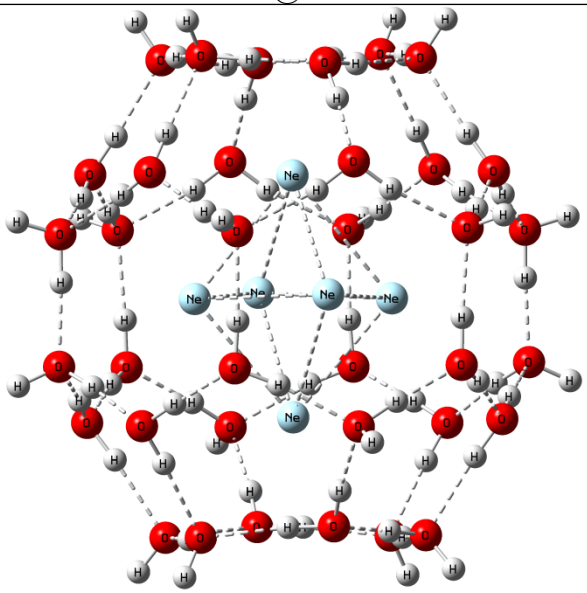
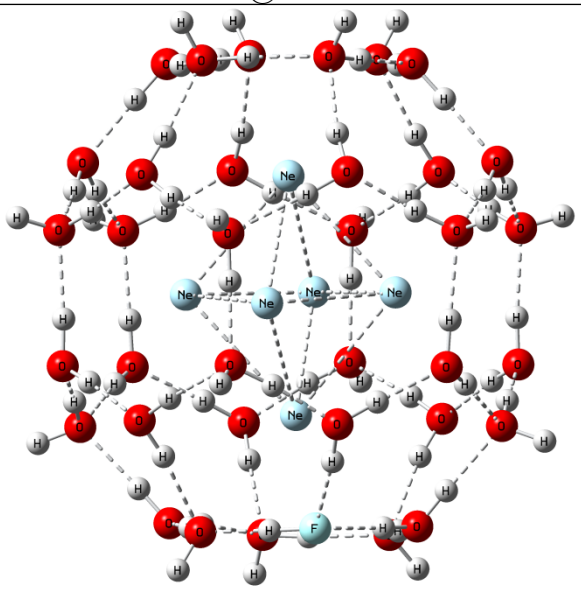
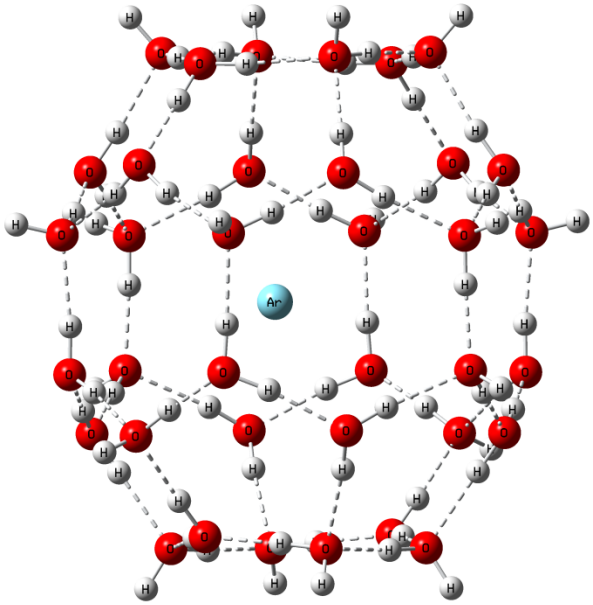
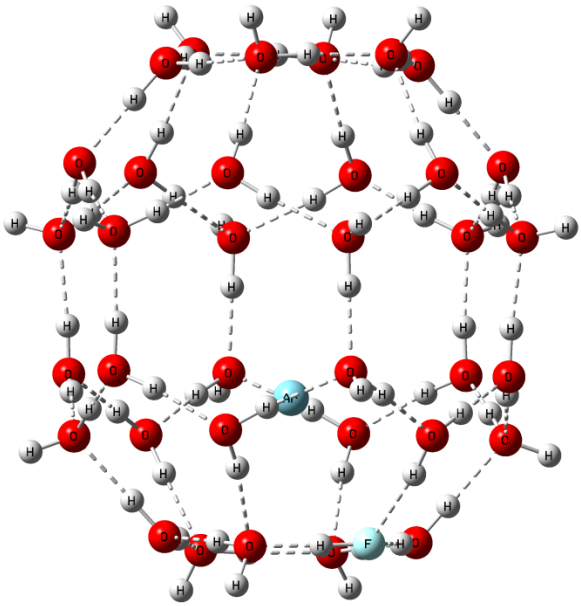
	
1Ne@$5^{12}6^{8}$	**1Ne@HF$5^{12}6^{8}$**
	
2Ne@$5^{12}6^{8}$	**2Ne@HF$5^{12}6^{8}$**

	
3Ne@$5^{12}6^8$	**3Ne@HF$5^{12}6^8$**
	
4Ne@$5^{12}6^8$	**4Ne@HF$5^{12}6^8$**

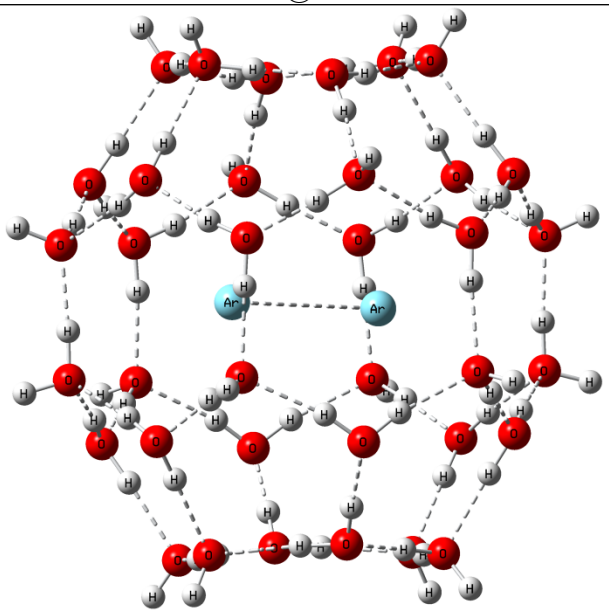
	
$5Ne@5^{12}6^{8}$	**$5Ne@HF5^{12}6^{8}$**
	
$6Ne@5^{12}6^{8}$	**$6Ne@HF5^{12}6^{8}$**



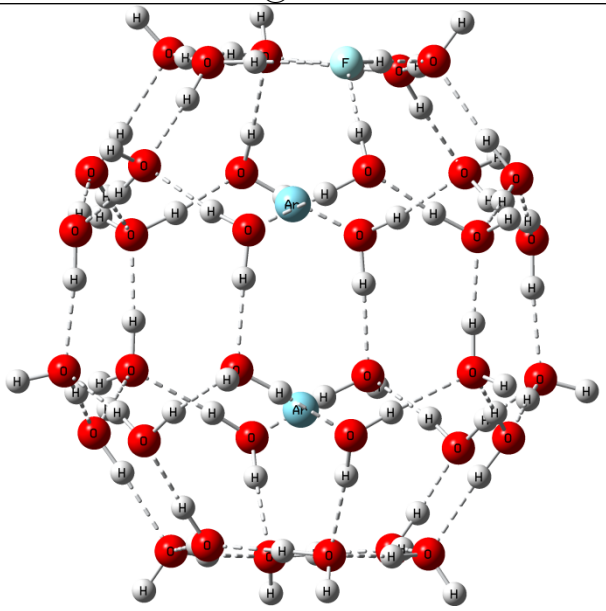
1Ar@$5^{12}6^8$



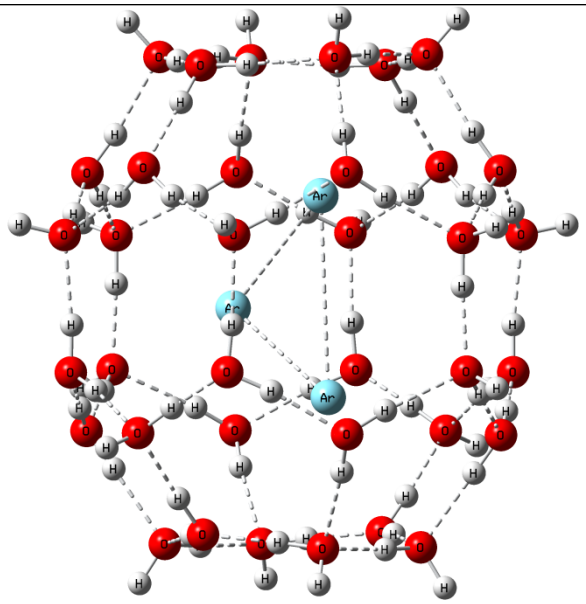
1Ar@HF$5^{12}6^8$



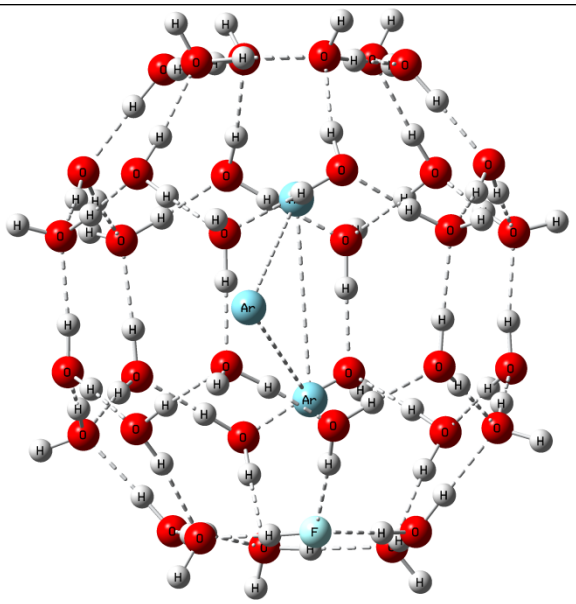
2Ar@$5^{12}6^8$



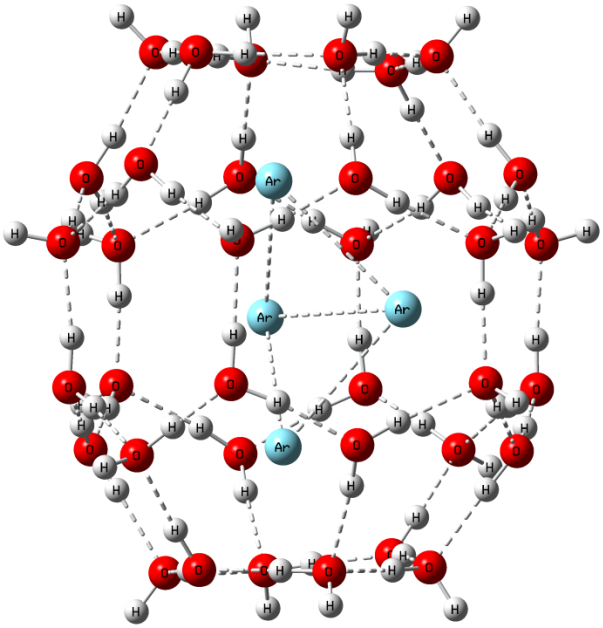
2Ar@HF$5^{12}6^8$



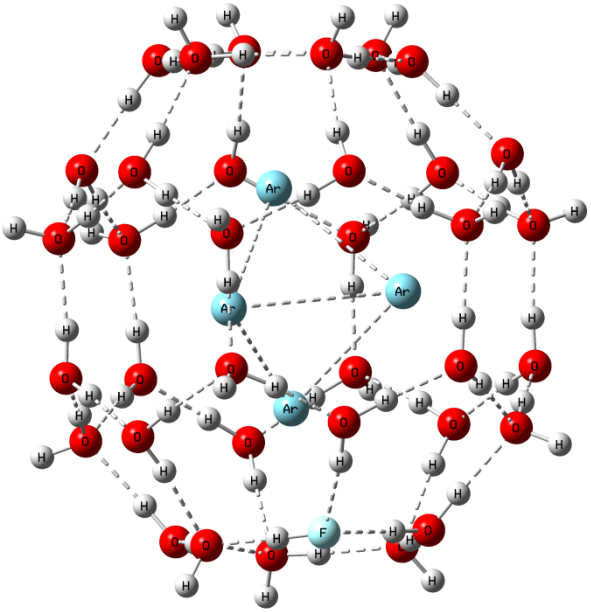
3Ar@$5^{12}6^8$



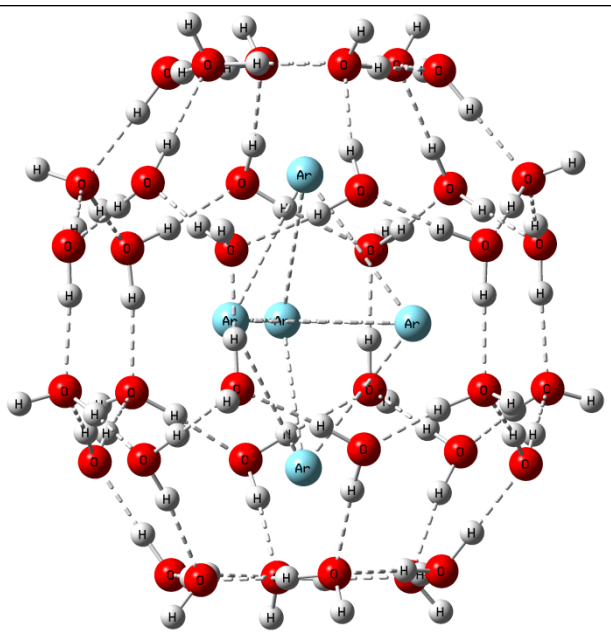
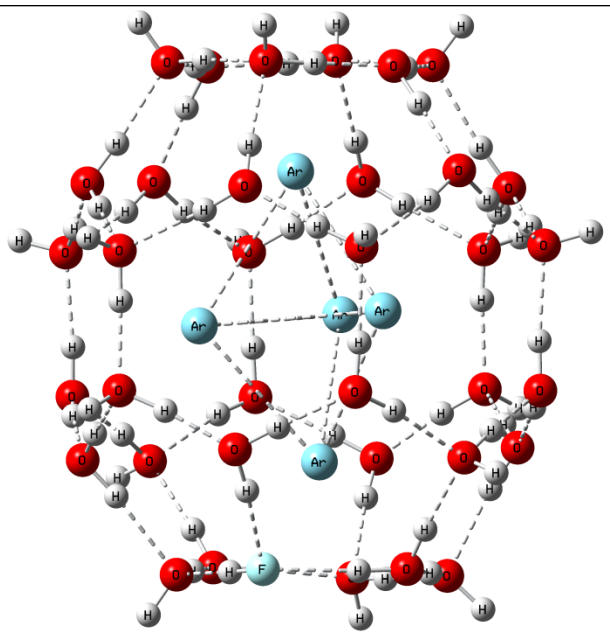
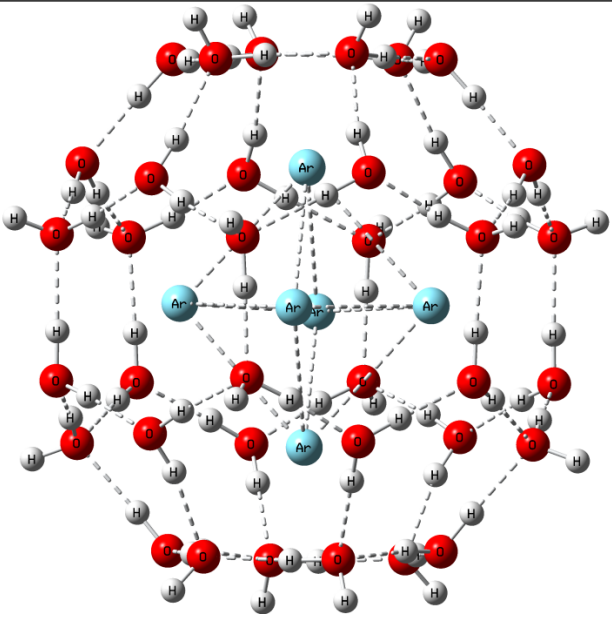
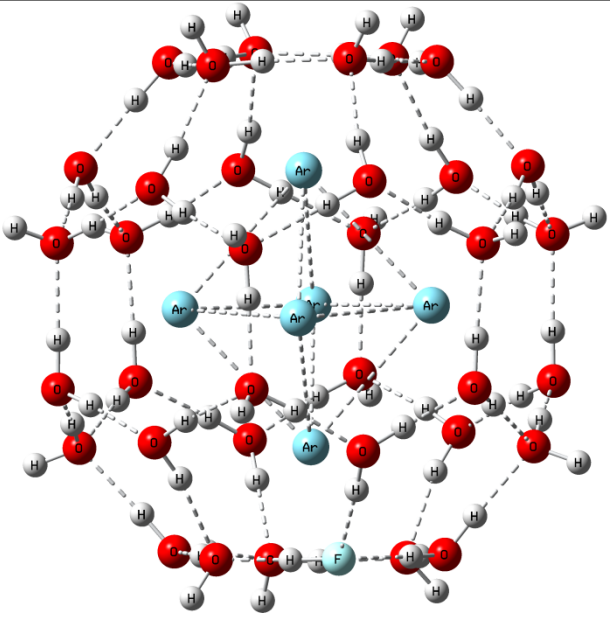
3Ar@HF$5^{12}6^8$



4Ar@$5^{12}6^8$



4Ar@HF$5^{12}6^8$

	
5Ar@$5^{12}6^8$	**5Ar@HF$5^{12}6^8$**
	
6Ar@$5^{12}6^8$	**6Ar@HF$5^{12}6^8$**