Non-paper Materials

All-metal and Nonmetal Clusters and their Gas Storage Potential

Thesis submitted to the

Indian Institute of Technology Kharagpur

For award of the degree

of

Doctor of Philosophy

by

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DECEMBER 2014

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Table 3.N1: Hardness (η, eV) and electrophilicity (ω, eV) values calculated at *ω*B97X-D/6-311+G(d,p) level of theory for the nNg@5^{12} and nNg@HF5^{12} systems.

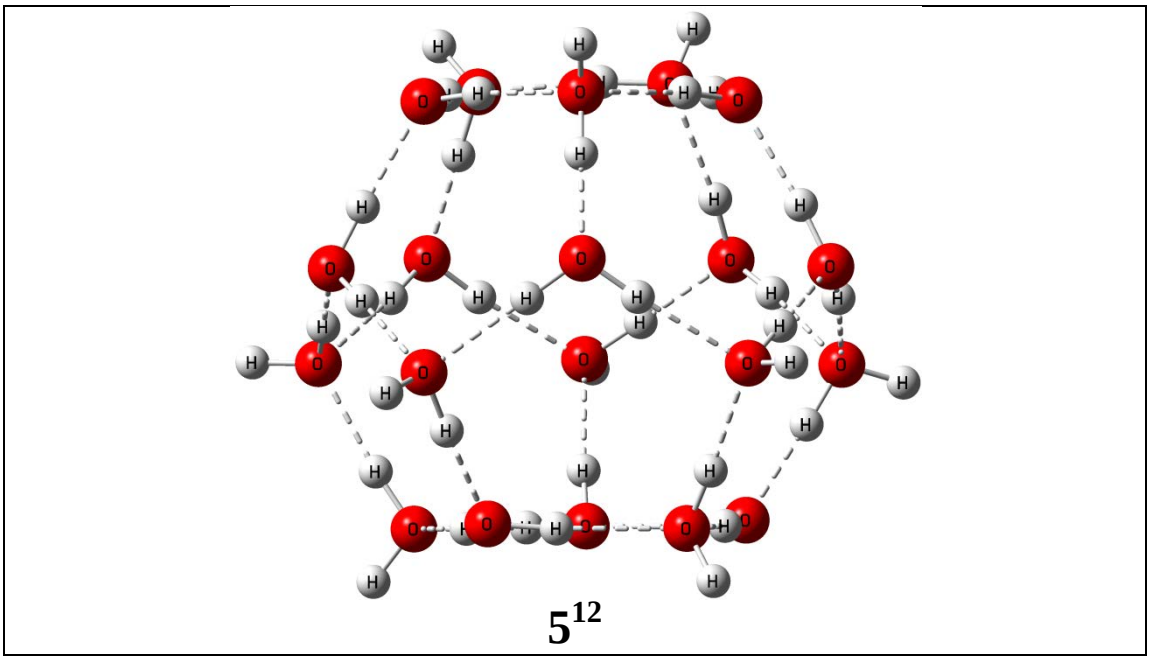
Systems	η	ω	Systems	η	ω
5^{12}	12.020	0.759	HF5^{12}	12.067	0.798
1He@5^{12}	12.173	0.724	1He@HF5^{12}	12.220	0.761
2He@5^{12}	12.242	0.717	2He@HF5^{12}	12.303	0.746
3He@5^{12}	12.323	0.694	3He@HF5^{12}	12.371	0.729
4He@5^{12}	12.361	0.693	4He@HF5^{12}	12.407	0.729
5He@5^{12}	12.374	0.697	5He@HF5^{12}	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 3.N2: Hardness (η, eV) and electrophilicity (ω, eV) values calculated at *ω*B97X-D/6-311+G(d,p) level of theory for the nNg@$5^{12}6^{8}$ and nNg@HF$5^{12}6^{8}$ systems.

Systems	η	ω	Systems	η	ω
$5^{12}6^{8}$	11.872	0.733	HF$5^{12}6^{8}$	11.887	0.747
1He@$5^{12}6^{8}$	11.890	0.728	1He@HF$5^{12}6^{8}$	11.903	0.744
2He@$5^{12}6^{8}$	11.929	0.720	2He@HF$5^{12}6^{8}$	11.944	0.734
3He@$5^{12}6^{8}$	11.922	0.721	3He@HF$5^{12}6^{8}$	11.936	0.736
4He@$5^{12}6^{8}$	11.974	0.710	4He@HF$5^{12}6^{8}$	11.981	0.726
5He@$5^{12}6^{8}$	11.990	0.707	5He@HF$5^{12}6^{8}$	12.007	0.721
6He@$5^{12}6^{8}$	12.006	0.703	6He@HF$5^{12}6^{8}$	12.022	0.716
7He@$5^{12}6^{8}$	12.026	0.702	7He@HF$5^{12}6^{8}$	12.067	0.707
8He@$5^{12}6^{8}$	12.042	0.702	8He@HF$5^{12}6^{8}$	12.061	0.716

9He@$5^{12}6^8$	12.084	0.696	9He@HF$5^{12}6^8$	12.108	0.708
10He@$5^{12}6^8$	-	-	10He@HF$5^{12}6^8$	12.132	0.698
1Ne@$5^{12}6^8$	11.853	0.737	1Ne@HF$5^{12}6^8$	11.877	0.750
2Ne@$5^{12}6^8$	11.855	0.738	2Ne@HF$5^{12}6^8$	11.867	0.753
3Ne@$5^{12}6^8$	11.852	0.737	3Ne@HF$5^{12}6^8$	11.871	0.754
4Ne@$5^{12}6^8$	11.888	0.733	4Ne@HF$5^{12}6^8$	11.893	0.749
5Ne@$5^{12}6^8$	11.900	0.732	5Ne@HF$5^{12}6^8$	11.916	0.745
6Ne@$5^{12}6^8$	11.920	0.724	6Ne@HF$5^{12}6^8$	11.933	0.738
1Ar@$5^{12}6^8$	11.744	0.763	1Ar@HF$5^{12}6^8$	11.792	0.771
2Ar@$5^{12}6^8$	11.798	0.749	2Ar@HF$5^{12}6^8$	11.822	0.765
3Ar@$5^{12}6^8$	11.840	0.737	3Ar@HF$5^{12}6^8$	11.851	0.752
4Ar@$5^{12}6^8$	11.887	0.738	4Ar@HF$5^{12}6^8$	11.901	0.755
5Ar@$5^{12}6^8$	11.924	0.741	5Ar@HF$5^{12}6^8$	11.938	0.754
6Ar@$5^{12}6^8$	11.938	0.736	6Ar@HF$5^{12}6^8$	11.953	0.750

Figure 3.N1: Minimum energy structures of 5^{12} and $5^{12}6^8$ at ωB97X-D/6-311+G(d,p) level of theory.



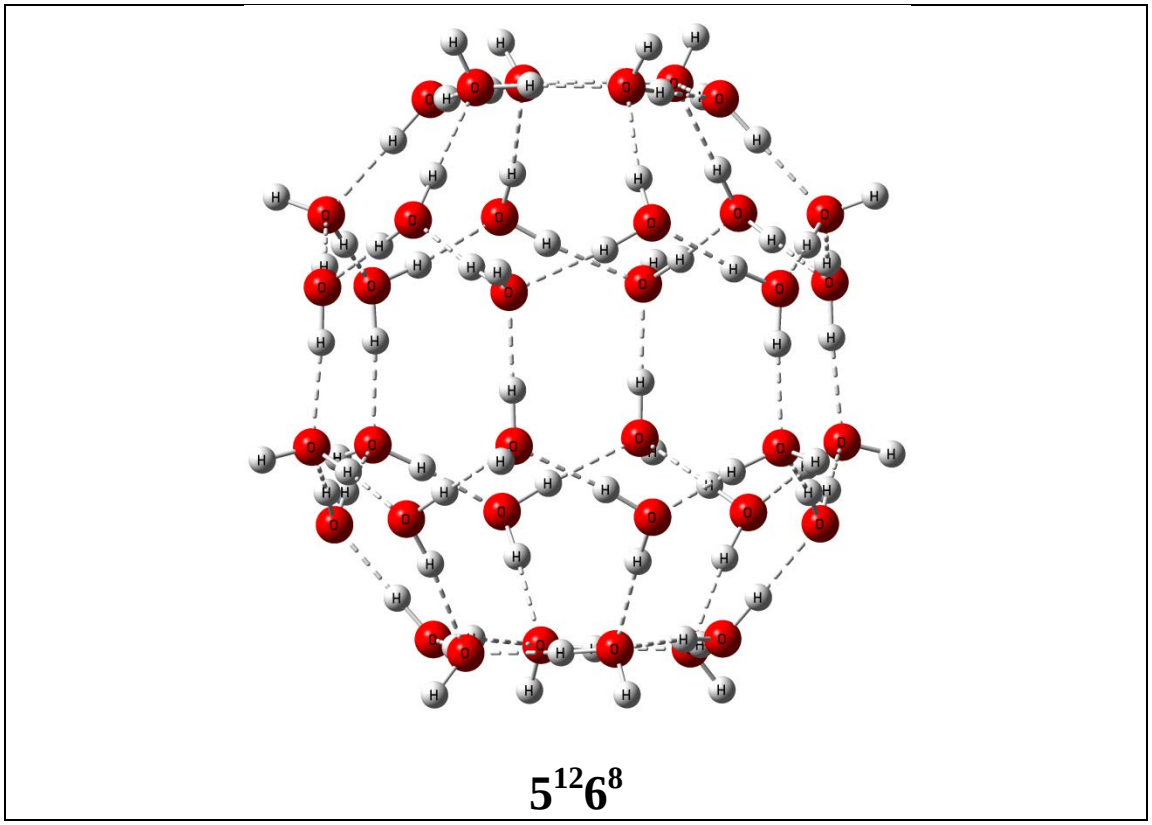
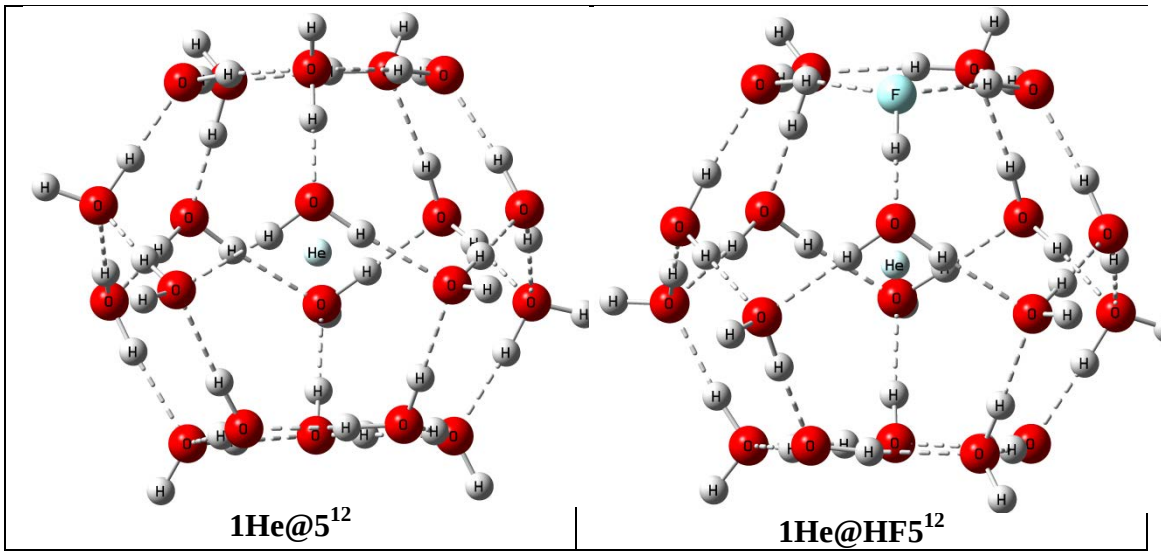
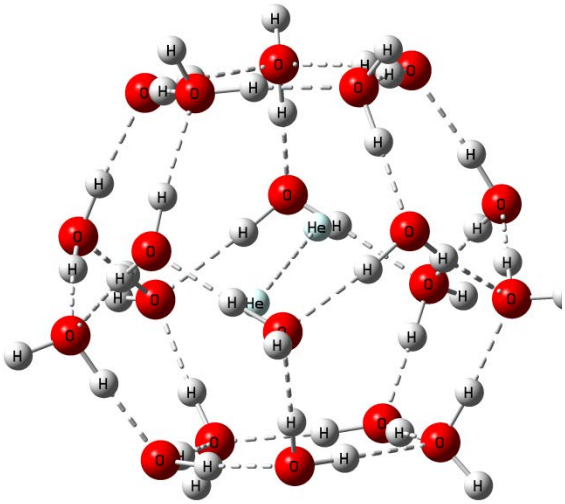
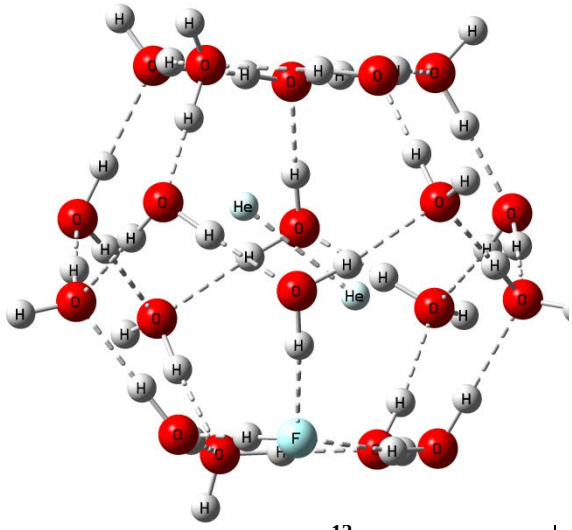


Figure 3.N2: Minimum energy structures of nNg@5^{12}, nNg@HF5^{12} {Ng = He (n = 1 - 5), Ne (n = 1 - 3), Ar (n = 1 - 2)} and nNg@$5^{12}6^{8}$, nNg@HF$5^{12}6^{8}$ {Ng = He (n = 1 – 9/10), Ne and Ar (n = 1 - 6)} at ωB97X-D/6-311+G(d,p) level of theory.





2He@5^{12}



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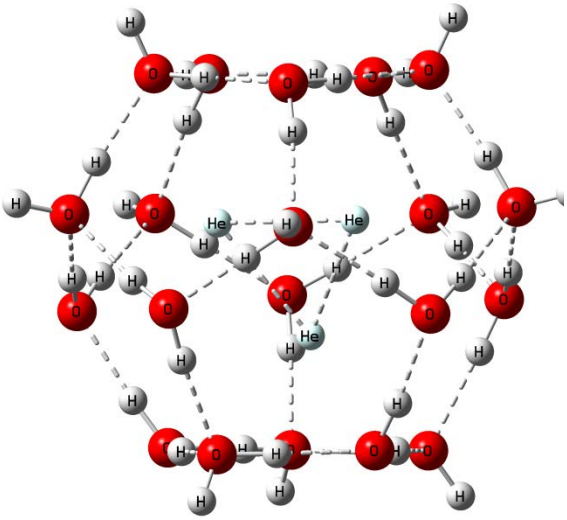

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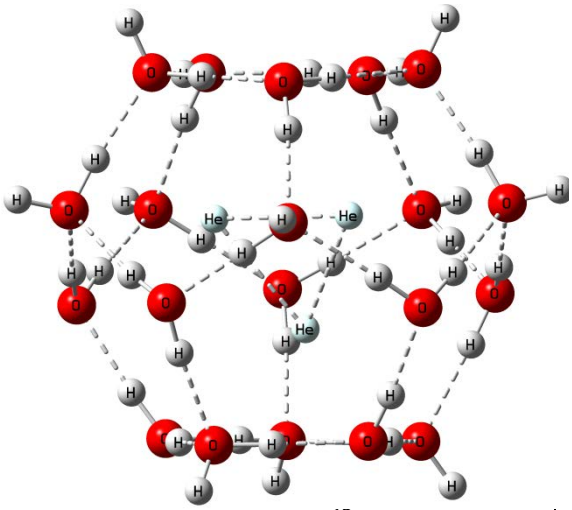
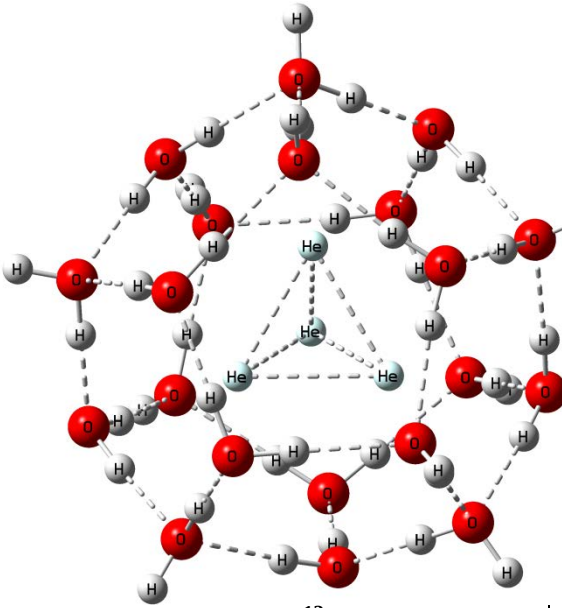
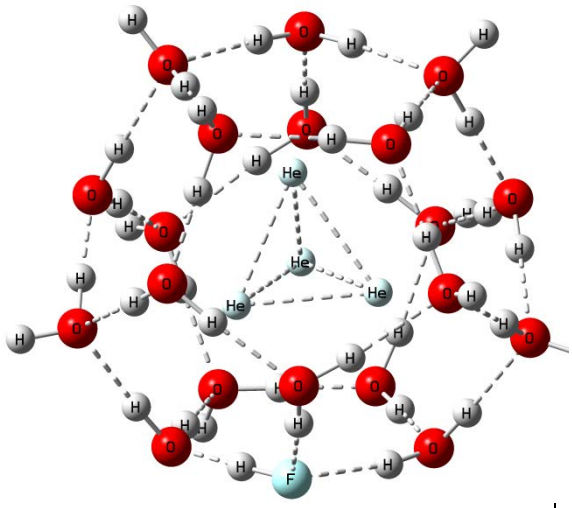


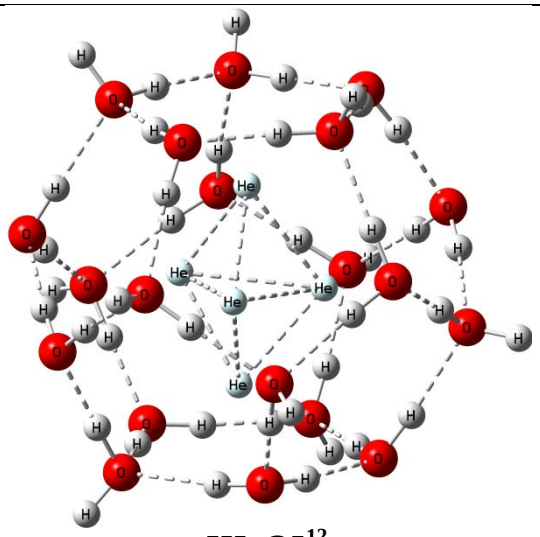
3He@HF5^{12}



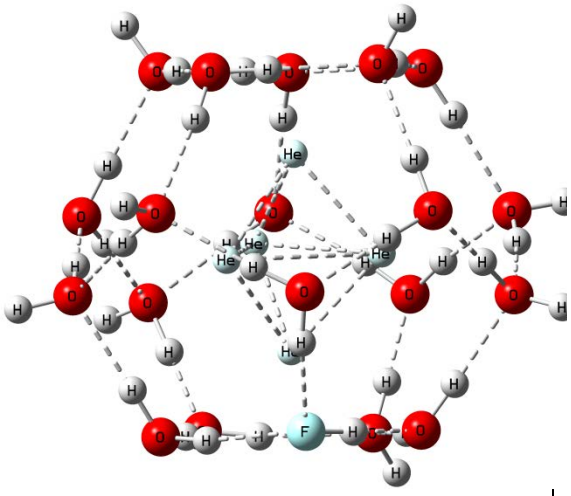
4He@5^{12}



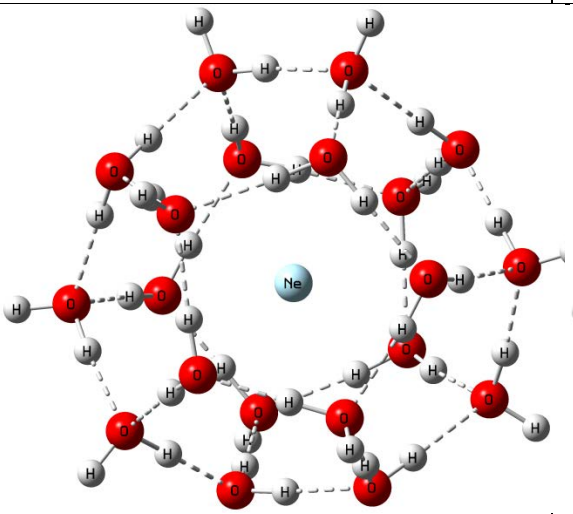
4He@HF5^{12}



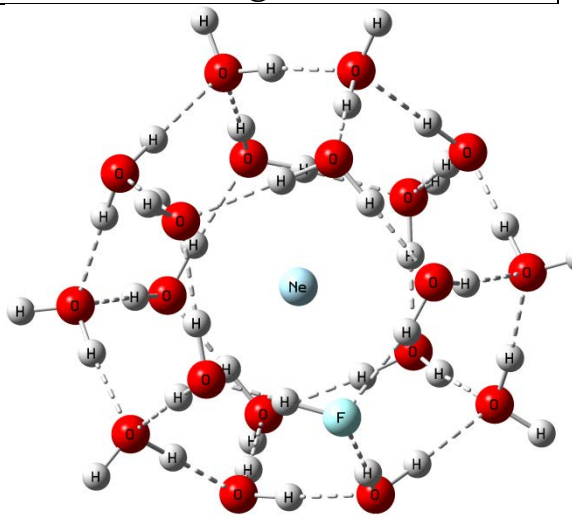
$5He@5^{12}$



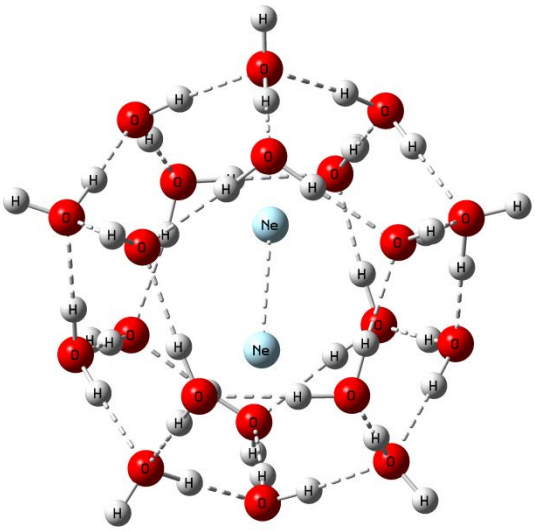
$5He@HF5^{12}$



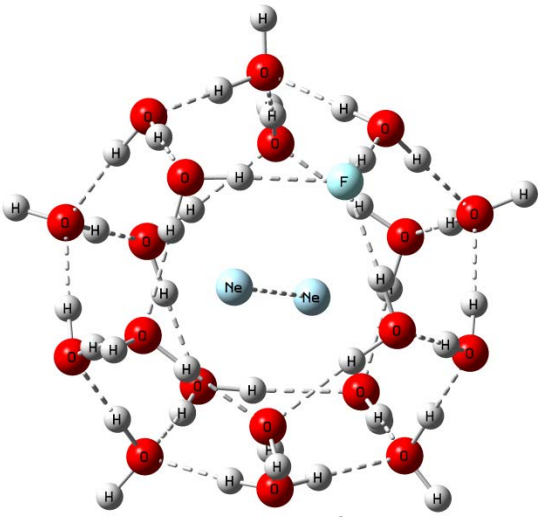
$1Ne@5^{12}$



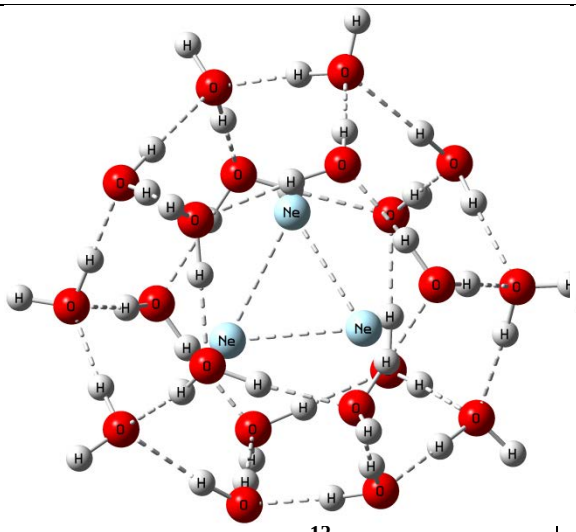
$1Ne@HF5^{12}$



$2Ne@5^{12}$



$2Ne@HF5^{12}$



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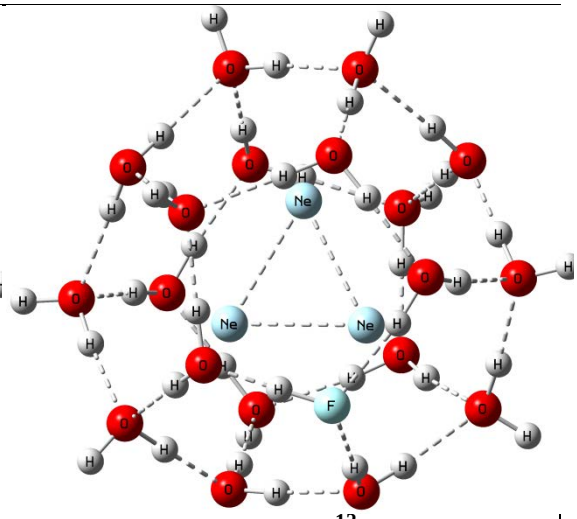
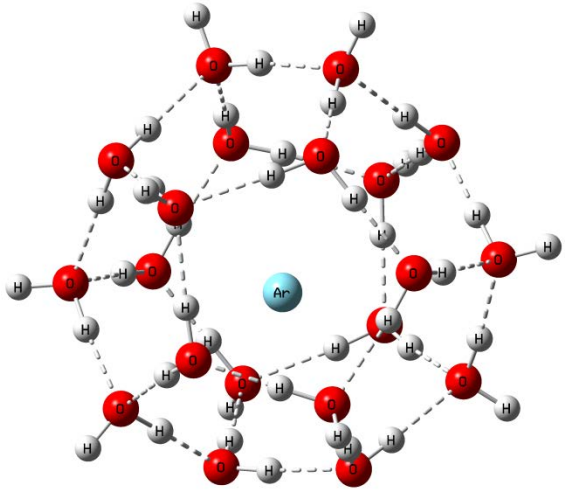
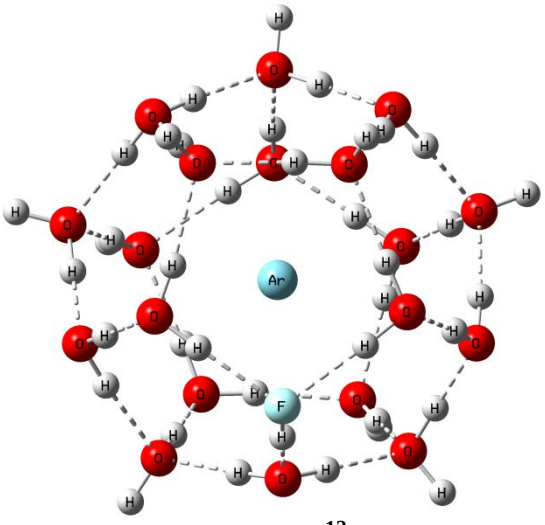


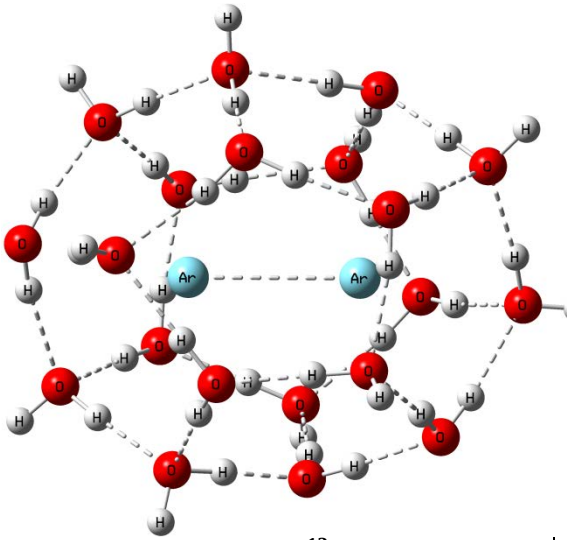
$3Ne@HF5^{12}$



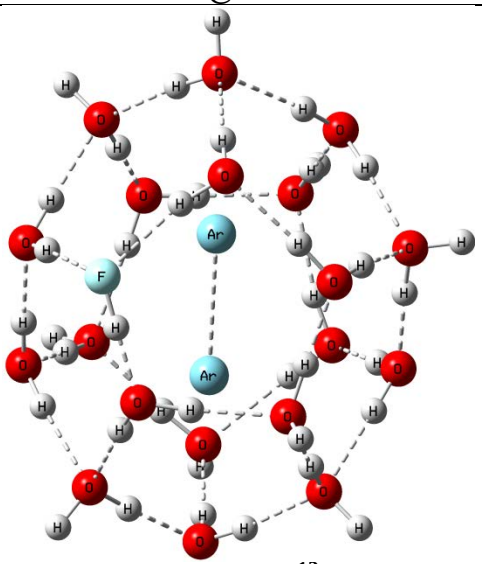
$1Ar@5^{12}$



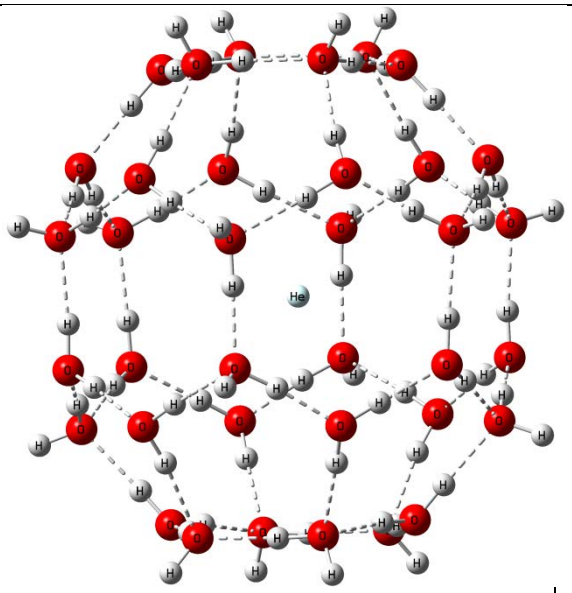
$1Ar@HF5^{12}$



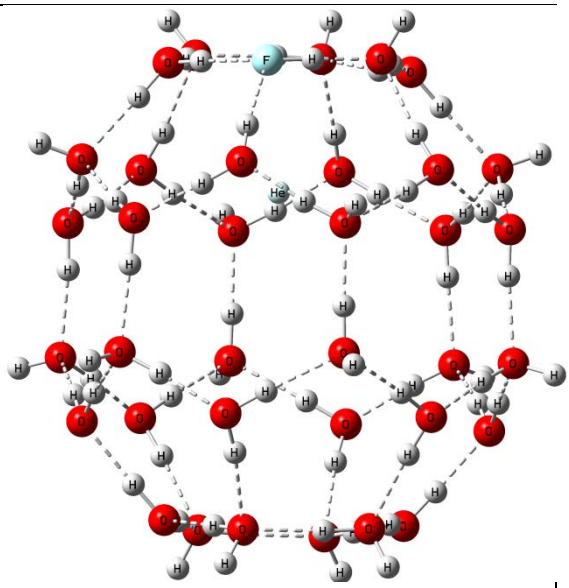
$2Ar@5^{12}$



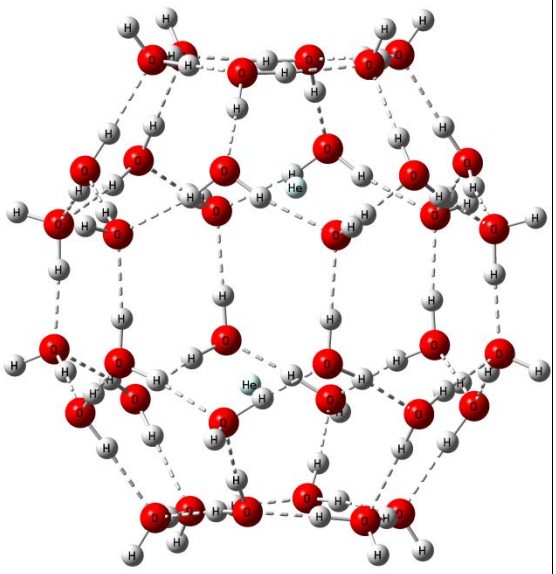
$2Ar@HF5^{12}$



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



$1He@HF5^{12}6^{8}$



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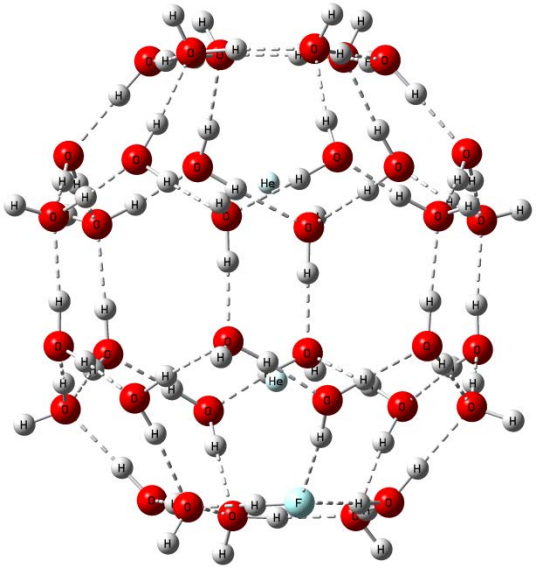
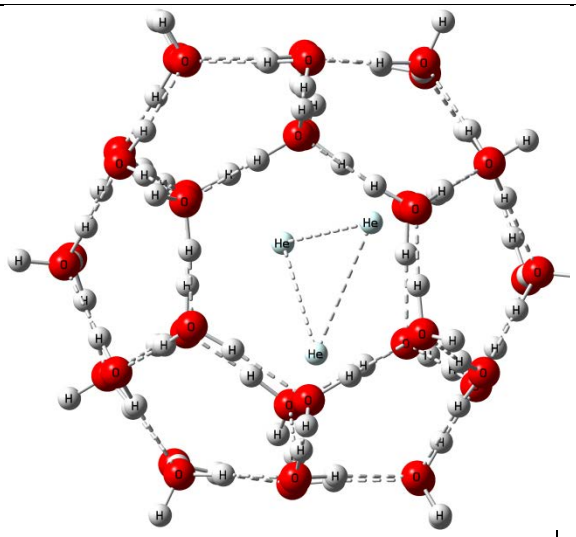


$2He@HF5^{12}6^{8}$



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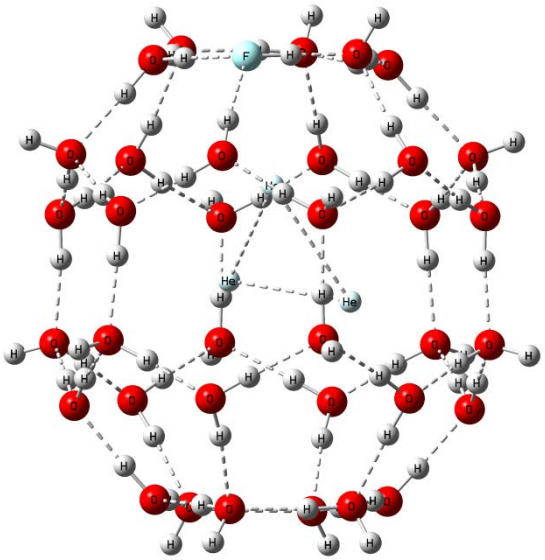
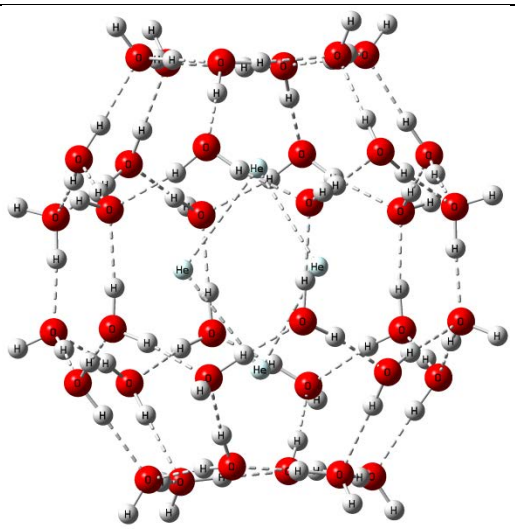


$3He@HF5^{12}6^8$



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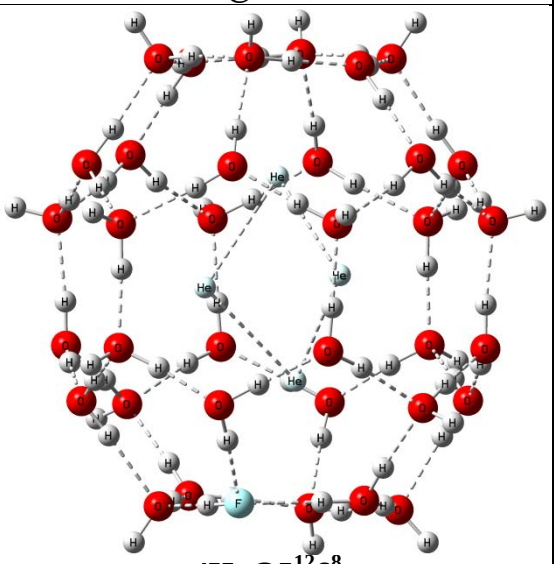
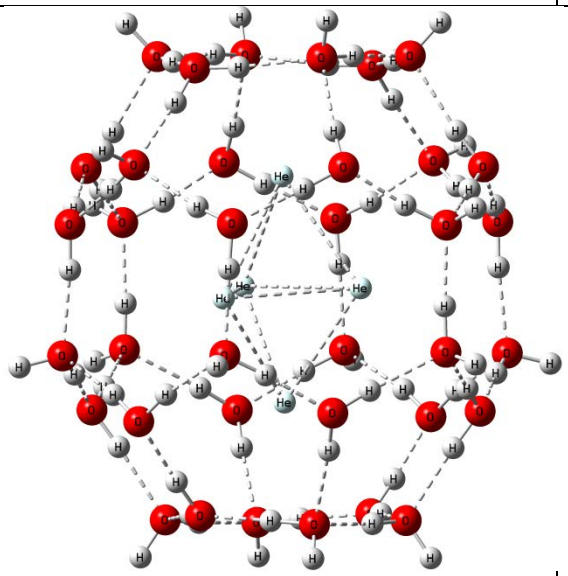
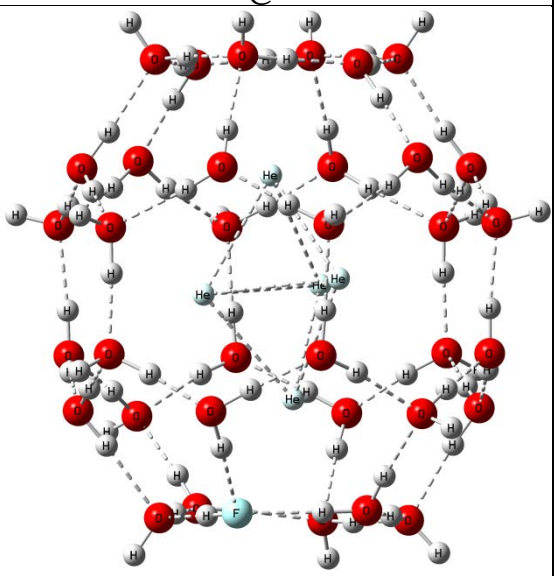


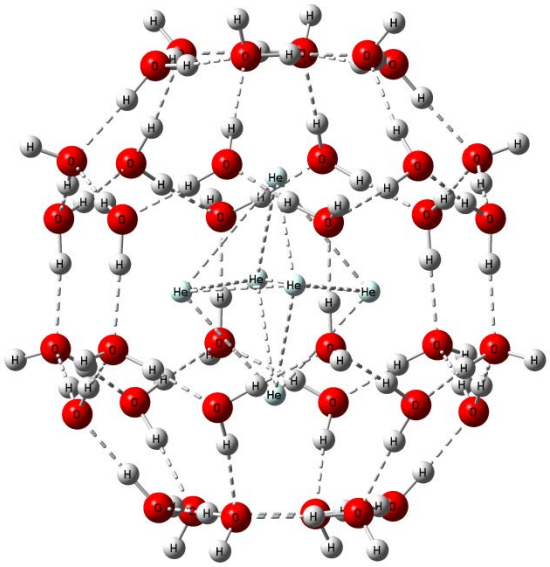
$4He@5^{12}6^8$



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



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



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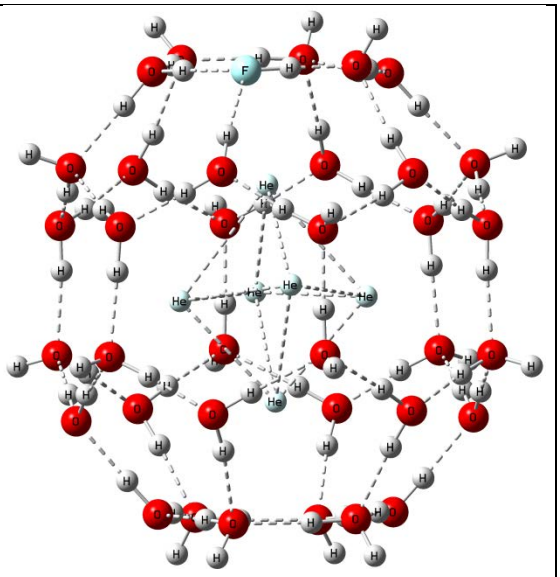
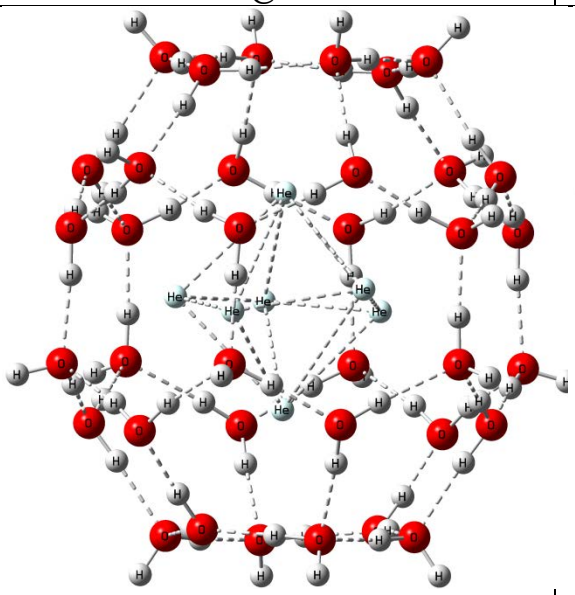
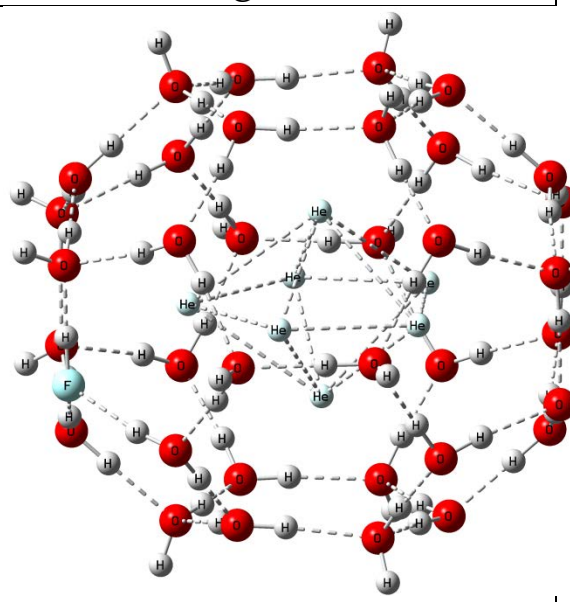


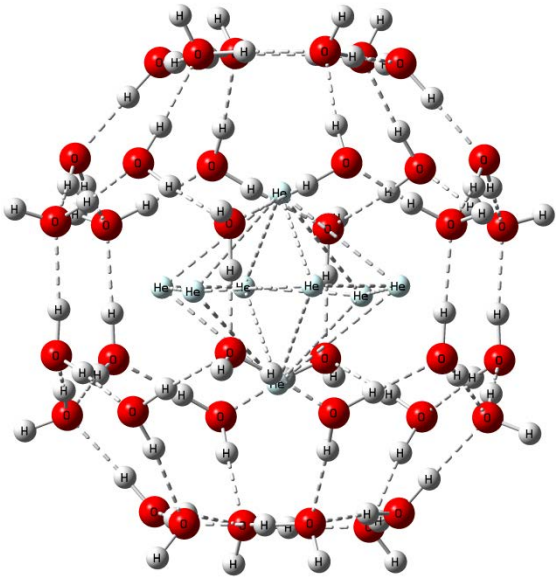
$6He@HF5^{12}6^{8}$



$7He@5^{12}6^{8}$



$7He@HF5^{12}6^{8}$



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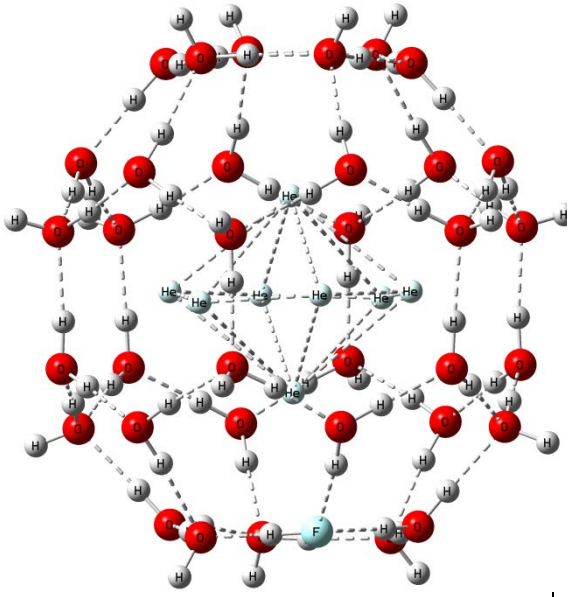
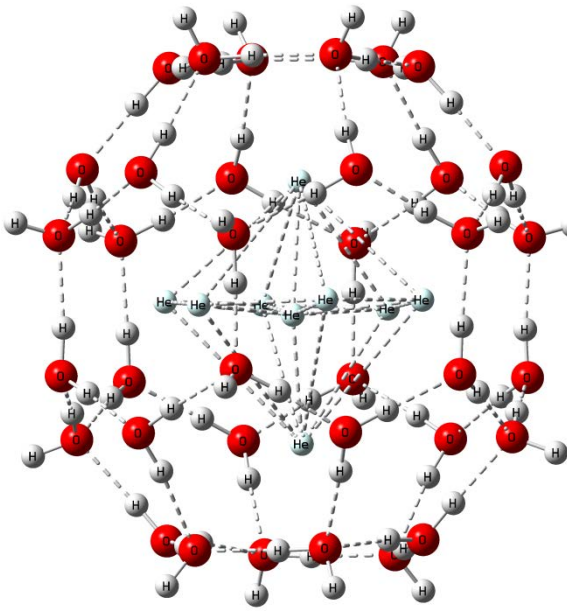


$8He@HF5^{12}6^8$



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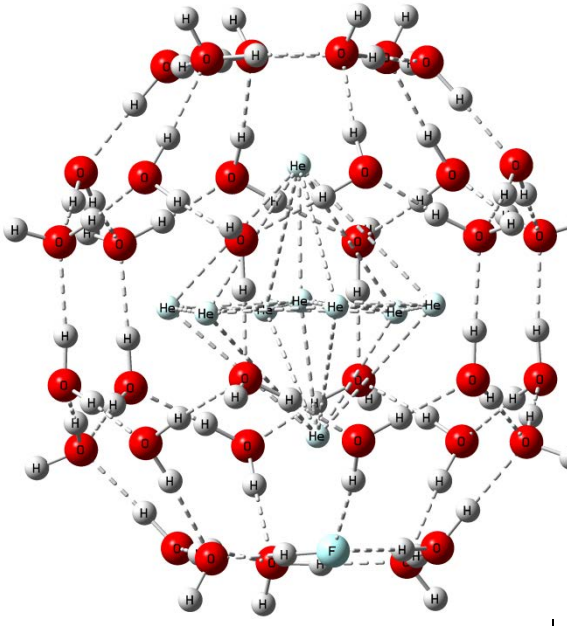
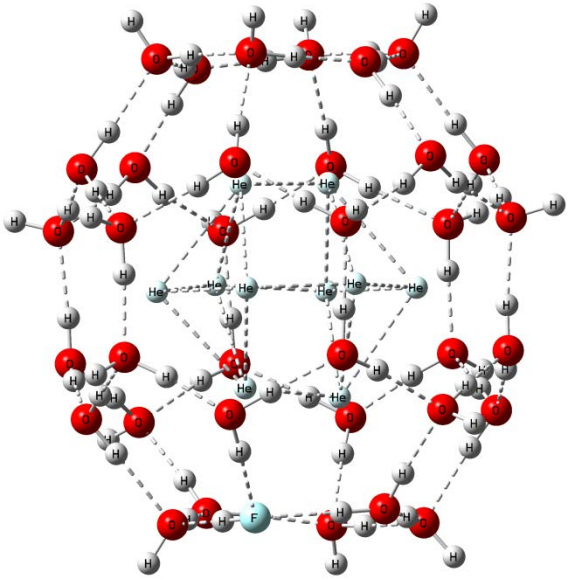
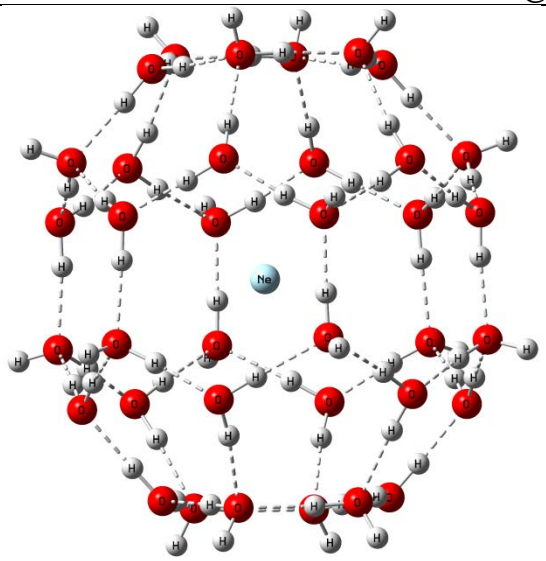


$9He@HF5^{12}6^8$



10He@HF5^{12}6^{8}



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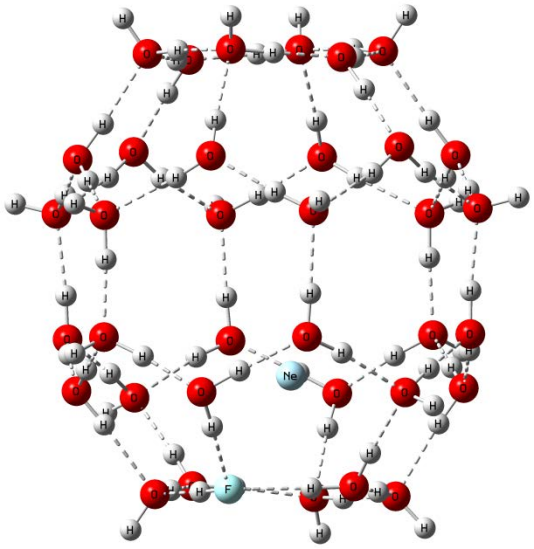
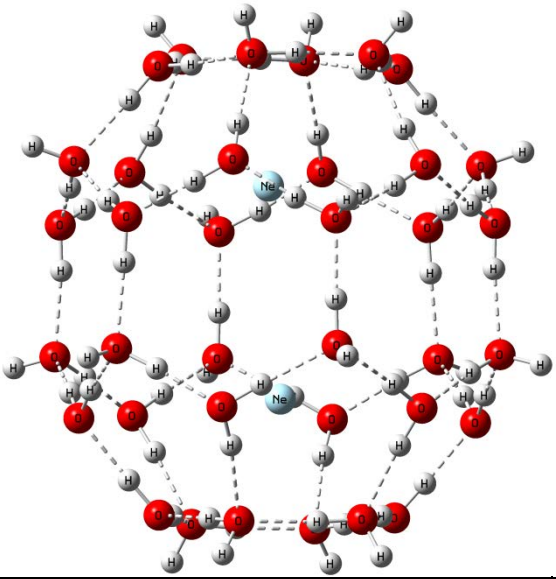
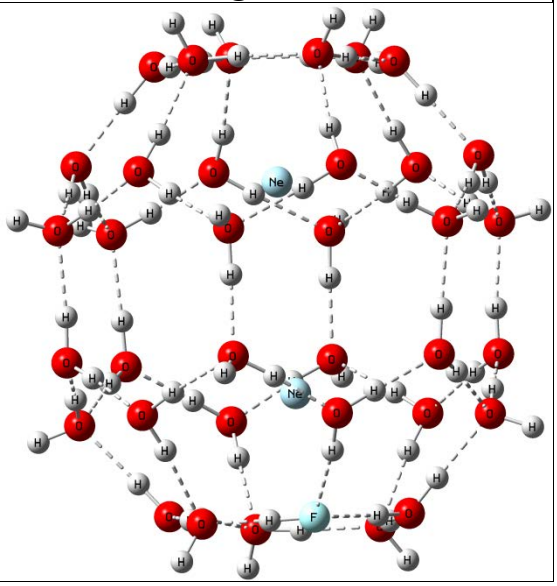
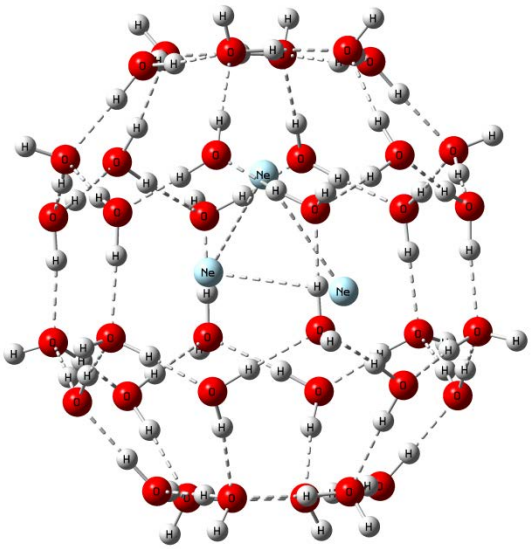
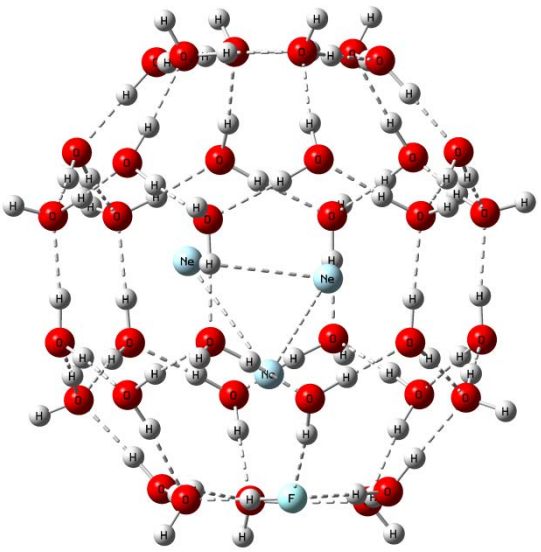


1Ne@HF5^{12}6^{8}





$2Ne@5^{12}6^{8}$	$2Ne@HF5^{12}6^{8}$
	
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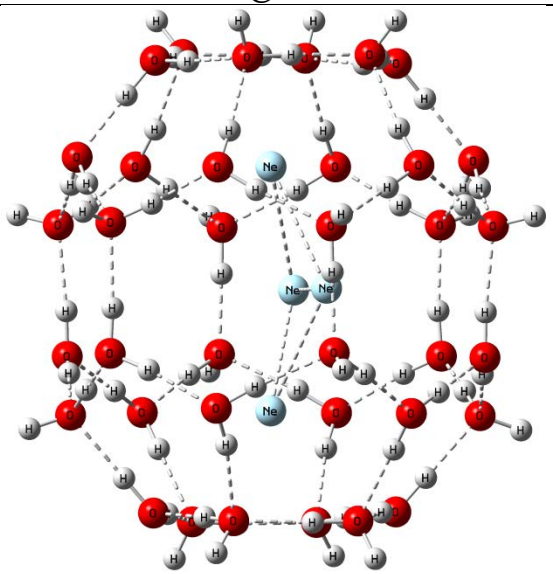	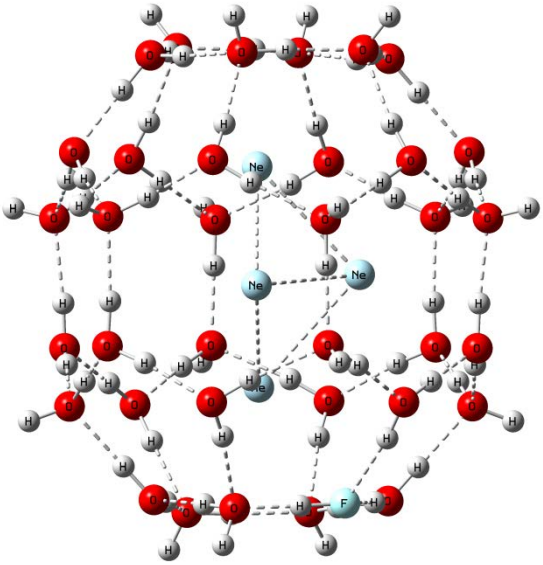
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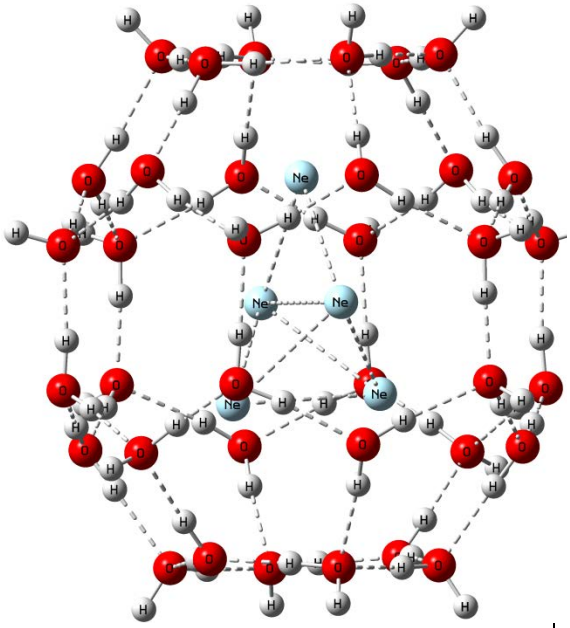

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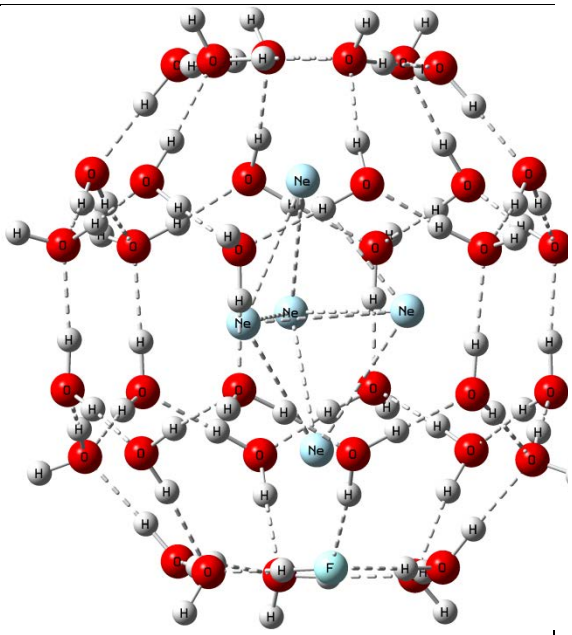

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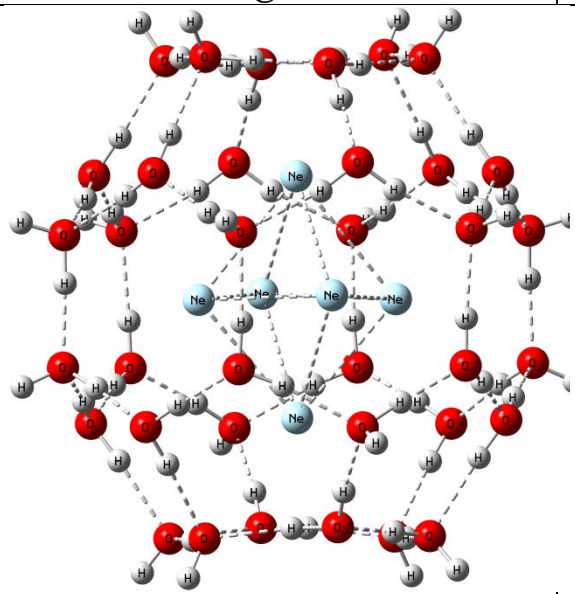

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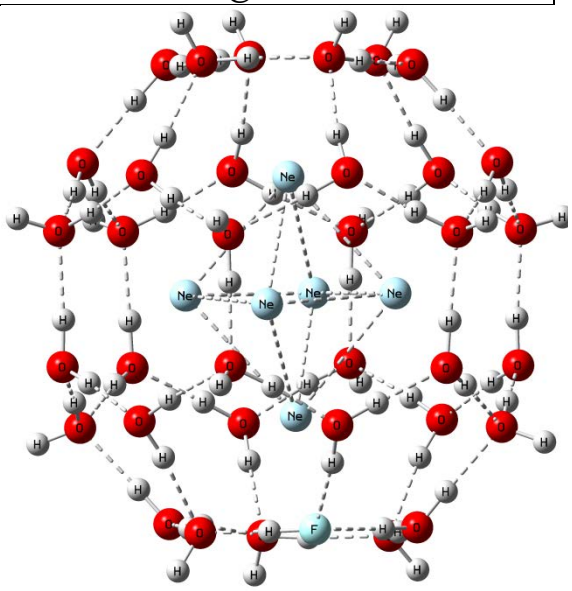

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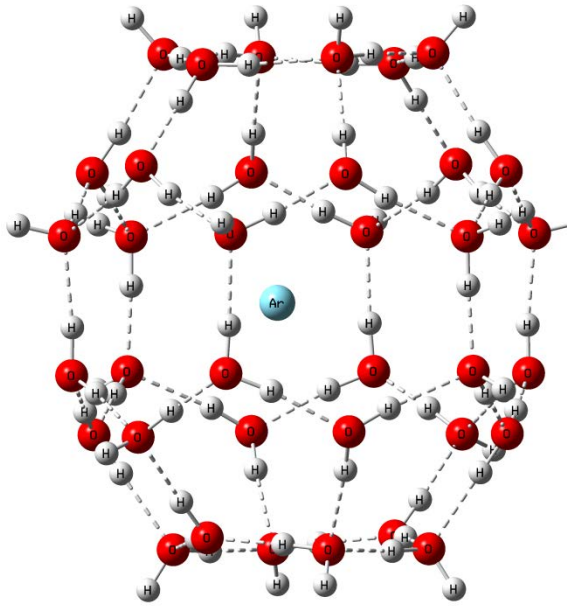

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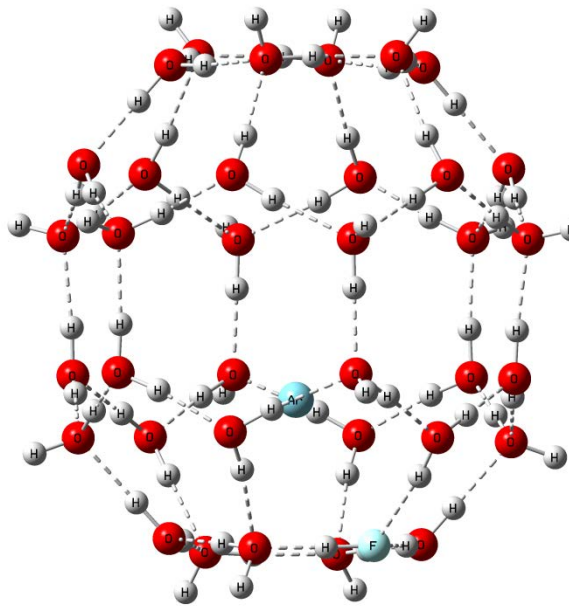

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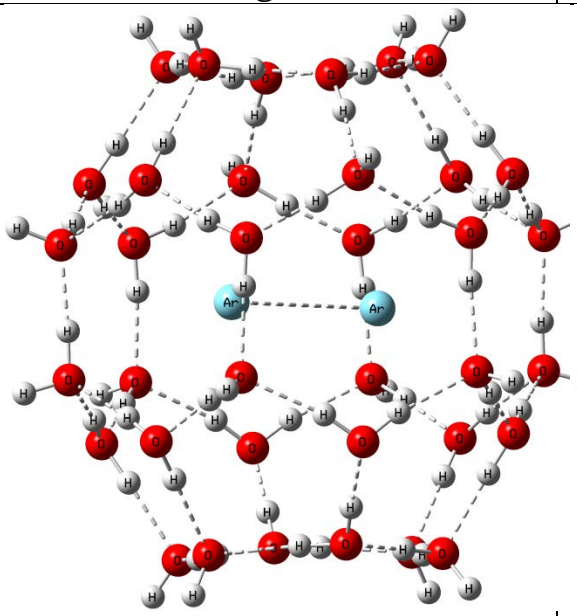

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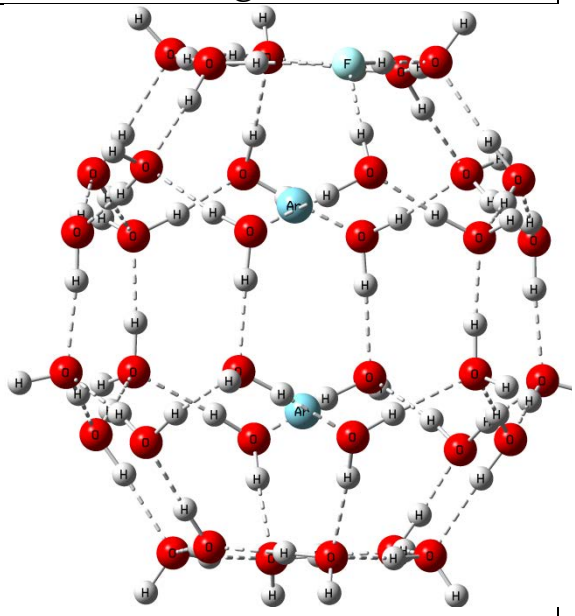

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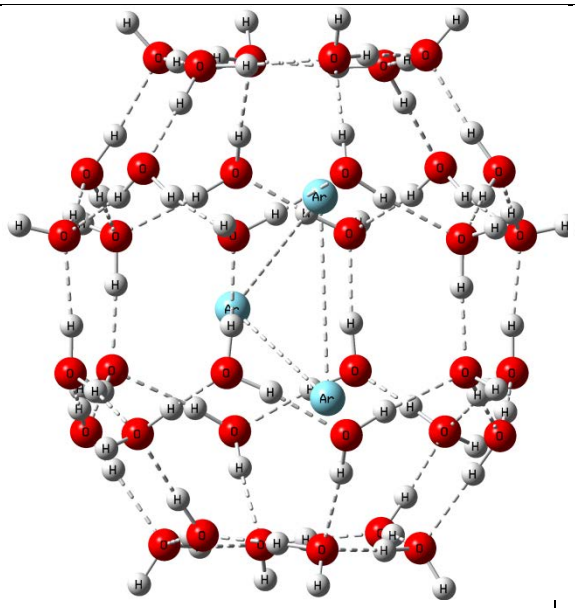

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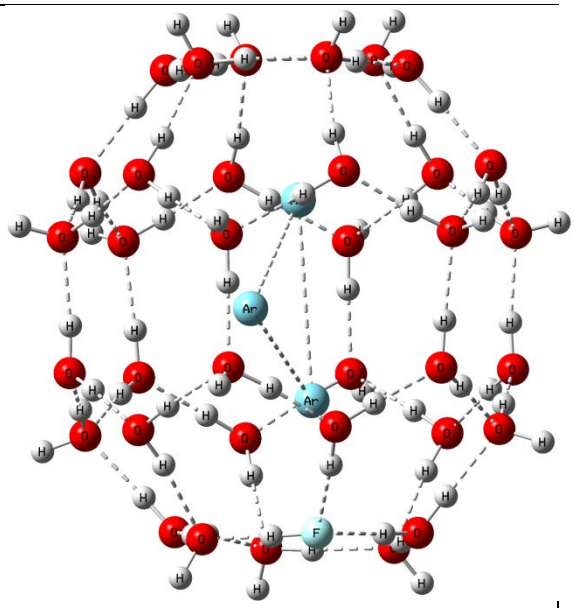

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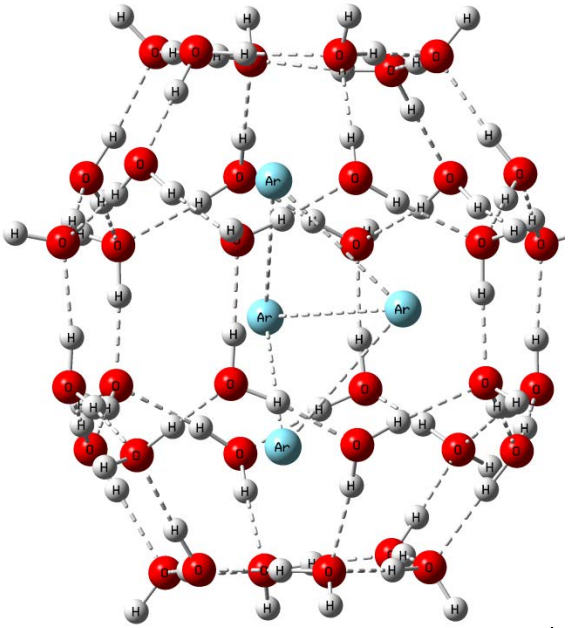

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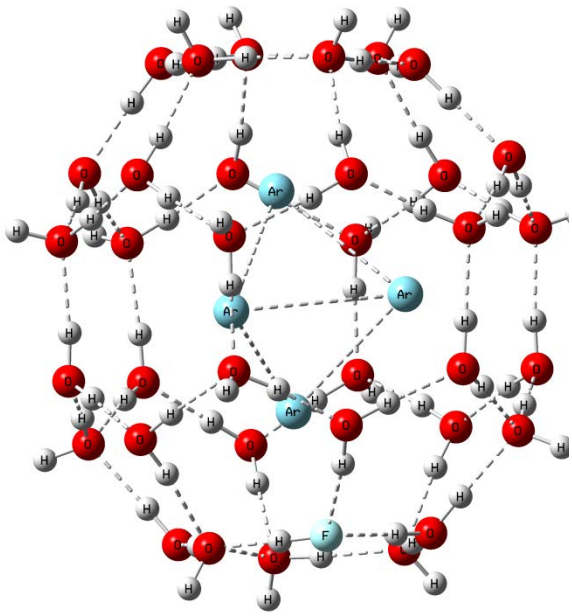

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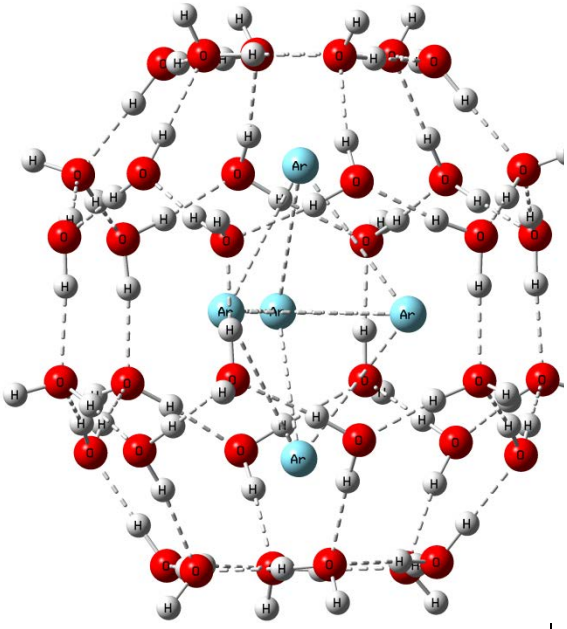

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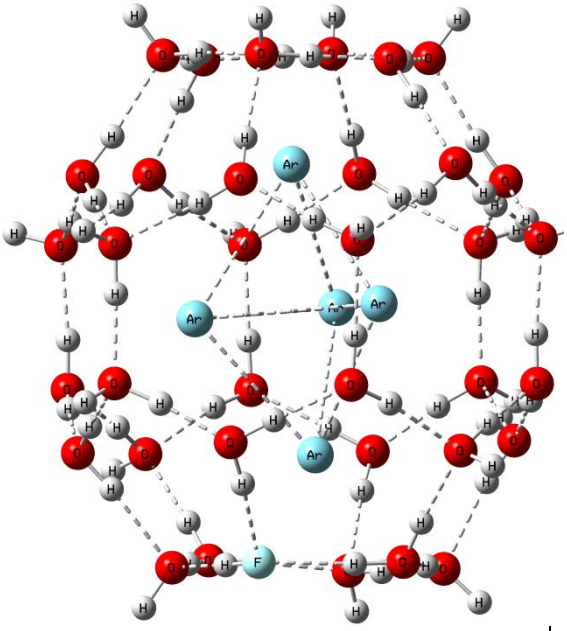

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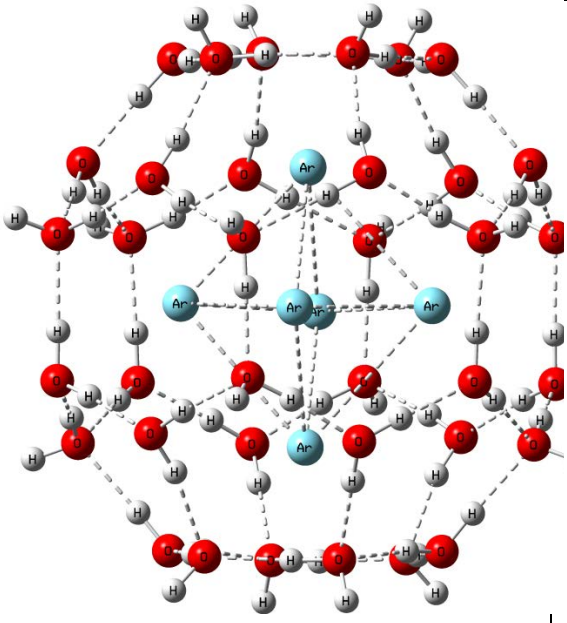

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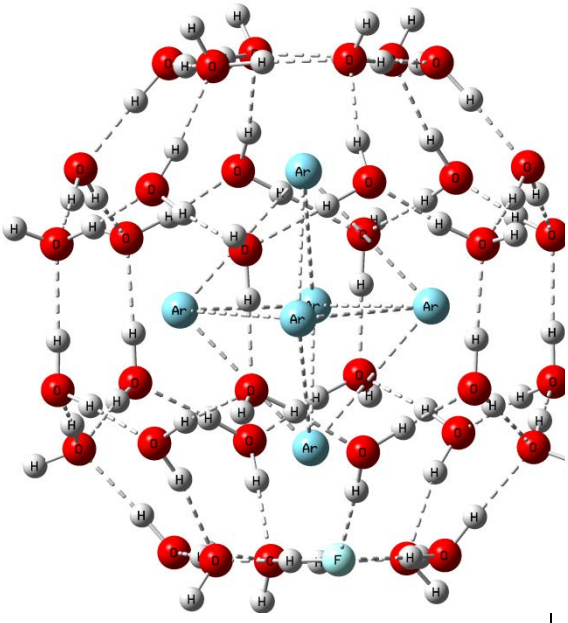

$6Ar@HF5^{12}6^8$