

Incremental DF-LCCSD(T) calculations for a water molecule inside and outside armchair carbon nanotubes

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TABLE I: $\text{H}_2\text{O}@(\text{5,5})\text{CNT}$

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C70H20H2O

C1	3.342639693	0.710500000	0.000000000
C1	3.121873739	1.389947741	1.228354249
C1	2.286630896	2.539560890	1.228354249
C1	1.708658126	2.959482687	0.000000000
C1	0.357206816	3.398595836	0.000000000
C1	-0.357206816	3.398595836	1.228354249
C1	-1.708658126	2.959482687	1.228354249
C1	-2.286630896	2.539560890	0.000000000
C1	-3.121873739	1.389947741	0.000000000
C1	-3.342639693	0.710500000	1.228354249
C1	-3.342639693	-0.710500000	1.228354249
C1	-3.121873739	-1.389947741	0.000000000
C1	-2.286630896	-2.539560890	0.000000000
C1	-1.708658126	-2.959482687	1.228354249
C1	-0.357206816	-3.398595836	1.228354249
C1	0.357206816	-3.398595836	0.000000000
C1	1.708658126	-2.959482687	0.000000000
C1	2.286630896	-2.539560890	1.228354249
C1	3.121873739	-1.389947741	1.228354249
C1	3.342639693	-0.710500000	0.000000000
C1	3.342639693	0.710500000	2.456708498
C1	3.121873739	1.389947741	3.685062748
C1	2.286630896	2.539560890	3.685062748
C1	1.708658126	2.959482687	2.456708498
C1	0.357206816	3.398595836	2.456708498
C1	-0.357206816	3.398595836	3.685062748
C1	-1.708658126	2.959482687	3.685062748

C1	-2.286630896	2.539560890	2.456708498
C1	-3.121873739	1.389947741	2.456708498
C1	-3.342639693	0.710500000	3.685062748
C1	-3.342639693	-0.710500000	3.685062748
C1	-3.121873739	-1.389947741	2.456708498
C1	-2.286630896	-2.539560890	2.456708498
C1	-1.708658126	-2.959482687	3.685062748
C1	-0.357206816	-3.398595836	3.685062748
C1	0.357206816	-3.398595836	2.456708498
C1	1.708658126	-2.959482687	2.456708498
C1	2.286630896	-2.539560890	3.685062748
C1	3.121873739	-1.389947741	3.685062748
C1	3.342639693	-0.710500000	2.456708498
C1	3.342639693	0.710500000	4.913416997
C1	3.121873739	1.389947741	6.141771246
C1	2.286630896	2.539560890	6.141771246
C1	1.708658126	2.959482687	4.913416997
C1	0.357206816	3.398595836	4.913416997
C1	-0.357206816	3.398595836	6.141771246
C1	-1.708658126	2.959482687	6.141771246
C1	-2.286630896	2.539560890	4.913416997
C1	-3.121873739	1.389947741	4.913416997
C1	-3.342639693	0.710500000	6.141771246
C1	-3.342639693	-0.710500000	6.141771246
C1	-3.121873739	-1.389947741	4.913416997
C1	-2.286630896	-2.539560890	4.913416997
C1	-1.708658126	-2.959482687	6.141771246
C1	-0.357206816	-3.398595836	6.141771246
C1	0.357206816	-3.398595836	4.913416997
C1	1.708658126	-2.959482687	4.913416997

C1	2.286630896	-2.539560890	6.141771246
C1	3.121873739	-1.389947741	6.141771246
C1	3.342639693	-0.710500000	4.913416997
C1	3.342639693	0.710500000	7.370125495
C1	1.708658126	2.959482687	7.370125495
C1	0.357206816	3.398595836	7.370125495
C1	-2.286630896	2.539560890	7.370125495
C1	-3.121873739	1.389947741	7.370125495
C1	-3.121873739	-1.389947741	7.370125495
C1	-2.286630896	-2.539560890	7.370125495
C1	0.357206816	-3.398595836	7.370125495
C1	1.708658126	-2.959482687	7.370125495
C1	3.342639693	-0.710500000	7.370125495
H1	3.187033889	1.233233699	8.306924467
H1	2.157722579	2.649959177	8.306924467
H1	-0.188027313	3.412139519	8.306924467
H1	-1.853487997	2.870998539	8.306924467
H1	-3.303241159	0.875584498	8.306924467
H1	-3.303241159	-0.875584498	8.306924467
H1	-1.853487997	-2.870998539	8.306924467
H1	-0.188027313	-3.412139519	8.306924467
H1	2.157722579	-2.649959177	8.306924467
H1	3.187033889	-1.233233699	8.306924467
H1	3.187033889	1.233233699	-0.936798972
H1	2.157722579	2.649959177	-0.936798972
H1	-0.188027313	3.412139519	-0.936798972
H1	-1.853487997	2.870998539	-0.936798972
H1	-3.303241159	0.875584498	-0.936798972
H1	-3.303241159	-0.875584498	-0.936798972
H1	-1.853487997	-2.870998539	-0.936798972

H1	-0.188027313	-3.412139519	-0.936798972
H1	2.157722579	-2.649959177	-0.936798972
H1	3.187033889	-1.233233699	-0.936798972
O2	0.342639693	0.000000000	3.685062748
H2	-0.244439944	0.000000000	4.442603546
H2	-0.244439944	0.000000000	2.927521950

TABLE II: H₂O@(6,6)CNT

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C84H24H2O

C1	4.029445733	-0.710500000	0.000000000
C1	4.029445733	0.710500000	0.000000000
C1	3.844852368	1.399411817	1.229051178
C1	3.134352368	2.630033916	1.229051178
C1	2.630033916	3.134352368	0.000000000
C1	1.399411817	3.844852368	0.000000000
C1	0.710500000	4.029445733	1.229051178
C1	-0.710500000	4.029445733	1.229051178
C1	-1.399411817	3.844852368	0.000000000
C1	-2.630033916	3.134352368	0.000000000
C1	-3.134352368	2.630033916	1.229051178
C1	-3.844852368	1.399411817	1.229051178
C1	-4.029445733	0.710500000	0.000000000
C1	-4.029445733	-0.710500000	0.000000000
C1	4.029445733	-0.710500000	2.458102356
C1	4.029445733	0.710500000	2.458102356
C1	3.844852368	1.399411817	3.687153534
C1	3.134352368	2.630033916	3.687153534
C1	2.630033916	3.134352368	2.458102356
C1	1.399411817	3.844852368	2.458102356

C1	0.710500000	4.029445733	3.687153534
C1	-0.710500000	4.029445733	3.687153534
C1	-1.399411817	3.844852368	2.458102356
C1	-2.630033916	3.134352368	2.458102356
C1	-3.134352368	2.630033916	3.687153534
C1	-3.844852368	1.399411817	3.687153534
C1	-4.029445733	0.710500000	2.458102356
C1	-4.029445733	-0.710500000	2.458102356
C1	4.029445733	-0.710500000	4.916204712
C1	4.029445733	0.710500000	4.916204712
C1	3.844852368	1.399411817	6.145255890
C1	3.134352368	2.630033916	6.145255890
C1	2.630033916	3.134352368	4.916204712
C1	1.399411817	3.844852368	4.916204712
C1	0.710500000	4.029445733	6.145255890
C1	-0.710500000	4.029445733	6.145255890
C1	-1.399411817	3.844852368	4.916204712
C1	-2.630033916	3.134352368	4.916204712
C1	-3.134352368	2.630033916	6.145255890
C1	-3.844852368	1.399411817	6.145255890
C1	-4.029445733	0.710500000	4.916204712
C1	-4.029445733	-0.710500000	4.916204712
C1	-3.844852368	-1.399411817	1.229051178
C1	-3.134352368	-2.630033916	1.229051178
C1	-2.630033916	-3.134352368	0.000000000
C1	-1.399411817	-3.844852368	0.000000000
C1	-0.710500000	-4.029445733	1.229051178
C1	0.710500000	-4.029445733	1.229051178
C1	1.399411817	-3.844852368	0.000000000
C1	2.630033916	-3.134352368	0.000000000

C1	3.134352368	-2.630033916	1.229051178
C1	3.844852368	-1.399411817	1.229051178
C1	-3.844852368	-1.399411817	3.687153534
C1	-3.134352368	-2.630033916	3.687153534
C1	-2.630033916	-3.134352368	2.458102356
C1	-1.399411817	-3.844852368	2.458102356
C1	-0.710500000	-4.029445733	3.687153534
C1	0.710500000	-4.029445733	3.687153534
C1	1.399411817	-3.844852368	2.458102356
C1	2.630033916	-3.134352368	2.458102356
C1	3.134352368	-2.630033916	3.687153534
C1	3.844852368	-1.399411817	3.687153534
C1	-3.844852368	-1.399411817	6.145255890
C1	-3.134352368	-2.630033916	6.145255890
C1	-2.630033916	-3.134352368	4.916204712
C1	-1.399411817	-3.844852368	4.916204712
C1	-0.710500000	-4.029445733	6.145255890
C1	0.710500000	-4.029445733	6.145255890
C1	1.399411817	-3.844852368	4.916204712
C1	2.630033916	-3.134352368	4.916204712
C1	3.134352368	-2.630033916	6.145255890
C1	3.844852368	-1.399411817	6.145255890
C1	4.029445733	0.710500000	7.374307068
C1	4.029445733	-0.710500000	7.374307068
C1	-4.029445733	-0.710500000	7.374307068
C1	-4.029445733	0.710500000	7.374307068
C1	2.630033916	3.134352368	7.374307068
C1	2.630033916	-3.134352368	7.374307068
C1	-2.630033916	-3.134352368	7.374307068
C1	-2.630033916	3.134352368	7.374307068

C1	1.399411817	3.844852368	7.374307068
C1	1.399411817	-3.844852368	7.374307068
C1	-1.399411817	-3.844852368	7.374307068
C1	-1.399411817	3.844852368	7.374307068
H1	3.899466684	-1.239113692	8.311712536
H1	3.899466684	1.239113692	8.311712536
H1	3.022837277	2.757480364	8.311712536
H1	0.876629407	3.996594056	8.311712536
H1	-0.876629407	3.996594056	8.311712536
H1	-3.022837277	2.757480364	8.311712536
H1	-3.899466684	1.239113692	8.311712536
H1	-3.899466684	-1.239113692	8.311712536
H1	-3.022837277	-2.757480364	8.311712536
H1	-0.876629407	-3.996594056	8.311712536
H1	3.022837277	-2.757480364	8.311712536
H1	0.876629407	-3.996594056	8.311712536
H1	3.899466684	-1.239113692	-0.937405468
H1	3.899466684	1.239113692	-0.937405468
H1	3.022837277	2.757480364	-0.937405468
H1	0.876629407	3.996594056	-0.937405468
H1	-0.876629407	3.996594056	-0.937405468
H1	-3.022837277	2.757480364	-0.937405468
H1	-3.899466684	1.239113692	-0.937405468
H1	-3.899466684	-1.239113692	-0.937405468
H1	-3.022837277	-2.757480364	-0.937405468
H1	-0.876629407	-3.996594056	-0.937405468
H1	3.022837277	-2.757480364	-0.937405468
H1	0.876629407	-3.996594056	-0.937405468
O2	1.029445733	0.000000000	3.687153534
H2	0.442366096	0.000000000	4.444694332

H2	0.442366096	0.000000000	2.929612736
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TABLE III: H₂O@(7,7)CNT

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C98H28H2O

C1	4.713859498	0.710500000	0.000000000
C1	4.555315052	1.405128604	1.229469707
C1	3.938766259	2.685405365	1.229469707
C1	3.494534593	3.242454255	0.000000000
C1	2.383552056	4.128433264	0.000000000
C1	1.741618700	4.437572075	1.229469707
C1	0.356246136	4.753774322	1.229469707
C1	-0.356246136	4.753774322	0.000000000
C1	-1.741618700	4.437572075	0.000000000
C1	-2.383552056	4.128433264	1.229469707
C1	-3.494534593	3.242454255	1.229469707
C1	-3.938766259	2.685405365	0.000000000
C1	-4.555315052	1.405128604	0.000000000
C1	-4.713859498	0.710500000	1.229469707
C1	-4.713859498	-0.710500000	1.229469707
C1	-4.555315052	-1.405128604	0.000000000
C1	-3.938766259	-2.685405365	0.000000000
C1	-3.494534593	-3.242454255	1.229469707
C1	-2.383552056	-4.128433264	1.229469707
C1	-1.741618700	-4.437572075	0.000000000
C1	-0.356246136	-4.753774322	0.000000000
C1	0.356246136	-4.753774322	1.229469707
C1	1.741618700	-4.437572075	1.229469707
C1	2.383552056	-4.128433264	0.000000000
C1	3.494534593	-3.242454255	0.000000000

C1	3.938766259	-2.685405365	1.229469707
C1	4.555315052	-1.405128604	1.229469707
C1	4.713859498	-0.710500000	0.000000000
C1	4.713859498	0.710500000	2.458939415
C1	4.555315052	1.405128604	3.688409122
C1	3.938766259	2.685405365	3.688409122
C1	3.494534593	3.242454255	2.458939415
C1	2.383552056	4.128433264	2.458939415
C1	1.741618700	4.437572075	3.688409122
C1	0.356246136	4.753774322	3.688409122
C1	-0.356246136	4.753774322	2.458939415
C1	-1.741618700	4.437572075	2.458939415
C1	-2.383552056	4.128433264	3.688409122
C1	-3.494534593	3.242454255	3.688409122
C1	-3.938766259	2.685405365	2.458939415
C1	-4.555315052	1.405128604	2.458939415
C1	-4.713859498	0.710500000	3.688409122
C1	-4.713859498	-0.710500000	3.688409122
C1	-4.555315052	-1.405128604	2.458939415
C1	-3.938766259	-2.685405365	2.458939415
C1	-3.494534593	-3.242454255	3.688409122
C1	-2.383552056	-4.128433264	3.688409122
C1	-1.741618700	-4.437572075	2.458939415
C1	-0.356246136	-4.753774322	2.458939415
C1	0.356246136	-4.753774322	3.688409122
C1	1.741618700	-4.437572075	3.688409122
C1	2.383552056	-4.128433264	2.458939415
C1	3.494534593	-3.242454255	2.458939415
C1	3.938766259	-2.685405365	3.688409122
C1	4.555315052	-1.405128604	3.688409122

C1	4.713859498	-0.710500000	2.458939415
C1	4.713859498	0.710500000	4.917878829
C1	4.555315052	1.405128604	6.147348536
C1	3.938766259	2.685405365	6.147348536
C1	3.494534593	3.242454255	4.917878829
C1	2.383552056	4.128433264	4.917878829
C1	1.741618700	4.437572075	6.147348536
C1	0.356246136	4.753774322	6.147348536
C1	-0.356246136	4.753774322	4.917878829
C1	-1.741618700	4.437572075	4.917878829
C1	-2.383552056	4.128433264	6.147348536
C1	-3.494534593	3.242454255	6.147348536
C1	-3.938766259	2.685405365	4.917878829
C1	-4.555315052	1.405128604	4.917878829
C1	-4.713859498	0.710500000	6.147348536
C1	-4.713859498	-0.710500000	6.147348536
C1	-4.555315052	-1.405128604	4.917878829
C1	-3.938766259	-2.685405365	4.917878829
C1	-3.494534593	-3.242454255	6.147348536
C1	-2.383552056	-4.128433264	6.147348536
C1	-1.741618700	-4.437572075	4.917878829
C1	-0.356246136	-4.753774322	4.917878829
C1	0.356246136	-4.753774322	6.147348536
C1	1.741618700	-4.437572075	6.147348536
C1	2.383552056	-4.128433264	4.917878829
C1	3.494534593	-3.242454255	4.917878829
C1	3.938766259	-2.685405365	6.147348536
C1	4.555315052	-1.405128604	6.147348536
C1	4.713859498	-0.710500000	4.917878829
C1	4.713859498	0.710500000	7.376818244

C1	3.494534593	3.242454255	7.376818244
C1	2.383552056	4.128433264	7.376818244
C1	-0.356246136	4.753774322	7.376818244
C1	-1.741618700	4.437572075	7.376818244
C1	-3.938766259	2.685405365	7.376818244
C1	-4.555315052	1.405128604	7.376818244
C1	-4.555315052	-1.405128604	7.376818244
C1	-3.938766259	-2.685405365	7.376818244
C1	-1.741618700	-4.437572075	7.376818244
C1	-0.356246136	-4.753774322	7.376818244
C1	2.383552056	-4.128433264	7.376818244
C1	3.494534593	-3.242454255	7.376818244
C1	4.713859498	-0.710500000	7.376818244
H1	4.602289925	1.242662087	8.314587801
H1	3.841033175	2.823428016	8.314587801
H1	1.897928492	4.373002293	8.314587801
H1	0.187400102	4.763419236	8.314587801
H1	-2.235611807	4.210382580	8.314587801
H1	-3.607349071	3.116458615	8.314587801
H1	-4.685690816	0.877258907	8.314587801
H1	-4.685690816	-0.877258907	8.314587801
H1	-3.607349071	-3.116458615	8.314587801
H1	-2.235611807	-4.210382580	8.314587801
H1	0.187400102	-4.763419236	8.314587801
H1	1.897928492	-4.373002293	8.314587801
H1	3.841033175	-2.823428016	8.314587801
H1	4.602289925	-1.242662087	8.314587801
H1	4.602289925	1.242662087	-0.937769558
H1	3.841033175	2.823428016	-0.937769558
H1	1.897928492	4.373002293	-0.937769558

H1	0.187400102	4.763419236	-0.937769558
H1	-2.235611807	4.210382580	-0.937769558
H1	-3.607349071	3.116458615	-0.937769558
H1	-4.685690816	0.877258907	-0.937769558
H1	-4.685690816	-0.877258907	-0.937769558
H1	-3.607349071	-3.116458615	-0.937769558
H1	-2.235611807	-4.210382580	-0.937769558
H1	0.187400102	-4.763419236	-0.937769558
H1	1.897928492	-4.373002293	-0.937769558
H1	3.841033175	-2.823428016	-0.937769558
H1	4.602289925	-1.242662087	-0.937769558
O2	1.713859498	0.000000000	3.688409122
H2	1.126779861	0.000000000	4.445949920
H2	1.126779861	0.000000000	2.930868324

TABLE IV: $\text{H}_2\text{O}@(\text{8,8})\text{CNT}$

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C112H32H2O

C1	5.396783297	-0.710500000	0.000000000
C1	5.396783297	0.710500000	0.000000000
C1	5.257874208	1.408843148	1.229740669
C1	4.714081051	2.721675964	1.229740669
C1	4.318501434	3.313702698	0.000000000
C1	3.313702698	4.318501434	0.000000000
C1	2.721675964	4.714081051	1.229740669
C1	1.408843148	5.257874208	1.229740669
C1	0.710500000	5.396783297	0.000000000
C1	-0.710500000	5.396783297	0.000000000
C1	-1.408843148	5.257874208	1.229740669
C1	-2.721675964	4.714081051	1.229740669

C1	-3.313702698	4.318501434	0.000000000
C1	-4.318501434	3.313702698	0.000000000
C1	-4.714081051	2.721675964	1.229740669
C1	-5.257874208	1.408843148	1.229740669
C1	-5.396783297	0.710500000	0.000000000
C1	-5.396783297	-0.710500000	0.000000000
C1	5.396783297	-0.710500000	2.459481338
C1	5.396783297	0.710500000	2.459481338
C1	5.257874208	1.408843148	3.689222007
C1	4.714081051	2.721675964	3.689222007
C1	4.318501434	3.313702698	2.459481338
C1	3.313702698	4.318501434	2.459481338
C1	2.721675964	4.714081051	3.689222007
C1	1.408843148	5.257874208	3.689222007
C1	0.710500000	5.396783297	2.459481338
C1	-0.710500000	5.396783297	2.459481338
C1	-1.408843148	5.257874208	3.689222007
C1	-2.721675964	4.714081051	3.689222007
C1	-3.313702698	4.318501434	2.459481338
C1	-4.318501434	3.313702698	2.459481338
C1	-4.714081051	2.721675964	3.689222007
C1	-5.257874208	1.408843148	3.689222007
C1	-5.396783297	0.710500000	2.459481338
C1	-5.396783297	-0.710500000	2.459481338
C1	5.396783297	-0.710500000	4.918962675
C1	5.396783297	0.710500000	4.918962675
C1	5.257874208	1.408843148	6.148703344
C1	4.714081051	2.721675964	6.148703344
C1	4.318501434	3.313702698	4.918962675
C1	3.313702698	4.318501434	4.918962675

C1	2.721675964	4.714081051	6.148703344
C1	1.408843148	5.257874208	6.148703344
C1	0.710500000	5.396783297	4.918962675
C1	-0.710500000	5.396783297	4.918962675
C1	-1.408843148	5.257874208	6.148703344
C1	-2.721675964	4.714081051	6.148703344
C1	-3.313702698	4.318501434	4.918962675
C1	-4.318501434	3.313702698	4.918962675
C1	-4.714081051	2.721675964	6.148703344
C1	-5.257874208	1.408843148	6.148703344
C1	-5.396783297	0.710500000	4.918962675
C1	-5.396783297	-0.710500000	4.918962675
C1	-5.257874208	-1.408843148	1.229740669
C1	-4.714081051	-2.721675964	1.229740669
C1	-4.318501434	-3.313702698	0.000000000
C1	-3.313702698	-4.318501434	0.000000000
C1	-2.721675964	-4.714081051	1.229740669
C1	-1.408843148	-5.257874208	1.229740669
C1	-0.710500000	-5.396783297	0.000000000
C1	0.710500000	-5.396783297	0.000000000
C1	1.408843148	-5.257874208	1.229740669
C1	2.721675964	-4.714081051	1.229740669
C1	3.313702698	-4.318501434	0.000000000
C1	4.318501434	-3.313702698	0.000000000
C1	4.714081051	-2.721675964	1.229740669
C1	5.257874208	-1.408843148	1.229740669
C1	-5.257874208	-1.408843148	3.689222007
C1	-4.714081051	-2.721675964	3.689222007
C1	-4.318501434	-3.313702698	2.459481338
C1	-3.313702698	-4.318501434	2.459481338

C1	-2.721675964	-4.714081051	3.689222007
C1	-1.408843148	-5.257874208	3.689222007
C1	-0.710500000	-5.396783297	2.459481338
C1	0.710500000	-5.396783297	2.459481338
C1	1.408843148	-5.257874208	3.689222007
C1	2.721675964	-4.714081051	3.689222007
C1	3.313702698	-4.318501434	2.459481338
C1	4.318501434	-3.313702698	2.459481338
C1	4.714081051	-2.721675964	3.689222007
C1	5.257874208	-1.408843148	3.689222007
C1	-5.257874208	-1.408843148	6.148703344
C1	-4.714081051	-2.721675964	6.148703344
C1	-4.318501434	-3.313702698	4.918962675
C1	-3.313702698	-4.318501434	4.918962675
C1	-2.721675964	-4.714081051	6.148703344
C1	-1.408843148	-5.257874208	6.148703344
C1	-0.710500000	-5.396783297	4.918962675
C1	0.710500000	-5.396783297	4.918962675
C1	1.408843148	-5.257874208	6.148703344
C1	2.721675964	-4.714081051	6.148703344
C1	3.313702698	-4.318501434	4.918962675
C1	4.318501434	-3.313702698	4.918962675
C1	4.714081051	-2.721675964	6.148703344
C1	5.257874208	-1.408843148	6.148703344
C1	5.396783297	0.710500000	7.378444013
C1	5.396783297	-0.710500000	7.378444013
C1	-5.396783297	-0.710500000	7.378444013
C1	-5.396783297	0.710500000	7.378444013
C1	4.318501434	3.313702698	7.378444013
C1	4.318501434	-3.313702698	7.378444013

C1	-4.318501434	-3.313702698	7.378444013
C1	-4.318501434	3.313702698	7.378444013
C1	3.313702698	4.318501434	7.378444013
C1	3.313702698	-4.318501434	7.378444013
C1	-3.313702698	-4.318501434	7.378444013
C1	-3.313702698	4.318501434	7.378444013
C1	0.710500000	5.396783297	7.378444013
C1	0.710500000	-5.396783297	7.378444013
C1	-0.710500000	-5.396783297	7.378444013
C1	-0.710500000	5.396783297	7.378444013
H1	5.299069642	-1.244966320	8.316449234
H1	5.299069642	1.244966320	8.316449234
H1	4.627332205	2.866683951	8.316449234
H1	2.866683951	4.627332205	8.316449234
H1	1.244966320	5.299069642	8.316449234
H1	-1.244966320	5.299069642	8.316449234
H1	-2.866683951	4.627332205	8.316449234
H1	-4.627332205	2.866683951	8.316449234
H1	-5.299069642	1.244966320	8.316449234
H1	-5.299069642	-1.244966320	8.316449234
H1	-4.627332205	-2.866683951	8.316449234
H1	-2.866683951	-4.627332205	8.316449234
H1	-1.244966320	-5.299069642	8.316449234
H1	4.627332205	-2.866683951	8.316449234
H1	2.866683951	-4.627332205	8.316449234
H1	1.244966320	-5.299069642	8.316449234
H1	5.299069642	-1.244966320	-0.938005221
H1	5.299069642	1.244966320	-0.938005221
H1	4.627332205	2.866683951	-0.938005221
H1	2.866683951	4.627332205	-0.938005221

H1	1.244966320	5.299069642	-0.938005221
H1	-1.244966320	5.299069642	-0.938005221
H1	-2.866683951	4.627332205	-0.938005221
H1	-4.627332205	2.866683951	-0.938005221
H1	-5.299069642	1.244966320	-0.938005221
H1	-5.299069642	-1.244966320	-0.938005221
H1	-4.627332205	-2.866683951	-0.938005221
H1	-2.866683951	-4.627332205	-0.938005221
H1	-1.244966320	-5.299069642	-0.938005221
H1	4.627332205	-2.866683951	-0.938005221
H1	2.866683951	-4.627332205	-0.938005221
H1	1.244966320	-5.299069642	-0.938005221
O2	2.396783297	0.000000000	3.689222007
H2	1.809703660	0.000000000	4.446762805
H2	1.809703660	0.000000000	2.931681209

TABLE V: $\text{H}_2\text{O}@(10,10)\text{CNT}$

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$\text{C}_{140}\text{H}_{40}\text{H}_2\text{O}$

C1	6.759955945	0.710500000	0.000000000
C1	6.648656726	1.413215613	1.230058637
C1	6.209543577	2.764666923	1.230058637
C1	5.886540662	3.398595836	0.000000000
C1	5.051297819	4.548208985	0.000000000
C1	4.548208985	5.051297819	1.230058637
C1	3.398595836	5.886540662	1.230058637
C1	2.764666923	6.209543577	0.000000000
C1	1.413215613	6.648656726	0.000000000
C1	0.710500000	6.759955945	1.230058637
C1	-0.710500000	6.759955945	1.230058637

C1	-1.413215613	6.648656726	0.000000000
C1	-2.764666923	6.209543577	0.000000000
C1	-3.398595836	5.886540662	1.230058637
C1	-4.548208985	5.051297819	1.230058637
C1	-5.051297819	4.548208985	0.000000000
C1	-5.886540662	3.398595836	0.000000000
C1	-6.209543577	2.764666923	1.230058637
C1	-6.648656726	1.413215613	1.230058637
C1	-6.759955945	0.710500000	0.000000000
C1	-6.759955945	-0.710500000	0.000000000
C1	-6.648656726	-1.413215613	1.230058637
C1	-6.209543577	-2.764666923	1.230058637
C1	-5.886540662	-3.398595836	0.000000000
C1	-5.051297819	-4.548208985	0.000000000
C1	-4.548208985	-5.051297819	1.230058637
C1	-3.398595836	-5.886540662	1.230058637
C1	-2.764666923	-6.209543577	0.000000000
C1	-1.413215613	-6.648656726	0.000000000
C1	-0.710500000	-6.759955945	1.230058637
C1	0.710500000	-6.759955945	1.230058637
C1	1.413215613	-6.648656726	0.000000000
C1	2.764666923	-6.209543577	0.000000000
C1	3.398595836	-5.886540662	1.230058637
C1	4.548208985	-5.051297819	1.230058637
C1	5.051297819	-4.548208985	0.000000000
C1	5.886540662	-3.398595836	0.000000000
C1	6.209543577	-2.764666923	1.230058637
C1	6.648656726	-1.413215613	1.230058637
C1	6.759955945	-0.710500000	0.000000000
C1	6.759955945	0.710500000	2.460117274

C1	6.648656726	1.413215613	3.690175911
C1	6.209543577	2.764666923	3.690175911
C1	5.886540662	3.398595836	2.460117274
C1	5.051297819	4.548208985	2.460117274
C1	4.548208985	5.051297819	3.690175911
C1	3.398595836	5.886540662	3.690175911
C1	2.764666923	6.209543577	2.460117274
C1	1.413215613	6.648656726	2.460117274
C1	0.710500000	6.759955945	3.690175911
C1	-0.710500000	6.759955945	3.690175911
C1	-1.413215613	6.648656726	2.460117274
C1	-2.764666923	6.209543577	2.460117274
C1	-3.398595836	5.886540662	3.690175911
C1	-4.548208985	5.051297819	3.690175911
C1	-5.051297819	4.548208985	2.460117274
C1	-5.886540662	3.398595836	2.460117274
C1	-6.209543577	2.764666923	3.690175911
C1	-6.648656726	1.413215613	3.690175911
C1	-6.759955945	0.710500000	2.460117274
C1	-6.759955945	-0.710500000	2.460117274
C1	-6.648656726	-1.413215613	3.690175911
C1	-6.209543577	-2.764666923	3.690175911
C1	-5.886540662	-3.398595836	2.460117274
C1	-5.051297819	-4.548208985	2.460117274
C1	-4.548208985	-5.051297819	3.690175911
C1	-3.398595836	-5.886540662	3.690175911
C1	-2.764666923	-6.209543577	2.460117274
C1	-1.413215613	-6.648656726	2.460117274
C1	-0.710500000	-6.759955945	3.690175911
C1	0.710500000	-6.759955945	3.690175911

C1	1.413215613	-6.648656726	2.460117274
C1	2.764666923	-6.209543577	2.460117274
C1	3.398595836	-5.886540662	3.690175911
C1	4.548208985	-5.051297819	3.690175911
C1	5.051297819	-4.548208985	2.460117274
C1	5.886540662	-3.398595836	2.460117274
C1	6.209543577	-2.764666923	3.690175911
C1	6.648656726	-1.413215613	3.690175911
C1	6.759955945	-0.710500000	2.460117274
C1	6.759955945	0.710500000	4.920234548
C1	6.648656726	1.413215613	6.150293185
C1	6.209543577	2.764666923	6.150293185
C1	5.886540662	3.398595836	4.920234548
C1	5.051297819	4.548208985	4.920234548
C1	4.548208985	5.051297819	6.150293185
C1	3.398595836	5.886540662	6.150293185
C1	2.764666923	6.209543577	4.920234548
C1	1.413215613	6.648656726	4.920234548
C1	0.710500000	6.759955945	6.150293185
C1	-0.710500000	6.759955945	6.150293185
C1	-1.413215613	6.648656726	4.920234548
C1	-2.764666923	6.209543577	4.920234548
C1	-3.398595836	5.886540662	6.150293185
C1	-4.548208985	5.051297819	6.150293185
C1	-5.051297819	4.548208985	4.920234548
C1	-5.886540662	3.398595836	4.920234548
C1	-6.209543577	2.764666923	6.150293185
C1	-6.648656726	1.413215613	6.150293185
C1	-6.759955945	0.710500000	4.920234548
C1	-6.759955945	-0.710500000	4.920234548

C1	-6.648656726	-1.413215613	6.150293185
C1	-6.209543577	-2.764666923	6.150293185
C1	-5.886540662	-3.398595836	4.920234548
C1	-5.051297819	-4.548208985	4.920234548
C1	-4.548208985	-5.051297819	6.150293185
C1	-3.398595836	-5.886540662	6.150293185
C1	-2.764666923	-6.209543577	4.920234548
C1	-1.413215613	-6.648656726	4.920234548
C1	-0.710500000	-6.759955945	6.150293185
C1	0.710500000	-6.759955945	6.150293185
C1	1.413215613	-6.648656726	4.920234548
C1	2.764666923	-6.209543577	4.920234548
C1	3.398595836	-5.886540662	6.150293185
C1	4.548208985	-5.051297819	6.150293185
C1	5.051297819	-4.548208985	4.920234548
C1	5.886540662	-3.398595836	4.920234548
C1	6.209543577	-2.764666923	6.150293185
C1	6.648656726	-1.413215613	6.150293185
C1	6.759955945	-0.710500000	4.920234548
C1	6.759955945	0.710500000	7.380351822
C1	6.759955945	-0.710500000	7.380351822
C1	-6.759955945	-0.710500000	7.380351822
C1	-6.759955945	0.710500000	7.380351822
C1	5.886540662	3.398595836	7.380351822
C1	5.886540662	-3.398595836	7.380351822
C1	-5.886540662	-3.398595836	7.380351822
C1	-5.886540662	3.398595836	7.380351822
C1	5.051297819	4.548208985	7.380351822
C1	5.051297819	-4.548208985	7.380351822
C1	-5.051297819	-4.548208985	7.380351822

C1	-5.051297819	4.548208985	7.380351822
C1	2.764666923	6.209543577	7.380351822
C1	2.764666923	-6.209543577	7.380351822
C1	-2.764666923	-6.209543577	7.380351822
C1	-2.764666923	6.209543577	7.380351822
C1	1.413215613	6.648656726	7.380351822
C1	1.413215613	-6.648656726	7.380351822
C1	-1.413215613	-6.648656726	7.380351822
C1	-1.413215613	6.648656726	7.380351822
H1	6.681700083	1.247677294	8.318633537
H1	6.138975231	2.918012635	8.318633537
H1	4.672242605	4.936796903	8.318633537
H1	3.251370497	5.969120916	8.318633537
H1	0.878147256	6.740227891	8.318633537
H1	-0.878147256	6.740227891	8.318633537
H1	-3.251370497	5.969120916	8.318633537
H1	-4.672242605	4.936796903	8.318633537
H1	-6.138975231	2.918012635	8.318633537
H1	-6.681700083	1.247677294	8.318633537
H1	-6.681700083	-1.247677294	8.318633537
H1	-6.138975231	-2.918012635	8.318633537
H1	-4.672242605	-4.936796903	8.318633537
H1	-3.251370497	-5.969120916	8.318633537
H1	-0.878147256	-6.740227891	8.318633537
H1	6.681700083	-1.247677294	8.318633537
H1	6.138975231	-2.918012635	8.318633537
H1	4.672242605	-4.936796903	8.318633537
H1	3.251370497	-5.969120916	8.318633537
H1	0.878147256	-6.740227891	8.318633537
H1	6.681700083	1.247677294	-0.938281714

H1	6.138975231	2.918012635	-0.938281714
H1	4.672242605	4.936796903	-0.938281714
H1	3.251370497	5.969120916	-0.938281714
H1	0.878147256	6.740227891	-0.938281714
H1	-0.878147256	6.740227891	-0.938281714
H1	-3.251370497	5.969120916	-0.938281714
H1	-4.672242605	4.936796903	-0.938281714
H1	-6.138975231	2.918012635	-0.938281714
H1	-6.681700083	1.247677294	-0.938281714
H1	-6.681700083	-1.247677294	-0.938281714
H1	-6.138975231	-2.918012635	-0.938281714
H1	-4.672242605	-4.936796903	-0.938281714
H1	-3.251370497	-5.969120916	-0.938281714
H1	-0.878147256	-6.740227891	-0.938281714
H1	6.681700083	-1.247677294	-0.938281714
H1	6.138975231	-2.918012635	-0.938281714
H1	4.672242605	-4.936796903	-0.938281714
H1	3.251370497	-5.969120916	-0.938281714
H1	0.878147256	-6.740227891	-0.938281714
O2	3.759955945	0.000000000	3.690175911
H2	3.172876308	0.000000000	4.447716709
H2	3.172876308	0.000000000	2.932635113