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Electronic Supplementary Information (ESI)for Hydrogen Bonding from a Valence Bond Theory Perspective: The Role of Covalency by Coleen T. Nemes†, Croix J. Laconsay and John Morrison Galbraith, Department of Chemistry, Biochemistry, and Physics, Marist College, Poughkeepsie NY 12601

PBEPBE/aug-cc-PVDZ geoms

FH

F	0.000000	0.000000	0.093408
H	0.000000	0.000000	-0.840671

FHFH

F	1.420150	0.019192	0.000000
H	0.488355	-0.132331	0.000005
F	-1.297745	-0.093106	0.000000
H	-1.590005	0.797555	0.000001

FHOH2

F	-1.394441	0.000020	0.015200
H	-0.436579	-0.000904	-0.056171
O	1.227805	-0.000060	-0.103668
H	1.582999	-0.770861	0.374717
H	1.581102	0.772064	0.374000

FHNH3

F	1.408105	-0.000018	0.000084
H	0.423270	-0.000003	0.000089
N	-1.194294	0.000008	0.000102
H	-1.577841	0.906647	-0.287145
H	-1.580639	-0.204974	0.927716
H	-1.577680	-0.701570	-0.642126

HOH

O	0.000000	0.120082	0.000000
H	0.765853	-0.480323	0.000000
H	-0.765853	-0.480334	0.000000

HOHFH
NA

HOHOH2

H	0	-1.909702	-0.185366	0.733577
O	0	-1.497492	0.029938	-0.120003
H	0	-0.531557	-0.012599	0.061045
O	0	1.381738	-0.027404	0.117225
H	0	1.684782	0.837408	-0.212656
H	0	1.682507	-0.659709	-0.559748

HOHNH3

H	-1.900135	0.790621	-0.000427
O	-1.530561	-0.108147	0.000019
H	-0.547362	0.029320	-0.000262
N	1.352335	0.019476	-0.000150
H	1.681941	-0.512415	-0.813151

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H                  1.682398   -0.488536    0.827794
H                  1.861305    0.909860   -0.013058

H2NH
N                  0.000000    0.119546    0.000000
H                 -0.946622   -0.277173    0.000000
H                  0.473311   -0.279823    0.819407
H                  0.473311   -0.279823   -0.819407

H2NHFH
NA

H2NHOH2
NA

H2NHNH3
H                  0.457984    2.066655   -0.816793
H                  0.457984    2.066655    0.816793
N                 -0.037488    1.689373    0.000000
H                  0.138842    0.670941    0.000000
N                 -0.037488   -1.551165    0.000000
H                 -1.063038   -1.594171    0.000000
H                  0.266529   -2.088767    0.819515
H                  0.266529   -2.088767   -0.819515
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