Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Cooperativity between hydrogen bonds and beryllium bonds in $(H_2O)_nBeX_2$ (n =1-3, X = H, F) complexes. A new perspective.

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Supporting Information

(A total of 16 pages)

Table S1. CCSD(T)/aug-cc-pVTQZ//CCSD/6-31+g(d,p) total energies (E, hartrees) and relative free energies (ΔG, kJ mol^{-1}) for **WD(BeH_2)a** and **WD(BeH_2)b** clusters.

Cluster	E	ΔG
WD(BeH_2)a	-168.6327986	0.0
WD(BeH_2)b	-168.6309422	5.6

Table S2. B3LYP/6-31+G(d,p) optimized geometries for the water dimer and trimer, and the $(H_2O)_n$ BeX_2 (n =1-3, X = H, F) complexes. Coordinates are in Å

$(H_2O)_2$			
8	0.007035	-0.004858	-0.097332
1	0.051539	-0.001213	0.871549
1	0.921804	0.004924	-0.391940
8	-0.036388	-0.000158	2.801888
1	-0.480854	0.761251	3.188979
1	-0.463204	-0.772899	3.186401

$(H_2O)_3$			
8	-0.101541	0.040752	-0.188709
8	-0.104155	0.112758	2.597583
8	2.297625	-0.086707	1.210611
1	-0.459409	0.144352	0.712880
1	0.855712	0.037268	2.435930
1	1.678129	-0.061769	0.456557
1	2.863824	-0.851074	1.071128
1	-0.216065	0.760200	3.298802
1	-0.521876	0.713425	-0.731370

H_2O:BeH_2			
8	-0.005288	-0.086058	0.031365
1	0.090649	0.043361	0.981203
1	0.831224	0.032487	-0.431610
4	-1.461878	-0.468328	-0.729727
1	-2.416897	-0.554075	0.227869
1	-1.217990	-0.569053	-2.058924

H_2O:BeF_2			
8	0.006243	-0.109381	0.039354
1	0.097696	0.050165	0.984616
1	0.828029	0.051275	-0.436231
4	-1.430742	-0.626080	-0.699025
9	-2.428713	-0.762837	0.313671
9	-1.189281	-0.761918	-2.100199

WD(BeH_2)a			
8	0.231893	-0.355351	0.065392
1	0.432347	-0.257056	1.032568
1	0.878889	-0.869867	-0.425130
8	-0.176819	0.133774	2.562190
1	0.071117	0.878418	3.118954
1	-1.031620	0.365476	2.137819
4	-1.310974	-0.039255	-0.407613
1	-1.970435	0.480978	0.690091
1	-1.574879	-0.353119	-1.694842

WD(BeF_2)a			
8	-0.010017	0.034757	-0.004271
1	-0.046112	0.009449	0.991300
1	0.877659	-0.015587	-0.368897
8	-0.883847	-0.272349	2.404471
1	-1.076897	0.353437	3.108835
1	-1.720902	-0.444878	1.929394
4	-1.386141	-0.441314	-0.782538
9	-2.428108	-0.585736	0.231617
9	-1.249944	-0.614030	-2.190441

WD(BeH_2)b			
8	0.304537	-0.040250	-0.037072
1	0.170000	-0.165803	0.909899
1	1.078731	0.522567	-0.157365
4	-1.126013	0.800783	-0.711415
1	-2.075746	0.721716	0.298837
1	-0.590441	1.849569	-1.447553
8	-1.703397	-0.356897	-1.950329
1	-1.704272	0.084302	-2.808197
1	-2.611625	-0.605349	-1.740576

WD(BeF_2)b			
8	0.017861	-0.006769	0.012679
1	0.015296	0.012662	0.978246
1	0.935105	0.014565	-0.288829
4	-0.801538	1.459704	-0.580612
8	-2.163994	0.881044	-1.569202
1	-2.064318	1.231212	-2.463671
1	-2.983005	1.230609	-1.195441
9	0.142248	2.005527	-1.572662
9	-1.453064	2.003772	0.624599

WT(BeH_2)a			
8	-0.827683	0.083689	0.074616
8	0.287437	0.887919	2.262396
8	2.199576	-0.877434	1.695828
1	-0.462637	0.444054	0.943649
1	1.092861	0.316417	2.258671
1	1.704271	-1.366450	0.996093
1	2.852349	-1.477902	2.065362
1	-0.136975	0.765965	3.117031
1	-1.429185	0.701403	-0.350782
4	-0.289252	-1.218040	-0.739715
1	0.677684	-1.897025	-0.031915
1	-0.891914	-1.379670	-1.941900

WT(BeF_2)a			
8	-0.028250	0.027247	-0.030927
8	0.072458	0.028553	2.532292
8	2.699190	-0.401141	2.545822
1	-0.072476	0.025687	0.982083
1	1.042671	-0.081777	2.706743
1	2.810317	-0.486046	1.575322
1	3.419055	0.150782	2.863962
1	-0.381606	-0.635957	3.059658
1	-0.839691	0.341338	-0.439828
4	1.308890	-0.195358	-0.933229
9	2.475327	-0.505945	-0.107312
9	1.085779	-0.028414	-2.335528

WT(BeH_2)b			
8	0.283775	0.054532	0.308774
1	0.107100	0.108950	1.272917
1	1.176398	0.297623	-0.019611
8	-1.167379	-0.276968	2.458295
1	-1.670910	0.294853	3.045302
1	-1.764328	-0.523872	1.723960
4	-0.863284	-0.429113	-0.710910
1	-2.032304	-0.733909	-0.055011
1	-0.420297	-0.430796	-2.012225
8	2.062638	0.515757	-1.551315
1	1.282838	0.184650	-2.040023
1	2.828460	0.052713	-1.903750

WT(BeF_2)b			
8	0.021612	0.034822	0.033028
1	-0.058286	-0.114557	1.001832
1	0.894945	-0.114750	-0.395060
8	-1.179101	0.041413	2.359225
1	-1.109237	0.471667	3.215979
1	-1.837810	0.539012	1.839335
4	-1.084826	0.933459	-0.724780
8	1.835702	0.211935	-1.847792
1	1.095799	0.663529	-2.295747
1	2.226300	-0.392317	-2.485442
9	-0.680538	1.262990	-2
9	-2.221351	1.237377	0.129047

WT(BeH_2)c			
8	0.159874	-0.449575	0.121021
1	0.076286	-0.157034	1.061387
1	0.692270	0.185488	-0.368030
8	-0.919111	0.035527	2.478394
1	-1.151170	0.850253	2.934092
1	-1.669413	-0.174614	1.867314
4	-1.406948	-0.675919	-0.581906
1	-2.333360	-0.599734	0.489155
1	-1.446556	-0.031491	-1.806540
8	-1.429830	-2.421233	-1.006456
1	-2.121690	-2.885423	-0.520600
1	-1.638583	-2.479684	-1.946537

WT(BeF_2)c			
8	-0.016461	0.013474	0.018584
1	-0.010186	0.044088	1.009334
1	0.888184	0.031171	-0.312244
8	-0.615930	0.581222	2.528472
1	-0.151209	1.036058	3.236433
1	-1.158324	1.251088	2.059041
4	-0.947961	1.304548	-0.635112
8	-2.268733	0.555991	-1.579772
1	-3.118613	0.844953	-1.224240
1	-2.188359	0.901825	-2.478376
9	-1.695164	1.909980	0.528584
9	-0.135357	1.960595	-1.674566

WT(BeF_2)d			
8	0.012415	-0.122697	0.049398
1	-0.092572	-0.168611	1.048406
1	0.904144	-0.286281	-0.268392
8	-0.957059	-0.332416	2.391789
1	-1.072113	0.397652	3.026301
1	-1.785612	-0.397808	1.883284
4	-1.357415	-0.334551	-0.823198
1	-2.415549	-0.320963	0.064688
1	-1.157889	-0.480706	-2.155757
8	-1.310468	1.770723	4.249033
1	-1.699249	2.620257	4.016735
1	-1.575835	1.592357	5.157053

WT(BeF_2)d			
8	-0.020480	0.104705	0.008291
1	-0.081595	0.055967	1.026376
1	0.869150	-0.008011	-0.344076
8	-0.734289	-0.226274	2.401041
1	-0.912178	0.503055	3.027897
1	-1.589775	-0.506165	2.020181
4	-1.336934	-0.549844	-0.725830
8	-1.240832	1.853233	4.214542
1	-1.855019	2.572044	4.018121
1	-1.337395	1.655869	5.154800
9	-2.388749	-0.729809	0.273745
9	-1.200535	-0.837213	-2.121250

Table S3. B3LYP/6-311+G(3df,2p)//B3LYP/6-31+G(d,p) total energies (hartrees)

water	-76.463373
water dimer	-152.934352
water trimer	-229.41373
BeH_2	-15.9234856
BeF_2	-214.689368
H_2O:BeH2	-92.4161175
H_2O:BeF2	-291.1860227
WD(BeH_2)a	-168.9017818
WD(BeH_2)b	-168.896473
WD(BeF_2)a	-367.674095
WD(BeF_2)b	-367.6694464
WT(BeH_2)a	-245.3850267
WT(BeH_2)b	-245.3837711
WT(BeH_2)c	-245.3815168
WT(BeH_2)d	-245.3753606
WT(BeF_2)a	-444.1586208
WT(BeF_2)b	-444.158092
WT(BeF_2)c	-444.1559868
WT(BeF_2)d	-444.1479908

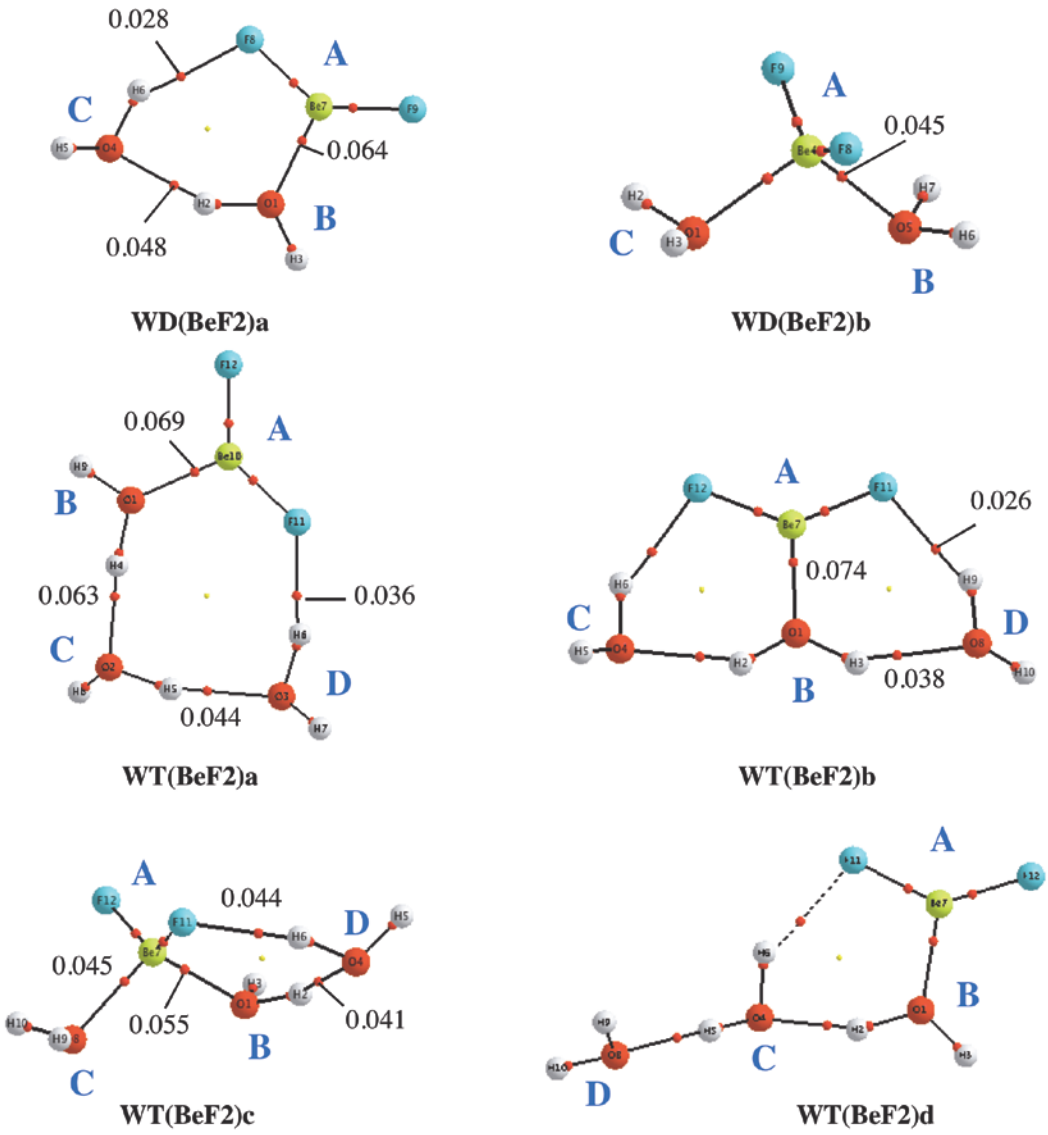

Figure S1. Molecular graphs of the optimized clusters formed by two and three water molecules with BeF_2. Red dots denote BCPs. Electron densities are in a.u.. **A** and **B** denote respectively the BeH_2 molecule and the water molecule attached to through a beryllium bond.

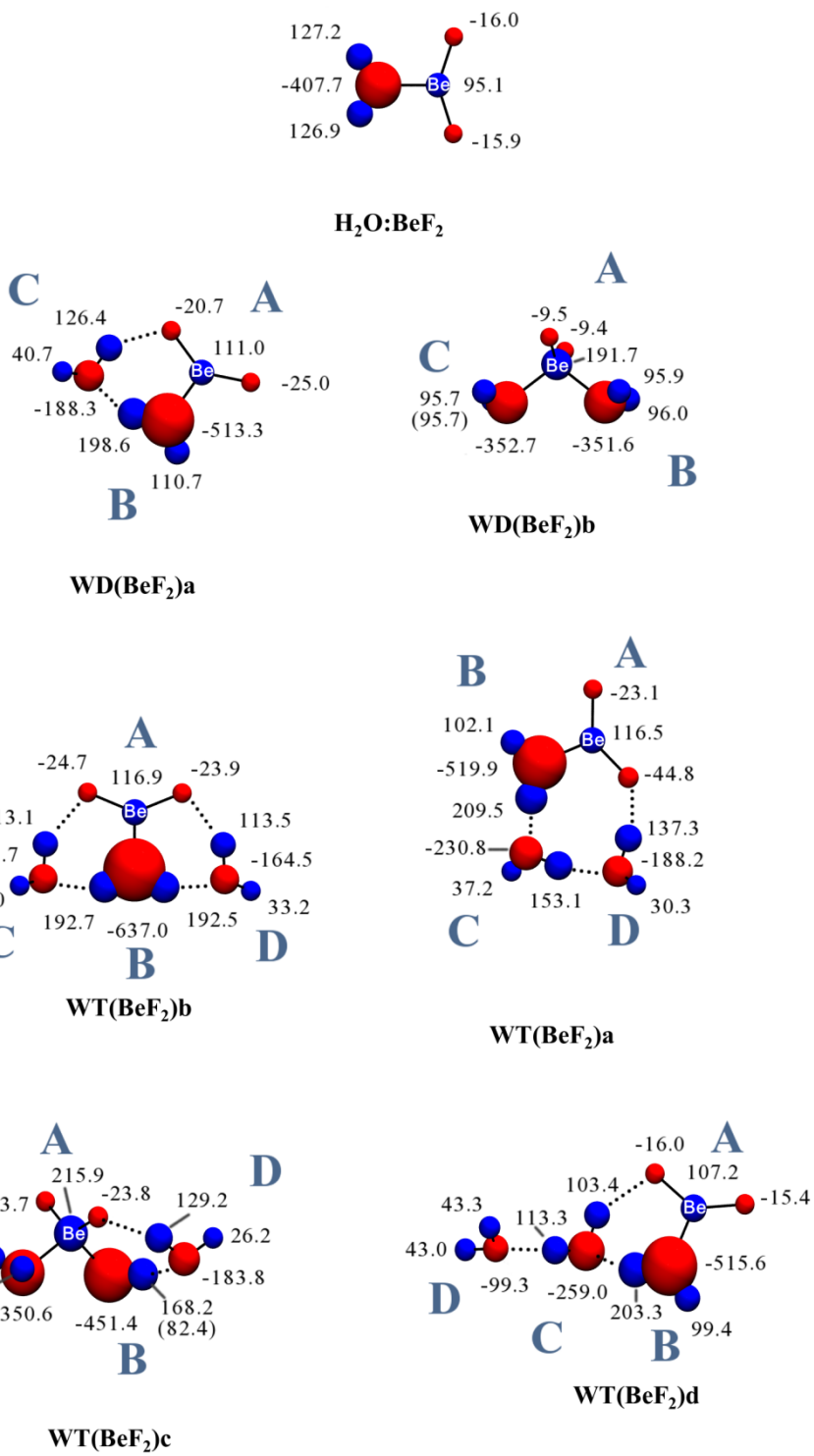

Figure S2. Change in atomic energy for the formation of $BeF_2:(H_2O)_n$, n=1-3, systems. Values for the relative energy change of each atom are labeled (kJ mol^{-1}). Stabilized atoms are red, destabilized atoms are blue. Atom size corresponds to the magnitude of energy change. **A**, **B**, **C**, and **D** denote labels as in Figure 1. For hydrogens which are hidden the energy is included in parentheses. The atomic energies for the atoms in BeF_2 and H_2O monomers are: Be (-3.7×10^5), F (-2.63×10^3), and O (1.98×10^5), H (1.03×10^3), respectively, in kJ mol^{-1}.

Table S4. QTAIM Atomic energies, charges, dipole moments and Lagrangian values for the water, BeH_2, and BeF_2 monomers, water dimer and trimer, and the $(H_2O)_n$ BeX_2 (n =1-3, X = H, F) complexes.

Note: **AIMAll vs. 12.06.03**. Default parameters were used except for special cases where it was necessary to improve integration. Instances where L(A) is $>10^4$ have been evaluated using "Sculpt" method for maximum accuracy possible.

Definitions of Some Atomic Properties:

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q(A) = Net Charge of Atom A

L(A) = Lagrangian of Atom A = -(1/4) Times Atomic Integral of the Laplacian of the Electron Density

K(A) = Electronic Kinetic Energy of Atom A (Hamiltonian Form)

K_Scaled(A) = K(A) * E(Mol)/K(Mol) = Approximation to Virial-Based Total Energy of Atom A.

|Mu_Intra(A)| = Magnitude of Intraatomic Dipole Moment of Atom A

Note. K_Scaled(A) = (1+V(Mol)/T(Mol))*K(A) = (E(Mol)/T(Mol))*K(A)

H_2O

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.096280696	-4.51579E-05	75.44435714	-75.67260469	0.130715883
H2	0.54813183	1.56412E-05	0.391741648	-0.392926814	0.173629559
H3	0.548129566	1.59059E-05	0.391741154	-0.392926319	0.173628936
Total	-1.92998E-05	-1.36108E-05	76.22783995	-76.45845782	

BeH_2

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
Be1	1.65491442	3.76922E-05	14.25869156	-14.38688405	1.90628E-07
H2	-0.827441221	-4.41243E-06	0.761108332	-0.767951061	0.529440009
H3	-0.827440802	-4.27755E-06	0.76110819	-0.767950918	0.529439247
Total	3.23976E-05	2.90022E-05	15.78090808	-15.92278603	

BeF_2

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|

Be1	1.712506237	8.80365E-05	14.21092092	-14.2536159	3.07946E-16
F2	-0.856223543	-1.46899E-05	99.91037514	-100.2105437	0.440669195
F3	-0.856223543	-1.46899E-05	99.91037514	-100.2105437	0.440669195
Total	5.91517E-05	5.86567E-05	214.0316712	-214.6747033	

BeH_2:H_2O

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.24534795	-3.58671E-05	75.58849609	-75.91560531	0.053034367
H2	0.61914358	1.36964E-05	0.348282315	-0.349789507	0.144153399
H3	0.619138534	1.42365E-05	0.348284995	-0.349792198	0.144157301
Be4	1.642716431	-7.31313E-05	14.22062468	-14.28216443	0.059948557
H5	-0.817938582	6.71822E-07	0.753454918	-0.756715494	0.345916976
H6	-0.81793669	7.26184E-07	0.753460728	-0.756721329	0.345905297
Total	-0.000224678	-7.96676E-05	92.01260373	-92.41078827	

BeF_2:H_2O

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
Be1	1.719669985	1.76629E-05	14.17327953	-14.21741131	0.005837175
O2	-1.221472658	-4.03901E-05	75.59251817	-75.82789291	0.099017431
H3	0.627489776	-6.14617E-06	0.343408695	-0.344477977	0.139083813
H4	0.627421297	-3.66906E-06	0.343517725	-0.344587347	0.139083863
F5	-0.876537179	-6.94879E-06	99.90551571	-100.2165946	0.32436472
F6	-0.876481851	1.04602E-05	99.90554706	-100.216626	0.325516454

Total	8.93711E-05	-2.90311E-05	290.2637869	-291.1675902

$(H_2O)_2$ ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.146960286	-3.48372E-05	75.46068494	-75.69470739	0.131064922
H2	0.589476136	-6.19491E-05	0.368472901	-0.369615628	0.134217803
H3	0.537102085	1.63975E-05	0.39791085	-0.399144871	0.179143306
O4	-1.113397261	-3.57648E-05	75.46576269	-75.69980089	0.192872776
H5	0.566867627	1.85576E-05	0.38028379	-0.381463145	0.165286442
H6	0.566854846	1.82933E-05	0.380288876	-0.381468247	0.165289566
Total	-5.68525E-05	-7.93028E-05	152.4534041	-152.9262002	

WD(BeH_2)a ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.305027705	-2.74227E-05	75.62938841	-75.91741613	0.058317613
H2	0.654589496	4.9594E-05	0.319133265	-0.320348655	0.109085305
H3	0.613402366	1.1946E-05	0.352597853	-0.35394069	0.145657814
O4	-1.159583794	-4.66958E-05	75.50074956	-75.78828737	0.178414486
H5	0.570125004	1.27622E-05	0.378226854	-0.379667297	0.163504577
H6	0.58599073	3.07089E-05	0.352162133	-0.353503311	0.157551702
Be7	1.641457878	2.07934E-05	14.21390584	-14.26803822	0.059188543
H8	-0.784088713	-1.14589E-05	0.753531505	-0.756401261	0.313009309
H9	-0.816817685	7.05398E-07	0.751886341	-0.754749833	0.349520331
Total	4.75776E-05	4.09324E-05	168.2515818	-168.8923528	

WD(BeH_2)b ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.201428488	3.40188E-05	75.56211037	-75.85179888	0.210974194
H2	0.600371298	2.08765E-05	0.358839703	-0.360215415	0.15426571
H3	0.600341524	2.13421E-05	0.358865458	-0.360241269	0.154259913
Be4	1.641451396	1.9971E-06	14.18160094	-14.23597008	0.047954018
H5	-0.819870162	1.15452E-05	0.750116072	-0.752991852	0.225668834
H6	-0.819885155	1.22061E-05	0.750121391	-0.752997191	0.225721163
O7	-1.201434331	3.93341E-05	75.56214637	-75.85183502	0.210983416
H8	0.600371624	2.29246E-05	0.358847336	-0.360223077	0.154258434
H9	0.600361328	2.22365E-05	0.358851226	-0.360226983	0.154264731
Total	0.000279034	0.000186481	168.2414989	-168.8864998	

WD(BeF_2)a

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.284864907	-6.55954E-06	75.63074143	-75.86810776	0.092889969
H2	0.657620287	-4.56735E-05	0.316282161	-0.317274809	0.104625464
H3	0.618075949	9.28571E-06	0.349682773	-0.350780249	0.143019862
O4	-1.16260427	-3.42048E-05	75.50733168	-75.74431069	0.189518517
H5	0.574419606	1.44523E-05	0.376237217	-0.377418034	0.161180059
H6	0.625302363	-4.10414E-05	0.343723005	-0.344801776	0.125897121
Be7	1.71952978	-8.46751E-05	14.16686881	-14.21133138	0.002449283
F8	-0.871346283	-3.38047E-06	99.9065122	-100.2200678	0.268928627
F9	-0.876376335	-1.02775E-05	99.90487708	-100.2184275	0.32666981
Total	-0.00024381	-0.000202074	366.5022564	-367.65252	

WD(BeF_2)b

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|

O1	-1.18248174	6.08492E-06	75.5679964	-75.80651394	0.196091292
H2	0.607046579	1.88421E-05	0.355363387	-0.356485031	0.147917813
H3	0.607079389	1.88337E-05	0.355344012	-0.356465595	0.147907887
Be4	1.723956282	-0.000113766	14.13600164	-14.18061953	0.000293909
O5	-1.182758307	1.89923E-05	75.56841027	-75.80692911	0.196069929
H6	0.607203595	1.84675E-05	0.355274366	-0.356395729	0.147855963
H7	0.607255015	1.84304E-05	0.355234846	-0.356356084	0.147838315
F8	-0.893550823	-1.67917E-05	99.89883127	-100.2141449	0.240325985
F9	-0.893553651	-1.64254E-05	99.89881607	-100.2141297	0.240256058

Total	0.000196338	-4.73323E-05	366.4912723	-367.6480397	

$(H_2O)_3$

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.162053349	-2.98449E-05	75.48697009	-75.72488766	0.178654606
O2	-1.165703617	-4.90548E-05	75.48673937	-75.72465621	0.17507886
O3	-1.162668692	-4.02691E-05	75.48716535	-75.72508354	0.171653399
H4	0.607301157	-1.746E-05	0.353522556	-0.354636778	0.133698177
H5	0.606871663	2.46315E-05	0.353846661	-0.354961904	0.132415315
H6	0.607483198	7.00798E-05	0.353809546	-0.354924672	0.131737551
H7	0.556617974	1.80533E-05	0.386467127	-0.387685183	0.169877562
H8	0.555730942	1.6489E-05	0.3870697	-0.388289655	0.170464957
H9	0.556436233	1.67905E-05	0.386597777	-0.387816244	0.170209071

Total	1.55097E-05	9.41522E-06	228.6821882	-229.4029418	

WT(BeH_2)c ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.260680822	-7.27888E-05	75.5981035	-75.873174	0.195390422
H2	0.638886884	5.29182E-05	0.330776773	-0.331980334	0.116070016
H3	0.594942348	1.97674E-05	0.363455828	-0.364778295	0.154840215
O4	-1.168915309	-2.26554E-05	75.49580611	-75.77050439	0.169040548
H5	0.559346473	1.32412E-05	0.384004497	-0.385401732	0.169337437
H6	0.577652472	1.76683E-05	0.353142193	-0.354427132	0.1554716
Be7	1.643532228	-2.0157E-05	14.17291544	-14.22448487	0.046748453
H8	-0.769931252	2.19703E-05	0.751854939	-0.754590631	0.227946058
H9	-0.817097215	1.24816E-05	0.749951826	-0.752680593	0.226444236
O10	-1.198100522	-1.88342E-06	75.55985517	-75.83478651	0.212655883
H11	0.598287424	1.39613E-05	0.36065394	-0.361966211	0.153757745
H12	0.602191017	2.39067E-05	0.357594901	-0.358896042	0.153932305
Total	0.000113725	5.84304E-05	244.4781151	-245.3676707	

WT(BeH_2)b ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.355763591	-8.75028E-06	75.67356109	-75.94733744	0.007513901
H2	0.653818676	-5.62283E-05	0.321458378	-0.32262137	0.115184775
H3	0.653856778	4.54394E-06	0.321472122	-0.322635163	0.115231558
O4	-1.157991751	-2.08058E-05	75.4918276	-75.76494647	0.177317527
H5	0.566722554	1.39569E-05	0.380357393	-0.381733473	0.16529717
H6	0.583304918	3.76632E-05	0.356021554	-0.35730959	0.159289123
Be7	1.640123043	-7.83735E-05	14.2105592	-14.26197101	0.062468419
H8	-0.788221075	-3.52893E-05	0.751350908	-0.75406919	0.317982466
H9	-0.788194721	-1.23747E-05	0.751365009	-0.754083342	0.317989333
O10	-1.157990284	-2.21804E-05	75.49179836	-75.76491712	0.177328908

H11	0.583220462	-2.88982E-05	0.356022613	-0.357310653	0.159302083
H12	0.566708392	1.41377E-05	0.380364067	-0.381740171	0.165305525
Total	-0.0004066	-0.000192599	244.4861583	-245.370675	

WT(BeH_2)d

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.313461124	-5.351E-05	75.63013433	-75.90330281	0.069312589
H2	0.654498368	6.48317E-05	0.317295241	-0.31844128	0.100119726
H3	0.606150435	1.08293E-05	0.356972473	-0.358261822	0.14915892
O4	-1.189417186	-5.79182E-06	75.5254021	-75.7981923	0.190525174
H5	0.617184053	4.27877E-05	0.350202139	-0.351467034	0.12145765
H6	0.579780703	4.7638E-05	0.360071491	-0.361372033	0.163998193
Be7	1.639095332	-1.16054E-05	14.21475427	-14.26609654	0.059943069
H8	-0.798743456	1.15123E-05	0.750341183	-0.753051341	0.302330797
H9	-0.82035092	4.23462E-07	0.750244674	-0.752954483	0.335719801
O10	-1.124011562	-3.77611E-05	75.47264846	-75.74524812	0.200282374
H11	0.574803432	1.72159E-05	0.375707861	-0.37706488	0.161563275
H12	0.57455212	1.76529E-05	0.375854021	-0.377211568	0.161799258
Total	8.01959E-05	0.000104223	244.4796283	-245.3626642	

WT(BeH_2)a

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.31726067	-7.79707E-05	75.6271126	-75.90147491	0.040686655
O2	-1.173816469	-1.87677E-05	75.51870596	-75.79267498	0.201535061
O3	-1.183842408	-2.95359E-05	75.50178565	-75.7756933	0.18330293
H4	0.65678255	5.16244E-05	0.316106193	-0.317252972	0.091715877
H5	0.635632481	-9.92265E-05	0.334389874	-0.335602984	0.112332604

H6	0.584676784	-4.18484E-05	0.350593256	-0.351865148	0.14806166
H7	0.567043229	1.29272E-05	0.380009216	-0.381387825	0.165848325
H8	0.568572706	1.49693E-05	0.379383498	-0.380759837	0.163782475
H9	0.60812077	1.28231E-05	0.356127573	-0.357419544	0.147771902
Be10	1.641756423	-4.24136E-05	14.21182232	-14.26338039	0.056160065
H11	-0.770981254	-7.79651E-06	0.757770052	-0.760519113	0.323530877
H12	-0.816914086	6.79707E-07	0.751771952	-0.754499253	0.335527406
Total	-0.000229944	-0.000224536	244.4855781	-245.3725303	

WT(BeF_2)b

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.339980772	-1.465E-05	75.6761808	-75.91523781	0.072614852
H2	0.657064226	-4.74575E-05	0.318598679	-0.319605115	0.111947639
H3	0.657376805	1.20499E-05	0.318525594	-0.319531799	0.112471042
O4	-1.162335879	-2.58405E-05	75.49678127	-75.73527157	0.185325684
H5	0.569599739	1.54964E-05	0.379101747	-0.380299309	0.163666919
H6	0.618048191	1.99938E-05	0.348582696	-0.34968385	0.129182058
Be7	1.720755096	0.000738442	14.16436388	-14.20910835	0.001934702
F8	-0.872142213	-3.09016E-07	99.90405566	-100.2196472	0.276681015
F9	-0.872176641	-8.64666E-06	99.90437462	-100.2199672	0.277450615
O10	-1.163099557	-2.71156E-05	75.4964704	-75.73495971	0.187176265
H11	0.617922233	3.08156E-05	0.348732685	-0.349834313	0.129272297
H12	0.569447662	1.54718E-05	0.379168734	-0.380366508	0.163930322
Total	0.00047889	0.000708251	442.7349368	-444.1335128	

WT(BeF_2)c

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.247000461	-9.64753E-06	75.60460462	-75.84455095	0.181788303

H2	0.642393775	-3.71357E-06	0.327820268	-0.328860671	0.112011355
H3	0.599626695	1.80795E-05	0.360400316	-0.361544118	0.151017487
O4	-1.171213441	-3.09015E-05	75.50297426	-75.74259805	0.186720099
H5	0.564693037	1.50936E-05	0.38175447	-0.382966044	0.16615663
H6	0.627838621	-2.8087E-05	0.342617548	-0.343704914	0.12053291
Be7	1.72519135	-3.85342E-05	14.12654024	-14.17137364	0.002624879
O8	-1.179364923	-3.60432E-06	75.5663329	-75.80615777	0.196401156
H9	0.604365384	2.03773E-05	0.357249909	-0.358383713	0.14864296
H10	0.607585209	2.07617E-05	0.354926684	-0.356053115	0.147816451
F11	-0.892814815	-1.55423E-05	99.89869777	-100.2157463	0.237868459
F12	-0.881367847	-8.51471E-06	99.90255998	-100.2196207	0.200888438
Total	-6.74154E-05	-6.42331E-05	442.726479	-444.13156	

WT(BeF_2)d

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.293606198	-9.52864E-05	75.63120656	-75.86897562	0.092748465
H2	0.65666266	5.58446E-05	0.314510631	-0.315499388	0.095023646
H3	0.61105024	8.65647E-06	0.353947308	-0.355060046	0.146339924
O4	-1.194116984	-5.63555E-06	75.5337708	-75.77123354	0.196791945
H5	0.619589657	-2.85513E-05	0.348694746	-0.349790971	0.120420587
H6	0.611533608	-1.75884E-05	0.3524415	-0.353549504	0.13435167
Be7	1.718476179	-1.28013E-05	14.16824368	-14.21278575	0.002370382
O8	-1.124530073	-3.6367E-05	75.47315489	-75.71042707	0.200990663
H9	0.575605177	1.39411E-05	0.375263092	-0.376442843	0.161118905
H10	0.575365299	1.77966E-05	0.375383703	-0.376563833	0.161388573
F11	-0.877036517	8.91861E-06	99.90257218	-100.2166455	0.265899665
F12	-0.879065681	-1.07033E-05	99.90232619	-100.2163987	0.317726296

Total	-7.26332E-05	-0.000101776	442.7315153	-444.1233727	

WT(BeF_2)a ----------

Atom A	q(A)	L(A)	K(A)	K_Scaled(A)	|Mu_Intra(A)|
O1	-1.178694696	-4.96803E-05	75.50602936	-75.74428772	0.193319654
O2	-1.298427184	3.66944E-05	75.63195786	-75.8706136	0.041642306
O3	-1.179459635	-4.21451E-05	75.52218662	-75.76049597	0.194834507
H4	0.635883289	-0.000114125	0.339569312	-0.340640819	0.111590585
H5	0.660885632	5.04574E-05	0.312156406	-0.313141412	0.087908619
H6	0.635426496	8.57304E-05	0.333570659	-0.334623237	0.108775927
H7	0.57147524	1.55337E-05	0.377580879	-0.378772331	0.16245996
H8	0.612697642	9.89965E-06	0.352914378	-0.354027995	0.145250196
H9	0.567604042	1.59886E-05	0.38017723	-0.381376874	0.164622545
Be10	1.72093422	5.29441E-06	14.16453238	-14.2092284	0.001787798
F11	-0.870392551	4.64649E-06	99.91234523	-100.2276174	0.260415316
F12	-0.877761722	-9.87396E-06	99.90410818	-100.2193544	0.3156862
Total	0.000170772	8.42052E-06	442.7371285	-444.1341802	