Supporting Information

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Fostering The Basic Instinct Of Boron In Boron−Beryllium Interactions

M, Merced Montero-Campillo,[a,*] Ibon Alkorta,[a] and José Elguero[a]

[a]Instituto de Química Médica (CSIC), Juan de la Cierva, 3, 28006 Madrid (Spain)

*Email: mm.montero@uam.es

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Table S1. Pyramidalization degree or departure from planarity (º) of L_2BH isolated and in the $HL_2B{:}BeX_2$ complexes, along with the difference between these two magnitudes (L = CO, CS, CNH, H_3CCN, N_2, NH_3, PH_3, PF_3, PMe_3, OH_2; X = H, F) at the M06-2X/6-31+G(d) level of theory.

		L_2BH	$HL_2B\cdots BeX_2$	Change
$HL_2B\cdots BeX_2$				
L	X			
CNH	H	0.0	0.0	0.0
	F	0.0	0.0	0.0
CO	H	0.0	0.5	0.5
	F	0.0	0.7	0.7
CS	H	0.0	0.0	0.0
	F	0.0	5.0	5.0
N_2	H	0.0	6.1	6.1
	F	0.0	7.3	7.3
NH_3	H	2.2	35.4	33.2
	F	2.2	28.0	25.8
$NCCH_3$	H	---	---	---
	F	0.1	10.1	10.0
PH_3	H	2.5	12.5	10.1
	F	2.5	14.3	11.8
PF_3	H	0.0	6.8	6.8
	F	0.0	10.5	10.5
PMe_3	H	2.2	20.5	18.3
	F	2.2	21.4	19.2
OH_2	H	73.9	52.5	21.4
	F	73.9	51.1	22.8

Figure S1. B-Be distances (Å) versus the degree of pyramidalization (º) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-31+G(d) level of theory.

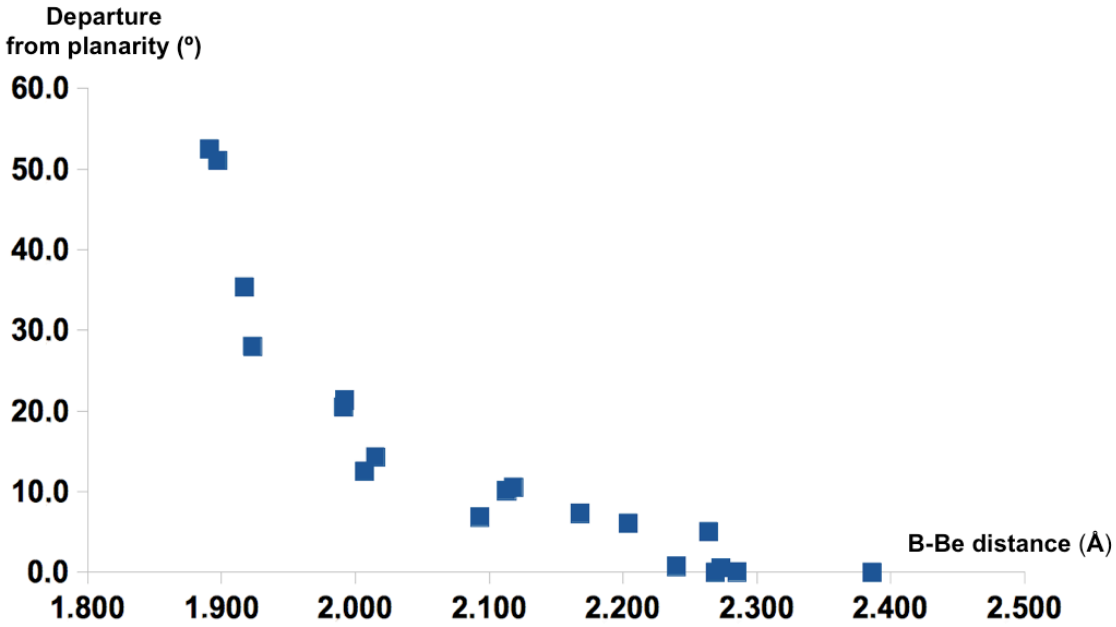

Figure S2. Linear correlation between binding energies and interaction energies (kJ/mol) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory.

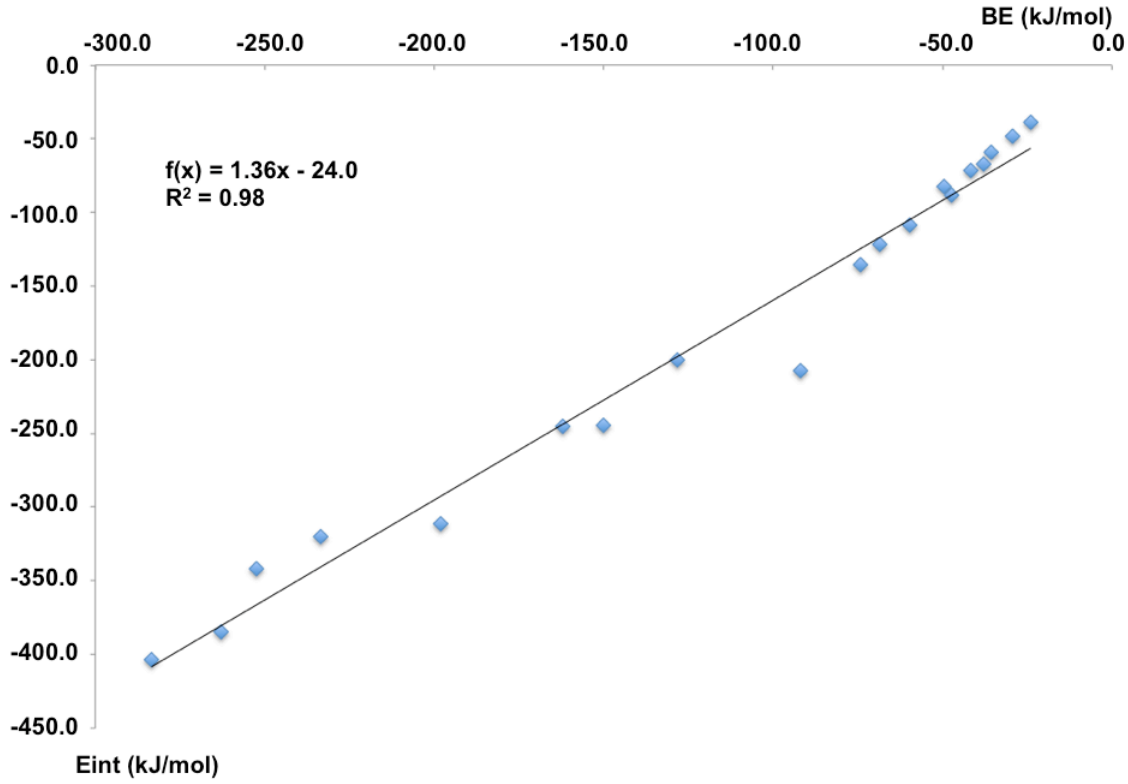

Figure S3. Exponential correlation between B-Be distances (Å) and electron density (a.u.) at the B-Be BCP for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory.

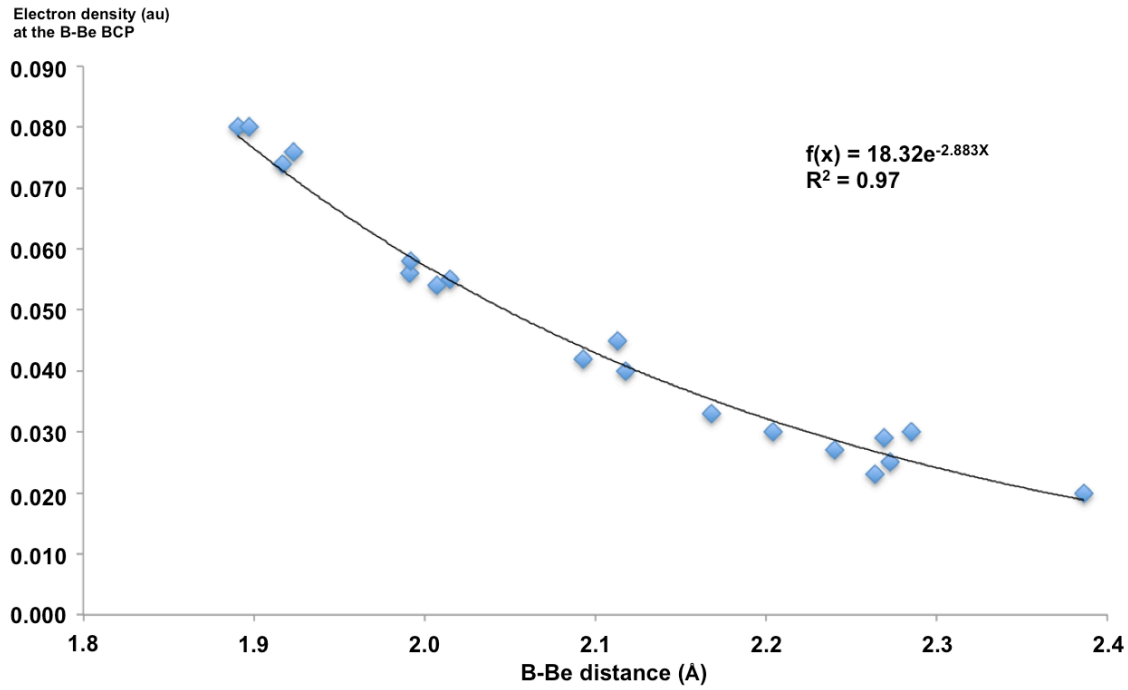

Figure S4. Linear correlation between B-Be distances (Å) and ELF population (e) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory.

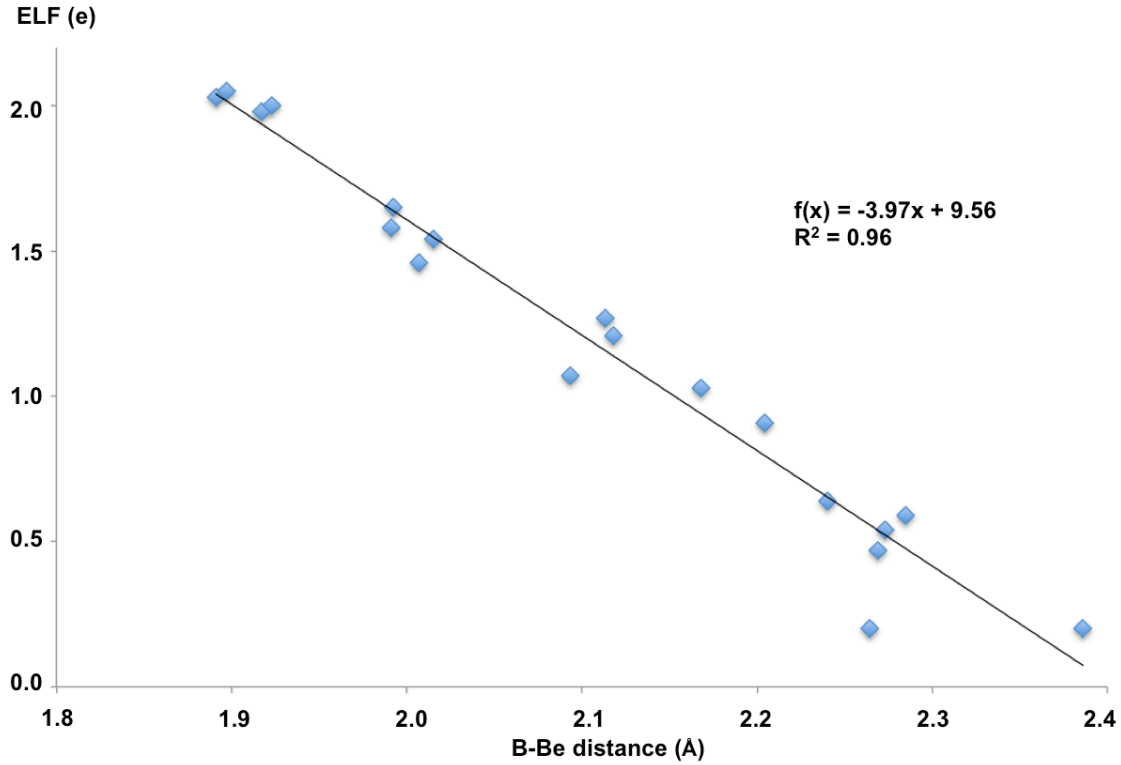

Figure S5. (First page) Molecular graphs (QTAIM calculations) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory.

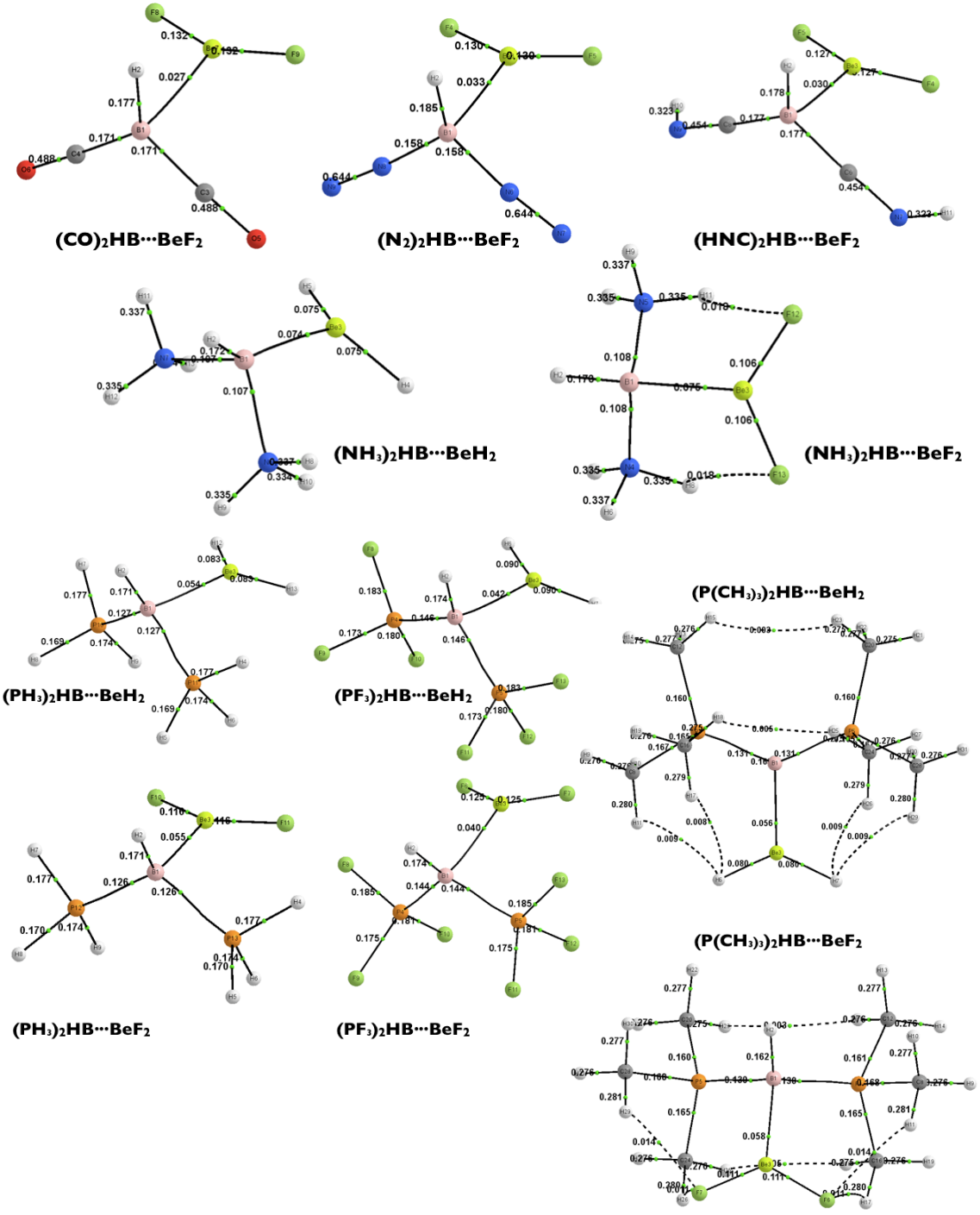

Figure S5. (Second page) Molecular graphs (QTAIM calculations) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory.

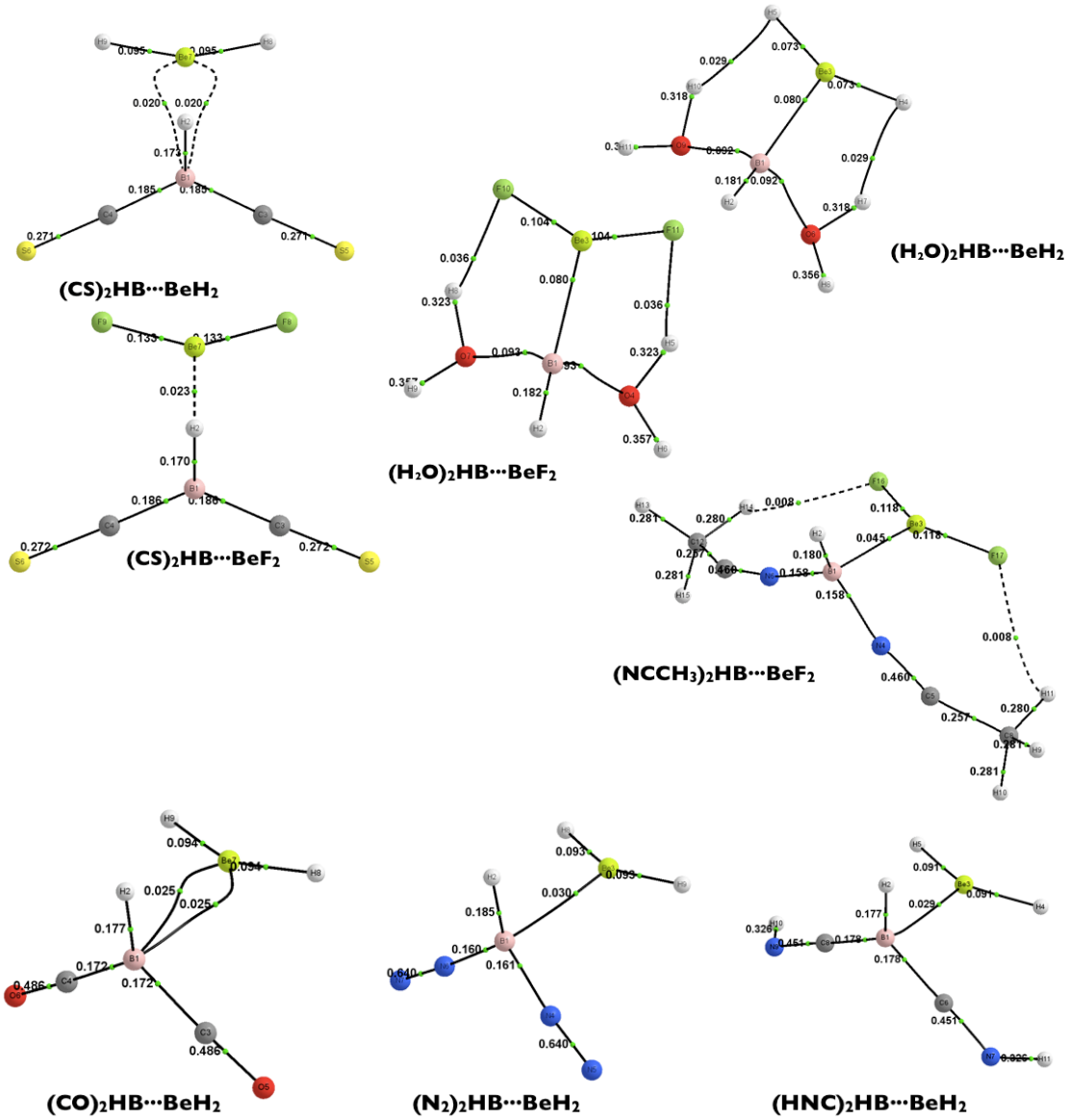

Table S2. Values at the B-Be BCP for the electron density (ρ), laplacian of the density ($\nabla^2\rho$) and total energy density (H) for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory. Values are given in atomic units.

		ρ	$\nabla^2\rho$	H
$HL_2B\cdots BeX_2$				
L	X			
CNH	H	0.029	0.053	-0.008
	F	0.030	0.039	-0.009
CO	H	0.025	0.012	-0.008
	F	0.027	0.052	-0.007
CS	H	0.020	0.009	-0.005
	F	0.023	0.059	-0.005
N_2	H	0.030	0.064	-0.008
	F	0.033	0.054	-0.011
NH_3	H	0.074	0.066	-0.038
	F	0.076	0.055	-0.040
$NCCH_3$	H	---	---	---
	F	0.045	0.035	-0.019
PH_3	H	0.054	0.069	-0.023
	F	0.055	0.057	-0.024
PF_3	H	0.042	0.077	-0.014
	F	0.040	0.065	-0.014
PMe_3	H	0.056	0.059	-0.025
	F	0.058	0.045	-0.027
OH_2	H	0.080	0.075	-0.043
	F	0.080	0.068	-0.044

Table S3. B and Be atomic charges from the NBO calculations for a set of $L_2HB\cdots BeX_2$ (L = CNH, CO, CS, N_2, NH_3, $NCCH_3$, PH_3, PF_3, PMe_3, OH_2; X = H, F) complexes at the M06-2X/6-311+G(3df,2pd)//M06-2X/6-31+G(d) level of theory. Values are given in atomic units.

		q(B)	q(Be)	Δq (qBe-qB)
$HL_2B\cdots BeX_2$				
L	X			
CNH	H	-0.475	0.650	1.125
	F	-0.502	1.289	1.791
CO	H	-0.697	0.660	1.356
	F	-0.735	1.301	2.037
CS	H	-0.391	0.754	1.145
	F	-0.413	1.329	1.741
N_2	H	-0.141	0.617	0.758
	F	-0.185	1.248	1.433
NH_3	H	-0.123	0.307	0.430
	F	-0.179	1.019	1.198
$NCCH_3$	H	-	-	-
	F	-0.080	1.180	1.259
PH_3	H	-1.156	0.476	1.632
	F	-1.173	1.166	2.339
PF_3	H	-1.438	0.484	1.922
	F	-1.482	1.219	2.702
PMe_3	H	-1.214	0.497	1.712
	F	-1.253	1.190	2.443
OH_2	H	0.102	0.331	0.229
	F	0.049	0.983	0.934

Table S4. Cartesian coordinates.

HB···BeH_2

H	0.039575	0.000000	-0.244761
H	0.039575	0.000000	2.288581
B	2.436574	0.000000	1.021910
H	3.634131	0.000000	1.021910
Be	0.560146	0.000000	1.021910

HB···BeF_2

F	-0.002517	0.000000	-0.313044
F	-0.002517	0.000000	2.356864
B	2.505890	0.000000	1.021910
H	3.704750	0.000000	1.021910
Be	0.504395	0.000000	1.021910

$(CNH)_2$HB···BeH_2

B	-0.285708	0.000000	0.039528
H	-0.388812	0.000000	1.224624
Be	1.973903	0.000000	-0.169061
H	2.405426	-1.287988	-0.234176
H	2.405426	1.287988	-0.234176
C	-0.221835	-1.239408	-0.751727
N	-0.207446	-2.258323	-1.374472
C	-0.221835	1.239408	-0.751727
N	-0.207446	2.258323	-1.374472
H	0.613456	2.798517	-1.640870
H	0.613456	-2.798517	-1.640870

$(CNH)_2$HB···BeF_2

B	-0.345040	0.000000	0.036898
H	-0.520115	0.000000	1.212942
Be	1.925231	0.000000	-0.220965
F	2.428032	-1.327918	-0.343423
F	2.428032	1.327918	-0.343423
C	-0.254492	-1.245009	-0.747279
N	-0.163829	-2.274830	-1.339216
C	-0.254492	1.245009	-0.747279
N	-0.163829	2.274830	-1.339216
H	0.699543	2.779691	-1.538218
H	0.699543	-2.779691	-1.538218

$(CO)_2HB\cdots BeH_2$

B	0.135015	-0.139625	-0.088487
H	0.263317	-0.330678	1.076214
C	1.268123	-0.214249	-1.023499
C	-1.186808	0.001867	-0.718033
O	2.170458	-0.232520	-1.723613
O	-2.221513	0.154121	-1.177372
Be	0.397213	2.041394	0.493668
H	1.731068	2.245906	0.430478
H	-0.856482	2.471424	0.754847

$(CO)_2HB\cdots BeF_2$

B	0.138671	-0.131056	-0.088568
H	0.272930	-0.317624	1.076369
C	1.267692	-0.221664	-1.030106
C	-1.189872	-0.014599	-0.713659
O	2.164083	-0.253237	-1.734396
O	-2.227168	0.116749	-1.168975
Be	0.393407	2.019781	0.484168
F	-0.898595	2.512657	0.771753
F	1.779244	2.286630	0.427616

$(CS)_2HB\cdots BeH_2$

B	0.136280	-0.190452	-0.040527
H	0.278256	-0.252937	1.145160
C	1.262717	-0.256657	-0.975356
C	-1.177738	-0.042491	-0.671860
S	2.452552	-0.282965	-1.938075
S	-2.552237	0.156206	-1.315728
Be	0.410308	2.105656	0.549114
H	1.745963	2.267164	0.473128
H	-0.855709	2.494117	0.798348

$(CS)_2HB\cdots BeF_2$

B	0.134690	-0.124848	-0.098237
H	0.291710	-0.013264	1.085150
C	1.268446	-0.268390	-1.014456
C	-1.195180	-0.052631	-0.707903
S	2.466194	-0.382246	-1.956392
S	-2.587207	0.059906	-1.327904
Be	0.408624	2.010997	0.599651
F	1.794970	2.266760	0.555657
F	-0.881854	2.501357	0.888639

$(N_2)_2HB\cdots BeH_2$

B	0.021787	-0.146747	-0.091734
H	-0.244111	-0.343723	1.042896
Be	2.113480	0.181058	0.520470
N	0.113002	-1.236706	-1.032871
N	0.269587	-2.110574	-1.710753
N	-0.339851	1.094694	-0.732602
N	-0.548708	2.101966	-1.167755
H	2.176032	1.509845	0.773579
H	2.672801	-1.049814	0.446373

$(N_2)_2HB\cdots BeF_2$

B	-0.000995	-0.155585	-0.077226
H	-0.357040	-0.374886	1.028198
Be	2.063871	0.172569	0.494786
F	2.216734	1.555601	0.764706
F	2.734299	-1.073831	0.421329
N	0.123599	-1.238145	-1.030832
N	0.305662	-2.106048	-1.706493
N	-0.333306	1.102218	-0.713523
N	-0.518805	2.118108	-1.133342

$(NH_3)_2HB\cdots BeH_2$

B	0.209291	0.000000	0.234826
H	-0.523919	0.000000	1.198707
Be	2.069727	0.000000	-0.228464
H	2.524415	-1.244362	-0.731208
H	2.524415	1.244362	-0.731208
N	-0.266767	-1.309602	-0.659692
N	-0.266767	1.309602	-0.659692
H	-0.114796	-2.084808	-0.010886
H	-1.222354	-1.395728	-1.022811
H	0.413127	-1.484419	-1.409074
H	-0.114796	2.084808	-0.010886
H	-1.222354	1.395728	-1.022811
H	0.413127	1.484419	-1.409074

$(NH_3)_2HB\cdots BeF_2$

B	0.203374	0.000000	0.251760
H	-0.528866	0.000000	1.214602
Be	2.052138	0.000000	-0.277903
N	-0.254056	-1.323539	-0.630865
N	-0.254056	1.323539	-0.630865
H	-0.140150	-2.089018	0.037203
H	-1.199268	-1.402071	-1.020712
H	0.446719	-1.524221	-1.353455
H	-0.140150	2.089018	0.037203
H	-1.199268	1.402071	-1.020712
H	0.446719	1.524221	-1.353455
F	2.494606	1.287103	-0.857537
F	2.494606	-1.287103	-0.857537

$(NCCH_3)_2HB\cdots BeF_2$

B	-0.104054	-0.000280	0.181137
H	-0.121981	-0.000630	1.371752
Be	1.752068	0.000194	-0.827664
N	-0.499663	-1.227270	-0.511943
C	-0.600701	-2.259191	-1.037509
N	-0.499736	1.226993	-0.511283
C	-0.600844	2.259225	-1.036289
C	-0.177623	-3.426156	-1.810093
H	-0.346529	-4.335711	-1.229812
H	-0.762324	-3.491362	-2.730411
H	0.888412	-3.310328	-2.040765
C	-0.176806	3.426254	-1.808321
H	-0.346536	4.335857	-1.228379
H	0.889466	3.310304	-2.037801
H	-0.760484	3.491306	-2.729320
F	2.193333	1.313627	-1.240469
F	2.192483	-1.312832	-1.242567

$(PH_3)_2HB\cdots BeH_2$

B	0.093746	0.000000	0.262391
H	-0.146665	0.000000	1.432876
Be	2.040824	0.000000	-0.224165
H	0.351933	-2.674271	-0.054686
H	-1.585501	-2.141402	-0.846519
H	0.175666	-1.609937	-1.956661
H	0.351933	2.674271	-0.054686
H	-1.585501	2.141402	-0.846519
H	0.175666	1.609937	-1.956661
P	-0.297667	1.581885	-0.637939
P	-0.297667	-1.581885	-0.637939
H	2.572790	1.254694	-0.470883
H	2.572790	-1.254694	-0.470883

$(PH_3)_2HB\cdots BeF_2$

B	0.087317	0.000000	0.266415
H	-0.205671	0.000000	1.425574
Be	2.051019	0.000000	-0.184917
H	0.403630	-2.663073	-0.113275
H	-1.586410	-2.165538	-0.795692
H	0.112499	-1.578942	-1.982877
H	0.403630	2.663073	-0.113275
H	-1.586410	2.165538	-0.795692
H	0.112499	1.578942	-1.982877
F	2.619897	1.309713	-0.448363
F	2.619897	-1.309713	-0.448363
P	-0.304775	1.582273	-0.644465
P	-0.304775	-1.582273	-0.644465

$(PF_3)_2HB\cdots BeH_2$

B	-0.264770	0.639356	0.000000
H	-0.832552	1.684359	0.000000
Be	1.792021	1.026718	0.000000
P	-0.229068	-0.265178	-1.540785
P	-0.229068	-0.265178	1.540785
H	2.275365	1.068541	-1.271396
H	2.275365	1.068541	1.271396
F	0.039163	0.610467	-2.789332
F	-1.477021	-1.047157	-2.095320
F	0.800284	-1.428600	-1.630541
F	-1.477021	-1.047157	2.095320
F	0.800284	-1.428600	1.630541
F	0.039163	0.610467	2.789332

$(PF_3)_2HB\cdots BeF_2$

B	-0.237624	0.656756	0.000000
H	-0.867711	1.665982	0.000000
Be	1.842383	1.057386	0.000000
P	-0.245070	-0.271494	-1.533925
P	-0.245070	-0.271494	1.533925
F	2.350563	1.074066	-1.335110
F	2.350563	1.074066	1.335110
F	-0.013896	0.604830	-2.785605
F	-1.501794	-1.066535	-2.037699
F	0.797746	-1.417639	-1.645537
F	-1.501794	-1.066535	2.037699
F	0.797746	-1.417639	1.645537
F	-0.013896	0.604830	2.785605

$(PMe_3)_2HB\cdots BeH_2$

B	0.053864	0.571924	-0.008985
H	-0.622906	1.572475	-0.003370
Be	1.992759	1.022382	-0.000325
P	-0.176276	-0.345716	-1.619017
P	-0.145294	-0.336845	1.610204
H	2.666048	0.980235	-1.221259
H	2.588665	1.224092	1.243448
C	0.085387	0.808256	-3.005344
H	-0.039685	0.294266	-3.963051
H	-0.638838	1.624616	-2.930906
H	1.096235	1.214622	-2.917114
C	-1.798944	-1.120207	-2.032908
H	-2.585315	-0.364154	-1.947990
H	-1.803562	-1.532998	-3.047749
H	-2.017128	-1.923567	-1.322341
C	1.002349	-1.711165	-1.910896
H	2.016264	-1.321240	-1.783464
H	0.828489	-2.522650	-1.197495
H	0.881566	-2.105901	-2.924378
C	-1.696334	-1.256779	2.003908
H	-1.697458	-1.621480	3.037050
H	-2.554562	-0.594966	1.853868
H	-1.799796	-2.112789	1.329006
C	1.146615	-1.580743	1.968152
H	1.115878	-2.387604	1.229925
H	2.120681	-1.084908	1.919670
H	0.996665	-2.008879	2.964119
C	-0.021813	0.865470	2.973758
H	0.939556	1.377284	2.880887
H	-0.830169	1.596344	2.882145
H	-0.094232	0.358386	3.940450

$(PMe_3)_2HB\cdots BeF_2$

B	0.006581	0.575620	-0.008614
H	-0.729231	1.533855	-0.004886
Be	1.947686	1.024491	-0.001224
P	-0.182368	-0.350479	-1.624971
P	-0.162403	-0.339969	1.616941
F	2.660653	0.999906	-1.279019
F	2.610220	1.159771	1.296915
C	0.090348	0.813457	-2.999757
H	-0.042953	0.309799	-3.961957
H	-0.622703	1.638715	-2.916735
H	1.107801	1.202593	-2.905953
C	-1.788283	-1.146101	-2.050885
H	-2.585739	-0.401196	-1.972506
H	-1.776109	-1.556583	-3.066308
H	-2.002012	-1.953676	-1.343911
C	1.027895	-1.688602	-1.908067
H	2.031895	-1.271865	-1.787846
H	0.875594	-2.500666	-1.190816
H	0.912700	-2.090050	-2.919633
C	-1.717425	-1.237333	2.032564
H	-1.706289	-1.599164	3.066361
H	-2.568400	-0.563957	1.894625
H	-1.841992	-2.092841	1.360885
C	1.128408	-1.588992	1.955637
H	1.087678	-2.395517	1.217740
H	2.102644	-1.094990	1.902280
H	0.984092	-2.017564	2.952284
C	0.011382	0.868331	2.968729
H	0.993151	1.338257	2.863780
H	-0.768216	1.629411	2.873917
H	-0.075896	0.373098	3.940431

$(OH_2)_2HB\cdots BeH_2$

B	-0.099377	1.180095	0.000000
H	-1.148019	1.769614	0.000000
Be	1.791441	1.184273	0.000000
H	2.275011	0.736037	1.263787
H	2.275011	0.736037	-1.263787
O	-0.229246	0.112956	1.253604
H	0.699917	0.174828	1.624680
H	-0.872881	0.368855	1.934355
O	-0.229246	0.112956	-1.253604
H	0.699917	0.174828	-1.624680
H	-0.872881	0.368855	-1.934355

$(OH_2)_2HB\cdots BeF_2$

B	-0.107053	1.188214	0.000000
H	-1.159619	1.767896	0.000000
Be	1.790100	1.195659	0.000000
O	-0.217483	0.136170	1.261921
H	0.690072	0.186337	1.669143
H	-0.897543	0.334009	1.925743
O	-0.217483	0.136170	-1.261921
H	0.690072	0.186337	-1.669143
H	-0.897543	0.334009	-1.925743
F	2.308063	0.727266	-1.310574
F	2.308063	0.727266	1.310574