Electronic Supplementary Information

Simulating the effect of triple bond to achieve the shortest main group metal–metal distance in diberyllium complexes: a computational study

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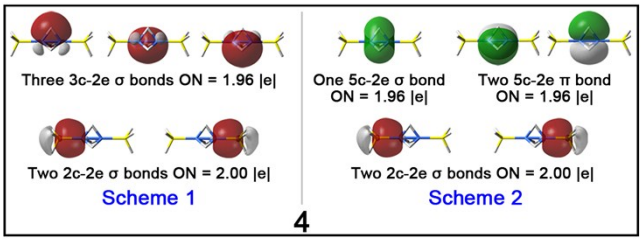
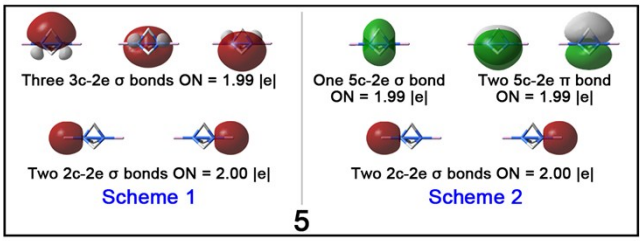
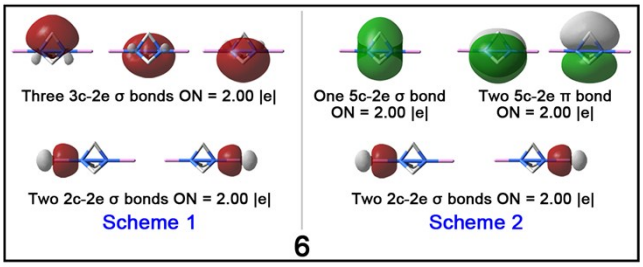
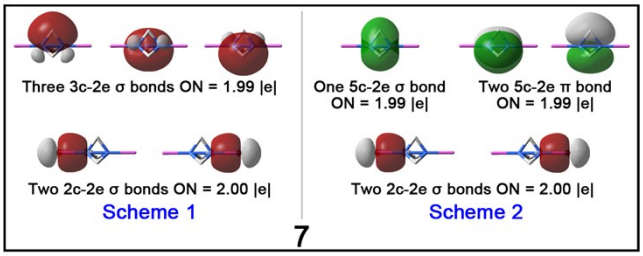
Contents

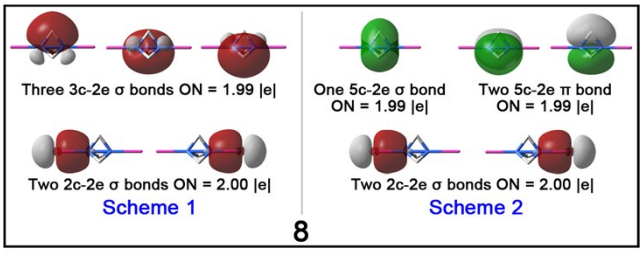
Fig. S1. AdNDP-generated orbitals (two phases shown in red/white or green/white) related to bonding to beryllium in **4**–**10**

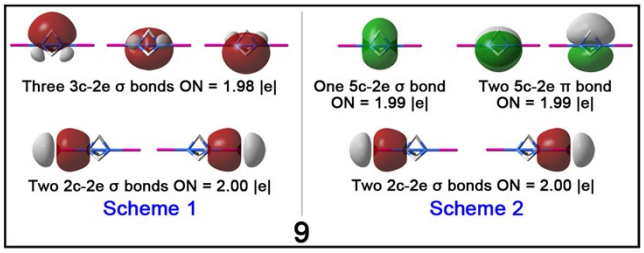












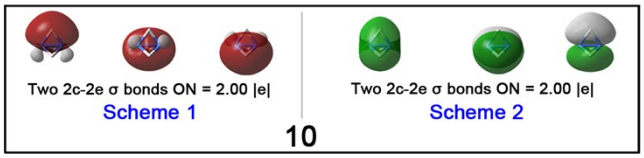


Fig. S2. B3LYP/BS1-optimized structures for **3–10** and their lowest isomers. The relative free energies (kcal/mol) were calculated using CCSD(T)/BS1 electronic energies plus B3LYP/BS1 Gibbs free energy corrections.

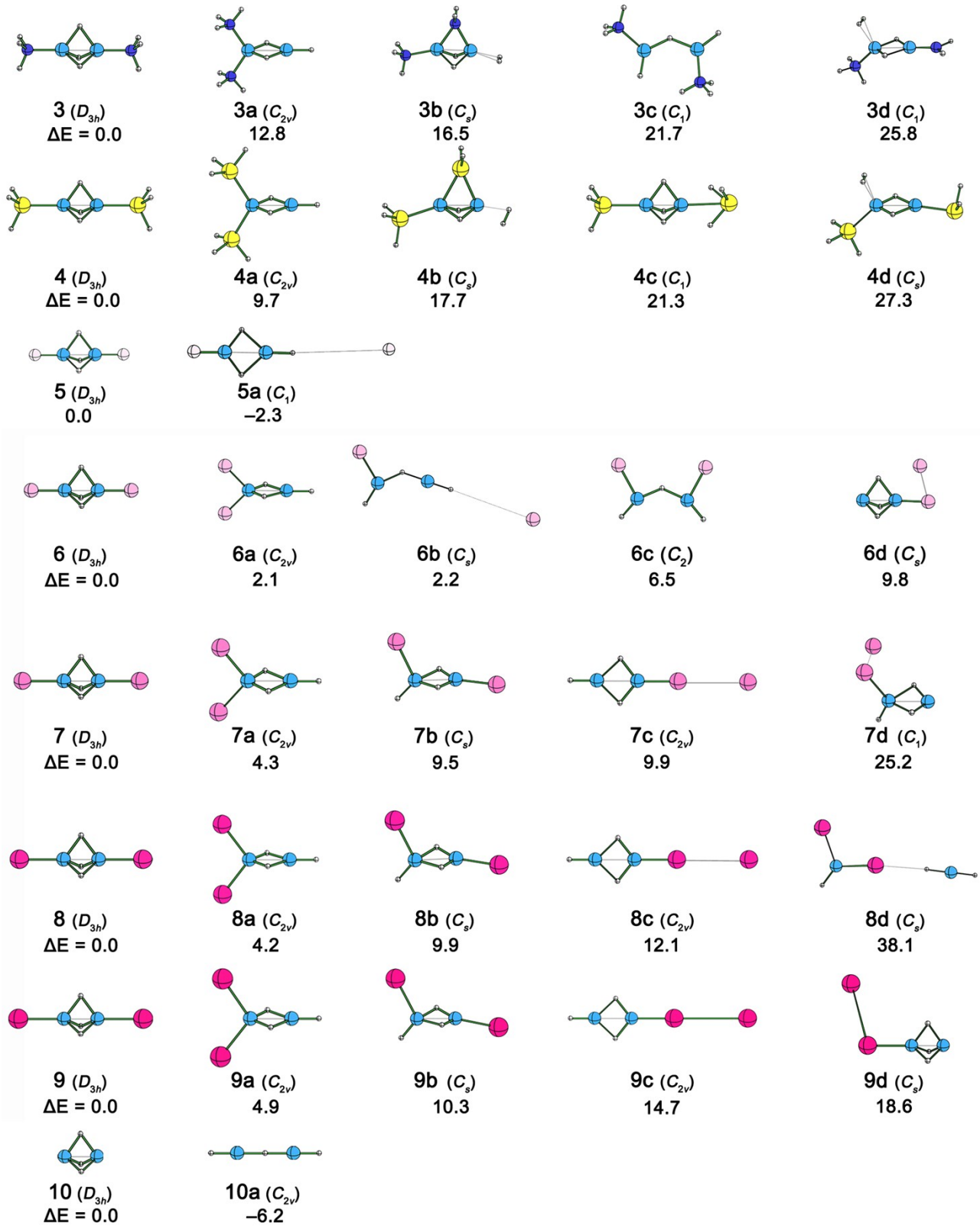
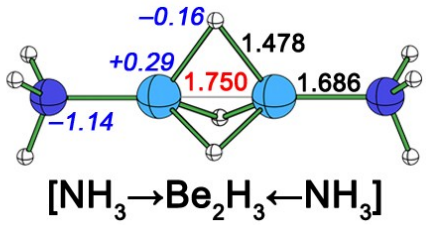


Fig. S3. B3LYP/BS1-optimized neutral free radical [NH_3→Be_2H_3←NH_3] with Be–Be distances, other interatomic distances, and NBO charges given in red, black, and italic blue fonts, respectively.



CCSD(T)/BS1-optimized structures (in Cartesian coordinates) for **1**–**10.**

1

Be	0.0000000000	0.8955577032	−0.0264642700
Be	0.0000000000	−0.8955577032	−0.0264642700
H	1.0377347228	0.0000000000	−0.7417433520
H	−1.0377347228	0.0000000000	−0.7417433520
N	0.0000000000	−2.5549356335	−0.5375099176
H	0.8153918192	−3.0228991818	−0.1564559664
H	−0.8153918192	−3.0228991818	−0.1564559664
N	0.0000000000	2.5549356335	−0.5375099176
H	−0.8153918192	3.0228991818	−0.1564559664
H	0.8153918192	3.0228991818	−0.1564559664
H	0.0000000000	−2.6857207339	−1.5436327867
H	0.0000000000	2.6857207339	−1.5436327867
C	0.0000000000	0.0000000000	1.4681863205
H	−0.8950994017	0.0000000000	2.1003880988
H	0.8950994017	0.0000000000	2.1003880988

2

Be	0.0000000000	0.8828906866	0.0432313685
Be	0.0000000000	-0.8828906866	0.0432313685
P	0.0000000000	2.9918109560	-0.3477244998
H	-1.0698477671	3.6757224501	0.2506584648
H	1.0698477671	3.6757224501	0.2506584648
H	0.0000000000	3.6315474575	-1.6045077464
P	0.0000000000	-2.9918109560	-0.3477244998
H	0.0000000000	-3.6315474575	-1.6045077464
H	1.0698477671	-3.6757224501	0.2506584648
H	-1.0698477671	-3.6757224501	0.2506584648
H	1.0256381008	0.0000000000	-0.6619305494
H	-1.0256381008	0.0000000000	-0.6619305494
C	0.0000000000	0.0000000000	1.5441335232
H	0.8964220335	0.0000000000	2.1702967360
H	-0.8964220335	0.0000000000	2.1702967360

3

Be	0.0000000000	–0.0004374572	0.8675467691
Be	0.0000000000	–0.0004374572	–0.8675467691
H	–1.0330192348	0.5978618856	0.0000000000
H	0.0000000000	–1.1943092702	0.0000000000
H	1.0330192348	0.5978618856	0.0000000000

H	–0.8149453679	–0.4705807417	–2.9438010514
H	0.0000000000	0.9409878788	–2.9436615704
H	0.8149453679	–0.4705807417	–2.9438010514
H	0.0000000000	0.9409878788	2.9436615704
H	–0.8149453679	–0.4705807417	2.9438010514
H	0.8149453679	–0.4705807417	2.9438010514
N	0.0000000000	–0.0000961936	–2.5566286382
N	0.0000000000	–0.0000961936	2.5566286382

4

Be	0.0000000000	0.0000435551	0.8668167861
Be	0.0000000000	0.0000435551	–0.8668167861
H	1.0306236509	0.5944243318	0.0000000000
H	–1.0306236509	0.5944243318	0.0000000000
H	0.0000000000	–1.1896950863	0.0000000000
H	0.0000000000	1.2604072995	–3.6040953269
H	1.0914526341	–0.6300552595	–3.6041237222
H	–1.0914526341	–0.6300552595	–3.6041237222
H	1.0914526341	–0.6300552595	3.6041237222
H	0.0000000000	1.2604072995	3.6040953269
H	–1.0914526341	–0.6300552595	3.6041237222
P	0.0000000000	0.0000828758	2.9934910760
P	0.0000000000	0.0000828758	–2.9934910760

5

Be	0.0000000000	-0.0000013773	0.8446889781
Be	0.0000000000	-0.0000013773	-0.8446889781
H	0.0000000000	1.1876879512	0.0000000000
H	-1.0285647579	-0.5938439734	0.0000000000
H	1.0285647579	-0.5938439734	0.0000000000
He	0.0000000000	0.0000008752	2.3436293352
He	0.0000000000	0.0000008752	-2.3436293352

6

Be	0.0000000000	0.0000000000	0.8461028577
Be	0.0000000000	0.0000000000	–0.8461028577
H	0.0000000000	1.1884163908	0.0000000000
H	–1.0291987863	–0.5942081954	0.0000000000
H	1.0291987863	–0.5942081954	0.0000000000
Ne	0.0000000000	0.0000000000	2.5732414979
Ne	0.0000000000	0.0000000000	–2.5732414979

7

Be	0.0000000000	–0.0000000000	0.8515932012
Be	0.0000000000	–0.0000000000	–0.8515932012
H	0.0000000000	1.1885134861	0.0000000000
H	–1.0292828674	–0.5942567430	0.0000000000
H	1.0292828674	–0.5942567430	0.0000000000
Ar	0.0000000000	–0.0000000001	2.8864806615
Ar	0.0000000000	–0.0000000001	–2.8864806615

8

Be	0.0000000000	–0.0000049942	0.8537329773
Be	0.0000000000	–0.0000049942	–0.8537329773
H	0.0000000000	1.1885913126	0.0000000000
H	–1.0293718951	–0.5942838213	0.0000000000
H	1.0293718951	–0.5942838213	0.0000000000
Kr	0.0000000000	–0.0000068407	3.0350374770
Kr	0.0000000000	–0.0000068407	–3.0350374770

9

Be	0.0000000000	0.0000000000	0.8566143898
Be	0.0000000000	0.0000000000	–0.8566143898
H	0.0000000000	1.1886036956	0.0000000000
H	–1.0293609934	–0.5943018478	0.0000000000
H	1.0293609934	–0.5943018478	0.0000000000
Xe	0.0000000000	0.0000000000	3.2254486773
Xe	0.0000000000	0.0000000000	–3.2254486773

10

Be	0.0000000000	-0.0000004544	0.8415724692
Be	0.0000000000	-0.0000004544	-0.8415724692
H	0.0000000000	1.1903007475	0.0000000000
H	1.0308283427	-0.5951499194	0.0000000000
H	-1.0308283427	-0.5951499194	0.0000000000

B3LYP/BS1-optimized structure (in Cartesian coordinates) for **11**.

11

Be	0.00000000	0.00000000	–0.87633289
Be	0.00000000	0.00000000	0.87683611
H	–0.48887680	–1.08013729	0.00025311
H	–0.69098793	0.96344837	0.00025311
H	1.17986473	0.11668892	0.00025311
N	0.00000000	0.00000000	2.56775511
N	0.00000000	0.00000000	–2.56727289
C	–0.05523904	1.41834378	–3.08853787
C	1.08792619	2.32113438	–2.64877090
C	–1.32576691	0.50707319	3.08900615
C	–2.54763585	–0.28532700	2.64813318
C	0.22374519	–1.40168442	3.08900615
C	1.52091835	–2.06365386	2.64813318
C	1.10202172	0.89461123	3.08900615
C	1.02671749	2.34898086	2.64813318
C	1.25594126	–0.66133348	–3.08853787
C	1.46619825	–2.10273891	–2.64877090
C	–1.20070222	–0.75701030	–3.08853787
C	–2.55412443	–0.21839548	–2.64877090
H	–0.99345043	1.84121425	–2.74328984
H	–0.09934829	1.36246031	–4.17876787
H	0.86430993	3.33577154	–2.97526088
H	1.19543792	2.34285781	–1.56491590
H	2.04353929	2.04540952	–3.08754792
H	–1.42501861	1.53164005	2.74453116
H	–1.25906491	0.53010910	4.17926915
H	–3.43683782	0.25176476	2.97516821
H	–2.60258036	–0.37877693	1.56415518
H	–2.59343074	–1.27943647	3.08562717
H	–0.61392989	–1.99992234	2.74453116
H	0.17044451	–1.35543674	4.17926915
H	1.50038423	–3.10227124	2.97516821
H	1.62932062	–2.06451225	1.56415518
H	2.40473985	–1.60625867	3.08562717
H	2.03894850	0.46828229	2.74453116
H	1.08862040	0.82532765	4.17926915
H	1.93645359	2.85050648	2.97516821
H	0.97325974	2.44328917	1.56415518
H	0.18869088	2.88569513	3.08562717
H	2.09126353	–0.06025382	–2.74328984
H	1.22959938	–0.59519201	–4.17876787
H	2.45670793	–2.41640012	–2.97526088

H	1.43125542	–2.20670851	–1.56491590
H	0.74960696	–2.79246170	–3.08754792
H	–1.09781310	–1.78096043	–2.74328984
H	–1.13025109	–0.76726830	–4.17876787
H	–3.32101786	–0.91937142	–2.97526088
H	–2.62669334	–0.13614929	–1.56491590
H	–2.79314625	0.74705218	–3.08754792

B3LYP/BS1-optimized structures (in Cartesian coordinates) for isomers shown in Figure S2. The free energies were calculated with CCSD(T)/BS1 electronic energies plus B3LYP/BS1 Gibbs free energy corrections.

3

Free energy = –143.9857192 a.u.

Be	0.00000000	0.00000000	0.86452000
Be	–0.00000000	0.00000000	–0.86452000
H	1.02879467	0.59397488	0.00000000
H	–1.02879467	0.59397488	0.00000000
H	0.00000000	–1.18794976	0.00000000
H	0.00000000	0.94185595	–2.93712500
H	0.81567118	–0.47092797	–2.93712500
H	–0.81567118	–0.47092797	–2.93712500
H	0.81567118	–0.47092797	2.93712500
H	0.00000000	0.94185595	2.93712500
H	–0.81567118	–0.47092797	2.93712500
N	0.00000000	0.00000000	–2.55060100
N	0.00000000	0.00000000	2.55060100

3a

Free energy = –143.9652573 a.u.

Be	0.00000000	0.00000000	0.20084623
Be	0.00000000	0.00000000	2.20644123
H	–1.06691800	0.00000000	1.18431823
H	0.00000000	2.27041800	–0.09255277
H	1.06691800	0.00000000	1.18431823
H	–0.81553400	–1.58773500	–1.31669477
H	0.81553400	1.58773500	–1.31669477
H	–0.81553400	1.58773500	–1.31669477
H	0.00000000	0.00000000	3.52148123
H	0.81553400	–1.58773500	–1.31669477
H	0.00000000	–2.27041800	–0.09255277
N	0.00000000	–1.46705200	–0.71909877
N	–0.00000000	1.46705200	–0.71909877

3b

Free energy = –143.9593683 a.u.

Be	0.18862436	0.26129485	0.00000000
Be	0.64731162	–1.44273989	0.00000000
H	1.46159444	–2.80049810	0.38331100
H	1.46159444	–2.80049810	–0.38331100
H	1.06209959	2.36194635	0.00000000

H	–0.35094044	2.33066015	0.81514500
H	–1.51437636	–1.16435238	0.81786500
H	1.04360722	–0.50472768	1.02550100
H	–0.35094044	2.33066015	–0.81514500
H	–1.51437636	–1.16435238	–0.81786500
H	1.04360722	–0.50472768	–1.02550100
N	0.12905413	1.95274796	0.00000000
N	–0.94128459	–1.00393799	0.00000000

3c

Free energy = –143.9511622 a.u.

Be	1.32689411	1.02468016	0.00000000
Be	–0.89167495	–0.34648473	0.00000000
H	2.92036306	–0.37450886	–0.80265892
H	2.92036306	–0.37450886	0.80265892
H	1.77612601	–1.25041386	0.00000000
N	–2.55185893	0.02373734	0.00000000
H	1.79035317	2.26367914	0.00000000
H	–3.01236296	–0.39806368	0.80785500
H	–2.78826889	1.01376935	0.00000000
N	2.29450605	–0.37194888	0.00000000
H	–3.01236296	–0.39806368	–0.80785500
H	–0.10851390	0.82747923	0.00000000
H	–0.41136501	–1.59254475	0.00000000

3d

Free energy = –143.9445977 a.u.

Be	0.08692460	–1.14120399	0.00000000
Be	0.42651675	0.80667067	0.00000000
H	2.04684564	1.08055922	0.38205500
H	0.28743191	–0.08438481	1.07898400
H	–0.30381241	–3.16770316	0.82100500
H	–0.23026337	2.86576742	0.81684000
H	–1.41447166	2.10778427	0.00000000
H	0.28743191	–0.08438481	–1.07898400
H	–0.23026337	2.86576742	–0.81684000
H	–0.30381241	–3.16770316	–0.82100500
H	2.04684564	1.08055922	–0.38205500
N	–0.40926604	2.28310204	0.00000000
N	–0.19640501	–2.59140609	0.00000000

4

Free energy = –716.378781 a.u.

Be	0.00000000	0.00000000	0.86429500
Be	–0.00000000	0.00000000	–0.86429500
H	1.02468870	0.59160430	0.00000000
H	–1.02468870	0.59160430	0.00000000
H	0.00000000	–1.18320860	0.00000000
H	0.00000000	1.25896980	–3.60592700
H	1.09029983	–0.62948490	–3.60592700
H	–1.09029983	–0.62948490	–3.60592700
H	1.09029983	–0.62948490	3.60592700
H	0.00000000	1.25896980	3.60592700
H	–1.09029983	–0.62948490	3.60592700
P	0.00000000	–0.00000000	2.98977700
P	–0.00000000	–0.00000000	–2.98977700

4a

Free energy = –716.3633994 a.u.

Be	0.00000000	0.00000000	0.59887015
Be	0.00000000	0.00000000	2.59225215
H	–1.06538400	0.00000000	1.54423215
H	0.00000000	3.01000800	0.31435415
H	1.06538400	0.00000000	1.54423215
P	0.00000000	1.86780100	–0.49982685
H	–1.08739100	–2.12453600	–1.34820285
H	1.08739100	2.12453600	–1.34820285
H	–1.08739100	2.12453600	–1.34820285
P	0.00000000	–1.86780100	–0.49982685
H	0.00000000	0.00000000	3.90595515
H	1.08739100	–2.12453600	–1.34820285
H	0.00000000	–3.01000800	0.31435415

4b

Free energy = –716.3506237 a.u.

Be	–0.10700872	0.39045784	0.00000000
Be	1.48604465	1.33494165	0.00000000
H	2.15509150	2.82102532	0.00000000
H	2.74766344	2.33042462	0.00000000
H	–3.09755440	1.03063999	0.00000000
P	1.71572446	–0.70386939	0.00000000
H	–2.65671886	–0.80759986	1.08943900
H	2.19373947	–1.39194065	1.11785400
H	0.46081300	1.31374041	1.02460400
P	–2.20352522	–0.05026979	0.00000000

H	–2.65671886	–0.80759986	–1.08943900
H	2.19373947	–1.39194065	–1.11785400
H	0.46081300	1.31374041	–1.02460400

4c

Free energy = –716.3447922 a.u.

Be	–0.87724400	–0.02698000	–0.00796700
Be	0.84844600	–0.05800300	–0.02375800
H	–3.63678400	–0.94498700	–0.79782000
H	2.82771200	0.08378900	1.32827600
H	0.01414100	0.85797100	0.74992100
P	3.23360400	0.00505100	–0.02877700
H	–3.60974300	–0.19377100	1.25167700
H	2.40644400	1.08822000	–0.46333000
H	–0.01196900	0.16685700	–1.17890300
P	–3.00165800	0.01171400	0.00573600
H	2.27485700	–1.01861900	–0.37597600
H	–3.59744600	1.20536700	–0.42390300
H	–0.03120700	–1.15636900	0.38257700

4d

Free energy = –716.3352825 a.u.

Be	–0.40755238	1.08547565	0.00000000
Be	–0.81793326	–0.86875785	0.00000000
H	–2.40252820	–1.12201721	0.38359100
H	–0.64185673	0.02131806	1.06874000
H	–0.45275807	3.45886763	1.06187500
P	0.33735032	2.95653101	0.00000000
H	0.15230754	–3.54964961	1.09562900
H	1.70451462	–2.45991940	0.00000000
H	–0.64185673	0.02131806	–1.06874000
P	0.32178960	–2.69146365	0.00000000
H	0.15230754	–3.54964961	–1.09562900
H	–0.45275807	3.45886763	–1.06187500
H	–2.40252820	–1.12201721	–0.38359100

5

Free energy = -36.65279819 a.u.

Be	-0.00000000	-0.00000000	0.84077500
Be	-0.00000000	-0.00000000	-0.84077500
H	0.00000000	1.18096307	0.00000000
H	-1.02274402	-0.59048153	0.00000000
H	1.02274402	-0.59048153	0.00000000

He	-0.00000000	-0.00000000	2.33144300
He	-0.00000000	-0.00000000	-2.33144300

5a

Free energy = -36.65639099 a.u.

Be	-0.16455100	0.23453100	0.17446400
Be	1.78957900	-0.08665600	-0.06008600
H	0.85494700	-1.01375800	0.30846200
H	-1.44157900	0.44583400	0.32670000
H	1.13732600	1.10142000	-0.23816900
He	-6.78920200	-0.23391900	-0.18959600
He	3.26380100	-0.32857900	-0.23765800

6

Free energy = –288.5534524 a.u.

Be	0.00000000	0.00000000	0.84257400
Be	–0.00000000	0.00000000	–0.84257400
H	0.00000000	1.18259600	0.00000000
H	–1.02415818	–0.59129800	0.00000000
H	1.02415818	–0.59129800	0.00000000
Ne	0.00000000	0.00000000	2.57446500
Ne	–0.00000000	0.00000000	–2.57446500

6a

Free energy = –288.5501035 a.u.

Be	0.00000000	0.00000000	2.36076741
Be	0.00000000	0.00000000	0.37148180
H	–1.08962300	0.00000000	1.21502214
H	0.00000000	0.00000000	3.66518894
H	1.08962300	0.00000000	1.21502214
Ne	0.00000000	1.31466202	–0.85121150
Ne	0.00000000	–1.31466202	–0.85121150

6b

Free energy = –288.5377976 a.u.

Be	–0.21598611	–0.12809705	0.00000000
Be	–2.68483205	0.81918007	0.00000000
H	–1.62956616	–0.15434627	0.00000000
H	1.08542352	–0.12265995	0.00000000
H	–2.98816102	2.08377775	0.00000000
Ne	5.62337416	–0.04100750	0.00000000
Ne	–4.10981653	–0.41610286	0.00000000

6c

Free energy = –288.5430356 a.u.

Be	–0.35223470	–1.24316381	0.96766610
Be	0.35223470	1.24316381	0.96766610
H	–0.82645926	–1.94971657	1.95136510
H	0.82645926	1.94971657	1.95136510
H	0.00000000	0.00000000	0.36335910
Ne	–0.14516535	2.31660180	–0.60037090
Ne	0.14516535	–2.31660180	–0.60037090

6d

Free energy = –288.5416642 a.u.

Be	–1.31006318	2.20329614	0.00000000
Be	–0.00915217	1.14134527	0.00000000
H	0.07181902	2.60265451	0.00000000
H	–1.04797757	1.22652525	1.02489300
H	–1.04797757	1.22652525	–1.02489300
Ne	–0.64093289	–1.95060102	0.00000000
Ne	1.37103264	0.10717395	0.00000000

7

Free energy = –1085.042436 a.u.

Be	0.00000000	0.00000000	0.84834800
Be	–0.00000000	0.00000000	–0.84834800
H	0.00000000	1.18149000	0.00000000
H	–1.02320035	–0.59074500	0.00000000
H	1.02320035	–0.59074500	0.00000000
Ar	0.00000000	0.00000000	2.89460200
Ar	–0.00000000	0.00000000	–2.89460200

7a

Free energy = –1085.035516 a.u.

Be	0.00000000	0.00000000	2.70326594
Be	0.00000000	0.00000000	0.71678294
H	0.00000000	0.00000000	4.01030894
H	–1.07785200	0.00000000	1.59905094
H	1.07785200	0.00000000	1.59905094
Ar	0.00000000	1.68416400	–0.58023906
Ar	0.00000000	–1.68416400	–0.58023906

7b

Free energy = –1085.027365 a.u.

Be	0.00000000	0.84955200	0.00000000

Be	1.31722600	–0.60162600	0.00000000
H	0.46068300	0.16530800	1.09287900
H	0.46068300	0.16530800	–1.09287900
H	2.62767800	–0.51028600	0.00000000
Ar	0.51184200	–2.65815800	0.00000000
Ar	–1.00172800	2.61304500	0.00000000

7c

Free energy = –1085.026727 a.u.

Be	0.00000000	0.00000000	–4.62197485
Be	0.00000000	0.00000000	–2.63577785
H	0.00000000	1.09192000	–3.48229785
H	0.00000000	0.00000000	–5.92702885
H	0.00000000	–1.09192000	–3.48229785
Ar	0.00000000	0.00000000	–0.62657285
Ar	0.00000000	0.00000000	2.95560815

7d

Free energy = –1085.002209 a.u.

Be	–1.40395422	0.92423267	0.62078701
Be	–1.79787551	2.43035044	–0.55138219
H	–1.19934705	1.22609290	1.88393493
H	–2.75579537	1.64739347	–0.00955791
H	–0.57298845	1.86934654	–0.43519128
Ar	–1.38119519	–1.07852845	–0.08245664
Ar	2.34427574	0.06957482	–0.01292141

8

Free energy = –5535.452102 a.u.

Be	–0.00000000	–0.00000000	0.85050300
Be	–0.00000000	–0.00000000	–0.85050300
H	0.00000000	1.18123800	0.00000000
H	–1.02298212	–0.59061900	0.00000000
H	1.02298212	–0.59061900	0.00000000
Kr	–0.00000000	–0.00000000	3.04665400
Kr	–0.00000000	–0.00000000	–3.04665400

8a

Free energy = –5535.445372 a.u.

Be	0.00000000	0.00000000	1.00420856
Be	0.00000000	0.00000000	2.99023110
H	–1.07538700	0.00000000	1.89697713
H	0.00000000	0.00000000	4.29793145

H	1.07538700	0.00000000	1.89697713
Kr	0.00000000	1.84507444	–0.33430062
Kr	0.00000000	–1.84507444	–0.33430062

8b

Free energy = –5535.436356 a.u.

Be	–0.36454562	0.79755909	0.00000000
Be	–1.20573418	–0.96742822	0.00000000
H	–2.50063557	–1.20358059	0.00000000
H	–0.60202523	0.00191856	1.09070600
H	–0.60202523	0.00191856	–1.09070600
Kr	0.10621736	2.92192881	0.00000000
Kr	0.17116612	–2.86972826	0.00000000

8c

Free energy = –5535.432767 a.u.

Be	0.00000000	0.00000000	–5.35520680
Be	0.00000000	0.00000000	–3.37034580
H	0.00000000	0.00000000	–6.66087880
H	0.00000000	1.08947600	–4.22582680
H	0.00000000	–1.08947600	–4.22582680
Kr	0.00000000	0.00000000	–1.21657680
Kr	0.00000000	0.00000000	2.60587520

8d

Free energy = –5535.391334 a.u.

Be	–0.60654878	1.27418399	0.00000000
Be	5.37251867	–1.10501036	0.00000000
H	–0.87809338	2.54757017	0.00000000
H	4.09969831	–0.69876049	0.00000000
H	6.62455453	–1.50906235	0.00000000
Kr	–2.19122912	–0.33639816	0.00000000
Kr	1.38817248	0.30816367	0.00000000

9

Free energy = –687.9046758 a.u.

Be	0.00000000	0.00000000	0.85308900
Be	0.00000000	0.00000000	–0.85308900
H	0.00000000	1.18124400	0.00000000
H	–1.02298800	–0.59062200	0.00000000
H	1.02298800	–0.59062200	0.00000000
Xe	0.00000000	0.00000000	3.23898900
Xe	0.00000000	0.00000000	–3.23898900

9a

Free energy = –687.8968934 a.u.

Be	0.00000000	0.00000000	3.14241713
Be	0.00000000	0.00000000	1.15983013
H	0.00000000	0.00000000	4.45213713
H	–1.07314700	0.00000000	2.06295613
H	1.07314700	0.00000000	2.06295613
Xe	0.00000000	2.04370800	–0.23876887
Xe	0.00000000	–2.04370800	–0.23876887

9b

Free energy = –687.8883272 a.u.

Be	–0.42825956	0.79655106	0.00000000
Be	–1.27251358	–0.96129805	0.00000000
H	–0.66326121	–0.00728548	1.08812500
H	–2.57953825	–1.14352570	0.00000000
H	–0.66326121	–0.00728548	–1.08812500
Xe	0.07917937	3.10710551	0.00000000
Xe	0.11913828	–3.07345580	0.00000000

9c

Free energy = –687.8812488 a.u.

Be	0.00000000	0.00000000	–3.87221524
Be	0.00000000	0.00000000	–5.85581724
H	0.00000000	1.08634000	–4.73973124
H	0.00000000	–1.08634000	–4.73973124
H	0.00000000	0.00000000	–7.16250124
Xe	0.00000000	0.00000000	–1.53228324
Xe	0.00000000	0.00000000	2.56106276

9d

Free energy = –687.8750167 a.u.

Be	–1.21972317	3.49321274	0.00000000
Be	–1.58253130	1.84143327	0.00000000
H	–2.54722746	2.97389379	0.00000000
H	–0.81704115	2.58967282	1.02776899
H	–0.81704115	2.58967282	–1.02776899
Xe	2.44130485	–0.09299026	0.00000000
Xe	–2.15629879	–0.45315462	0.00000000

10

Free energy = -30.82411066 a.u.

Be	-0.00000000	-0.00000000	0.83653500

Be	-0.00000000	-0.00000000	-0.83653500
H	0.00000000	1.18397309	0.00000000
H	1.02535077	-0.59198655	0.00000000
H	-1.02535077	-0.59198655	0.00000000

10a

Free energy = -30.83405838 a.u.

Be	0.00000000	0.00000000	-1.41890300
Be	0.00000000	0.00000000	1.41890300
H	0.00000000	0.00000000	-2.72156300
H	0.00000000	0.00000000	2.72156300
H	0.00000000	0.00000000	0.00000000