Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2019

Electronic Supplementary Information

Neutral nano-polygons with ultrashort Be-Be distances

Wen-Yan Tong,[a,‡] Tao-Tao Zhao,[a,‡] Xue-Feng Zhao,[a] Xiaotai Wang,[a,b] Yan-Bo Wu*[a] and Caixia Yuan*[a]

[a] Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan, 030006, People's Republic of China.

[b] Department of Chemistry, University of Colorado Denver, Campus Box 194, P.O. Box 173364, Denver, Colorado 80217-3364, United States.

‡These authors contribute equally to this work.

*To whom correspondence should be addressed.

E-mail: wyb@sxu.edu.cn (Y.B.W.) or cxyuan@sxu.edu.cn (C.X.Y.)

Contents

Fig. S1. B3LYP/def2-TZVPP-optimized polygonal structures of heptagons and octagons with NH_2 and PH_2. 1

Fig. S2. B3LYP/def2-TZVPP-optimized structures of trigons and tetragons with OH, SH, F, Cl, and Br moieties as the vertexes.....2

Fig. S3. B3LYP/def2-TZVPP-optimized structures of trigons, tetragons and pentagons with $N(CH_3)_2$, $N(CH_3)_2$, OCH_3, and SCH_3 moieties as the vertexes.....3

Fig. S4. AdNDP view of chemical bonding in ***n*-NH₂** (*n* = 3, 4) 5

Fig. S5. AdNDP view of chemical bonding in ***n*-NH₂** (*n* = 5, 6) 5

Fig. S6. AdNDP view of chemical bonding in ***n*-PH₂** (*n* = 3, 4).....6

Fig. S7. AdNDP view of chemical bonding in ***n*-PH₂** (*n* = 5, 6).....7

Fig. S8. AdNDP view of chemical bonding in **5-E** (E = F, Cl).....8

Fig. S9 AdNDP view of chemical bonding in **5-E** (E = Br).....9

Fig. S10. AdNDP view of chemical bonding in **5-E** (E =OH, SH).....10

Table. S1. NBO results including natural charges (*Q*) on selected atoms and the total Wiberg bond index (WBI) for selected atoms and atom-atom interactions... 11

Cartesian Coordinates for optimized structures shown in the figures in the text and ESI 12

Fig. S1. B3LYP/def2-TZVPP-optimized polygonal structures of heptagons and octagons with NH_2 and PH_2.The Be-Be distances (in Å), other interatomic distances (in Å), and natural charges (in |e|) are shown in red, black, and italic blue fonts, respectively.

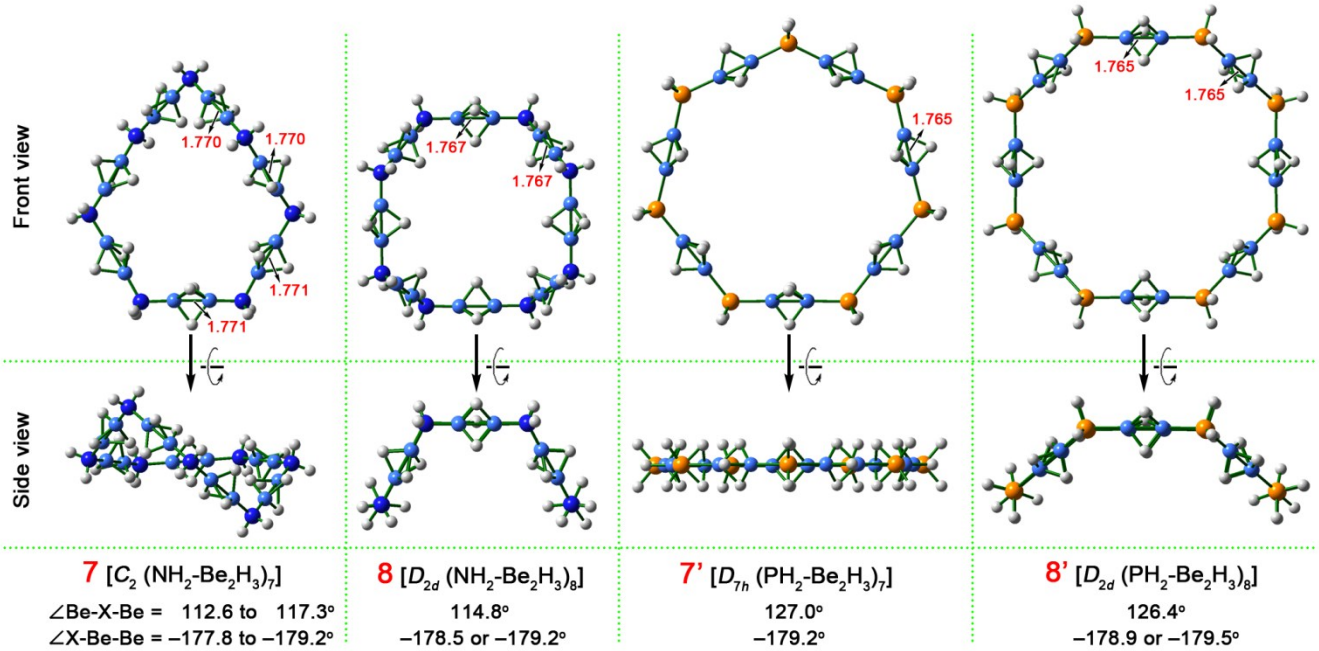

Fig. S2. B3LYP/def2-TZVPP-optimized structures of trigons and tetragons with OH, SH, F, Cl, and Br moieties as the vertexes.

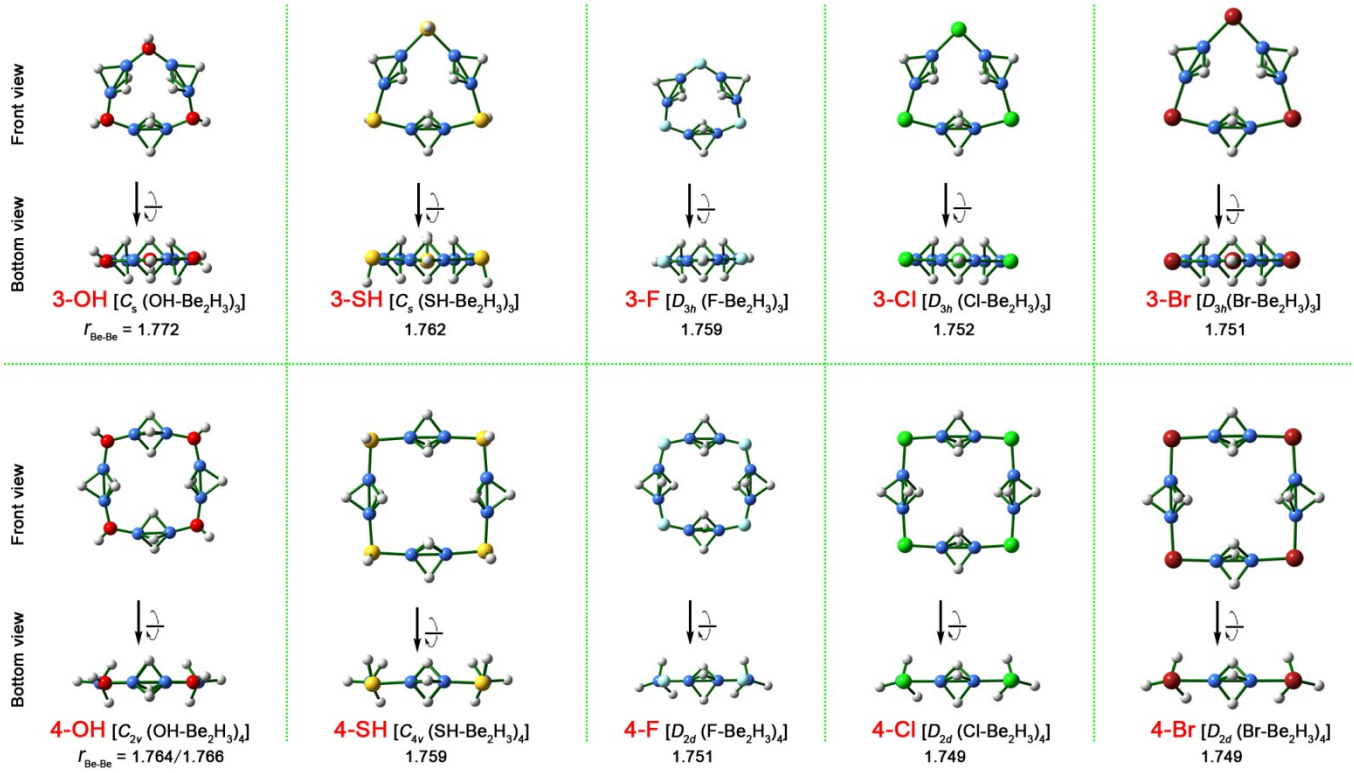

Fig. S3. B3LYP/def2-TZVPP-optimized structures of trigons, tetragons and pentagons with $N(CH_3)_2$, $N(CH_3)_2$, OCH_3, and SCH_3 moieties as the vertexes.

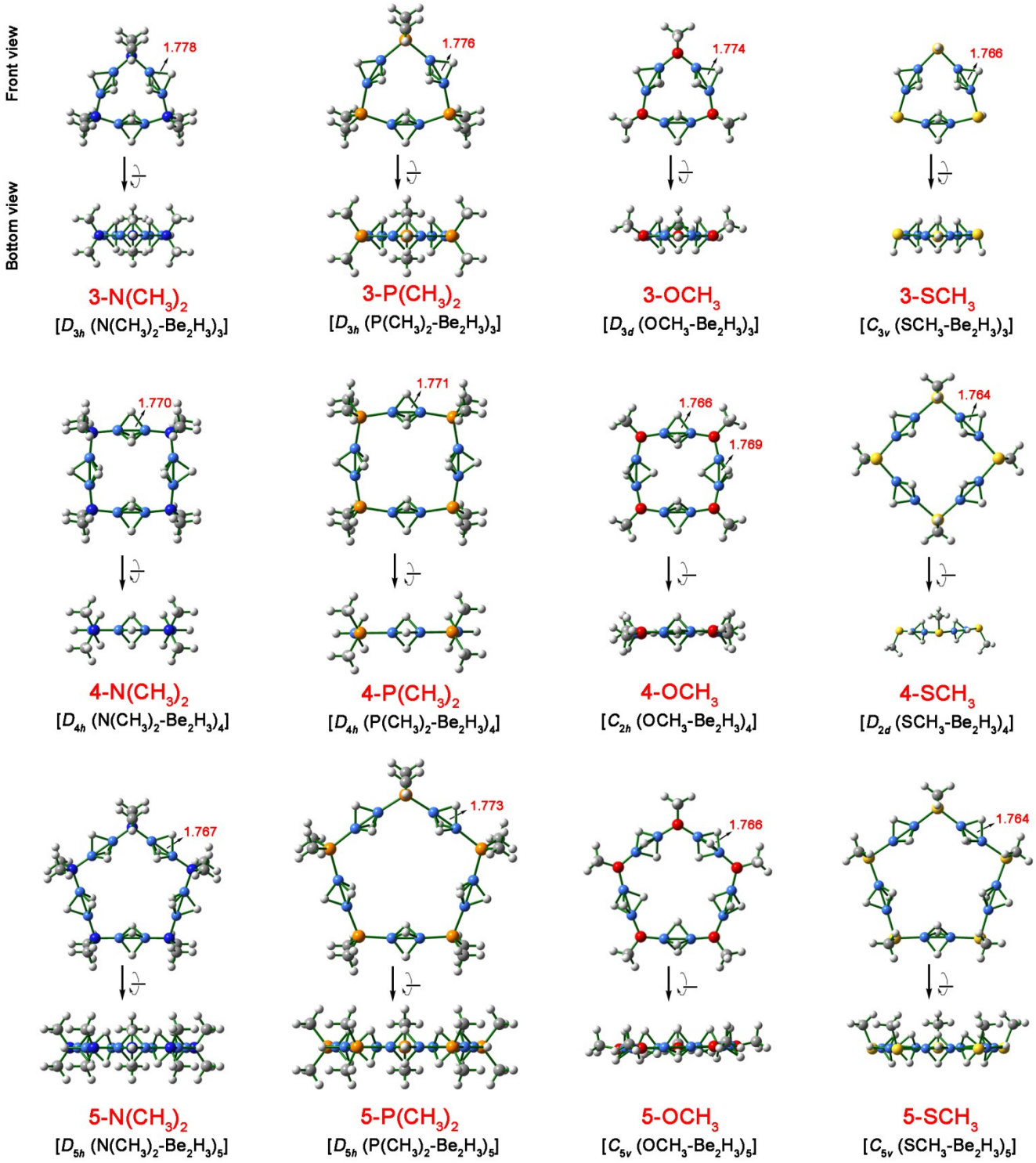

Fig. S4. AdNDP view of chemical bonding in n-NH_2 (n = 3, 4)

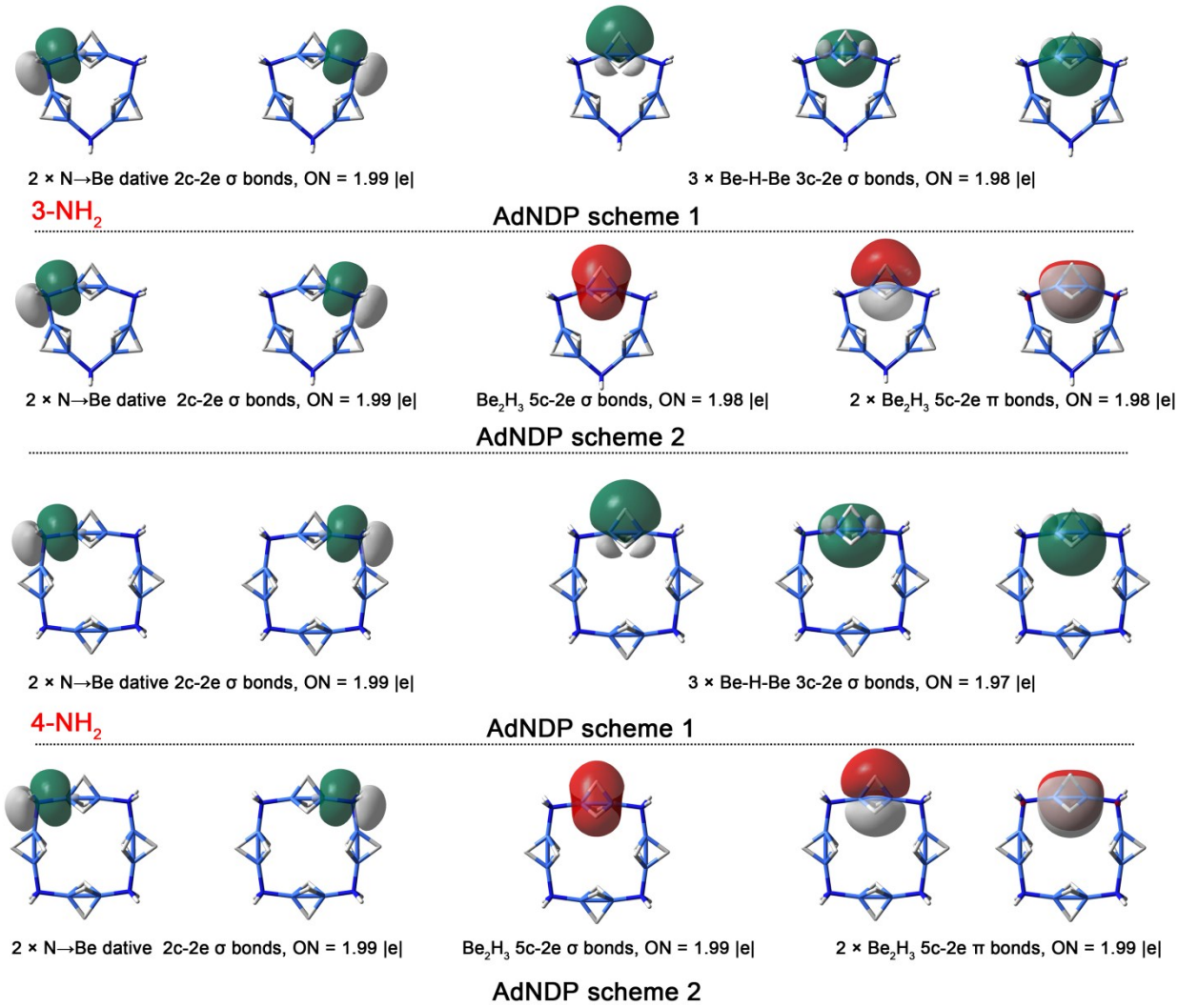

Fig. S5. AdNDP view of chemical bonding in n-NH_2 (n = 5, 6)

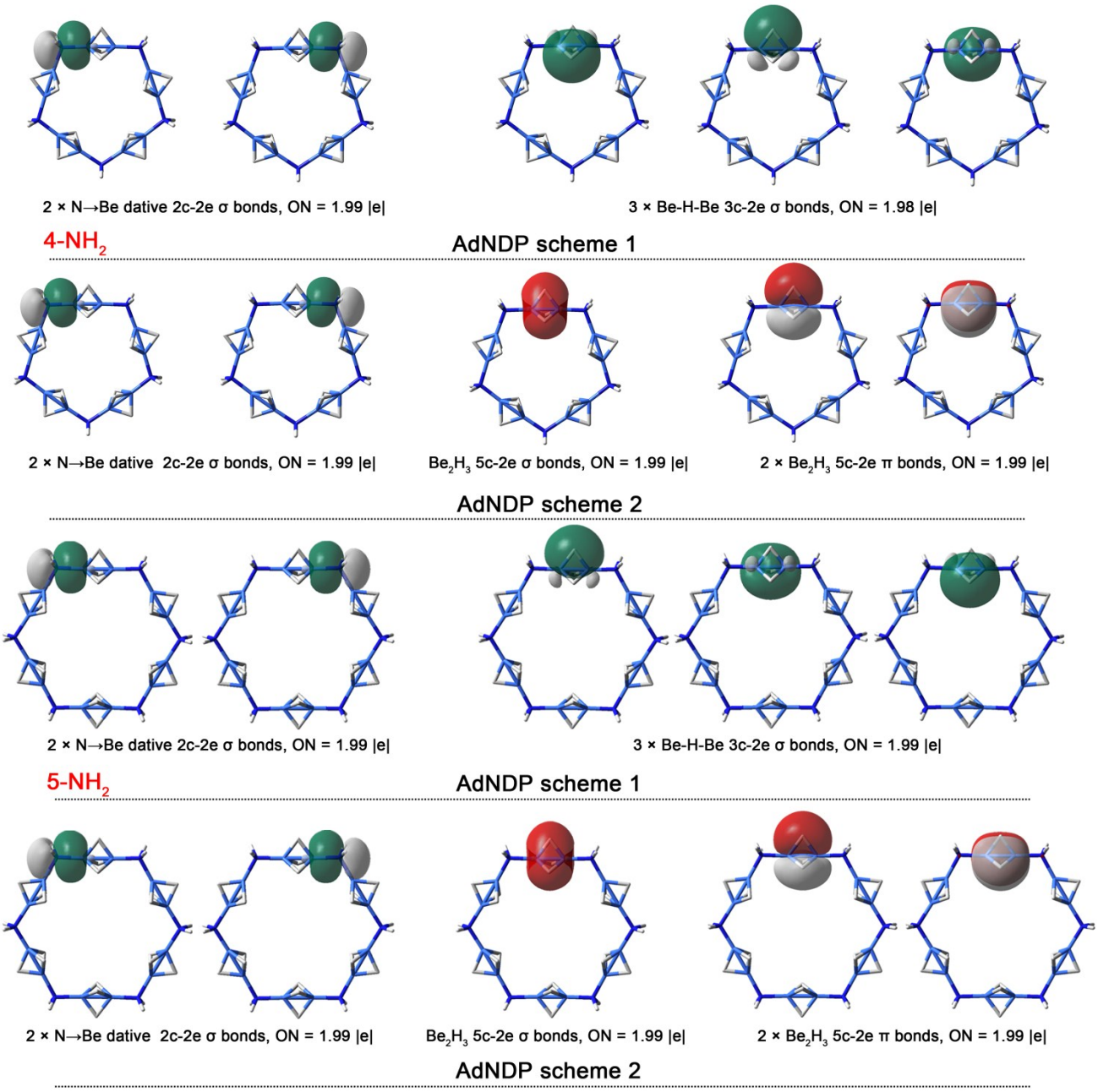

Fig. S6. AdNDP view of chemical bonding in n-PH_2 (n = 3, 4)

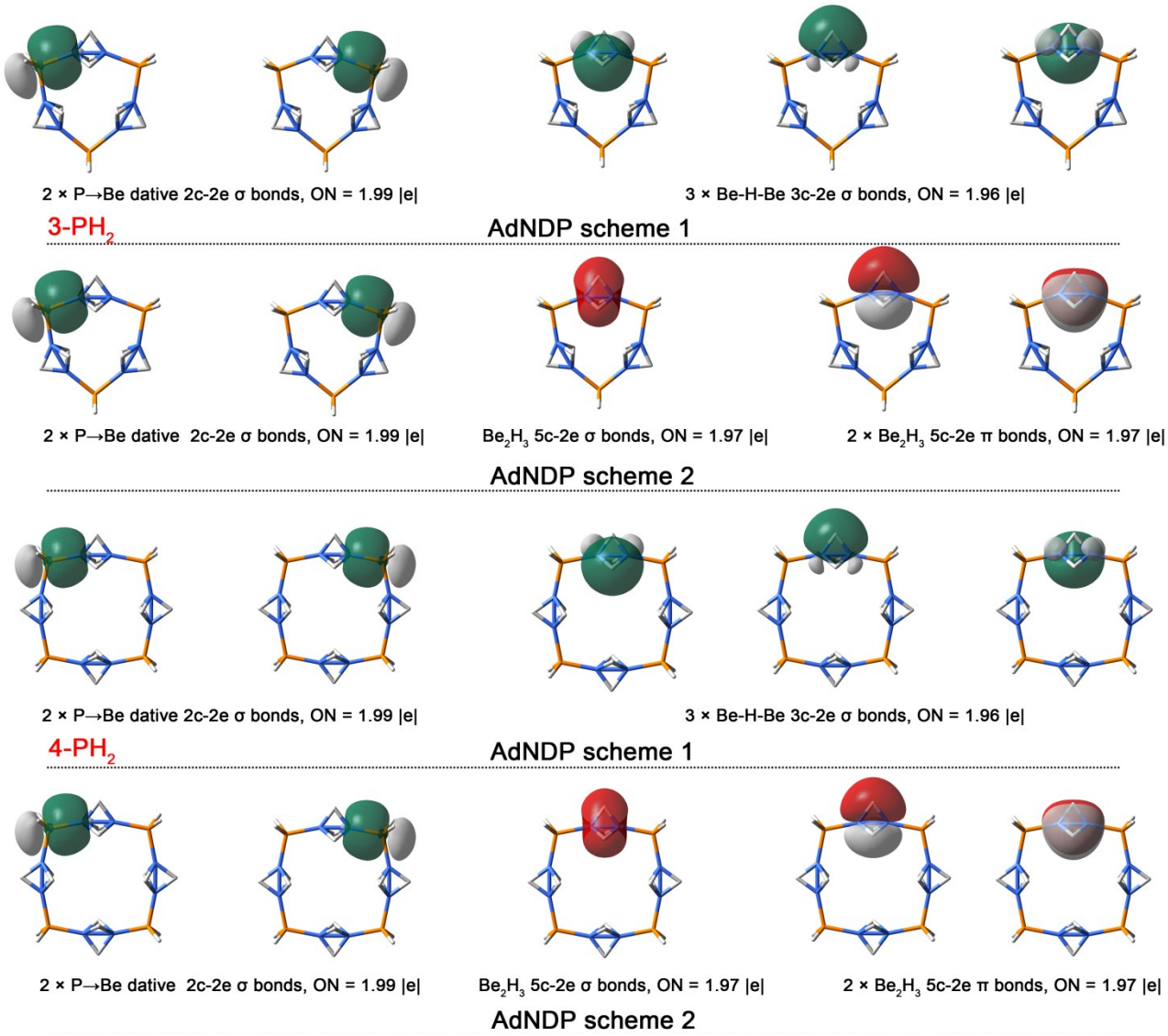

Fig. S7. AdNDP view of chemical bonding in *n*-PH_2 (*n* = 5, 6)

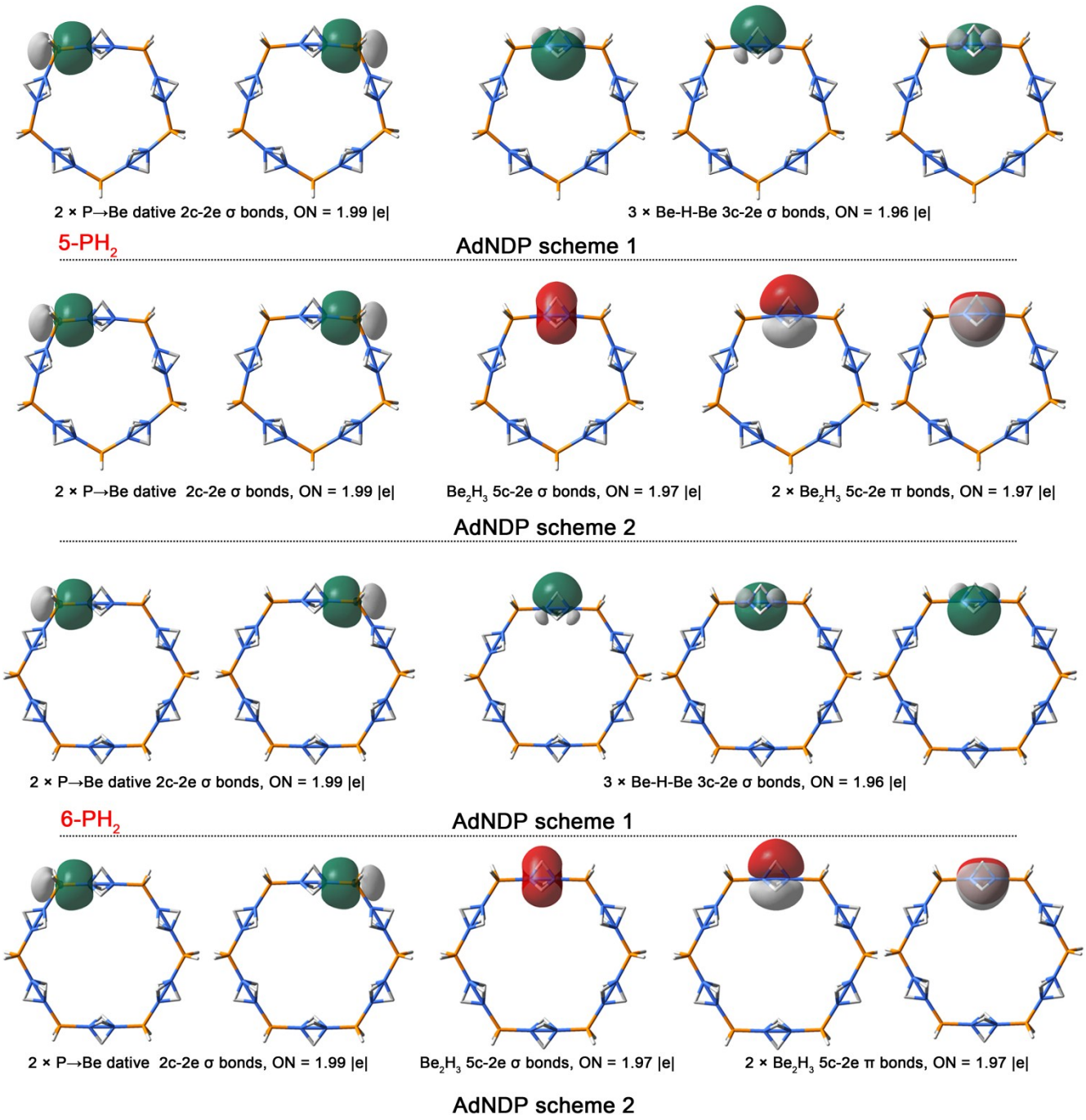

Fig. S8. AdNDP view of chemical bonding in 5-E (E = F, Cl)

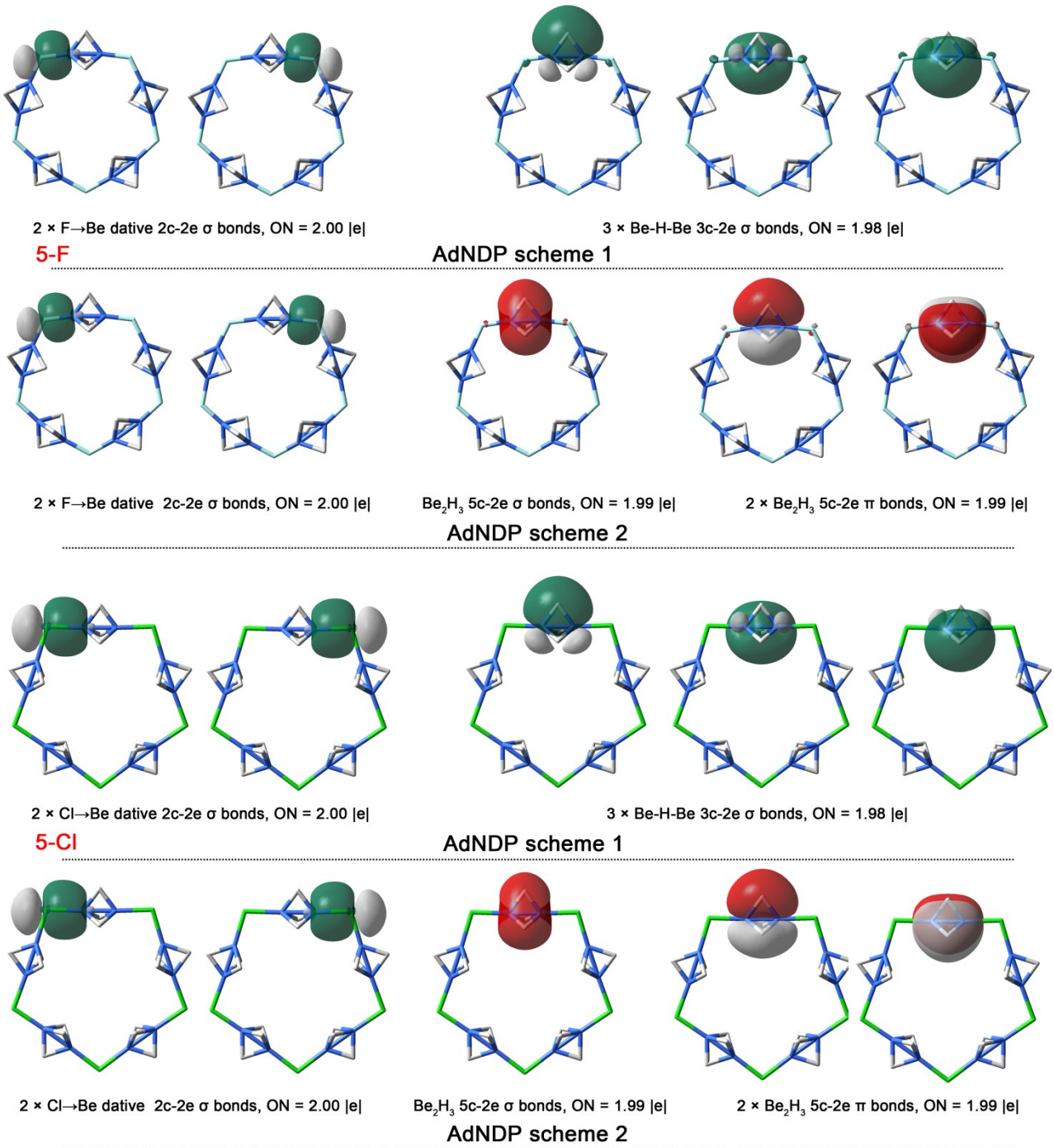

Fig. S9. AdNDP view of chemical bonding in 5-E (E = Br)

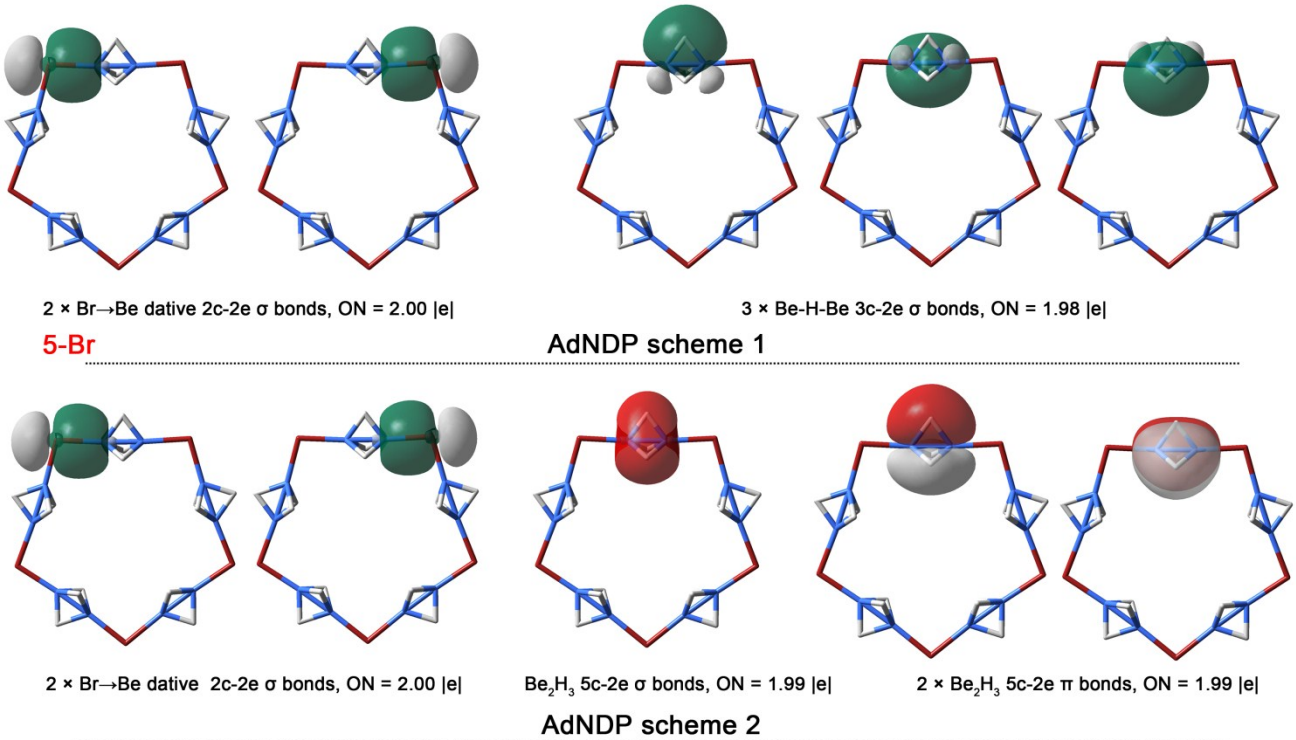

Fig. S10. AdNDP view of chemical bonding in 5-E (E = OH, SH)

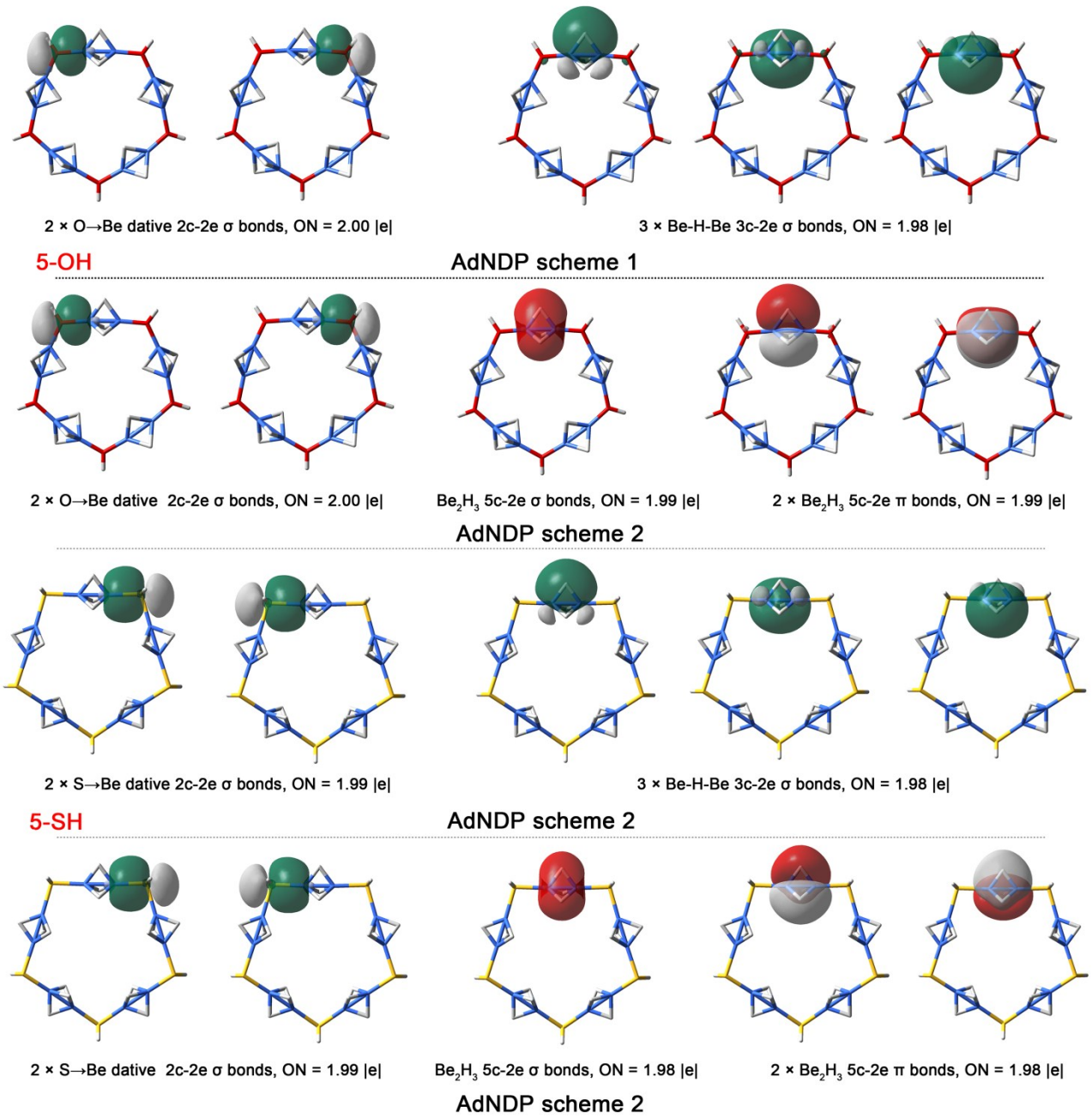

Table. S1. NBO results including natural charges (*Q*) on selected atoms and the total Wiberg bond index (WBI) for selected atoms and atom-atom interactions.

	Q				WBI					
	H_{BR}	Be	X	H_{TE}/C	H_{BR}	Be	X	X-Be	Be-H_{BR}	Be-Be
1	-0.23	+0.46	-1.27	+0.33	0.95	2.48	2.46	0.66	0.40-0.51	0.42
2	-0.21--0.22	+0.36/+0.58	-1.18/-1.28	+0.34-+0.38	0.95-0.96	2.33/2.58	2.46/2.68	0.49/0.68	0.36-0.44	0.44
3-NH_2	-0.18/-0.21	+0.50	-1.22	+0.40	0.96/0.97	2.42	2.65	0.48	0.46	0.48
4-NH_2	-0.18/-0.20	+0.48	-1.21	+0.40	0.96/0.97	2.44	2.66	0.49	0.47	0.49
5-NH_2	-0.18/-0.20	+0.49	-1.21	+0.40	0.96/0.97	2.44	2.66	0.49	0.47	0.49
6-NH_2	-0.19/-0.20	+0.50	-1.21	+0.40	0.96/0.97	2.44	2.66	0.50	0.47	0.49
7-NH_2	-0.18/-0.20	+0.48-+0.49	-1.21	+0.40	0.96-0.97	2.43-2.44	2.66	0.49-0.50	0.46-0.48	0.49
8-NH_2	-0.18/-0.20	+0.49	-1.21	+0.40	0.96-0.97	2.44	2.66	0.49-0.50	0.46-0.48	0.49
1'	-0.19	+0.18	-0.35	-0.02	0.97	2.80	2.87	0.87	0.45-0.48	0.49
2'	-0.17/-0.18	+0.11/+0.27	-0.34/-0.04	-0.01/+0.02	0.97	2.68/2.88	2.90/3.51	0.76/0.90	0.41-0.42	0.50
3-PH_2	-0.16/-0.17	+0.23	-0.07	+0.04	0.98	2.74	3.54	0.77	0.47	0.52
4-PH_2	-0.15/-0.17	+0.22	-0.06	+0.04	0.98	2.75	3.54	0.77	0.47	0.53
5-PH_2	-0.16	+0.22	-0.06	+0.05	0.98	2.75	3.53	0.77	0.48	0.53
6-PH_2	-0.16	+0.22	-0.06	+0.05	0.98/1.00	2.75	3.53	0.77	0.48	0.53
7-PH_2	-0.16	+0.22	-0.06/-0.07	+0.05	0.98/1.00	2.75	3.53	0.77	0.48	0.53
8-PH_2	-0.16	+0.22	-0.07	+0.05	0.98/1.00	2.75	3.53	0.78	0.48	0.53
3-OH	-0.19--0.22	+0.57	-1.02	+0.51	0.96-0.97	2.32/2.32	1.62/1.62	0.42-0.42	0.45-0.48	0.46
4-OH	-0.18--0.21	+0.55-+0.56	-1.02	+0.51	0.96/0.97	2.34/2.34	1.64	0.43/0.43	0.46/0.47	0.46/0.47
5-OH	-0.19--0.21	+0.55	-1.01	+0.51	0.96-0.97	2.34-2.34	1.64-1.64	0.43-0.44	0.46-0.47	0.47
6-OH	-0.19--0.21	+0.55	-1.01	+0.51	0.96-0.98	2.34	1.65	0.44	0.46-0.47	0.47
3-SH	-0.16--0.18	+0.32	-0.29	+0.18	0.97-0.98	2.66-2.66	2.38/2.38	0.69-0.69	0.46-0.48	0.50/0.50
4-SH	-0.16--0.17	+0.30	-0.28	+0.18	0.97-0.98	2.67	2.40	0.70	0.47/0.47	0.51
5-SH	-0.17	+0.30	-0.27	+0.18	0.98-0.98	2.68-2.68	2.41-2.41	0.71-0.71	0.46-0.49	0.51-0.51
6-SH	-0.17	+0.30	-0.27	+0.18	0.98/0.98	2.67	2.41	0.71	0.45-0.49	0.51
3-F	-0.21/-0.23	+0.62	-0.59		0.95/0.96	2.24	0.77	0.36	0.46/0.46	0.45
4-F	-0.20--0.22	+0.60	-0.57		0.96-0.96	2.27	0.79	0.37	0.46-0.46	0.46
5-F	-0.21--0.22	+0.60	-0.57		0.96	2.27	0.80	0.38-0.38	0.46-0.47	0.46-0.46
6-F	-0.21	+0.60	-0.56		0.96-0.96	2.27	0.81	0.38	0.47-0.47	0.46
3-Cl	-0.18--0.19	+0.38	-0.23		0.97	2.57	1.31	0.62	0.47/0.47	0.49
4-Cl	-0.17--0.18	+0.37	-0.21		0.97/0.98	2.59	1.34	0.64	0.47-0.47	0.50
6-Cl	-0.17	+0.36	-0.21		0.97-0.98	2.59	1.35	0.64	0.47/0.47	0.50
6-Cl	-0.17--0.18	+0.37	-0.21		0.97-0.97	2.59/2.59	1.35	0.64/0.64	0.46-0.48	0.50
3-Br	-0.17--0.18	+0.33	-0.13		0.97/0.97	2.64	1.44	0.69	0.47/0.47	0.49
4-Br	-0.17	+0.31	-0.11		0.97-0.98	2.66	1.47	0.70	0.47-0.47	0.50
5-Br	-0.17	+0.31	-0.11		0.97-0.98	2.66	1.47	0.70	0.47-0.47	0.50
6-Br	-0.17	+0.31-+0.32	-0.11		0.97/0.97	2.66/2.66	1.47	0.70/0.70	0.46-0.48	0.50
3-$N(CH_3)_2$	-0.19--0.20	+0.52	-0.84	-0.39	0.96/0.97	2.39	2.91	0.40	0.46/0.46	0.47
4-$N(CH_3)_2$	-0.18--0.20	+0.50	-0.84	-0.39	0.97/0.97	2.42	2.91	0.41	0.46/0.47	0.48
5-$N(CH_3)_2$	-0.18--0.20	+0.50	-0.84	-0.39	0.97/0.97	2.42	2.91	0.42	0.47/0.47	0.49
6-$N(CH_3)_2$	-0.18--0.20	+0.50	-0.84	-0.39	0.97/0.97	2.41	2.91	0.42	0.47/047	0.49
3-$P(CH_3)_2$	-0.16--0.18	+0.20	+0.49	-0.88	0.97/0.98	2.77	3.56	0.77	0.47/0.47	0.52
4-$P(CH_3)_2$	-0.16--0.17	+0.19	+0.49	-0.87	0.98/0.98	2.78	3.56	0.77	0.47/0.48	0.52
5-$P(CH_3)_2$	-0.16--0.17	+0.19	+0.48	-0.87	0.98/0.98	2.78	3.56	0.77	0.47/0.48	0.52
6-$P(CH_3)_2$	-0.16--0.17	+0.20	+0.48	-0.87	0.98/0.98	2.78	3.56	0.77	0.47/0.48	0.52
3-OCH_3	-0.19--0.23	+0.57	-0.84	-0.23	0.96-0.97	2.32	1.81	0.39	0.46/0.46	0.46
4-OCH_3	-0.18--0.21	+0.55	-0.83	-0.22	0.96/0.98	2.34/2.33	1.83	0.40/0.41	0.46-0.47	0.46/0.47
5-OCH_3	-0.18--0.21	+0.55	-0.83	-0.23	0.96-0.97	2.34	1.84	0.41	0.46-0.47	0.47
6-OCH_3	-0.18/-0.21	+0.55	-0.83	-0.23	0.96/0.97	2.34	1.84	0.41	0.46-0.47	0.47
3-SCH_3	-0.16--0.19	+0.30	-0.06	-0.68	0.97-0.98	2.67	2.50	0.69	0.47-0.47	0.50
4-SCH_3	-0.16--0.18	+0.28	-0.05	-0.68	0.97/0.98	2.69	2.52	0.71	0.45-0.49	0.51
5-SCH_3	-0.16--0.18	+0.28	-0.05	-0.68	0.97-0.98	2.69	2.53	0.71	0.47-0.48	0.51
6-SCH_3	-0.17/-0.17	+0.28	-0.05	-0.68	0.97-0.98	2.69	2.54	0.71	0.45-0.50	0.51

Cartesian Coordinates for optimized structures of **1**, **1'**, **2**, **2'**, ***n*-XH$_2$** (*n* = 3–8, X = N, P), ***n*-E** (*n* = 5, 6 and E = OH, SH, F, Cl, Br), ***n*-X(CH$_3$)$_2$** (*n* = 3–6, X = N, P), ***n*-X(CH$_3$)** (*n* = 3–6, X = O, S).

B3LYP/def2-TZVPP-optimized structures

1

Be	-0.01098400	0.92258300	0.00342300
Be	0.01098400	-0.92258300	0.00342300
H	1.05144900	-0.06909100	-0.61833500
H	-1.05144900	0.06909100	-0.61833500
H	0.00000000	0.00000000	1.20523400
H	0.19395200	-3.01939200	-0.80709500
H	-0.82239900	-2.97303100	0.45485700
H	0.82239900	2.97303100	0.45485700
H	-0.19395200	3.01939200	-0.80709500
N	-0.01098400	-2.52360000	0.05060900
N	0.01098400	2.52360000	0.05060900

1'

Be	0.90438300	-0.01373600	0.00341400
Be	-0.90438400	-0.01374400	-0.00341700
H	0.01719400	-0.60765700	-1.03497800
H	-0.00000300	1.17965600	0.00004100
H	-0.01719400	-0.60772500	1.03495000
H	-3.28226200	0.44338200	-1.24701800
H	-3.28766800	-1.31283400	-0.15973200
H	3.28763700	-1.31285400	0.15962000
H	3.28224500	0.44326200	1.24706400
P	3.02956900	0.06282700	-0.10150000
P	-3.02956600	0.06281900	0.10150500

2

Be	0.00000000	3.10019200	-0.22883700
Be	-0.00058900	1.47394900	0.57207000
H	-0.05658900	2.74222100	1.31202800
H	-1.01636400	1.96378300	-0.37638600
H	1.07149400	2.00021500	-0.28679400
H	0.79991000	0.00123800	1.98774900
H	-0.79991000	-0.00123800	1.98774900
H	-0.83241400	5.04822100	-1.03679400
H	0.79082400	5.11580000	-0.90555700
N	0.00431000	4.48771600	-0.97577800
N	0.00000000	0.00000000	1.36093300
Be	0.00058900	-1.47394900	0.57207000

Be	0.00000000	-3.10019200	-0.22883700
H	1.01636400	-1.96378300	-0.37638600
H	0.05658900	-2.74222100	1.31202800
H	-1.07149400	-2.00021500	-0.28679400
N	-0.00431000	-4.48771600	-0.97577800
H	0.83241400	-5.04822100	-1.03679400
H	-0.79082400	-5.11580000	-0.90555700

2'

Be	0.00000000	3.57515700	-0.10430200
Be	0.00000000	1.92925500	0.60304200
H	1.03113400	2.46995900	-0.27945200
H	0.00000000	3.17622900	1.36612600
H	-1.03113400	2.46995900	-0.27945200
Be	0.00000000	-3.57515700	-0.10430200
Be	0.00000000	-1.92925500	0.60304200
H	0.00000000	-3.17622900	1.36612600
H	1.03113400	-2.46995900	-0.27945200
H	-1.03113400	-2.46995900	-0.27945200
P	0.00000000	-5.46171100	-1.05645100
P	0.00000000	5.46171100	-1.05645100
P	0.00000000	0.00000000	1.48880900
H	-1.03338000	6.04838000	-0.27363400
H	1.03338000	6.04838000	-0.27363400
H	-1.05454800	0.00000000	2.42578400
H	1.05454800	0.00000000	2.42578400
H	-1.03338000	-6.04838000	-0.27363400
H	1.03338000	-6.04838000	-0.27363400

***n*-NH_2** (n = 3–8)

3-NH_2

Be	-0.88808800	1.97782100	0.00000000
Be	0.88808800	1.97782100	0.00000000
H	0.00000000	3.23604600	0.00000000
H	0.00000000	1.45336900	1.03114700
H	0.00000000	1.45336900	-1.03114700
H	3.00222300	1.73333400	-0.80974300
H	3.00222300	1.73333400	0.80974300
H	-3.00222300	1.73333400	0.80974300
H	-3.00222300	1.73333400	-0.80974300
N	-2.47315900	1.42787900	0.00000000
N	2.47315900	1.42787900	0.00000000
Be	-2.15688700	-0.21980400	0.00000000
Be	-1.26879900	-1.75801700	0.00000000

H	-1.25865500	-0.72668500	1.03114700
H	-2.80249800	-1.61802300	0.00000000
H	-1.25865500	-0.72668500	-1.03114700
N	0.00000000	-2.85575800	0.00000000
H	0.00000000	-3.46666900	0.80974300
H	0.00000000	-3.46666900	-0.80974300
Be	1.26879900	-1.75801700	0.00000000
Be	2.15688700	-0.21980400	0.00000000
H	2.80249800	-1.61802300	0.00000000
H	1.25865500	-0.72668500	-1.03114700
H	1.25865500	-0.72668500	1.03114700

4-NH_2

Be	-0.88466200	2.75255600	0.00000000
Be	0.88466200	2.75255600	0.00000000
H	0.00000000	3.97672800	0.00000000
H	0.00000000	2.18020300	1.03264200
H	0.00000000	2.18020300	-1.03264200
H	2.96406100	2.96406100	-0.80808300
H	2.96406100	2.96406100	0.80808300
H	-2.96406100	2.96406100	0.80808300
H	-2.96406100	2.96406100	-0.80808300
N	-2.52994200	2.52994200	0.00000000
N	2.52994200	2.52994200	0.00000000
Be	2.75255600	0.88466200	0.00000000
Be	2.75255600	-0.88466200	0.00000000
H	2.18020300	0.00000000	-1.03264200
H	3.97672800	0.00000000	0.00000000
H	2.18020300	0.00000000	1.03264200
Be	-2.75255600	0.88466200	0.00000000
Be	-2.75255600	-0.88466200	0.00000000
H	-2.18020300	0.00000000	1.03264200
H	-3.97672800	0.00000000	0.00000000
H	-2.18020300	0.00000000	-1.03264200
N	-2.52994200	-2.52994200	0.00000000
H	-2.96406100	-2.96406100	0.80808300
H	-2.96406100	-2.96406100	-0.80808300
N	2.52994200	-2.52994200	0.00000000
H	2.96406100	-2.96406100	-0.80808300
H	2.96406100	-2.96406100	0.80808300
Be	-0.88466200	-2.75255600	0.00000000
Be	0.88466200	-2.75255600	0.00000000
H	0.00000000	-3.97672800	0.00000000
H	0.00000000	-2.18020300	-1.03264200

H	0.00000000	-2.18020300	1.03264200

5-NH_2

Be	-0.88460800	3.55357400	0.00000000
Be	0.88460800	3.55357400	0.00000000
H	0.00000000	4.76567500	0.00000000
H	0.00000000	2.96959000	1.03536100
H	0.00000000	2.96959000	-1.03536100
H	2.90314900	3.99584200	-0.80585100
H	2.90314900	3.99584200	0.80585100
H	-2.90314900	3.99584200	0.80585100
H	-2.90314900	3.99584200	-0.80585100
N	-2.53973600	3.49564600	0.00000000
N	2.53973600	3.49564600	0.00000000
Be	3.10629100	1.93942700	0.00000000
Be	3.65300900	0.25680300	0.00000000
H	2.82424800	0.91765400	-1.03536100
H	4.53242600	1.47267500	0.00000000
H	2.82424800	0.91765400	1.03536100
N	4.10937800	-1.33521800	0.00000000
H	4.69739400	-1.52627600	-0.80585100
H	4.69739400	-1.52627600	0.80585100
Be	-3.10629100	1.93942700	0.00000000
Be	-3.65300900	0.25680300	0.00000000
H	-2.82424800	0.91765400	1.03536100
H	-4.53242600	1.47267500	0.00000000
H	-2.82424800	0.91765400	-1.03536100
N	-4.10937800	-1.33521800	0.00000000
H	-4.69739400	-1.52627600	0.80585100
H	-4.69739400	-1.52627600	-0.80585100
Be	2.80440100	-2.35494200	0.00000000
Be	1.37307600	-3.39486100	0.00000000
H	1.74548100	-2.40244900	-1.03536100
H	2.80119400	-3.85551200	0.00000000
H	1.74548100	-2.40244900	1.03536100
N	0.00000000	-4.32085600	0.00000000
H	0.00000000	-4.93913300	-0.80585100
H	0.00000000	-4.93913300	0.80585100
Be	-2.80440100	-2.35494200	0.00000000
Be	-1.37307600	-3.39486100	0.00000000
H	-2.80119400	-3.85551200	0.00000000
H	-1.74548100	-2.40244900	-1.03536100
H	-1.74548100	-2.40244900	1.03536100

6-NH_2

Be	0.88509500	4.35627500	0.00000000
Be	-0.88509500	4.35627500	0.00000000
H	0.00000000	3.76648600	1.03678600
H	0.00000000	5.56143700	0.00000000
H	0.00000000	3.76648600	-1.03678600
N	-2.53967500	4.39884600	0.00000000
H	-2.85062900	4.93743300	0.80400300
H	-2.85062900	4.93743300	-0.80400300
Be	3.33009700	-2.94465200	0.00000000
Be	4.21519200	-1.41162300	0.00000000
H	4.81634600	-2.78071900	0.00000000
H	3.26187300	-1.88324300	-1.03678600
H	3.26187300	-1.88324300	1.03678600
H	5.70125700	0.00000000	0.80400300
H	5.70125700	0.00000000	-0.80400300
H	2.85062900	-4.93743300	-0.80400300
H	2.85062900	-4.93743300	0.80400300
N	2.53967500	-4.39884600	0.00000000
N	5.07934900	0.00000000	0.00000000
Be	4.21519200	1.41162300	0.00000000
Be	3.33009700	2.94465200	0.00000000
H	3.26187300	1.88324300	1.03678600
H	4.81634600	2.78071900	0.00000000
H	3.26187300	1.88324300	-1.03678600
N	2.53967500	4.39884600	0.00000000
H	2.85062900	4.93743300	0.80400300
H	2.85062900	4.93743300	-0.80400300
Be	0.88509500	-4.35627500	0.00000000
Be	-0.88509500	-4.35627500	0.00000000
H	0.00000000	-3.76648600	-1.03678600
H	0.00000000	-5.56143700	0.00000000
H	0.00000000	-3.76648600	1.03678600
N	-2.53967500	-4.39884600	0.00000000
H	-2.85062900	-4.93743300	-0.80400300
H	-2.85062900	-4.93743300	0.80400300
Be	-3.33009700	2.94465200	0.00000000
Be	-4.21519200	1.41162300	0.00000000
H	-3.26187300	1.88324300	1.03678600
H	-4.81634600	2.78071900	0.00000000
H	-3.26187300	1.88324300	-1.03678600
N	-5.07934900	0.00000000	0.00000000
H	-5.70125700	0.00000000	0.80400300
H	-5.70125700	0.00000000	-0.80400300
Be	-3.33009700	-2.94465200	0.00000000

Be	-4.21519200	-1.41162300	0.00000000
H	-4.81634600	-2.78071900	0.00000000
H	-3.26187300	-1.88324300	1.03678600
H	-3.26187300	-1.88324300	-1.03678600

7-NH_2

Be	0.00000000	4.56641600	0.40676300
Be	1.03183300	4.09479700	1.76503700
H	1.44210100	4.86742400	0.53852200
H	-0.15785000	4.96629700	1.85030000
H	0.27071600	3.18858700	0.87305700
N	2.01592800	3.65766600	3.02218300
H	2.90697700	3.33190200	2.65892800
H	2.24193000	4.47926700	3.57464600
Be	0.24877200	-0.84961900	-5.12985800
Be	-0.24877200	0.84961900	-5.12985800
H	0.00000000	0.00000000	-6.33443500
H	-0.99543500	-0.29099300	-4.54062400
H	0.99543500	0.29099300	-4.54062400
H	-0.11463700	2.94126800	-5.81022800
H	-1.64244900	2.47727800	-5.62159000
H	0.85454700	-6.01580100	-1.01952900
H	1.96789400	-4.97889400	-0.49447900
N	1.00710100	-5.03098900	-0.82178800
N	-0.72842600	2.43334100	-5.17905200
Be	-0.79693900	3.25063700	-3.74080900
Be	-0.88584900	4.16594800	-2.22779400
H	0.35131200	3.73921200	-2.93903600
H	-1.43710000	4.58917000	-3.55060200
H	-1.44780400	2.81624300	-2.47846700
N	-1.00710100	5.03098900	-0.82178800
H	-0.85454700	6.01580100	-1.01952900
H	-1.96789400	4.97889400	-0.49447900
Be	0.00000000	-4.56641600	0.40676300
Be	-1.03183300	-4.09479700	1.76503700
H	-1.44210100	-4.86742400	0.53852200
H	0.15785000	-4.96629700	1.85030000
H	-0.27071600	-3.18858700	0.87305700
N	-2.01592800	-3.65766600	3.02218300
H	-2.90697700	-3.33190200	2.65892800
H	-2.24193000	-4.47926700	3.57464600
Be	1.36662100	2.48167300	3.98947900
Be	0.67147500	1.20271800	4.99600100
H	1.43813800	1.02791400	3.73417300

H	1.70251700	2.20188000	5.42186700
H	-0.06917100	2.30846300	4.35084300
N	0.00000000	0.00000000	5.91480300
H	0.70008700	-0.39895900	6.53294700
H	-0.70008700	0.39895900	6.53294700
Be	-1.36662100	-2.48167300	3.98947900
Be	-0.67147500	-1.20271800	4.99600100
H	-1.70251700	-2.20188000	5.42186700
H	0.06917100	-2.30846300	4.35084300
H	-1.43813800	-1.02791400	3.73417300
Be	0.88584900	-4.16594800	-2.22779400
Be	0.79693900	-3.25063700	-3.74080900
H	1.43710000	-4.58917000	-3.55060200
H	-0.35131200	-3.73921200	-2.93903600
H	1.44780400	-2.81624300	-2.47846700
H	1.64244900	-2.47727800	-5.62159000
H	0.11463700	-2.94126800	-5.81022800
N	0.72842600	-2.43334100	-5.17905200

8-NH_2

Be	-3.99434800	3.26536900	0.69135100
Be	-3.21010200	4.03772700	-0.69467400
H	-4.61794700	3.50548600	-0.62752900
H	-3.44381500	4.66608700	0.62310900
H	-2.76885500	2.80729200	-0.00058100
H	-2.81866200	4.25969300	-2.85548200
H	-2.85559900	5.69123600	-2.11902500
H	-4.22387800	2.87949700	2.85236600
H	-5.65393100	2.93377100	2.11412700
N	-4.70969300	2.57287400	2.01414800
N	-2.50692000	4.74259300	-2.01746700
Be	-0.85189200	4.75409100	-1.99835000
Be	0.91811300	4.74259300	-1.99720200
H	0.02544400	3.56395600	-2.10533200
H	0.03828600	5.43775700	-2.98852600
H	0.03581400	5.26557800	-0.92178000
Be	3.26536900	3.99434800	-0.69135100
Be	4.03772700	3.21010200	0.69467400
H	4.66608700	3.44381500	-0.62310900
H	3.50548600	4.61794700	0.62752900
H	2.80729200	2.76885500	0.00058100
N	4.74259300	2.50692000	2.01746700
H	5.69123600	2.85559900	2.11902500
H	4.25969300	2.81866200	2.85548200

Be	-3.26536900	-3.99434800	-0.69135100
Be	-4.03772700	-3.21010200	0.69467400
H	-3.50548600	-4.61794700	0.62752900
H	-2.80729200	-2.76885500	0.00058100
H	-4.66608700	-3.44381500	-0.62310900
H	-5.69123600	-2.85559900	2.11902500
H	-4.25969300	-2.81866200	2.85548200
H	-2.93377100	-5.65393100	-2.11412700
H	-2.87949700	-4.22387800	-2.85236600
N	-2.57287400	-4.70969300	-2.01414800
N	-4.74259300	-2.50692000	2.01746700
Be	-4.75409100	-0.85189200	1.99835000
Be	-4.74259300	0.91811300	1.99720200
H	-5.26557800	0.03581400	0.92178000
H	-5.43775700	0.03828600	2.98852600
H	-3.56395600	0.02544400	2.10533200
N	2.57287400	4.70969300	-2.01414800
H	2.87949700	4.22387800	-2.85236600
H	2.93377100	5.65393100	-2.11412700
Be	-0.91811300	-4.74259300	-1.99720200
Be	0.85189200	-4.75409100	-1.99835000
H	-0.03581400	-5.26557800	-0.92178000
H	-0.03828600	-5.43775700	-2.98852600
H	-0.02544400	-3.56395600	-2.10533200
N	2.50692000	-4.74259300	-2.01746700
H	2.85559900	-5.69123600	-2.11902500
H	2.81866200	-4.25969300	-2.85548200
Be	4.75409100	0.85189200	1.99835000
Be	4.74259300	-0.91811300	1.99720200
H	5.26557800	-0.03581400	0.92178000
H	5.43775700	-0.03828600	2.98852600
H	3.56395600	-0.02544400	2.10533200
N	4.70969300	-2.57287400	2.01414800
H	5.65393100	-2.93377100	2.11412700
H	4.22387800	-2.87949700	2.85236600
Be	3.21010200	-4.03772700	-0.69467400
Be	3.99434800	-3.26536900	0.69135100
H	4.61794700	-3.50548600	-0.62752900
H	2.76885500	-2.80729200	-0.00058100
H	3.44381500	-4.66608700	0.62310900

***n*-PH$_2$** (n = 3–8)

3-PH$_2$

Be	-0.88408900	2.40604600	0.00000000

Be	0.88408900	2.40604600	0.00000000
H	0.00000000	3.62070000	0.00000000
H	0.00000000	1.82010400	1.01525500
H	0.00000000	1.82010400	-1.01525500
H	3.64689200	2.10553400	-1.07276400
H	3.64689200	2.10553400	1.07276400
H	-3.64689200	2.10553400	1.07276400
H	-3.64689200	2.10553400	-1.07276400
Be	-2.52574200	-0.43738000	0.00000000
Be	-1.64165300	-1.96866600	0.00000000
H	-1.57625600	-0.91005200	1.01525500
H	-3.13561800	-1.81035000	0.00000000
H	-1.57625600	-0.91005200	-1.01525500
H	0.00000000	-4.21106900	1.07276400
H	0.00000000	-4.21106900	-1.07276400
Be	1.64165300	-1.96866600	0.00000000
Be	2.52574200	-0.43738000	0.00000000
H	3.13561800	-1.81035000	0.00000000
H	1.57625600	-0.91005200	-1.01525500
H	1.57625600	-0.91005200	1.01525500
P	0.00000000	-3.30282000	0.00000000
P	2.86032600	1.65141000	0.00000000
P	-2.86032600	1.65141000	0.00000000

4-PH_2

Be	-0.88261300	3.35803100	0.00000000
Be	0.88261300	3.35803100	0.00000000
H	0.00000000	4.55899300	0.00000000
H	0.00000000	2.76346400	1.02106900
H	0.00000000	2.76346400	-1.02106900
H	3.59973800	3.59973800	-1.06934500
H	3.59973800	3.59973800	1.06934500
H	-3.59973800	3.59973800	1.06934500
H	-3.59973800	3.59973800	-1.06934500
Be	3.35803100	0.88261300	0.00000000
Be	3.35803100	-0.88261300	0.00000000
H	2.76346400	0.00000000	-1.02106900
H	4.55899300	0.00000000	0.00000000
H	2.76346400	0.00000000	1.02106900
Be	-3.35803100	0.88261300	0.00000000
Be	-3.35803100	-0.88261300	0.00000000
H	-2.76346400	0.00000000	1.02106900
H	-4.55899300	0.00000000	0.00000000
H	-2.76346400	0.00000000	-1.02106900

H	-3.59973800	-3.59973800	1.06934500
H	-3.59973800	-3.59973800	-1.06934500
H	3.59973800	-3.59973800	-1.06934500
H	3.59973800	-3.59973800	1.06934500
Be	-0.88261300	-3.35803100	0.00000000
Be	0.88261300	-3.35803100	0.00000000
H	0.00000000	-4.55899300	0.00000000
H	0.00000000	-2.76346400	-1.02106900
H	0.00000000	-2.76346400	1.02106900
P	2.95380200	2.95380200	0.00000000
P	2.95380200	-2.95380200	0.00000000
P	-2.95380200	-2.95380200	0.00000000
P	-2.95380200	2.95380200	0.00000000

5-PH_2

Be	-0.88247200	4.30420400	0.00000000
Be	0.88247200	4.30420400	0.00000000
H	0.00000000	5.49953400	0.00000000
H	0.00000000	3.70879600	1.02529700
H	0.00000000	3.70879600	-1.02529700
Be	3.82084200	2.16935300	0.00000000
Be	4.36624000	0.49079200	0.00000000
H	3.52727500	1.14608100	-1.02529700
H	5.23036800	1.69945000	0.00000000
H	3.52727500	1.14608100	1.02529700
Be	-3.82084200	2.16935300	0.00000000
Be	-4.36624000	0.49079200	0.00000000
H	-3.52727500	1.14608100	1.02529700
H	-5.23036800	1.69945000	0.00000000
H	-3.52727500	1.14608100	-1.02529700
Be	3.24388200	-2.96347000	0.00000000
Be	1.81601300	-4.00087800	0.00000000
H	2.17997600	-3.00047900	-1.02529700
H	3.23254500	-4.44921700	0.00000000
H	2.17997600	-3.00047900	1.02529700
Be	-3.24388200	-2.96347000	0.00000000
Be	-1.81601300	-4.00087800	0.00000000
H	-3.23254500	-4.44921700	0.00000000
H	-2.17997600	-3.00047900	-1.02529700
H	-2.17997600	-3.00047900	1.02529700
P	-4.82671400	-1.56829400	0.00000000
P	-2.98307300	4.10584800	0.00000000
P	2.98307300	4.10584800	0.00000000
P	4.82671400	-1.56829400	0.00000000

P	0.00000000	-5.07510700	0.00000000
H	-3.52239900	4.84816600	1.06644800
H	-3.52239900	4.84816600	-1.06644800
H	3.52239900	4.84816600	1.06644800
H	3.52239900	4.84816600	-1.06644800
H	5.69936100	-1.85183500	1.06644800
H	5.69936100	-1.85183500	-1.06644800
H	0.00000000	-5.99266200	1.06644800
H	0.00000000	-5.99266200	-1.06644800
H	-5.69936100	-1.85183500	1.06644800
H	-5.69936100	-1.85183500	-1.06644800

6-PH_2

Be	0.88237700	5.24909400	0.00000000
Be	-0.88237700	5.24909400	0.00000000
H	0.00000000	4.65347000	1.02711300
H	0.00000000	6.44018300	0.00000000
H	0.00000000	4.65347000	-1.02711300
H	-3.45230700	5.97957200	1.06452100
H	-3.45230700	5.97957200	-1.06452100
Be	4.10466000	-3.38870800	0.00000000
Be	4.98703800	-1.86038600	0.00000000
H	5.57736200	-3.22009100	0.00000000
H	4.03002300	-2.32673500	-1.02711300
H	4.03002300	-2.32673500	1.02711300
H	6.90461500	0.00000000	1.06452100
H	6.90461500	0.00000000	-1.06452100
H	3.45230700	-5.97957200	-1.06452100
H	3.45230700	-5.97957200	1.06452100
Be	4.98703800	1.86038600	0.00000000
Be	4.10466000	3.38870800	0.00000000
H	4.03002300	2.32673500	1.02711300
H	5.57736200	3.22009100	0.00000000
H	4.03002300	2.32673500	-1.02711300
H	3.45230700	5.97957200	1.06452100
H	3.45230700	5.97957200	-1.06452100
Be	0.88237700	-5.24909400	0.00000000
Be	-0.88237700	-5.24909400	0.00000000
H	0.00000000	-4.65347000	-1.02711300
H	0.00000000	-6.44018300	0.00000000
H	0.00000000	-4.65347000	1.02711300
H	-3.45230700	-5.97957200	-1.06452100
H	-3.45230700	-5.97957200	1.06452100
Be	-4.10466000	3.38870800	0.00000000

Be	-4.98703800	1.86038600	0.00000000
H	-4.03002300	2.32673500	1.02711300
H	-5.57736200	3.22009100	0.00000000
H	-4.03002300	2.32673500	-1.02711300
H	-6.90461500	0.00000000	1.06452100
H	-6.90461500	0.00000000	-1.06452100
Be	-4.10466000	-3.38870800	0.00000000
Be	-4.98703800	-1.86038600	0.00000000
H	-5.57736200	-3.22009100	0.00000000
H	-4.03002300	-2.32673500	1.02711300
H	-4.03002300	-2.32673500	-1.02711300
P	-2.99176000	5.18188100	0.00000000
P	2.99176000	-5.18188100	0.00000000
P	5.98352000	0.00000000	0.00000000
P	2.99176000	5.18188100	0.00000000
P	-2.99176000	-5.18188100	0.00000000
P	-5.98352000	0.00000000	0.00000000

7-PH_2

Be	0.88231100	6.18647400	0.00000000
Be	-0.88231100	6.18647400	0.00000000
H	0.00000000	5.59109200	1.02866700
H	0.00000000	7.37476700	0.00000000
H	0.00000000	5.59109200	-1.02866700
H	-3.39394700	7.04760400	1.06267800
H	-3.39394700	7.04760400	-1.06267800
Be	5.83503400	-2.23681000	0.00000000
Be	6.22769900	-0.51643000	0.00000000
H	7.18986700	-1.64104000	0.00000000
H	5.45091200	-1.24413500	-1.02866700
H	5.45091200	-1.24413500	1.02866700
H	7.62613000	1.74061400	1.06267800
H	7.62613000	1.74061400	-1.06267800
H	0.00000000	-7.82225000	-1.06267800
H	0.00000000	-7.82225000	1.06267800
Be	5.38689200	3.16738500	0.00000000
Be	4.28666800	4.54702200	0.00000000
H	4.37129200	3.48598900	1.02866700
H	5.76582500	4.59809200	0.00000000
H	4.37129200	3.48598900	-1.02866700
H	3.39394700	7.04760400	1.06267800
H	3.39394700	7.04760400	-1.06267800
Be	-1.88927600	-5.95664100	0.00000000
Be	-3.47914500	-5.19100000	0.00000000

H	-2.42588400	-5.03740000	-1.02866700
H	-3.19979200	-6.64443600	0.00000000
H	-2.42588400	-5.03740000	1.02866700
H	-6.11568100	-4.87709300	-1.06267800
H	-6.11568100	-4.87709300	1.06267800
Be	-4.28666800	4.54702200	0.00000000
Be	-5.38689200	3.16738500	0.00000000
H	-4.37129200	3.48598900	1.02866700
H	-5.76582500	4.59809200	0.00000000
H	-4.37129200	3.48598900	-1.02866700
H	-7.62613000	1.74061400	1.06267800
H	-7.62613000	1.74061400	-1.06267800
Be	-5.83503400	-2.23681000	0.00000000
Be	-6.22769900	-0.51643000	0.00000000
H	-7.18986700	-1.64104000	0.00000000
H	-5.45091200	-1.24413500	1.02866700
H	-5.45091200	-1.24413500	-1.02866700
Be	1.88927600	-5.95664100	0.00000000
Be	3.47914500	-5.19100000	0.00000000
H	3.19979200	-6.64443600	0.00000000
H	2.42588400	-5.03740000	-1.02866700
H	2.42588400	-5.03740000	1.02866700
H	6.11568100	-4.87709300	1.06267800
H	6.11568100	-4.87709300	-1.06267800
P	5.39342400	-4.30111200	0.00000000
P	-2.99312500	6.21528800	0.00000000
P	0.00000000	-6.89844900	0.00000000
P	6.72549000	1.53504900	0.00000000
P	2.99312500	6.21528800	0.00000000
P	-5.39342400	-4.30111200	0.00000000
P	-6.72549000	1.53504900	0.00000000

8-PH_2

Be	-0.88247900	6.56805400	1.59249900
Be	0.88247900	6.56805400	1.59249900
H	0.00000000	7.47302300	2.36361100
H	0.00000000	5.44664500	1.98730500
H	0.00000000	6.78354900	0.42423600
H	3.36642300	7.92538800	1.24373400
H	3.44129600	6.59116400	2.89699500
H	-3.44129600	6.59116400	2.89699500
H	-3.36642300	7.92538800	1.24373400
Be	4.25303900	5.31815000	0.46003900
Be	5.31815000	4.25303900	-0.46003900

H	3.98950400	4.74058200	-0.88081400
H	5.62594100	5.62594100	0.00000000
H	4.74058200	3.98950400	0.88081400
Be	6.56805400	0.88247900	-1.59249900
Be	6.56805400	-0.88247900	-1.59249900
H	5.44664500	0.00000000	-1.98730500
H	7.47302300	0.00000000	-2.36361100
H	6.78354900	0.00000000	-0.42423600
H	6.59116400	-3.44129600	-2.89699500
H	7.92538800	-3.36642300	-1.24373400
Be	-6.56805400	-0.88247900	-1.59249900
Be	-6.56805400	0.88247900	-1.59249900
H	-7.47302300	0.00000000	-2.36361100
H	-6.78354900	0.00000000	-0.42423600
H	-5.44664500	0.00000000	-1.98730500
H	-6.59116400	3.44129600	-2.89699500
H	-7.92538800	3.36642300	-1.24373400
H	-7.92538800	-3.36642300	-1.24373400
H	-6.59116400	-3.44129600	-2.89699500
Be	-5.31815000	4.25303900	-0.46003900
Be	-4.25303900	5.31815000	0.46003900
H	-3.98950400	4.74058200	-0.88081400
H	-5.62594100	5.62594100	0.00000000
H	-4.74058200	3.98950400	0.88081400
H	6.59116400	3.44129600	-2.89699500
H	7.92538800	3.36642300	-1.24373400
Be	-5.31815000	-4.25303900	-0.46003900
Be	-4.25303900	-5.31815000	0.46003900
H	-4.74058200	-3.98950400	0.88081400
H	-5.62594100	-5.62594100	0.00000000
H	-3.98950400	-4.74058200	-0.88081400
H	-3.44129600	-6.59116400	2.89699500
H	-3.36642300	-7.92538800	1.24373400
Be	5.31815000	-4.25303900	-0.46003900
Be	4.25303900	-5.31815000	0.46003900
H	3.98950400	-4.74058200	-0.88081400
H	5.62594100	-5.62594100	0.00000000
H	4.74058200	-3.98950400	0.88081400
H	3.36642300	-7.92538800	1.24373400
H	3.44129600	-6.59116400	2.89699500
Be	-0.88247900	-6.56805400	1.59249900
Be	0.88247900	-6.56805400	1.59249900
H	0.00000000	-7.47302300	2.36361100
H	0.00000000	-6.78354900	0.42423600

H	0.00000000	-5.44664500	1.98730500
P	-2.99267600	-6.60591400	1.56267200
P	-6.60591400	-2.99267600	-1.56267200
P	-6.60591400	2.99267600	-1.56267200
P	-2.99267600	6.60591400	1.56267200
P	2.99267600	6.60591400	1.56267200
P	6.60591400	2.99267600	-1.56267200
P	6.60591400	-2.99267600	-1.56267200
P	2.99267600	-6.60591400	1.56267200

***n*-F** (*n* = 3–6)

3-F

Be	-0.87953700	1.95251600	0.00000000
Be	0.87953700	1.95251600	0.00000000
H	0.00000000	3.20595100	0.00000000
H	0.00000000	1.43149100	1.03213800
H	0.00000000	1.43149100	-1.03213800
Be	-2.13069700	-0.21455700	0.00000000
Be	-1.25116000	-1.73795900	0.00000000
H	-1.23970700	-0.71574500	1.03213800
H	-2.77643500	-1.60297500	0.00000000
H	-1.23970700	-0.71574500	-1.03213800
Be	1.25116000	-1.73795900	0.00000000
Be	2.13069700	-0.21455700	0.00000000
H	2.77643500	-1.60297500	0.00000000
H	1.23970700	-0.71574500	-1.03213800
H	1.23970700	-0.71574500	1.03213800
F	2.31611700	1.33721100	0.00000000
F	-2.31611700	1.33721100	0.00000000
F	0.00000000	-2.67442200	0.00000000

4-F

Be	2.70406600	-0.87542900	0.00754200
Be	2.70406600	0.87542900	0.00754200
H	3.86658400	0.00000000	-0.35796200
H	1.85094000	0.00000000	-0.79762800
H	2.46612700	0.00000000	1.17122700
Be	0.87542900	2.70406600	-0.00754200
Be	-0.87542900	2.70406600	-0.00754200
H	0.00000000	1.85094000	0.79762800
H	0.00000000	3.86658400	0.35796200
H	0.00000000	2.46612700	-1.17122700
Be	0.87542900	-2.70406600	-0.00754200
Be	-0.87542900	-2.70406600	-0.00754200

H	0.00000000	-2.46612700	-1.17122700
H	0.00000000	-3.86658400	0.35796200
H	0.00000000	-1.85094000	0.79762800
Be	-2.70406600	-0.87542900	0.00754200
Be	-2.70406600	0.87542900	0.00754200
H	-3.86658400	0.00000000	-0.35796200
H	-2.46612700	0.00000000	1.17122700
H	-1.85094000	0.00000000	-0.79762800
F	2.38007700	2.38007700	0.00000000
F	-2.38007700	2.38007700	0.00000000
F	-2.38007700	-2.38007700	0.00000000
F	2.38007700	-2.38007700	0.00000000

5-F

Be	0.00000000	1.34222600	3.33294400
Be	-0.00806700	2.75730300	2.30471800
H	-0.41756400	2.71470200	3.73770200
H	1.17174900	1.93798800	2.65605500
H	-0.76995300	1.51636200	2.09019400
Be	-0.01546800	3.59150700	-0.24613300
Be	0.00189000	3.05231100	-1.90999300
H	-1.19942700	3.26194100	-1.07034200
H	0.53489000	4.34909300	-1.40653800
H	0.64680600	2.38692700	-0.76759100
Be	0.00000000	-1.34222600	3.33294400
Be	0.00806700	-2.75730300	2.30471800
H	0.76995300	-1.51636200	2.09019400
H	0.41756400	-2.71470200	3.73770200
H	-1.17174900	-1.93798800	2.65605500
Be	0.01031100	0.87448700	-3.48294300
Be	-0.01031100	-0.87448700	-3.48294300
H	-1.03312200	0.01243700	-2.89722200
H	0.00000000	0.00000000	-4.69127900
H	1.03312200	-0.01243700	-2.89722200
Be	0.01546800	-3.59150700	-0.24613300
Be	-0.00189000	-3.05231100	-1.90999300
H	-0.53489000	-4.34909300	-1.40653800
H	-0.64680600	-2.38692700	-0.76759100
H	1.19942700	-3.26194100	-1.07034200
F	0.00000000	0.00000000	4.06800800
F	0.02046000	-3.87353800	1.25789300
F	-0.02046000	3.87353800	1.25789300
F	0.02036900	2.39285400	-3.29089600
F	-0.02036900	-2.39285400	-3.29089600

6-F

Be	-0.87450400	4.27380200	0.00599200
Be	0.87450400	4.27380200	0.00599200
H	0.00000000	3.32401700	-0.70888000
H	0.00000000	5.37870100	-0.46736500
H	0.00000000	4.13771700	1.19235500
Be	-3.26396900	-2.89424300	0.00599200
Be	-4.13847200	-1.37955800	0.00599200
H	-4.65809200	-2.68935000	-0.46736500
H	-3.58336800	-2.06885900	1.19235500
H	-2.87868300	-1.66200800	-0.70888000
Be	-4.13847200	1.37955800	-0.00599200
Be	-3.26396900	2.89424300	-0.00599200
H	-3.58336800	2.06885900	-1.19235500
H	-4.65809200	2.68935000	0.46736500
H	-2.87868300	1.66200800	0.70888000
Be	-0.87450400	-4.27380200	-0.00599200
Be	0.87450400	-4.27380200	-0.00599200
H	0.00000000	-3.32401700	0.70888000
H	0.00000000	-5.37870100	0.46736500
H	0.00000000	-4.13771700	-1.19235500
Be	3.26396900	2.89424300	-0.00599200
Be	4.13847200	1.37955800	-0.00599200
H	3.58336800	2.06885900	-1.19235500
H	4.65809200	2.68935000	0.46736500
H	2.87868300	1.66200800	0.70888000
Be	3.26396900	-2.89424300	0.00599200
Be	4.13847200	-1.37955800	0.00599200
H	4.65809200	-2.68935000	-0.46736500
H	2.87868300	-1.66200800	-0.70888000
H	3.58336800	-2.06885900	1.19235500
F	2.39531500	4.14880700	0.00000000
F	-2.39531500	4.14880700	0.00000000
F	-4.79063000	0.00000000	0.00000000
F	-2.39531500	-4.14880700	0.00000000
F	2.39531500	-4.14880700	0.00000000
F	4.79063000	0.00000000	0.00000000

***n*-Cl** (*n* = 3–6)

3-Cl

Be	-0.87594100	2.12793200	0.00000000
Be	0.87594100	2.12793200	0.00000000
H	0.00000000	3.35054300	0.00000000

H	0.00000000	1.57061700	1.02418200
H	0.00000000	1.57061700	-1.02418200
Be	-2.28081400	-0.30537900	0.00000000
Be	-1.40487300	-1.82255300	0.00000000
H	-1.36019400	-0.78530900	1.02418200
H	-2.90165500	-1.67527200	0.00000000
H	-1.36019400	-0.78530900	-1.02418200
Be	1.40487300	-1.82255300	0.00000000
Be	2.28081400	-0.30537900	0.00000000
H	2.90165500	-1.67527200	0.00000000
H	1.36019400	-0.78530900	-1.02418200
H	1.36019400	-0.78530900	1.02418200
Cl	2.81313800	1.62416600	0.00000000
Cl	0.00000000	-3.24833200	0.00000000
Cl	-2.81313800	1.62416600	0.00000000

4-Cl

Be	2.97629000	-0.87451200	0.01448200
Be	2.97629000	0.87451200	0.01448200
H	4.13537900	0.00000000	-0.29154200
H	2.14985100	0.00000000	-0.82953400
H	2.67118300	0.00000000	1.16012000
Be	0.87451200	2.97629000	-0.01448200
Be	-0.87451200	2.97629000	-0.01448200
H	0.00000000	2.14985100	0.82953400
H	0.00000000	4.13537900	0.29154200
H	0.00000000	2.67118300	-1.16012000
Be	0.87451200	-2.97629000	-0.01448200
Be	-0.87451200	-2.97629000	-0.01448200
H	0.00000000	-2.67118300	-1.16012000
H	0.00000000	-4.13537900	0.29154200
H	0.00000000	-2.14985100	0.82953400
Be	-2.97629000	-0.87451200	0.01448200
Be	-2.97629000	0.87451200	0.01448200
H	-4.13537900	0.00000000	-0.29154200
H	-2.67118300	0.00000000	1.16012000
H	-2.14985100	0.00000000	-0.82953400
Cl	2.85309000	2.85309000	0.00000000
Cl	-2.85309000	2.85309000	0.00000000
Cl	2.85309000	-2.85309000	0.00000000
Cl	-2.85309000	-2.85309000	0.00000000

5-Cl

Be	-0.87408800	3.86520700	0.00000000

Be	0.87408800	3.86520700	0.00000000
H	0.00000000	5.05545200	0.00000000
H	0.00000000	3.27334600	1.03084900
H	0.00000000	3.27334600	-1.03084900
Be	3.40592300	2.02572100	0.00000000
Be	3.94613800	0.36310800	0.00000000
H	3.11313700	1.01152000	-1.03084900
H	4.80802000	1.56222000	0.00000000
H	3.11313700	1.01152000	1.03084900
Be	-3.40592300	2.02572100	0.00000000
Be	-3.94613800	0.36310800	0.00000000
H	-3.11313700	1.01152000	1.03084900
H	-4.80802000	1.56222000	0.00000000
H	-3.11313700	1.01152000	-1.03084900
Be	2.97906400	-2.61324300	0.00000000
Be	1.56476000	-3.64079400	0.00000000
H	1.92402400	-2.64819300	-1.03084900
H	2.97152000	-4.08994600	0.00000000
H	1.92402400	-2.64819300	1.03084900
Be	-2.97906400	-2.61324300	0.00000000
Be	-1.56476000	-3.64079400	0.00000000
H	-2.97152000	-4.08994600	0.00000000
H	-1.92402400	-2.64819300	-1.03084900
H	-1.92402400	-2.64819300	1.03084900
Cl	-2.85070800	3.92366400	0.00000000
Cl	2.85070800	3.92366400	0.00000000
Cl	4.61254300	-1.49870600	0.00000000
Cl	0.00000000	-4.84991500	0.00000000
Cl	-4.61254300	-1.49870600	0.00000000

6-Cl

Be	0.00000000	4.60632200	0.31242300
Be	-1.60033200	4.32192200	-0.33392600
H	-0.82253700	3.38900800	0.49428700
H	-1.20137100	5.40987200	0.58962800
H	-0.37856300	4.59714100	-1.11444300
Be	3.98919200	-2.30316100	0.31242300
Be	4.54306000	-0.77503300	-0.33392600
H	5.28577200	-1.66451800	0.58962800
H	4.17052200	-1.97072500	-1.11444300
H	3.34623600	-0.98216600	0.49428700
Be	3.98919200	2.30316100	-0.31242300
Be	2.94272800	3.54688900	0.33392600
H	3.79195900	2.62641500	1.11444300

H	4.08440100	3.74535400	-0.58962800
H	2.52369900	2.40684200	-0.49428700
Be	1.60033200	-4.32192200	0.33392600
Be	0.00000000	-4.60632200	-0.31242300
H	0.82253700	-3.38900800	-0.49428700
H	1.20137100	-5.40987200	-0.58962800
H	0.37856300	-4.59714100	1.11444300
Be	-3.98919200	2.30316100	-0.31242300
Be	-4.54306000	0.77503300	0.33392600
H	-4.17052200	1.97072500	1.11444300
H	-5.28577200	1.66451800	-0.58962800
H	-3.34623600	0.98216600	-0.49428700
Be	-2.94272800	-3.54688900	-0.33392600
Be	-3.98919200	-2.30316100	0.31242300
H	-4.08440100	-3.74535400	0.58962800
H	-2.52369900	-2.40684200	0.49428700
H	-3.79195900	-2.62641500	-1.11444300
Cl	1.78628300	4.96858000	1.07876700
Cl	5.19605800	0.93732400	-1.07876700
Cl	3.40977500	-4.03125600	1.07876700
Cl	-1.78628300	-4.96858000	-1.07876700
Cl	-5.19605800	-0.93732400	1.07876700
Cl	-3.40977500	4.03125600	-1.07876700

***n*-Br** (*n* = 3–6)

3-Br

Be	-0.87549400	2.20430300	0.00000000
Be	0.87549400	2.20430300	0.00000000
H	0.00000000	3.42071100	0.00000000
H	0.00000000	1.63914400	1.02392700
H	0.00000000	1.63914400	-1.02392700
Be	-2.34673000	-0.34395200	0.00000000
Be	-1.47123600	-1.86035200	0.00000000
H	-1.41954100	-0.81957200	1.02392700
H	-2.96242300	-1.71035600	0.00000000
H	-1.41954100	-0.81957200	-1.02392700
Be	1.47123600	-1.86035200	0.00000000
Be	2.34673000	-0.34395200	0.00000000
H	2.96242300	-1.71035600	0.00000000
H	1.41954100	-0.81957200	-1.02392700
H	1.41954100	-0.81957200	1.02392700
Br	2.97579400	1.71807500	0.00000000
Br	0.00000000	-3.43615100	0.00000000
Br	-2.97579400	1.71807500	0.00000000

4-Br

Be	3.10019600	-0.87456900	0.01285400
Be	3.10019600	0.87456900	0.01285400
H	4.26723000	0.00000000	-0.24802400
H	2.30509800	0.00000000	-0.86235600
H	2.75092600	0.00000000	1.14546500
Be	0.87456900	3.10019600	-0.01285400
Be	-0.87456900	3.10019600	-0.01285400
H	0.00000000	2.30509800	0.86235600
H	0.00000000	4.26723000	0.24802400
H	0.00000000	2.75092600	-1.14546500
Be	0.87456900	-3.10019600	-0.01285400
Be	-0.87456900	-3.10019600	-0.01285400
H	0.00000000	-2.75092600	-1.14546500
H	0.00000000	-4.26723000	0.24802400
H	0.00000000	-2.30509800	0.86235600
Be	-3.10019600	-0.87456900	0.01285400
Be	-3.10019600	0.87456900	0.01285400
H	-4.26723000	0.00000000	-0.24802400
H	-2.75092600	0.00000000	1.14546500
H	-2.30509800	0.00000000	-0.86235600
Br	3.01088300	3.01088300	0.00000000
Br	-3.01088300	3.01088300	0.00000000
Br	-3.01088300	-3.01088300	0.00000000
Br	3.01088300	-3.01088300	0.00000000

5-Br

Be	-0.05521800	3.07543500	2.74443900
Be	-0.02891400	1.66085800	3.77311000
H	-0.11767600	3.06460400	4.21834900
H	-1.03339000	1.97061400	2.73816100
H	1.02387200	2.07311700	2.82517700
Be	0.02891400	-1.66085800	3.77311000
Be	0.05521800	-3.07543500	2.74443900
H	1.03339000	-1.97061400	2.73816100
H	0.11767600	-3.06460400	4.21834900
H	-1.02387200	-2.07311700	2.82517700
Be	0.00000000	4.10109000	-0.41452600
Be	0.07541900	3.55977200	-2.07619500
H	-1.01570100	3.29563600	-1.12015700
H	0.08734600	4.95974500	-1.61104900
H	1.04210400	3.24223100	-1.00687500
Be	0.00000000	-4.10109000	-0.41452600

Be	-0.07541900	-3.55977200	-2.07619500
H	1.01570100	-3.29563600	-1.12015700
H	-0.08734600	-4.95974500	-1.61104900
H	-1.04210400	-3.24223100	-1.00687500
Be	0.04929600	0.87322900	-4.02840400
Be	-0.04929600	-0.87322900	-4.02840400
H	0.00000000	0.00000000	-5.21653200
H	1.02908100	-0.05958000	-3.43770300
H	-1.02908100	0.05958000	-3.43770300
Br	-0.09268300	4.86094100	1.57702700
Br	0.00000000	0.00000000	5.11217500
Br	0.09268300	-4.86094100	1.57702700
Br	-0.17432500	-3.00062500	-4.13286700
Br	0.17432500	3.00062500	-4.13286700

6-Br

Be	0.00000000	4.71591200	0.36681000
Be	-1.55810100	4.45356100	-0.38420200
H	-0.79874500	3.47217200	0.40216000
H	-1.23251900	5.46800200	0.64640200
H	-0.30763300	4.82015300	-1.07388700
Be	4.08410000	-2.35795600	0.36681000
Be	4.63594700	-0.87742500	-0.38420200
H	5.35168900	-1.66660800	0.64640200
H	4.32819200	-2.14365900	-1.07388700
H	3.40636100	-1.04435300	0.40216000
Be	4.08410000	2.35795600	-0.36681000
Be	3.07784600	3.57613600	0.38420200
H	4.02055900	2.67649400	1.07388700
H	4.11916900	3.80139400	-0.64640200
H	2.60761600	2.42781900	-0.40216000
Be	1.55810100	-4.45356100	0.38420200
Be	0.00000000	-4.71591200	-0.36681000
H	0.79874500	-3.47217200	-0.40216000
H	1.23251900	-5.46800200	-0.64640200
H	0.30763300	-4.82015300	1.07388700
Be	-4.08410000	2.35795600	-0.36681000
Be	-4.63594700	0.87742500	0.38420200
H	-4.32819200	2.14365900	1.07388700
H	-5.35168900	1.66660800	-0.64640200
H	-3.40636100	1.04435300	-0.40216000
Be	-3.07784600	-3.57613600	-0.38420200
Be	-4.08410000	-2.35795600	0.36681000
H	-4.11916900	-3.80139400	0.64640200

H	-2.60761600	-2.42781900	0.40216000
H	-4.02055900	-2.67649400	-1.07388700
Br	1.87582000	5.07182000	1.32082000
Br	-3.45441500	4.16041800	-1.32082000
Br	-5.33023500	-0.91140200	1.32082000
Br	-1.87582000	-5.07182000	-1.32082000
Br	3.45441500	-4.16041800	1.32082000
Br	5.33023500	0.91140200	-1.32082000

***n*- N(CH$_3$)$_2$** (*n* = 3–6)

3-N(CH$_3$)$_2$

Be	-0.88877600	1.94427600	0.00000000
Be	0.88877600	1.94427600	0.00000000
H	0.00000000	3.20529400	0.00000000
H	0.00000000	1.42761700	1.03429700
H	0.00000000	1.42761700	-1.03429700
N	-2.48784700	1.43635900	0.00000000
N	2.48784700	1.43635900	0.00000000
Be	-2.12818000	-0.20243500	0.00000000
Be	-1.23940400	-1.74184000	0.00000000
H	-1.23635300	-0.71380800	1.03429700
H	-2.77586600	-1.60264700	0.00000000
H	-1.23635300	-0.71380800	-1.03429700
N	0.00000000	-2.87271800	0.00000000
Be	1.23940400	-1.74184000	0.00000000
Be	2.12818000	-0.20243500	0.00000000
H	2.77586600	-1.60264700	0.00000000
H	1.23635300	-0.71380800	-1.03429700
H	1.23635300	-0.71380800	1.03429700
C	3.22263500	1.86058900	-1.21114200
H	3.33722100	2.94837100	-1.24113500
H	4.22197500	1.41593200	-1.24113500
H	2.67903900	1.54674400	-2.10104400
C	3.22263500	1.86058900	1.21114200
H	4.22197500	1.41593200	1.24113500
H	3.33722100	2.94837100	1.24113500
H	2.67903900	1.54674400	2.10104400
C	0.00000000	-3.72117800	-1.21114200
H	0.88475400	-4.36430400	-1.24113500
H	-0.88475400	-4.36430400	-1.24113500
H	0.00000000	-3.09348700	-2.10104400
C	0.00000000	-3.72117800	1.21114200
H	-0.88475400	-4.36430400	1.24113500
H	0.88475400	-4.36430400	1.24113500

H	0.00000000	-3.09348700	2.10104400
C	-3.22263500	1.86058900	1.21114200
H	-3.33722100	2.94837100	1.24113500
H	-4.22197500	1.41593200	1.24113500
H	-2.67903900	1.54674400	2.10104400
C	-3.22263500	1.86058900	-1.21114200
H	-4.22197500	1.41593200	-1.24113500
H	-3.33722100	2.94837100	-1.24113500
H	-2.67903900	1.54674400	-2.10104400

4-N(CH_3)$_2$

Be	-0.88475400	2.69598800	0.00000000
Be	0.88475400	2.69598800	0.00000000
H	0.00000000	3.92161200	0.00000000
H	0.00000000	2.12713200	1.03456800
H	0.00000000	2.12713200	-1.03456800
N	-2.53614500	2.53614500	0.00000000
N	2.53614500	2.53614500	0.00000000
Be	2.69598800	0.88475400	0.00000000
Be	2.69598800	-0.88475400	0.00000000
H	2.12713200	0.00000000	-1.03456800
H	3.92161200	0.00000000	0.00000000
H	2.12713200	0.00000000	1.03456800
Be	-2.69598800	0.88475400	0.00000000
Be	-2.69598800	-0.88475400	0.00000000
H	-2.12713200	0.00000000	1.03456800
H	-3.92161200	0.00000000	0.00000000
H	-2.12713200	0.00000000	-1.03456800
N	-2.53614500	-2.53614500	0.00000000
N	2.53614500	-2.53614500	0.00000000
Be	-0.88475400	-2.69598800	0.00000000
Be	0.88475400	-2.69598800	0.00000000
H	0.00000000	-3.92161200	0.00000000
H	0.00000000	-2.12713200	-1.03456800
H	0.00000000	-2.12713200	1.03456800
C	3.13819000	3.13819000	-1.21151100
H	2.96483200	4.21769600	-1.23836400
H	4.21769600	2.96483200	-1.23836400
H	2.69580200	2.69580200	-2.10251600
C	3.13819000	3.13819000	1.21151100
H	4.21769600	2.96483200	1.23836400
H	2.96483200	4.21769600	1.23836400
H	2.69580200	2.69580200	2.10251600
C	3.13819000	-3.13819000	1.21151100

H	2.96483200	-4.21769600	1.23836400
H	4.21769600	-2.96483200	1.23836400
H	2.69580200	-2.69580200	2.10251600
C	3.13819000	-3.13819000	-1.21151100
H	4.21769600	-2.96483200	-1.23836400
H	2.96483200	-4.21769600	-1.23836400
H	2.69580200	-2.69580200	-2.10251600
C	-3.13819000	-3.13819000	1.21151100
H	-4.21769600	-2.96483200	1.23836400
H	-2.96483200	-4.21769600	1.23836400
H	-2.69580200	-2.69580200	2.10251600
C	-3.13819000	-3.13819000	-1.21151100
H	-2.96483200	-4.21769600	-1.23836400
H	-4.21769600	-2.96483200	-1.23836400
H	-2.69580200	-2.69580200	-2.10251600
C	-3.13819000	3.13819000	1.21151100
H	-2.96483200	4.21769600	1.23836400
H	-4.21769600	2.96483200	1.23836400
H	-2.69580200	2.69580200	2.10251600
C	-3.13819000	3.13819000	-1.21151100
H	-4.21769600	2.96483200	-1.23836400
H	-2.96483200	4.21769600	-1.23836400
H	-2.69580200	2.69580200	-2.10251600

5-N(CH_3)$_2$

Be	-0.88358900	3.47362200	0.00000000
Be	0.88358900	3.47362200	0.00000000
H	0.00000000	4.68512300	0.00000000
H	0.00000000	2.88976800	1.03666000
H	0.00000000	2.88976800	-1.03666000
N	-2.53878100	3.49433200	0.00000000
N	2.53878100	3.49433200	0.00000000
Be	3.03056700	1.91375100	0.00000000
Be	3.57665500	0.23306500	0.00000000
H	2.74833300	0.89298800	-1.03666000
H	4.45581700	1.44778300	0.00000000
H	2.74833300	0.89298800	1.03666000
N	4.10783400	-1.33471600	0.00000000
Be	-3.03056700	1.91375100	0.00000000
Be	-3.57665500	0.23306500	0.00000000
H	-2.74833300	0.89298800	1.03666000
H	-4.45581700	1.44778300	0.00000000
H	-2.74833300	0.89298800	-1.03666000
N	-4.10783400	-1.33471600	0.00000000

Be	2.75658200	-2.29085800	0.00000000
Be	1.32690500	-3.32958000	0.00000000
H	1.69856300	-2.33787200	-1.03666000
H	2.75384600	-3.79034400	0.00000000
H	1.69856300	-2.33787200	1.03666000
N	0.00000000	-4.31923200	0.00000000
Be	-2.75658200	-2.29085800	0.00000000
Be	-1.32690500	-3.32958000	0.00000000
H	-2.75384600	-3.79034400	0.00000000
H	-1.69856300	-2.33787200	-1.03666000
H	-1.69856300	-2.33787200	1.03666000
C	3.04226800	4.18732300	-1.21108200
H	2.70057500	5.22540200	-1.23518000
H	4.13512900	4.18313700	-1.23518000
H	2.67594900	3.68312800	-2.10371300
C	3.04226800	4.18732300	1.21108200
H	2.67594900	3.68312800	2.10371300
H	4.13512900	4.18313700	1.23518000
H	2.70057500	5.22540200	1.23518000
C	-3.04226800	4.18732300	-1.21108200
H	-4.13512900	4.18313700	-1.23518000
H	-2.70057500	5.22540200	-1.23518000
H	-2.67594900	3.68312800	-2.10371300
C	-3.04226800	4.18732300	1.21108200
H	-2.67594900	3.68312800	2.10371300
H	-2.70057500	5.22540200	1.23518000
H	-4.13512900	4.18313700	1.23518000
C	-4.92249300	-1.59941500	1.21108200
H	-5.80417600	-0.95366100	1.23518000
H	-5.25622500	-2.64008100	1.23518000
H	-4.32977700	-1.40683000	2.10371300
C	-4.92249300	-1.59941500	-1.21108200
H	-5.80417600	-0.95366100	-1.23518000
H	-4.32977700	-1.40683000	-2.10371300
H	-5.25622500	-2.64008100	-1.23518000
C	0.00000000	-5.17581600	1.21108200
H	-0.88660300	-5.81479700	1.23518000
H	0.88660300	-5.81479700	1.23518000
H	0.00000000	-4.55259700	2.10371300
C	0.00000000	-5.17581600	-1.21108200
H	-0.88660300	-5.81479700	-1.23518000
H	0.00000000	-4.55259700	-2.10371300
H	0.88660300	-5.81479700	-1.23518000
C	4.92249300	-1.59941500	-1.21108200

H	5.80417600	-0.95366100	-1.23518000
H	5.25622500	-2.64008100	-1.23518000
H	4.32977700	-1.40683000	-2.10371300
C	4.92249300	-1.59941500	1.21108200
H	4.32977700	-1.40683000	2.10371300
H	5.25622500	-2.64008100	1.23518000
H	5.80417600	-0.95366100	1.23518000

6-N(CH_3)$_2$

Be	0.88538600	4.25688200	0.00000000
Be	-0.88538600	4.25688200	0.00000000
H	0.00000000	3.66778200	1.03843600
H	0.00000000	5.46067100	0.00000000
H	0.00000000	3.66778200	-1.03843600
N	-2.53406000	4.38912100	0.00000000
Be	3.24387500	-2.89520700	0.00000000
Be	4.12926100	-1.36167500	0.00000000
H	4.72908000	-2.73033500	0.00000000
H	3.17639200	-1.83389100	-1.03843600
H	3.17639200	-1.83389100	1.03843600
N	2.53406000	-4.38912100	0.00000000
N	5.06812000	0.00000000	0.00000000
Be	4.12926100	1.36167500	0.00000000
Be	3.24387500	2.89520700	0.00000000
H	3.17639200	1.83389100	1.03843600
H	4.72908000	2.73033500	0.00000000
H	3.17639200	1.83389100	-1.03843600
N	2.53406000	4.38912100	0.00000000
Be	0.88538600	-4.25688200	0.00000000
Be	-0.88538600	-4.25688200	0.00000000
H	0.00000000	-3.66778200	-1.03843600
H	0.00000000	-5.46067100	0.00000000
H	0.00000000	-3.66778200	1.03843600
N	-2.53406000	-4.38912100	0.00000000
Be	-3.24387500	2.89520700	0.00000000
Be	-4.12926100	1.36167500	0.00000000
H	-3.17639200	1.83389100	1.03843600
H	-4.72908000	2.73033500	0.00000000
H	-3.17639200	1.83389100	-1.03843600
N	-5.06812000	0.00000000	0.00000000
Be	-3.24387500	-2.89520700	0.00000000
Be	-4.12926100	-1.36167500	0.00000000
H	-4.72908000	-2.73033500	0.00000000
H	-3.17639200	-1.83389100	1.03843600

H	-3.17639200	-1.83389100	-1.03843600
C	2.96374100	-5.13335000	-1.21058700
H	4.05105600	-5.24224800	-1.23212500
H	2.51439200	-6.12944200	-1.23212500
H	2.65323300	-4.59553500	-2.10475100
C	2.96374100	-5.13335000	1.21058700
H	4.05105600	-5.24224800	1.23212500
H	2.65323300	-4.59553500	2.10475100
H	2.51439200	-6.12944200	1.23212500
C	-2.96374100	-5.13335000	1.21058700
H	-2.51439200	-6.12944200	1.23212500
H	-2.65323300	-4.59553500	2.10475100
H	-4.05105600	-5.24224800	1.23212500
C	-2.96374100	-5.13335000	-1.21058700
H	-4.05105600	-5.24224800	-1.23212500
H	-2.65323300	-4.59553500	-2.10475100
H	-2.51439200	-6.12944200	-1.23212500
C	-5.92748200	0.00000000	-1.21058700
H	-5.30646600	0.00000000	-2.10475100
H	-6.56544800	-0.88719400	-1.23212500
H	-6.56544800	0.88719400	-1.23212500
C	-5.92748200	0.00000000	1.21058700
H	-6.56544800	-0.88719400	1.23212500
H	-5.30646600	0.00000000	2.10475100
H	-6.56544800	0.88719400	1.23212500
C	-2.96374100	5.13335000	-1.21058700
H	-2.65323300	4.59553500	-2.10475100
H	-4.05105600	5.24224800	-1.23212500
H	-2.51439200	6.12944200	-1.23212500
C	-2.96374100	5.13335000	1.21058700
H	-4.05105600	5.24224800	1.23212500
H	-2.65323300	4.59553500	2.10475100
H	-2.51439200	6.12944200	1.23212500
C	2.96374100	5.13335000	-1.21058700
H	2.51439200	6.12944200	-1.23212500
H	4.05105600	5.24224800	-1.23212500
H	2.65323300	4.59553500	-2.10475100
C	2.96374100	5.13335000	1.21058700
H	2.65323300	4.59553500	2.10475100
H	4.05105600	5.24224800	1.23212500
H	2.51439200	6.12944200	1.23212500
C	5.92748200	0.00000000	1.21058700
H	6.56544800	0.88719400	1.23212500
H	5.30646600	0.00000000	2.10475100

H	6.56544800	-0.88719400	1.23212500
C	5.92748200	0.00000000	-1.21058700
H	5.30646600	0.00000000	-2.10475100
H	6.56544800	0.88719400	-1.23212500
H	6.56544800	-0.88719400	-1.23212500

***n*- P(CH$_3$)$_2$** (*n* = 3–6)

3-P(CH$_3$)$_2$

Be	-0.88806400	2.36257900	0.00000000
Be	0.88806400	2.36257900	0.00000000
H	0.00000000	3.58231400	0.00000000
H	0.00000000	1.78340200	1.01900400
H	0.00000000	1.78340200	-1.01900400
Be	-2.49008500	-0.41220300	0.00000000
Be	-1.60202100	-1.95037500	0.00000000
H	-1.54447100	-0.89170100	1.01900400
H	-3.10237500	-1.79115700	0.00000000
H	-1.54447100	-0.89170100	-1.01900400
Be	1.60202100	-1.95037500	0.00000000
Be	2.49008500	-0.41220300	0.00000000
H	3.10237500	-1.79115700	0.00000000
H	1.54447100	-0.89170100	-1.01900400
H	1.54447100	-0.89170100	1.01900400
P	0.00000000	-3.32667700	0.00000000
P	2.88098700	1.66333900	0.00000000
P	-2.88098700	1.66333900	0.00000000
C	3.86399800	2.23088000	1.45269200
H	3.96882400	3.31581200	1.45098600
H	3.35097000	1.93468300	2.36669700
H	4.85599000	1.77919600	1.45098600
C	3.86399800	2.23088000	-1.45269200
H	3.35097000	1.93468300	-2.36669700
H	3.96882400	3.31581200	-1.45098600
H	4.85599000	1.77919600	-1.45098600
C	-3.86399800	2.23088000	1.45269200
H	-4.85599000	1.77919600	1.45098600
H	-3.35097000	1.93468300	2.36669700
H	-3.96882400	3.31581200	1.45098600
C	-3.86399800	2.23088000	-1.45269200
H	-3.35097000	1.93468300	-2.36669700
H	-4.85599000	1.77919600	-1.45098600
H	-3.96882400	3.31581200	-1.45098600
C	0.00000000	-4.46176000	1.45269200
H	0.88716600	-5.09500900	1.45098600

H	0.00000000	-3.86936600	2.36669700
H	-0.88716600	-5.09500900	1.45098600
C	0.00000000	-4.46176000	-1.45269200
H	0.00000000	-3.86936600	-2.36669700
H	0.88716600	-5.09500900	-1.45098600
H	-0.88716600	-5.09500900	-1.45098600

4-P(CH_3)$_2$

Be	-0.88568200	3.29582000	0.00000000
Be	0.88568200	3.29582000	0.00000000
H	0.00000000	4.50179500	0.00000000
H	0.00000000	2.70775000	1.02471700
H	0.00000000	2.70775000	-1.02471700
Be	3.29582000	0.88568200	0.00000000
Be	3.29582000	-0.88568200	0.00000000
H	2.70775000	0.00000000	-1.02471700
H	4.50179500	0.00000000	0.00000000
H	2.70775000	0.00000000	1.02471700
Be	-3.29582000	0.88568200	0.00000000
Be	-3.29582000	-0.88568200	0.00000000
H	-2.70775000	0.00000000	1.02471700
H	-4.50179500	0.00000000	0.00000000
H	-2.70775000	0.00000000	-1.02471700
Be	-0.88568200	-3.29582000	0.00000000
Be	0.88568200	-3.29582000	0.00000000
H	0.00000000	-4.50179500	0.00000000
H	0.00000000	-2.70775000	-1.02471700
H	0.00000000	-2.70775000	1.02471700
P	2.96590100	2.96590100	0.00000000
P	2.96590100	-2.96590100	0.00000000
P	-2.96590100	-2.96590100	0.00000000
P	-2.96590100	2.96590100	0.00000000
C	3.77170900	3.77170900	-1.45156700
H	3.35457800	3.35457800	-2.36714800
H	3.59113700	4.84637000	-1.44751400
H	4.84637000	3.59113700	-1.44751400
C	3.77170900	3.77170900	1.45156700
H	3.59113700	4.84637000	1.44751400
H	3.35457800	3.35457800	2.36714800
H	4.84637000	3.59113700	1.44751400
C	-3.77170900	3.77170900	-1.45156700
H	-3.35457800	3.35457800	-2.36714800
H	-4.84637000	3.59113700	-1.44751400
H	-3.59113700	4.84637000	-1.44751400

C	-3.77170900	3.77170900	1.45156700
H	-4.84637000	3.59113700	1.44751400
H	-3.35457800	3.35457800	2.36714800
H	-3.59113700	4.84637000	1.44751400
C	-3.77170900	-3.77170900	1.45156700
H	-3.35457800	-3.35457800	2.36714800
H	-4.84637000	-3.59113700	1.44751400
H	-3.59113700	-4.84637000	1.44751400
C	-3.77170900	-3.77170900	-1.45156700
H	-4.84637000	-3.59113700	-1.44751400
H	-3.35457800	-3.35457800	-2.36714800
H	-3.59113700	-4.84637000	-1.44751400
C	3.77170900	-3.77170900	-1.45156700
H	3.59113700	-4.84637000	-1.44751400
H	3.35457800	-3.35457800	-2.36714800
H	4.84637000	-3.59113700	-1.44751400
C	3.77170900	-3.77170900	1.45156700
H	3.35457800	-3.35457800	2.36714800
H	3.59113700	-4.84637000	1.44751400
H	4.84637000	-3.59113700	1.44751400

5-P(CH_3)$_2$

Be	-0.88635200	4.23026700	0.00000000
Be	0.88635200	4.23026700	0.00000000
H	0.00000000	5.43076400	0.00000000
H	0.00000000	3.64073000	1.02818900
H	0.00000000	3.64073000	-1.02818900
Be	3.74932500	2.15019600	0.00000000
Be	4.29712100	0.46425300	0.00000000
H	3.46254000	1.12504700	-1.02818900
H	5.16496400	1.67819900	0.00000000
H	3.46254000	1.12504700	1.02818900
Be	-3.74932500	2.15019600	0.00000000
Be	-4.29712100	0.46425300	0.00000000
H	-3.46254000	1.12504700	1.02818900
H	-5.16496400	1.67819900	0.00000000
H	-3.46254000	1.12504700	-1.02818900
Be	3.20356200	-2.90137300	0.00000000
Be	1.76941400	-3.94334200	0.00000000
H	2.13996800	-2.94541300	-1.02818900
H	3.19212300	-4.39358100	0.00000000
H	2.13996800	-2.94541300	1.02818900
Be	-3.20356200	-2.90137300	0.00000000
Be	-1.76941400	-3.94334200	0.00000000

H	-3.19212300	-4.39358100	0.00000000
H	-2.13996800	-2.94541300	-1.02818900
H	-2.13996800	-2.94541300	1.02818900
P	-4.83485400	-1.57093900	0.00000000
P	-2.98810400	4.11277200	0.00000000
P	2.98810400	4.11277200	0.00000000
P	4.83485400	-1.57093900	0.00000000
P	0.00000000	-5.08366600	0.00000000
C	3.66017300	5.03779700	1.45022300
H	3.31512700	4.56288000	2.36769700
H	4.74998500	5.02667700	1.44393000
H	3.31282800	6.07083200	1.44393000
C	3.66017300	5.03779700	-1.45022300
H	4.74998500	5.02667700	-1.44393000
H	3.31512700	4.56288000	-2.36769700
H	3.31282800	6.07083200	-1.44393000
C	5.92228500	-1.92426700	1.45022300
H	5.36398800	-1.74286500	2.36769700
H	6.24848000	-2.96417500	1.44393000
H	6.79742500	-1.27469700	1.44393000
C	5.92228500	-1.92426700	-1.45022300
H	6.24848000	-2.96417500	-1.44393000
H	5.36398800	-1.74286500	-2.36769700
H	6.79742500	-1.27469700	-1.44393000
C	0.00000000	-6.22705900	1.45022300
H	0.00000000	-5.64003000	2.36769700
H	-0.88821100	-6.85863800	1.44393000
H	0.88821100	-6.85863800	1.44393000
C	0.00000000	-6.22705900	-1.45022300
H	0.00000000	-5.64003000	-2.36769700
H	0.88821100	-6.85863800	-1.44393000
H	-0.88821100	-6.85863800	-1.44393000
C	-5.92228500	-1.92426700	1.45022300
H	-5.36398800	-1.74286500	2.36769700
H	-6.79742500	-1.27469700	1.44393000
H	-6.24848000	-2.96417500	1.44393000
C	-5.92228500	-1.92426700	-1.45022300
H	-6.79742500	-1.27469700	-1.44393000
H	-5.36398800	-1.74286500	-2.36769700
H	-6.24848000	-2.96417500	-1.44393000
C	-3.66017300	5.03779700	1.45022300
H	-4.74998500	5.02667700	1.44393000
H	-3.31512700	4.56288000	2.36769700
H	-3.31282800	6.07083200	1.44393000

C	-3.66017300	5.03779700	-1.45022300
H	-3.31512700	4.56288000	-2.36769700
H	-4.74998500	5.02667700	-1.44393000
H	-3.31282800	6.07083200	-1.44393000

6-P(CH_3)$_2$

Be	3.34645200	4.02287300	-0.00012500
Be	1.81068500	4.90954900	-0.00012500
H	2.28378700	3.95563500	1.03014700
H	3.17718500	5.50304600	-0.00008500
H	2.28381000	3.95567500	-1.03041400
Be	1.81068500	-4.90954900	-0.00012500
Be	3.34645200	-4.02287300	-0.00012500
H	3.17718500	-5.50304600	-0.00008500
H	2.28381000	-3.95567500	-1.03041400
H	2.28378700	-3.95563500	1.03014700
Be	5.15713600	-0.88667500	-0.00012500
Be	5.15713600	0.88667500	-0.00012500
H	4.56757400	0.00000000	1.03014700
H	6.35437000	0.00000000	-0.00008500
H	4.56762100	0.00000000	-1.03041400
Be	-1.81068500	-4.90954900	-0.00012500
Be	-3.34645200	-4.02287300	-0.00012500
H	-2.28381000	-3.95567500	-1.03041400
H	-3.17718500	-5.50304600	-0.00008500
H	-2.28378700	-3.95563500	1.03014700
Be	-1.81068500	4.90954900	-0.00012500
Be	-3.34645200	4.02287300	-0.00012500
H	-2.28378700	3.95563500	1.03014700
H	-3.17718500	5.50304600	-0.00008500
H	-2.28381000	3.95567500	-1.03041400
Be	-5.15713600	-0.88667500	-0.00012500
Be	-5.15713600	0.88667500	-0.00012500
H	-6.35437000	0.00000000	-0.00008500
H	-4.56757400	0.00000000	1.03014700
H	-4.56762100	0.00000000	-1.03041400
P	0.00000000	5.98251600	-0.00002400
P	0.00000000	-5.98251600	-0.00002400
P	5.18101100	-2.99125800	-0.00002400
P	5.18101100	2.99125800	-0.00002400
P	-5.18101100	-2.99125800	-0.00002400
P	-5.18101100	2.99125800	-0.00002400
C	6.17366600	3.56436800	1.44920700
H	5.66710400	3.27190400	2.36803500

H	7.16428900	3.11050200	1.44123300
H	6.27591800	4.64920500	1.44123300
C	6.17391300	3.56451000	-1.44903200
H	7.16453500	3.11064600	-1.44093200
H	5.66750800	3.27213700	-2.36797200
H	6.27616600	4.64934700	-1.44093200
C	6.17366600	-3.56436800	1.44920700
H	5.66710400	-3.27190400	2.36803500
H	6.27591800	-4.64920500	1.44123300
H	7.16428900	-3.11050200	1.44123300
C	6.17391300	-3.56451000	-1.44903200
H	6.27616600	-4.64934700	-1.44093200
H	5.66750800	-3.27213700	-2.36797200
H	7.16453500	-3.11064600	-1.44093200
C	0.00000000	-7.12873500	1.44920700
H	0.00000000	-6.54380800	2.36803500
H	-0.88837100	-7.75970700	1.44123300
H	0.88837100	-7.75970700	1.44123300
C	0.00000000	-7.12902100	-1.44903200
H	0.00000000	-6.54427500	-2.36797200
H	0.88837000	-7.75999200	-1.44093200
H	-0.88837000	-7.75999200	-1.44093200
C	-6.17366600	-3.56436800	1.44920700
H	-6.27591800	-4.64920500	1.44123300
H	-5.66710400	-3.27190400	2.36803500
H	-7.16428900	-3.11050200	1.44123300
C	-6.17391300	-3.56451000	-1.44903200
H	-5.66750800	-3.27213700	-2.36797200
H	-6.27616600	-4.64934700	-1.44093200
H	-7.16453500	-3.11064600	-1.44093200
C	-6.17366600	3.56436800	1.44920700
H	-7.16428900	3.11050200	1.44123300
H	-5.66710400	3.27190400	2.36803500
H	-6.27591800	4.64920500	1.44123300
C	-6.17391300	3.56451000	-1.44903200
H	-5.66750800	3.27213700	-2.36797200
H	-7.16453500	3.11064600	-1.44093200
H	-6.27616600	4.64934700	-1.44093200
C	0.00000000	7.12873500	1.44920700
H	0.00000000	6.54380800	2.36803500
H	0.88837100	7.75970700	1.44123300
H	-0.88837100	7.75970700	1.44123300
C	0.00000000	7.12902100	-1.44903200
H	0.88837000	7.75999200	-1.44093200

H	0.00000000	6.54427500	-2.36797200
H	-0.88837000	7.75999200	-1.44093200

***n*-O(CH$_3$)** (*n* = 3–6)

3-OCH$_3$

Be	-2.12418200	0.20217800	-0.25453200
Be	-1.23718200	1.73850700	-0.25453200
H	-2.77424500	1.60171100	-0.35492000
H	-1.31346400	0.75832900	0.83364100
H	-1.17143900	0.67633100	-1.23371200
Be	-0.88700000	-1.94068400	-0.25453200
Be	0.88700000	-1.94068400	-0.25453200
H	0.00000000	-1.51665800	0.83364100
H	0.00000000	-3.20342200	-0.35492000
H	0.00000000	-1.35266200	-1.23371200
Be	2.12418200	0.20217800	-0.25453200
Be	1.23718200	1.73850700	-0.25453200
H	2.77424500	1.60171100	-0.35492000
H	1.17143900	0.67633100	-1.23371200
H	1.31346400	0.75832900	0.83364100
O	0.00000000	2.73268300	-0.25429700
O	2.36657300	-1.36634100	-0.25429700
O	-2.36657300	-1.36634100	-0.25429700
C	0.00000000	3.96297400	0.47489300
H	0.00000000	3.77571700	1.55110700
H	0.88540800	4.54123300	0.21257600
H	-0.88540800	4.54123300	0.21257600
C	3.43203600	-1.98148700	0.47489300
H	4.37552700	-1.50383100	0.21257600
H	3.26986600	-1.88785800	1.55110700
H	3.49011900	-3.03740200	0.21257600
C	-3.43203600	-1.98148700	0.47489300
H	-3.49011900	-3.03740200	0.21257600
H	-3.26986600	-1.88785800	1.55110700
H	-4.37552700	-1.50383100	0.21257600

4-OCH$_3$

Be	0.01852800	2.65013900	0.88443000
Be	0.01852800	2.65013900	-0.88443000
H	1.09956900	2.16810700	0.00000000
H	-0.97776400	2.02960400	0.00000000
H	-0.06394500	3.88388100	0.00000000
Be	-0.00091700	0.88297900	-2.75158700
Be	0.00091700	-0.88297900	-2.75158700

H	0.00000000	0.00000000	-1.59927700
H	-1.04322900	-0.00668500	-3.38030100
H	1.04322900	0.00668500	-3.38030100
Be	-0.00091700	0.88297900	2.75158700
Be	0.00091700	-0.88297900	2.75158700
H	1.04322900	0.00668500	3.38030100
H	-1.04322900	-0.00668500	3.38030100
H	0.00000000	0.00000000	1.59927700
Be	-0.01852800	-2.65013900	0.88443000
Be	-0.01852800	-2.65013900	-0.88443000
H	-1.09956900	-2.16810700	0.00000000
H	0.97776400	-2.02960400	0.00000000
H	0.06394500	-3.88388100	0.00000000
O	0.00091700	2.41246900	-2.43231000
O	0.00091700	2.41246900	2.43231000
O	-0.00091700	-2.41246900	2.43231000
O	-0.00091700	-2.41246900	-2.43231000
C	0.23919200	3.42751600	-3.40980500
H	-0.07558900	4.39275400	-3.01610000
H	1.30029500	3.47047800	-3.66043100
H	-0.33399700	3.20897400	-4.31060900
C	-0.23919200	-3.42751600	3.40980500
H	0.33399700	-3.20897400	4.31060900
H	-1.30029500	-3.47047800	3.66043100
H	0.07558900	-4.39275400	3.01610000
C	0.23919200	3.42751600	3.40980500
H	-0.33399700	3.20897400	4.31060900
H	1.30029500	3.47047800	3.66043100
H	-0.07558900	4.39275400	3.01610000
C	-0.23919200	-3.42751600	-3.40980500
H	-1.30029500	-3.47047800	-3.66043100
H	0.33399700	-3.20897400	-4.31060900
H	0.07558900	-4.39275400	-3.01610000

5-OCH_3

Be	-0.88280700	-3.48443800	-0.09078700
Be	0.88280700	-3.48443800	-0.09078700
H	0.00000000	-4.41905900	-0.87036300
H	0.00000000	-2.38286700	-0.48342300
H	0.00000000	-3.73078300	1.09146800
Be	3.04109500	-1.91635100	-0.09078700
Be	3.58670000	-0.23715100	-0.09078700
H	3.54818600	-1.15287500	1.09146800
H	4.20277500	-1.36556400	-0.87036300

H	2.26624100	-0.73634600	-0.48342300
Be	-3.04109500	-1.91635100	-0.09078700
Be	-3.58670000	-0.23715100	-0.09078700
H	-2.26624100	-0.73634600	-0.48342300
H	-4.20277500	-1.36556400	-0.87036300
H	-3.54818600	-1.15287500	1.09146800
Be	2.76230800	2.30006900	-0.09078700
Be	1.33389500	3.33787100	-0.09078700
H	2.19289900	3.01826700	1.09146800
H	2.59745800	3.57509400	-0.87036300
H	1.40061400	1.92778000	-0.48342300
Be	-2.76230800	2.30006900	-0.09078700
Be	-1.33389500	3.33787100	-0.09078700
H	-2.59745800	3.57509400	-0.87036300
H	-2.19289900	3.01826700	1.09146800
H	-1.40061400	1.92778000	-0.48342300
O	3.94099100	1.28050600	-0.09891300
O	2.43566600	-3.35240700	-0.09891300
O	-2.43566600	-3.35240700	-0.09891300
O	-3.94099100	1.28050600	-0.09891300
O	0.00000000	4.14380300	-0.09891300
C	0.00000000	5.55058400	0.17574900
H	0.00000000	5.72443000	1.25269100
H	0.88696900	6.00526300	-0.26363400
H	-0.88696900	6.00526300	-0.26363400
C	5.27891900	1.71522500	0.17574900
H	5.43725600	2.69928600	-0.26363400
H	5.44425600	1.76894600	1.25269100
H	5.98543300	1.01217100	-0.26363400
C	3.26255100	-4.49051700	0.17574900
H	4.24737800	-4.33701300	-0.26363400
H	3.36473500	-4.63116100	1.25269100
H	2.81223200	-5.37970700	-0.26363400
C	-3.26255100	-4.49051700	0.17574900
H	-2.81223200	-5.37970700	-0.26363400
H	-3.36473500	-4.63116100	1.25269100
H	-4.24737800	-4.33701300	-0.26363400
C	-5.27891900	1.71522500	0.17574900
H	-5.98543300	1.01217100	-0.26363400
H	-5.44425600	1.76894600	1.25269100
H	-5.43725600	2.69928600	-0.26363400

6-OCH_3

Be	-2.88861300	3.24039600	-0.05273000

Be	-1.36195900	4.12181100	0.05273000
H	-2.38598300	4.24464400	-1.03699600
H	-2.48297800	4.18864400	1.03699600
H	-1.53545000	2.65947800	0.00000000
Be	-1.36195900	-4.12181100	-0.05273000
Be	-2.88861300	-3.24039600	0.05273000
H	-2.38598300	-4.24464400	1.03699600
H	-1.53545000	-2.65947800	0.00000000
H	-2.48297800	-4.18864400	-1.03699600
Be	-4.25057200	-0.88141400	0.05273000
Be	-4.25057200	0.88141400	-0.05273000
H	-4.86896100	-0.05600000	-1.03699600
H	-4.86896100	0.05600000	1.03699600
H	-3.07090100	0.00000000	0.00000000
Be	1.36195900	-4.12181100	-0.05273000
Be	2.88861300	-3.24039600	0.05273000
H	1.53545000	-2.65947800	0.00000000
H	2.38598300	-4.24464400	1.03699600
H	2.48297800	-4.18864400	-1.03699600
Be	1.36195900	4.12181100	0.05273000
Be	2.88861300	3.24039600	-0.05273000
H	1.53545000	2.65947800	0.00000000
H	2.38598300	4.24464400	-1.03699600
H	2.48297800	4.18864400	1.03699600
Be	4.25057200	-0.88141400	0.05273000
Be	4.25057200	0.88141400	-0.05273000
H	4.86896100	-0.05600000	-1.03699600
H	3.07090100	0.00000000	0.00000000
H	4.86896100	0.05600000	1.03699600
O	-4.21404900	2.43298200	-0.14956400
O	-4.21404900	-2.43298200	0.14956400
O	0.00000000	-4.86596500	-0.14956400
O	4.21404900	-2.43298200	0.14956400
O	4.21404900	2.43298200	-0.14956400
O	0.00000000	4.86596500	0.14956400
C	-5.45519800	3.14956000	-0.23491300
H	-5.83042400	3.36619700	0.76578600
H	-5.29815000	4.08328900	-0.77332900
H	-6.18530700	2.54668800	-0.77332900
C	0.00000000	6.29912000	0.23491300
H	0.00000000	6.73239400	-0.76578600
H	-0.88715700	6.62997700	0.77332900
H	0.88715700	6.62997700	0.77332900
C	5.45519800	3.14956000	-0.23491300

H	5.29815000	4.08328900	-0.77332900
H	5.83042400	3.36619700	0.76578600
H	6.18530700	2.54668800	-0.77332900
C	5.45519800	-3.14956000	0.23491300
H	5.83042400	-3.36619700	-0.76578600
H	6.18530700	-2.54668800	0.77332900
H	5.29815000	-4.08328900	0.77332900
C	0.00000000	-6.29912000	-0.23491300
H	0.88715700	-6.62997700	-0.77332900
H	0.00000000	-6.73239400	0.76578600
H	-0.88715700	-6.62997700	-0.77332900
C	-5.45519800	-3.14956000	0.23491300
H	-6.18530700	-2.54668800	0.77332900
H	-5.83042400	-3.36619700	-0.76578600
H	-5.29815000	-4.08328900	0.77332900

***n*-S(CH$_3$)** (*n* = 3–6)

3-SCH$_3$

Be	-0.88314600	2.16442900	-0.42018000
Be	0.88314600	2.16442900	-0.42018000
H	0.00000000	3.38904200	-0.43668000
H	0.00000000	1.61406100	0.61671700
H	0.00000000	1.58800300	-1.43239800
Be	-2.31602400	-0.31738800	-0.42018000
Be	-1.43287800	-1.84704200	-0.42018000
H	-1.39781800	-0.80703000	0.61671700
H	-2.93499600	-1.69452100	-0.43668000
H	-1.37525100	-0.79400100	-1.43239800
Be	1.43287800	-1.84704200	-0.42018000
Be	2.31602400	-0.31738800	-0.42018000
H	2.93499600	-1.69452100	-0.43668000
H	1.37525100	-0.79400100	-1.43239800
H	1.39781800	-0.80703000	0.61671700
C	3.45016100	1.99195100	1.23952500
H	2.75352600	1.58974900	1.96924600
H	4.42662000	1.53183400	1.36443900
H	3.53991800	3.06764800	1.36443900
C	0.00000000	-3.98390300	1.23952500
H	0.88670300	-4.59948300	1.36443900
H	0.00000000	-3.17949800	1.96924600
H	-0.88670300	-4.59948300	1.36443900
C	-3.45016100	1.99195100	1.23952500
H	-4.42662000	1.53183400	1.36443900
H	-2.75352600	1.58974900	1.96924600

H	-3.53991800	3.06764800	1.36443900
S	2.86880700	1.65630700	-0.47009200
S	-2.86880700	1.65630700	-0.47009200
S	0.00000000	-3.31261300	-0.47009200

4-SCH_3

Be	2.77044700	-1.52513800	-0.04688700
Be	1.52513800	-2.77044700	0.04688700
H	2.99830000	-2.99830000	0.00000000
H	1.75706000	-1.70846300	1.02878200
H	1.70846300	-1.75706000	-1.02878200
Be	-1.52513800	-2.77044700	0.04688700
Be	-2.77044700	-1.52513800	-0.04688700
H	-1.70846300	-1.75706000	-1.02878200
H	-2.99830000	-2.99830000	0.00000000
H	-1.75706000	-1.70846300	1.02878200
Be	2.77044700	1.52513800	-0.04688700
Be	1.52513800	2.77044700	0.04688700
H	1.75706000	1.70846300	1.02878200
H	2.99830000	2.99830000	0.00000000
H	1.70846300	1.75706000	-1.02878200
Be	-1.52513800	2.77044700	0.04688700
Be	-2.77044700	1.52513800	-0.04688700
H	-2.99830000	2.99830000	0.00000000
H	-1.70846300	1.75706000	-1.02878200
H	-1.75706000	1.70846300	1.02878200
C	4.89264500	0.00000000	1.50446600
H	4.13862800	0.00000000	2.28573100
H	5.51387000	-0.88761300	1.58677600
H	5.51387000	0.88761300	1.58677600
C	0.00000000	4.89264500	-1.50446600
H	0.00000000	4.13862800	-2.28573100
H	-0.88761300	5.51387000	-1.58677600
H	0.88761300	5.51387000	-1.58677600
C	-4.89264500	0.00000000	1.50446600
H	-5.51387000	-0.88761300	1.58677600
H	-4.13862800	0.00000000	2.28573100
H	-5.51387000	0.88761300	1.58677600
C	0.00000000	-4.89264500	-1.50446600
H	0.00000000	-4.13862800	-2.28573100
H	0.88761300	-5.51387000	-1.58677600
H	-0.88761300	-5.51387000	-1.58677600
S	0.00000000	-4.11143500	0.15839500
S	4.11143500	0.00000000	-0.15839500

S	0.00000000	4.11143500	0.15839500
S	-4.11143500	0.00000000	-0.15839500

5-SCH_3

Be	0.88177300	3.94243500	-0.42376600
Be	-0.88177300	3.94243500	-0.42376600
H	0.00000000	5.12924700	-0.28250300
H	0.00000000	3.47947500	-1.51478700
H	0.00000000	3.23278800	0.53453200
Be	-3.47699600	2.05689500	-0.42376600
Be	-4.02196100	0.37966400	-0.42376600
H	-3.07456400	0.99898600	0.53453200
H	-4.87820400	1.58502400	-0.28250300
H	-3.30917700	1.07521700	-1.51478700
Be	3.47699600	2.05689500	-0.42376600
Be	4.02196100	0.37966400	-0.42376600
H	3.30917700	1.07521700	-1.51478700
H	4.87820400	1.58502400	-0.28250300
H	3.07456400	0.99898600	0.53453200
Be	-3.03067400	-2.67120400	-0.42376600
Be	-1.60393600	-3.70779000	-0.42376600
H	-1.90018500	-2.61538000	0.53453200
H	-3.01489600	-4.14964800	-0.28250300
H	-2.04518400	-2.81495400	-1.51478700
Be	3.03067400	-2.67120400	-0.42376600
Be	1.60393600	-3.70779000	-0.42376600
H	3.01489600	-4.14964800	-0.28250300
H	1.90018500	-2.61538000	0.53453200
H	2.04518400	-2.81495400	-1.51478700
C	0.00000000	-5.66188100	1.23189100
H	0.00000000	-4.87626000	1.98153800
H	-0.88778900	-6.27896000	1.33976400
H	0.88778900	-6.27896000	1.33976400
C	-5.38476900	-1.74961800	1.23189100
H	-5.69730400	-2.78464300	1.33976400
H	-4.63759900	-1.50684700	1.98153800
H	-6.24598800	-1.09596700	1.33976400
C	-3.32797000	4.58055800	1.23189100
H	-4.40891700	4.55795600	1.33976400
H	-2.86619400	3.94497800	1.98153800
H	-2.97244300	5.60161500	1.33976400
C	3.32797000	4.58055800	1.23189100
H	2.97244300	5.60161500	1.33976400
H	2.86619400	3.94497800	1.98153800

H	4.40891700	4.55795600	1.33976400
C	5.38476900	-1.74961800	1.23189100
H	6.24598800	-1.09596700	1.33976400
H	4.63759900	-1.50684700	1.98153800
H	5.69730400	-2.78464300	1.33976400
S	0.00000000	-4.95302000	-0.46247000
S	4.71060200	-1.53056700	-0.46247000
S	2.91131200	4.00707800	-0.46247000
S	-2.91131200	4.00707800	-0.46247000
S	-4.71060200	-1.53056700	-0.46247000

6-SCH_3

Be	1.64377800	4.58508700	0.15167000
Be	3.14891300	3.71609700	-0.15167000
H	1.96868000	3.71550100	-1.02265100
H	2.99231400	5.18284000	0.00000000
H	2.23337800	3.56267800	1.02265100
Be	-4.79269100	-0.86899000	0.15167000
Be	-4.79269100	0.86899000	-0.15167000
H	-5.98462800	0.00000000	0.00000000
H	-4.20205800	0.15282300	1.02265100
H	-4.20205800	-0.15282300	-1.02265100
Be	-3.14891300	3.71609700	-0.15167000
Be	-1.64377800	4.58508700	0.15167000
H	-1.96868000	3.71550100	-1.02265100
H	-2.99231400	5.18284000	0.00000000
H	-2.23337800	3.56267800	1.02265100
Be	-3.14891300	-3.71609700	0.15167000
Be	-1.64377800	-4.58508700	-0.15167000
H	-1.96868000	-3.71550100	1.02265100
H	-2.99231400	-5.18284000	0.00000000
H	-2.23337800	-3.56267800	-1.02265100
Be	4.79269100	0.86899000	-0.15167000
Be	4.79269100	-0.86899000	0.15167000
H	4.20205800	-0.15282300	-1.02265100
H	5.98462800	0.00000000	0.00000000
H	4.20205800	0.15282300	1.02265100
Be	1.64377800	-4.58508700	-0.15167000
Be	3.14891300	-3.71609700	0.15167000
H	2.99231400	-5.18284000	0.00000000
H	2.23337800	-3.56267800	-1.02265100
H	1.96868000	-3.71550100	1.02265100
S	0.00000000	5.72052500	0.50229500
S	4.95412000	2.86026200	-0.50229500

S	4.95412000	-2.86026200	0.50229500
S	0.00000000	-5.72052500	-0.50229500
S	-4.95412000	-2.86026200	0.50229500
S	-4.95412000	2.86026200	-0.50229500
C	-5.94452600	-3.43207400	-0.93519300
H	-6.03862300	-4.51252200	-0.87084000
H	-6.92727100	-2.97334000	-0.87084000
H	-5.46652800	-3.15610100	-1.87024200
C	0.00000000	6.86414700	-0.93519300
H	-0.88864700	7.48586200	-0.87084000
H	0.88864700	7.48586200	-0.87084000
H	0.00000000	6.31220300	-1.87024200
C	-5.94452600	3.43207400	0.93519300
H	-6.03862300	4.51252200	0.87084000
H	-6.92727100	2.97334000	0.87084000
H	-5.46652800	3.15610100	1.87024200
C	5.94452600	3.43207400	0.93519300
H	6.92727100	2.97334000	0.87084000
H	6.03862300	4.51252200	0.87084000
H	5.46652800	3.15610100	1.87024200
C	5.94452600	-3.43207400	-0.93519300
H	6.92727100	-2.97334000	-0.87084000
H	6.03862300	-4.51252200	-0.87084000
H	5.46652800	-3.15610100	-1.87024200
C	0.00000000	-6.86414700	0.93519300
H	-0.88864700	-7.48586200	0.87084000
H	0.88864700	-7.48586200	0.87084000
H	0.00000000	-6.31220300	1.87024200

MP2/def2-TZVPP-optimized structures

1

Be	-0.00528700	0.92576700	0.00418800
Be	0.00528700	-0.92576700	0.00418800
H	1.05005200	-0.06296300	-0.61569300
H	-1.05005200	0.06296300	-0.61569300
H	0.00000000	0.00000000	1.20663300
H	0.14195300	-3.00697200	-0.83098000
H	-0.83080500	-2.96697400	0.45169400
H	0.83080500	2.96697400	0.45169400
H	-0.14195300	3.00697200	-0.83098000
N	-0.00528700	-2.53983300	0.05355900
N	0.00528700	2.53983300	0.05355900

1’

Be	-0.04294600	-0.90806700	-0.00537400
Be	0.04294600	0.90806700	-0.00537400
H	1.03396900	-0.06047200	-0.60034300
H	0.00000000	0.00000000	1.18881000
H	-1.03396900	0.06047200	-0.60034300
H	1.39809000	3.19849600	0.43544600
H	0.32304800	3.24745700	-1.31140300
H	-0.32304800	-3.24745700	-1.31140300
H	-1.39809000	-3.19849600	0.43544600
P	-0.04294600	-3.04365200	0.06022600
P	0.04294600	3.04365200	0.06022600

2

Be	0.00000200	3.10236400	-0.23103100
Be	-0.00000100	1.47369400	0.58201300
H	-0.00004300	2.75630300	1.30982900
H	-1.04615300	1.97859100	-0.32559500
H	1.04619500	1.97862100	-0.32552800
H	0.79815100	0.00000100	2.00845700
H	-0.79815100	-0.00000100	2.00845700
H	-0.80954100	5.08888400	-0.93516800
H	0.80950200	5.08893300	-0.93508900
N	0.00000200	4.49117400	-1.00515600
N	0.00000000	0.00000000	1.38150100
Be	0.00000100	-1.47369400	0.58201300
Be	-0.00000200	-3.10236400	-0.23103100
H	1.04615300	-1.97859100	-0.32559500
H	0.00004300	-2.75630300	1.30982900
H	-1.04619500	-1.97862100	-0.32552800

N	-0.00000200	-4.49117400	-1.00515600
H	0.80954100	-5.08888400	-0.93516800
H	-0.80950200	-5.08893300	-0.93508900

2’

Be	0.00000000	3.59251600	-0.11350800
Be	0.00000000	1.93794500	0.59548000
H	1.03259800	2.48296200	-0.28745200
H	0.00000000	3.18882100	1.35920100
H	-1.03259800	2.48296200	-0.28745200
Be	0.00000000	-3.59251600	-0.11350800
Be	0.00000000	-1.93794500	0.59548000
H	0.00000000	-3.18882100	1.35920100
H	1.03259800	-2.48296200	-0.28745200
H	-1.03259800	-2.48296200	-0.28745200
P	0.00000000	-5.49413900	-1.05201300
P	0.00000000	5.49413900	-1.05201300
P	0.00000000	0.00000000	1.48681200
H	-1.02629100	6.04358500	-0.24907500
H	1.02629100	6.04358500	-0.24907500
H	-1.05148800	0.00000000	2.41506800
H	1.05148800	0.00000000	2.41506800
H	-1.02629100	-6.04358500	-0.24907500
H	1.02629100	-6.04358500	-0.24907500

***n*-NH$_2$** (n = 3–5)

3-NH$_2$

Be	-0.89161800	1.98039600	0.00000000
Be	0.89161800	1.98039600	0.00000000
H	0.00000000	3.23528800	0.00000000
H	0.00000000	1.44943400	1.03192500
H	0.00000000	1.44943400	-1.03192500
H	3.01275500	1.73941500	-0.80803400
H	3.01275500	1.73941500	0.80803400
H	-3.01275500	1.73941500	0.80803400
H	-3.01275500	1.73941500	-0.80803400
N	-2.48343700	1.43381300	0.00000000
N	2.48343700	1.43381300	0.00000000
Be	-2.16088200	-0.21803400	0.00000000
Be	-1.26926400	-1.76236200	0.00000000
H	-1.25524700	-0.72471700	1.03192500
H	-2.80184200	-1.61764400	0.00000000
H	-1.25524700	-0.72471700	-1.03192500
N	0.00000000	-2.86762600	0.00000000

H	0.00000000	-3.47882900	0.80803400
H	0.00000000	-3.47882900	-0.80803400
Be	1.26926400	-1.76236200	0.00000000
Be	2.16088200	-0.21803400	0.00000000
H	2.80184200	-1.61764400	0.00000000
H	1.25524700	-0.72471700	-1.03192500
H	1.25524700	-0.72471700	1.03192500

4-NH_2

Be	2.75586400	0.88850500	0.01102500
Be	2.75586400	-0.88850500	0.01102500
H	3.95804200	0.00000000	0.22804400
H	2.00198000	0.00000000	0.92012200
H	2.37403600	0.00000000	-1.11380900
H	2.98137500	-2.96663600	-0.80641500
H	2.96663600	-2.98137500	0.80641500
H	2.96663600	2.98137500	0.80641500
H	2.98137500	2.96663600	-0.80641500
N	2.54002400	2.54002400	0.00000000
N	2.54002400	-2.54002400	0.00000000
Be	0.88850500	-2.75586400	-0.01102500
Be	-0.88850500	-2.75586400	-0.01102500
H	0.00000000	-2.00198000	-0.92012200
H	0.00000000	-3.95804200	-0.22804400
H	0.00000000	-2.37403600	1.11380900
Be	0.88850500	2.75586400	-0.01102500
Be	-0.88850500	2.75586400	-0.01102500
H	0.00000000	2.37403600	1.11380900
H	0.00000000	3.95804200	-0.22804400
H	0.00000000	2.00198000	-0.92012200
N	-2.54002400	2.54002400	0.00000000
H	-2.96663600	2.98137500	0.80641500
H	-2.98137500	2.96663600	-0.80641500
N	-2.54002400	-2.54002400	0.00000000
H	-2.98137500	-2.96663600	-0.80641500
H	-2.96663600	-2.98137500	0.80641500
Be	-2.75586400	0.88850500	0.01102500
Be	-2.75586400	-0.88850500	0.01102500
H	-3.95804200	0.00000000	0.22804400
H	-2.37403600	0.00000000	-1.11380900
H	-2.00198000	0.00000000	0.92012200

5-NH_2

Be	-0.88846400	3.56579700	0.00000000

Be	0.88846400	3.56579700	0.00000000
H	0.00000000	4.77616000	0.00000000
H	0.00000000	2.97936100	1.03596300
H	0.00000000	2.97936100	-1.03596300
H	2.91326300	4.00976300	-0.80392600
H	2.91326300	4.00976300	0.80392600
H	-2.91326300	4.00976300	0.80392600
H	-2.91326300	4.00976300	-0.80392600
N	-2.54967100	3.50932100	0.00000000
N	2.54967100	3.50932100	0.00000000
Be	3.11672400	1.94687100	0.00000000
Be	3.66582500	0.25691200	0.00000000
H	2.83354100	0.92067300	-1.03596300
H	4.54239800	1.47591500	0.00000000
H	2.83354100	0.92067300	1.03596300
N	4.12545400	-1.34044100	0.00000000
H	4.71375900	-1.53159300	-0.80392600
H	4.71375900	-1.53159300	0.80392600
Be	-3.11672400	1.94687100	0.00000000
Be	-3.66582500	0.25691200	0.00000000
H	-2.83354100	0.92067300	1.03596300
H	-4.54239800	1.47591500	0.00000000
H	-2.83354100	0.92067300	-1.03596300
N	-4.12545400	-1.34044100	0.00000000
H	-4.71375900	-1.53159300	0.80392600
H	-4.71375900	-1.53159300	-0.80392600
Be	2.81470500	-2.36256400	0.00000000
Be	1.37714000	-3.40701600	0.00000000
H	1.75122400	-2.41035400	-1.03596300
H	2.80735600	-3.86399500	0.00000000
H	1.75122400	-2.41035400	1.03596300
N	0.00000000	-4.33775900	0.00000000
H	0.00000000	-4.95633900	-0.80392600
H	0.00000000	-4.95633900	0.80392600
Be	-2.81470500	-2.36256400	0.00000000
Be	-1.37714000	-3.40701600	0.00000000
H	-2.80735600	-3.86399500	0.00000000
H	-1.75122400	-2.41035400	-1.03596300
H	-1.75122400	-2.41035400	1.03596300

***n*-PH$_2$** (n = 3–5)

3-PH$_2$

Be	-0.88773300	2.38537700	0.00000000
Be	0.88773300	2.38537700	0.00000000

H	0.00000000	3.59877000	0.00000000
H	0.00000000	1.79386400	1.01678600
H	0.00000000	1.79386400	-1.01678600
H	3.65932300	2.11271100	-1.07350000
H	3.65932300	2.11271100	1.07350000
H	-3.65932300	2.11271100	1.07350000
H	-3.65932300	2.11271100	-1.07350000
Be	-2.50966300	-0.42388900	0.00000000
Be	-1.62193100	-1.96148700	0.00000000
H	-1.55353200	-0.89693200	1.01678600
H	-3.11662600	-1.79938500	0.00000000
H	-1.55353200	-0.89693200	-1.01678600
H	0.00000000	-4.22542200	1.07350000
H	0.00000000	-4.22542200	-1.07350000
Be	1.62193100	-1.96148700	0.00000000
Be	2.50966300	-0.42388900	0.00000000
H	3.11662600	-1.79938500	0.00000000
H	1.55353200	-0.89693200	-1.01678600
H	1.55353200	-0.89693200	1.01678600
P	0.00000000	-3.33092500	0.00000000
P	2.88466500	1.66546200	0.00000000
P	-2.88466500	1.66546200	0.00000000

4-PH_2

Be	-0.88651600	3.35260400	0.00000000
Be	0.88651600	3.35260400	0.00000000
H	0.00000000	4.55338100	0.00000000
H	0.00000000	2.75666600	1.02287600
H	0.00000000	2.75666600	-1.02287600
H	3.60880800	3.60880800	-1.06871600
H	3.60880800	3.60880800	1.06871600
H	-3.60880800	3.60880800	1.06871600
H	-3.60880800	3.60880800	-1.06871600
Be	3.35260400	0.88651600	0.00000000
Be	3.35260400	-0.88651600	0.00000000
H	2.75666600	0.00000000	-1.02287600
H	4.55338100	0.00000000	0.00000000
H	2.75666600	0.00000000	1.02287600
Be	-3.35260400	0.88651600	0.00000000
Be	-3.35260400	-0.88651600	0.00000000
H	-2.75666600	0.00000000	1.02287600
H	-4.55338100	0.00000000	0.00000000
H	-2.75666600	0.00000000	-1.02287600
H	-3.60880800	-3.60880800	1.06871600

H	-3.60880800	-3.60880800	-1.06871600
H	3.60880800	-3.60880800	-1.06871600
H	3.60880800	-3.60880800	1.06871600
Be	-0.88651600	-3.35260400	0.00000000
Be	0.88651600	-3.35260400	0.00000000
H	0.00000000	-4.55338100	0.00000000
H	0.00000000	-2.75666600	-1.02287600
H	0.00000000	-2.75666600	1.02287600
P	2.97105100	2.97105100	0.00000000
P	2.97105100	-2.97105100	0.00000000
P	-2.97105100	-2.97105100	0.00000000
P	-2.97105100	2.97105100	0.00000000

5-PH_2

Be	-0.88640700	4.31487200	0.00000000
Be	0.88640700	4.31487200	0.00000000
H	0.00000000	5.50997400	0.00000000
H	0.00000000	3.71889400	1.02614200
H	0.00000000	3.71889400	-1.02614200
Be	3.82977200	2.17639200	0.00000000
Be	4.37760200	0.49034500	0.00000000
H	3.53687800	1.14920100	-1.02614200
H	5.24029700	1.70267600	0.00000000
H	3.53687800	1.14920100	1.02614200
Be	-3.82977200	2.17639200	0.00000000
Be	-4.37760200	0.49034500	0.00000000
H	-3.53687800	1.14920100	1.02614200
H	-5.24029700	1.70267600	0.00000000
H	-3.53687800	1.14920100	-1.02614200
Be	3.25333600	-2.96978700	0.00000000
Be	1.81910000	-4.01182200	0.00000000
H	2.18591100	-3.00864800	-1.02614200
H	3.23868200	-4.45766300	0.00000000
H	2.18591100	-3.00864800	1.02614200
Be	-3.25333600	-2.96978700	0.00000000
Be	-1.81910000	-4.01182200	0.00000000
H	-3.23868200	-4.45766300	0.00000000
H	-2.18591100	-3.00864800	-1.02614200
H	-2.18591100	-3.00864800	1.02614200
P	-4.85056100	-1.57604300	0.00000000
P	-2.99781200	4.12613400	0.00000000
P	2.99781200	4.12613400	0.00000000
P	4.85056100	-1.57604300	0.00000000
P	0.00000000	-5.10018200	0.00000000

H	-3.53150200	4.86069500	1.06480200
H	-3.53150200	4.86069500	-1.06480200
H	3.53150200	4.86069500	1.06480200
H	3.53150200	4.86069500	-1.06480200
H	5.71409000	-1.85662000	1.06480200
H	5.71409000	-1.85662000	-1.06480200
H	0.00000000	-6.00815000	1.06480200
H	0.00000000	-6.00815000	-1.06480200
H	-5.71409000	-1.85662000	1.06480200
H	-5.71409000	-1.85662000	-1.06480200

M06-2X-D3/def2-TZVPP-optimized structures

1

Be	-0.00734800	0.92321400	0.01124300
Be	0.00734800	-0.92321400	0.01124300
H	1.04676500	-0.05772400	-0.60579400
H	-1.04676500	0.05772400	-0.60579400
H	0.00000000	0.00000000	1.21099000
H	0.18988900	-3.00203900	-0.82047800
H	-0.82407400	-2.96996900	0.44193700
H	0.82407400	2.96996900	0.44193700
H	-0.18988900	3.00203900	-0.82047800
N	-0.00734800	-2.52296600	0.04769500
N	0.00734800	2.52296600	0.04769500

1’

Be	0.90455800	-0.00027200	-0.00067100
Be	-0.90455800	-0.00027300	0.00067000
H	0.01113100	-0.59283900	-1.03192400
H	-0.00000100	1.18942000	-0.00001200
H	-0.01112900	-0.59282100	1.03193200
H	-3.24886700	0.43518300	-1.24624200
H	-3.23903200	-1.31506600	-0.17321400
H	3.23903000	-1.31506700	0.17321100
H	3.24886600	0.43517900	1.24624400
P	3.02263100	0.05860700	-0.10136800
P	-3.02263100	0.05860600	0.10136900

2

Be	0.00000000	3.05742400	-0.24048000
Be	-0.00084000	1.44943700	0.59935700
H	-0.05638900	2.73775800	1.30118800
H	-1.01382000	1.91591000	-0.35924500
H	1.06855600	1.95477700	-0.27071600
H	0.80201000	0.00157200	2.04103000
H	-0.80201000	-0.00157200	2.04103000
H	-0.83421600	4.98672500	-1.07307700
H	0.78820800	5.05816800	-0.94266900
N	0.00360600	4.42867100	-1.01360400
N	0.00000000	0.00000000	1.41806000
Be	0.00084000	-1.44943700	0.59935700
Be	0.00000000	-3.05742400	-0.24048000
H	1.01382000	-1.91591000	-0.35924500
H	0.05638900	-2.73775800	1.30118800
H	-1.06855600	-1.95477700	-0.27071600

N	-0.00360600	-4.42867100	-1.01360400
H	0.83421600	-4.98672500	-1.07307700
H	-0.78820800	-5.05816800	-0.94266900

2'

Be	0.00000000	3.56649000	-0.10930900
Be	0.00000000	1.92294400	0.60044000
H	1.02802700	2.46263700	-0.28051900
H	0.00000000	3.16980000	1.35902400
H	-1.02802700	2.46263700	-0.28051900
Be	0.00000000	-3.56649000	-0.10930900
Be	0.00000000	-1.92294400	0.60044000
H	0.00000000	-3.16980000	1.35902400
H	1.02802700	-2.46263700	-0.28051900
H	-1.02802700	-2.46263700	-0.28051900
P	0.00000000	-5.44735700	-1.05362400
P	0.00000000	5.44735700	-1.05362400
P	0.00000000	0.00000000	1.48585000
H	-1.02769800	6.01434400	-0.26018000
H	1.02769800	6.01434400	-0.26018000
H	-1.05098500	0.00000000	2.41833900
H	1.05098500	0.00000000	2.41833900
H	-1.02769800	-6.01434400	-0.26018000
H	1.02769800	-6.01434400	-0.26018000

***n*-NH_2** (*n* = 3–5)

3-NH_2

Be	-0.88833400	1.96622600	0.00000000
Be	0.88833400	1.96622600	0.00000000
H	0.00000000	3.21469900	0.00000000
H	0.00000000	1.43414800	1.02916000
H	0.00000000	1.43414800	-1.02916000
H	2.99672500	1.73016000	-0.81050300
H	2.99672500	1.73016000	0.81050300
H	-2.99672500	1.73016000	0.81050300
H	-2.99672500	1.73016000	-0.81050300
N	-2.46902400	1.42549200	0.00000000
N	2.46902400	1.42549200	0.00000000
Be	-2.14696900	-0.21379300	0.00000000
Be	-1.25863500	-1.75243300	0.00000000
H	-1.24200800	-0.71707400	1.02916000
H	-2.78401100	-1.60734900	0.00000000
H	-1.24200800	-0.71707400	-1.02916000
N	0.00000000	-2.85098400	0.00000000

H	0.00000000	-3.46032000	0.81050300
H	0.00000000	-3.46032000	-0.81050300
Be	1.25863500	-1.75243300	0.00000000
Be	2.14696900	-0.21379300	0.00000000
H	2.78401100	-1.60734900	0.00000000
H	1.24200800	-0.71707400	-1.02916000
H	1.24200800	-0.71707400	1.02916000

4-NH_2

Be	2.72614500	0.88441100	0.01354300
Be	2.72614500	-0.88441100	0.01354300
H	3.91294900	0.00000000	0.27003800
H	1.93721900	0.00000000	0.89033100
H	2.38006400	0.00000000	-1.12039400
H	2.96643400	-2.94832200	-0.80934000
H	2.94832200	-2.96643400	0.80934000
H	2.94832200	2.96643400	0.80934000
H	2.96643400	2.94832200	-0.80934000
N	2.52516700	2.52516700	0.00000000
N	2.52516700	-2.52516700	0.00000000
Be	0.88441100	-2.72614500	-0.01354300
Be	-0.88441100	-2.72614500	-0.01354300
H	0.00000000	-1.93721900	-0.89033100
H	0.00000000	-3.91294900	-0.27003800
H	0.00000000	-2.38006400	1.12039400
Be	0.88441100	2.72614500	-0.01354300
Be	-0.88441100	2.72614500	-0.01354300
H	0.00000000	2.38006400	1.12039400
H	0.00000000	3.91294900	-0.27003800
H	0.00000000	1.93721900	-0.89033100
N	-2.52516700	2.52516700	0.00000000
H	-2.94832200	2.96643400	0.80934000
H	-2.96643400	2.94832200	-0.80934000
N	-2.52516700	-2.52516700	0.00000000
H	-2.96643400	-2.94832200	-0.80934000
H	-2.94832200	-2.96643400	0.80934000
Be	-2.72614500	0.88441100	0.01354300
Be	-2.72614500	-0.88441100	0.01354300
H	-3.91294900	0.00000000	0.27003800
H	-2.38006400	0.00000000	-1.12039400
H	-1.93721900	0.00000000	0.89033100

5-NH_2

Be	-0.88436100	3.52630900	0.00000000

Be	0.88436100	3.52630900	0.00000000
H	0.00000000	4.72976300	0.00000000
H	0.00000000	2.93705800	1.03183300
H	0.00000000	2.93705800	-1.03183300
H	2.89504500	3.98468800	-0.80730300
H	2.89504500	3.98468800	0.80730300
H	-2.89504500	3.98468800	0.80730300
H	-2.89504500	3.98468800	-0.80730300
N	-2.53314600	3.48657600	0.00000000
N	2.53314600	3.48657600	0.00000000
Be	3.08043700	1.93076700	0.00000000
Be	3.62700200	0.24861200	0.00000000
H	2.79330800	0.90760100	-1.03183300
H	4.49827200	1.46157700	0.00000000
H	2.79330800	0.90760100	1.03183300
N	4.09871600	-1.33175300	0.00000000
H	4.68428100	-1.52201500	-0.80730300
H	4.68428100	-1.52201500	0.80730300
Be	-3.08043700	1.93076700	0.00000000
Be	-3.62700200	0.24861200	0.00000000
H	-2.79330800	0.90760100	1.03183300
H	-4.49827200	1.46157700	0.00000000
H	-2.79330800	0.90760100	-1.03183300
N	-4.09871600	-1.33175300	0.00000000
H	-4.68428100	-1.52201500	0.80730300
H	-4.68428100	-1.52201500	-0.80730300
Be	2.78817600	-2.33303000	0.00000000
Be	1.35724900	-3.37265900	0.00000000
H	1.72635900	-2.37613000	-1.03183300
H	2.78008500	-3.82645900	0.00000000
H	1.72635900	-2.37613000	1.03183300
N	0.00000000	-4.30964500	0.00000000
H	0.00000000	-4.92534500	-0.80730300
H	0.00000000	-4.92534500	0.80730300
Be	-2.78817600	-2.33303000	0.00000000
Be	-1.35724900	-3.37265900	0.00000000
H	-2.78008500	-3.82645900	0.00000000
H	-1.72635900	-2.37613000	-1.03183300
H	-1.72635900	-2.37613000	1.03183300

***n*-PH$_2$** (*n* = 3–5)

3-PH$_2$

Be	-0.88267800	2.36998700	0.00000000

Be	0.88267800	2.36998700	0.00000000
H	0.00000000	3.57446100	0.00000000
H	0.00000000	1.77371200	1.01227900
H	0.00000000	1.77371200	-1.01227900
H	3.64251400	2.10300600	-1.07201000
H	3.64251400	2.10300600	1.07201000
H	-3.64251400	2.10300600	1.07201000
H	-3.64251400	2.10300600	-1.07201000
Be	-2.49380800	-0.42057200	0.00000000
Be	-1.61113000	-1.94941500	0.00000000
H	-1.53608000	-0.88685600	1.01227900
H	-3.09557400	-1.78723100	0.00000000
H	-1.53608000	-0.88685600	-1.01227900
H	0.00000000	-4.20601300	1.07201000
H	0.00000000	-4.20601300	-1.07201000
Be	1.61113000	-1.94941500	0.00000000
Be	2.49380800	-0.42057200	0.00000000
H	3.09557400	-1.78723100	0.00000000
H	1.53608000	-0.88685600	-1.01227900
H	1.53608000	-0.88685600	1.01227900
P	0.00000000	-3.30584900	0.00000000
P	2.86294900	1.65292400	0.00000000
P	-2.86294900	1.65292400	0.00000000

4-PH_2

Be	2.97747900	1.73109000	0.00004700
Be	1.73109000	2.97747900	-0.00004700
H	3.19864300	3.19864300	0.00000000
H	1.93138300	1.93154600	-1.01845400
H	1.93154600	1.93138300	1.01845400
H	0.00000000	5.07736600	1.06840000
H	0.00000000	5.07780800	-1.06717300
H	5.07736600	0.00000000	-1.06840000
H	5.07780800	0.00000000	1.06717300
Be	-1.73109000	2.97747900	-0.00004700
Be	-2.97747900	1.73109000	0.00004700
H	-1.93154600	1.93138300	1.01845400
H	-3.19864300	3.19864300	0.00000000
H	-1.93138300	1.93154600	-1.01845400
Be	2.97747900	-1.73109000	0.00004700
Be	1.73109000	-2.97747900	-0.00004700
H	1.93138300	-1.93154600	-1.01845400
H	3.19864300	-3.19864300	0.00000000
H	1.93154600	-1.93138300	1.01845400

H	0.00000000	-5.07780800	-1.06717300
H	0.00000000	-5.07736600	1.06840000
H	-5.07780800	0.00000000	1.06717300
H	-5.07736600	0.00000000	-1.06840000
Be	-1.73109000	-2.97747900	-0.00004700
Be	-2.97747900	-1.73109000	0.00004700
H	-3.19864300	-3.19864300	0.00000000
H	-1.93154600	-1.93138300	1.01845400
H	-1.93138300	-1.93154600	-1.01845400
P	0.00000000	4.17093900	0.00043200
P	-4.17093900	0.00000000	-0.00043200
P	0.00000000	-4.17093900	0.00043200
P	4.17093900	0.00000000	-0.00043200

5-PH_2

Be	-0.88112300	4.28842700	0.00000000
Be	0.88112300	4.28842700	0.00000000
H	0.00000000	5.47828400	0.00000000
H	0.00000000	3.69300000	1.02171700
H	0.00000000	3.69300000	-1.02171700
Be	3.80625400	2.16319400	0.00000000
Be	4.35081800	0.48719900	0.00000000
H	3.51225100	1.14120000	-1.02171700
H	5.21015800	1.69288300	0.00000000
H	3.51225100	1.14120000	1.02171700
Be	-3.80625400	2.16319400	0.00000000
Be	-4.35081800	0.48719900	0.00000000
H	-3.51225100	1.14120000	1.02171700
H	-5.21015800	1.69288300	0.00000000
H	-3.51225100	1.14120000	-1.02171700
Be	3.23351700	-2.95149900	0.00000000
Be	1.80783100	-3.98732100	0.00000000
H	2.17069100	-2.98769900	-1.02171700
H	3.22005500	-4.43202500	0.00000000
H	2.17069100	-2.98769900	1.02171700
Be	-3.23351700	-2.95149900	0.00000000
Be	-1.80783100	-3.98732100	0.00000000
H	-3.22005500	-4.43202500	0.00000000
H	-2.17069100	-2.98769900	-1.02171700
H	-2.17069100	-2.98769900	1.02171700
P	-4.81566600	-1.56470500	0.00000000
P	-2.97624500	4.09645000	0.00000000
P	2.97624500	4.09645000	0.00000000
P	4.81566600	-1.56470500	0.00000000

P	0.00000000	-5.06349100	0.00000000
H	-3.51250400	4.83454600	1.06432500
H	-3.51250400	4.83454600	-1.06432500
H	3.51250400	4.83454600	1.06432500
H	3.51250400	4.83454600	-1.06432500
H	5.68335000	-1.84663200	1.06432500
H	5.68335000	-1.84663200	-1.06432500
H	0.00000000	-5.97582800	1.06432500
H	0.00000000	-5.97582800	-1.06432500
H	-5.68335000	-1.84663200	1.06432500
H	-5.68335000	-1.84663200	-1.06432500

6-E (E = F, Cl, Br, OH, SH)

6-F

Be	0.00972600	4.23099800	0.87364900
Be	0.00972600	4.23099800	-0.87364900
H	-0.67938000	3.26120400	0.00000000
H	-0.48793200	5.31633000	0.00000000
H	1.19511900	4.11704400	0.00000000
Be	0.01029300	-2.87235500	3.22363500
Be	0.01007000	-1.35799500	4.09527700
H	-0.51129800	-2.65102400	4.59019400
H	1.19789800	-2.07138800	3.58357100
H	-0.65736000	-1.62397600	2.80603500
Be	-0.01007000	1.35799500	4.09527700
Be	-0.01029300	2.87235500	3.22363500
H	-1.19789800	2.07138800	3.58357100
H	0.51129800	2.65102400	4.59019400
H	0.65736000	1.62397600	2.80603500
Be	-0.00972600	-4.23099800	0.87364900
Be	-0.00972600	-4.23099800	-0.87364900
H	0.67938000	-3.26120400	0.00000000
H	0.48793200	-5.31633000	0.00000000
H	-1.19511900	-4.11704400	0.00000000
Be	-0.01029300	2.87235500	-3.22363500
Be	-0.01007000	1.35799500	-4.09527700
H	-1.19789800	2.07138800	-3.58357100
H	0.51129800	2.65102400	-4.59019400
H	0.65736000	1.62397600	-2.80603500
Be	0.01029300	-2.87235500	-3.22363500
Be	0.01007000	-1.35799500	-4.09527700
H	-0.51129800	-2.65102400	-4.59019400
H	-0.65736000	-1.62397600	-2.80603500

H	1.19789800	-2.07138800	-3.58357100
F	0.00000000	4.13406400	-2.38533000
F	0.00000000	4.13406400	2.38533000
F	0.00000000	0.00000000	4.76626900
F	0.00000000	-4.13406400	2.38533000
F	0.00000000	-4.13406400	-2.38533000
F	0.00000000	0.00000000	-4.76626900

6-Cl

Be	1.49448200	4.09699200	0.42392900
Be	0.00000000	4.36903300	-0.44023600
H	0.32086800	3.20136300	0.39076500
H	0.57669500	5.22643100	0.61825400
H	1.34205800	4.27139500	-1.03391900
Be	2.80085800	-3.34275600	0.42392900
Be	3.78369400	-2.18451700	-0.44023600
H	4.23787400	-3.11264800	0.61825400
H	3.02810700	-3.29795400	-1.03391900
H	2.61202800	-1.87856200	0.39076500
Be	4.29534100	0.75423700	-0.42392900
Be	3.78369400	2.18451700	0.44023600
H	4.37016600	0.97344100	1.03391900
H	4.81456900	2.11378300	-0.61825400
H	2.93289600	1.32280100	-0.39076500
Be	0.00000000	-4.36903300	0.44023600
Be	-1.49448200	-4.09699200	-0.42392900
H	-0.32086800	-3.20136300	-0.39076500
H	-0.57669500	-5.22643100	-0.61825400
H	-1.34205800	-4.27139500	1.03391900
Be	-2.80085800	3.34275600	-0.42392900
Be	-3.78369400	2.18451700	0.44023600
H	-3.02810700	3.29795400	1.03391900
H	-4.23787400	3.11264800	-0.61825400
H	-2.61202800	1.87856200	-0.39076500
Be	-3.78369400	-2.18451700	-0.44023600
Be	-4.29534100	-0.75423700	0.42392900
H	-4.81456900	-2.11378300	0.61825400
H	-2.93289600	-1.32280100	0.39076500
H	-4.37016600	-0.97344100	-1.03391900
Cl	3.17970900	3.79604500	1.39614300
Cl	4.87732600	-0.85568600	-1.39614300
Cl	1.69761700	-4.65173100	1.39614300
Cl	-3.17970900	-3.79604500	-1.39614300
Cl	-4.87732600	0.85568600	1.39614300

Cl	-1.69761700	4.65173100	-1.39614300

6-Br

Be	1.44658700	4.20406100	0.46686000
Be	0.00000000	4.45414900	-0.48163900
H	0.30031200	3.28260400	0.35062500
H	0.49199500	5.30822300	0.62072600
H	1.37657200	4.39829200	-0.99438600
Be	2.91753000	-3.35481200	0.46686000
Be	3.85740600	-2.22707500	-0.48163900
H	4.35105800	-3.08019100	0.62072600
H	3.12074600	-3.39129300	-0.99438600
H	2.69266200	-1.90138000	0.35062500
Be	4.36411700	0.84924900	-0.46686000
Be	3.85740600	2.22707500	0.48163900
H	4.49731900	1.00699900	0.99438600
H	4.84305300	2.22803100	-0.62072600
H	2.99297400	1.38122400	-0.35062500
Be	0.00000000	-4.45414900	0.48163900
Be	-1.44658700	-4.20406100	-0.46686000
H	-0.30031200	-3.28260400	-0.35062500
H	-0.49199500	-5.30822300	-0.62072600
H	-1.37657200	-4.39829200	0.99438600
Be	-2.91753000	3.35481200	-0.46686000
Be	-3.85740600	2.22707500	0.48163900
H	-3.12074600	3.39129300	0.99438600
H	-4.35105800	3.08019100	-0.62072600
H	-2.69266200	1.90138000	-0.35062500
Be	-3.85740600	-2.22707500	-0.48163900
Be	-4.36411700	-0.84924900	0.46686000
H	-4.84305300	-2.22803100	0.62072600
H	-2.99297400	-1.38122400	0.35062500
H	-4.49731900	-1.00699900	-0.99438600
Br	3.20968200	3.90430300	1.61697600
Br	-1.77638500	4.73181800	-1.61697600
Br	-4.98606700	0.82751500	1.61697600
Br	-3.20968200	-3.90430300	-1.61697600
Br	1.77638500	-4.73181800	1.61697600
Br	4.98606700	-0.82751500	-1.61697600

6-OH

Be	4.28262100	0.88158900	0.00878400
Be	4.28298700	-0.88082400	-0.04431400

H	3.12371000	-0.00847800	0.21008700
H	4.68515900	0.03039700	-1.14711200
H	5.07781100	-0.02124600	0.88405500
Be	-2.90478900	3.26806400	0.00878400
Be	-1.37867800	4.14958700	-0.04431400
H	-2.36890500	4.04226800	-1.14711200
H	-2.52050600	4.40813700	0.88405500
H	-1.55451200	2.70945100	0.21008700
Be	1.37783200	4.14965400	-0.00878400
Be	2.90430900	3.26876400	0.04431400
H	2.55730600	4.38689100	-0.88405500
H	2.31625500	4.07266600	1.14711200
H	1.56919700	2.70097300	-0.21008700
Be	-4.28298700	0.88082400	0.04431400
Be	-4.28262100	-0.88158900	-0.00878400
H	-4.68515900	-0.03039700	1.14711200
H	-5.07781100	0.02124600	-0.88405500
H	-3.12371000	0.00847800	-0.21008700
Be	2.90478900	-3.26806400	-0.00878400
Be	1.37867800	-4.14958700	0.04431400
H	1.55451200	-2.70945100	-0.21008700
H	2.52050600	-4.40813700	-0.88405500
H	2.36890500	-4.04226800	1.14711200
Be	-2.90430900	-3.26876400	-0.04431400
Be	-1.37783200	-4.14965400	0.00878400
H	-2.55730600	-4.38689100	0.88405500
H	-2.31625500	-4.07266600	-1.14711200
H	-1.56919700	-2.70097300	0.21008700
O	4.21559400	2.43387400	0.06903400
O	0.00000000	4.86774900	-0.06903400
O	-4.21559400	2.43387400	0.06903400
O	-4.21559400	-2.43387400	-0.06903400
O	0.00000000	-4.86774900	0.06903400
O	4.21559400	-2.43387400	-0.06903400
H	5.04227100	2.90953900	0.14610700
H	0.00140100	5.82150500	-0.14610700
H	-5.04087100	2.91196500	0.14610700
H	5.04087100	-2.91196500	-0.14610700
H	-0.00140100	-5.82150500	0.14610700
H	-5.04227100	-2.90953900	-0.14610700

6-SH

Be	-1.48708400	4.18787500	0.36781900

Be	0.02928000	4.42229000	-0.48967400
H	-0.30477600	3.32926500	0.45894300
H	-1.30424800	4.22802900	-1.09539400
H	-0.57883100	5.36435900	0.45834000
Be	-2.81791300	-3.39738700	0.47654400
Be	-3.81062600	-2.23886000	-0.39620400
H	-2.99576500	-3.32167200	-0.98530500
H	-4.28672900	-3.19574900	0.61110800
H	-2.66553500	-1.94022600	0.49969000
Be	-4.35346600	0.77218900	-0.40769600
Be	-3.83084600	2.22787300	0.42751500
H	-4.95311400	2.13006600	-0.51463100
H	-4.29475200	0.97294100	1.05305700
H	-3.03423100	1.39894800	-0.51333000
Be	0.03473500	-4.43338100	0.43733000
Be	1.49852600	-4.15497100	-0.49474800
H	1.40701600	-4.29761100	0.97029600
H	0.56885400	-5.31203000	-0.61214000
H	0.32454400	-3.27999900	-0.44890200
Be	2.86925400	3.33651000	-0.39265700
Be	3.79963100	2.16232400	0.52642600
H	2.64967800	1.88800400	-0.36909200
H	4.32833500	3.06171200	-0.50695100
H	3.03074300	3.30228600	1.07187100
Be	3.80670400	-2.20685800	-0.50459300
Be	4.31523500	-0.82105100	0.44894400
H	4.81460200	-2.21920600	0.56401800
H	4.41749800	-0.95921300	-1.01477100
H	2.95744900	-1.36633800	0.37194200
H	-3.95935100	4.77114500	0.68672000
H	-6.07741600	-1.09386200	-0.72266700
H	-2.07994200	-5.81470800	0.86274100
H	2.18658900	5.76304700	-0.81909500
H	6.03341000	1.00367900	0.99981400
H	3.94504500	-4.71582400	-1.01677500
S	1.79130500	4.67428200	-1.49100200
S	4.85491800	0.77706800	1.59360500
S	3.16812400	-3.80077100	-1.60998000
S	-1.67235100	-4.72213400	1.52082900
S	-4.95319400	-0.89179200	-1.42111900
S	-3.22130300	3.91475200	1.40417300