Electronic Supplementary Information (ESI)

Digitization of Electron Shell via Localized Orbital Locator Formalism: Trends in the Size and Electronegativity changes of Atoms across Periodic Table

Andrei V. Afonin*, Valentin A. Semenov and Alexander V. Vashchenko

A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of Russian Academy of Sciences,
1 Favorsky St., 664033 Irkutsk, Russian Federation.
* E-mail: andvalaf@irioch.irk.ru (Andrei V. Afonin)

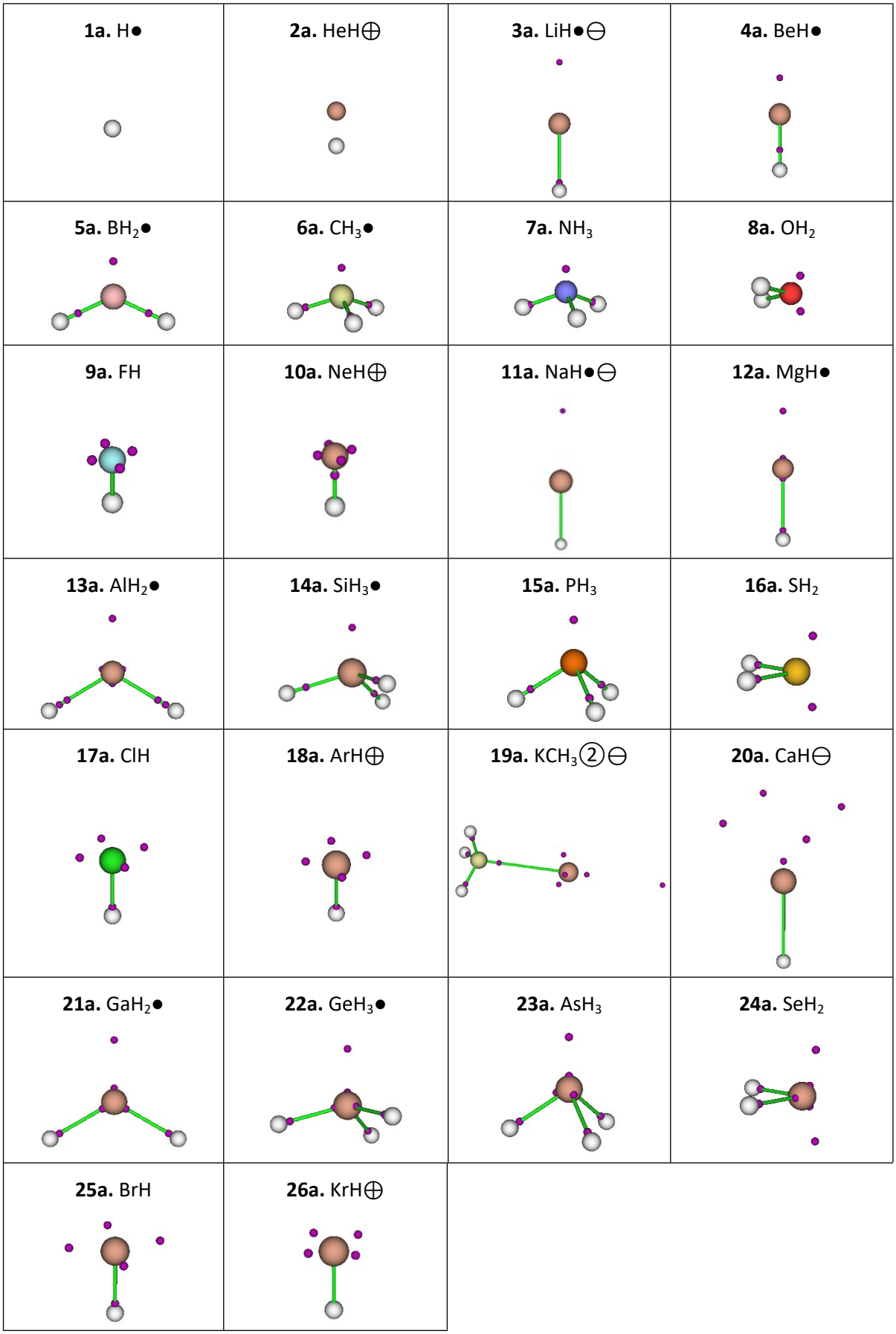
Contents	Page
1. Details of calculations	S2
2. Figure S1. Location of the (3,–3) critical points in the LOL topology of some studied compounds.	S3
3. Table S1. Structure of studied compounds **1a; 2a; 3a,b; 4a,b; 5a–c; 6a–d; 7a–d; 8a–c; 9a,b; 10a; 11a–d; 12a,b; 13a–c; 14a–c; 15a–d; 16a–c; 17a,b; 18a; 19a–d; 20a–c; 21a–c; 22a–d; 23a–d; 24a–d; 25a,b; 26a,b**	S4
4. Table S2. The values of the calculated parameters for the (3,–3) critical point in the LOL space topology related to the electron shell of element hydrides and methyls **1a–26a**	S6, S6
5. Table S3. The values of the calculated parameters for the (3,–3) critical point in the LOL space topology related to the electron shell of element hydrides and methyls **1a; 2a; 3a,b; 4a,b; 5a–c; 6a–d; 7a–d; 8a–c; 9a,b; 10a; 11a–d; 12a,b; 13a–c; 14a–c; 15a–d; 16a–c; 17a,b; 18a; 19a–d; 20a–c; 21a–c; 22a–d; 23a–d; 24a–d; 25a,b; 26a,b**	S7 – S9
6. Table S4. Filled and empty ranges for the r(LOL-shell), ρ(LOL-shell), V(LOL-shell), K(LOL-shell) and H(LOL-shell) parameters of the (3,–3) LOL-shell critical point for the elements of 2nd period of periodic table.	S10
7. Table S5. Filled and empty ranges for the r(LOL-shell), ρ(LOL-shell), V(LOL-shell), K(LOL-shell) and H(LOL-shell) parameters of the (3,–3) LOL-shell critical point for the elements of 3rd period of periodic table.	S11
8. Table S6. Filled and empty ranges for the r(LOL-shell), ρ(LOL-shell), V(LOL-shell), K(LOL-shell) and H(LOL-shell) parameters of the (3,–3) LOL-shell critical point for the elements of 4th period of periodic table.	S12, S13
9. Table S7. The value of electronegativity, atomic, covalent, van der Waals radii and energy of ionization for elements of 1st, 2nd, 3rd and 4th periods of periodic table.	S14
10. Table S8. The values of the calculated parameters for the (3,–3) LOL and ELF critical points related to the electron shells of element hydrides and methyls **3a–26a**	S15, S16
11. Cartesian coordinates of studied compounds, optimized at the (u)B3LYP/AQZP//ATZP level in gas phase	S17 – S23

1. Details of calculations

Geometry optimization of all compounds and complexes was performed with GAUSSIAN 09 program package[1] at the B3LYP/AQZP//ATZP level. All calculated structures are minima on the potential energy surfaces as proved by the absence of imaginary frequencies. Open-shell electronic structures were calculated within the framework of unrestricted DFT (uB3LYP). Analysis of the electron density using the obtained wave functions were performed with the Multiwfn program[2] in order to locate the (3,–3) critical points of the Localized Orbital Locator (LOL) for elements hydrides and methyls **1a; 2a; 3a,b; 4a,b; 5a–c; 6a–d; 7a–d; 8a–c; 9a,b; 10a; 11a–d; 12a,b; 13a–c; 14a–c; 15a–d; 16a–c; 17a,b; 18a; 19a–d; 20a–c; 21a–c; 22a–d; 23a–d; 24a–d; 25a,b; 26a,b.** The search for the critical points was carried out from nuclear positions and the batch of points within a sphere with the gradient-norm convergence criterion equal to $1 \cdot 10^{-5}$ and the number of points in the sphere equal to 3000.
For the detailed consideration of the mathematical apparatus to calculate the localized orbital locator function see ref. 3.

References

1. Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2011. See http://www.gaussian.com.
2. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.
3. H. L. Schmider and A. D. Becke, *J. Mol. Struct. (THEOCHEM)*, 2000, **527**, 51–61.



2. Figure S1. Location of the (3,–3) critical points in the LOL topology of some studied compounds. The (3,–3) LOL critical points are indicated by purple circles inside the positions of nuclei, covalent bonds and near the element atom. Critical points located near the atomic nucleus (less than 0.3 Å) are masked by the image of the element. Designations: ● – radical; ⊕ – cation; ⊖– anion; ●⊖ – anion radical; ●⊕ – cation radical, ②⊕ – dication, ②⊖ – dianion.

3. Table S1. Structures of studied compounds **1a; 2a; 3a,b; 4a,b; 5a–c; 6a–d; 7a–d; 8a–c; 9a,b; 10a; 11a–d; 12a,b; 13a–c; 14a–c; 15a–d; 16a–c; 17a,b; 18a; 19a–d; 20a–c; 21a–c; 22a–d; 23a–d; 24a–d; 25a,b; 26a,b**. Designations: ● – radical; ⊕ – cation; ⊖– anion; ●⊖ – anion radical; ●⊕ – cation radical, ②⊕ – dication, ②⊖ – dianion.

No	Structure	No	Structure	No	Structure	No	Structure	No	Structure
1st period		**7a**	NH_3	**12a**	$MgH●$	**17a**	ClH	**22b**	$GeH_3⊖$
1a	$H●$	**7b**	$NH_3●⊕$	**12b**	$MgH⊖$	**17b**	$ClH_2⊕$	**22c**	GeH_2
2a	$HeH⊕$	**7c**	$NH_2⊖$	**13a**	$AlH_2●$	**18a**	$ArH⊕$	**22d**	$GeH_2②⊖$
2nd period		**7d**	$NH_2⊕$	**13b**	$AlH_2⊖$	**4th period**		**23a**	AsH_3
3a	$LiH●⊖$	**8a**	OH_2	**13c**	AlH	**19a**	$KCH_3②⊖$	**23b**	$AsH_3●$
3b	$LiCH_3②⊖$	**8b**	$OH⊕$	**14a**	$SiH_3●$	**19b**	$KH●⊖$	**23c**	$AsH_2⊖$
4a	$BeH●$	**8c**	$OH_2②⊕$	**14b**	$SiH_3⊖$	**19c**	$K–i–Pr②⊖$	**23d**	$AsH_2⊕$
4b	$BeH⊖$	**9a**	FH	**14c**	SiH_2	**19d**	$KCH_3●⊖$	**24a**	SeH_2
5a	$BH_2●$	**9b**	$FH_2⊕$	**15a**	PH_3	**20a**	$CaH⊖$	**24b**	$SeH⊖$
5b	$BH_2⊖$	**10a**	$NeH⊕$	**15b**	$PH_3●$	**20b**	$CaH●$	**24c**	$SeH⊕$
5c	BH	**3rd period**		**15c**	$PH_2⊖$	**20c**	$CaCH_3⊖$	**24d**	$SeH_2②⊕$
6a	$CH_3●$	**11a**	$NaH●⊖$	**15d**	$PH_2⊕$	**21a**	$GaH_2●$	**25a**	BrH
6b	$CH_3⊖$	**11b**	$NaCH_3②⊖$	**16a**	SH_2	**21b**	$GaH_2⊖$	**25b**	$BrH_2⊕$
6c	CH_2	**11c**	$NaH②⊖$	**16b**	$SH⊕$	**21c**	GaH	**26a**	$KrH⊕$
6d	$CH_2②⊖$	**11d**	$NaCH_3●⊖$	**16c**	$SH_2②⊕$	**22a**	$GeH_3●$	**26b**	$KrCH_3⊕$

4. Table S2. The values of the calculated parameters for the (3,–3) critical point in the LOL space topology related to the electron shell of element hydrides and methyls **1a–26a**: the distance between the (3,–3) LOL critical point and the element nucleus (r(LOL-shell) in pm), the value of LOL at the (3,–3) LOL-shell critical point, the value of ρ electron density at the (3,–3) LOL-shell critical point (ρ(LOL-shell), in a.u., 1 a.u. = 6.7483 eÅ^{-3}), the value of potential V electron energy density at the (3,–3) LOL-shell critical point (V(LOL-shell), in a.u., 1 a.u. = 1 Hartree), the value of kinetic K electron energy density at the (3,–3) LOL-shell critical point (K(LOL-shell), in a.u., 1 a.u. = 1 Hartree) and the value of total H electron energy density at the (3,–3) LOL-shell critical point (H(LOL-shell), in a.u., 1 a.u. = 1 Hartree).

No	structure	r(LOL–shell)	LOL–shell	ρ(LOL–shell)	V(LOL–shell)	K(LOL–shell)	H(LOL–shell)
1st period							
1a	H	8.6	0.77361	0.235706	–1.379736	0.119961	–1.259776
2a	HeH⊕	4.2	0.77110	2.637644	–61.044998	4.291500	–56.753499
2nd period							
3a	LiH●⊖	159.7	0.83583	0.003370	–0.000588	0.000068	–0.000521
4a	BeH●	90.9	0.79328	0.031525	–0.019778	0.003702	–0.016076
5a	BH_2●	71.4	0.70851	0.079912	–0.095575	0.025826	–0.069750
6a	CH_3●	59.9	0.58975	0.143062	–0.283892	0.111020	–0.172871
7a	NH_3	47.1	0.62301	0.433379	–1.246359	0.431206	–0.815153
8a	OH_2	40.5	0.59972	0.737219	–3.080308	1.152935	–1.927373
9a	FH	35.8	0.57947	1.153258	–6.593179	2.642722	–3.950457
10a	NeH⊕	31.4	0.57783	1.825768	–13.979907	5.721411	–8.258497
3rd period[a]							
11a	NaH●⊖	216.9	0.74142	0.002036	–0.000225	0.000050	–0.000175
		28.2	0.56889	2.648198	–26.020247	11.029371	–14.990877
12a	MgH●	141.2	0.65696	0.010438	–0.003528	0.001103	–0.002426
		25.0	0.57309	3.956147	–50.431881	21.168405	–29.263476
13a	AlH_2●	117.2	0.71808	0.026050	–0.014256	0.003752	–0.010504
		22.6	0.57484	5.568760	–87.721242	37.154764	–50.566478
14a	SiH_3●	101.4	0.69177	0.046218	–0.037801	0.010872	–0.026929
		20.5	0.57459	7.572301	–146.578010	62.073158	–84.504852
15a	PH_3	85.3	0.69053	0.105765	–0.108668	0.030438	–0.078230
		18.6	0.57700	10.361623	–246.822943	103.658739	–143.164204
16a	SH_2	76.5	0.65976	0.162196	–0.231199	0.071427	–0.159772
		17.2	0.57642	13.412808	–379.575770	159.757841	–219.817929
17a	ClH	69.2	0.62076	0.231341	–0.441498	0.152927	–0.288571
		15.9	0.57510	17.047062	–567.917354	239.534994	–328.382360
18a	ArH⊕	62.2	0.61675	0.340758	–0.854533	0.296605	–0.557928
		14.9	0.57473	21.293736	–818.364883	347.551464	–470.813419
4th period[b]							
19a	$KCH_3$②⊖	268.2	0.30933	0.000665	–0.000075	0.000033	–0.000043
		57.1	0.59914	0.468889	–1.511413	0.543639	–0.967774
		14.0	0.57248	25.960089	–1137.546925	488.019500	–649.527425
20a	CaH⊖	218.2	0.60399	0.003596	–0.000372	0.000159	–0.000213
		51.6	0.60558	0.669117	–2.728220	0.957251	–1.770969
		13.1	0.57183	31.966382	–1613.925010	692.210787	–921.714223
21a	GaH_2●	133.5	0.48415	0.020488	–0.010958	0.006398	–0.004560
		29.6	0.56866	6.773438	–119.595316	52.812283	–66.783033
		7.8	0.56469	157.974324	–23736.946580	10218.022490	–13518.749780
22a	GeH_3●	123.0	0.53633	0.029948	–0.019234	0.009926	–0.009308
		28.2	0.57051	8.029421	–158.945125	69.595124	–89.350001
		7.6	0.56348	175.946670	–28311.995730	12288.304150	–16023.691580
23a	AsH_3	105.4	0.54625	0.067020	–0.052902	0.026374	–0.026528
		26.8	0.57358	9.591482	–212.901362	92.423042	–120.478320
		7.3	0.56281	196.953579	–34204.711870	14870.374390	–19334.337480
24a	SeH_2	97.3	0.57123	0.097376	–0.096929	0.044418	–0.052511
		25.7	0.57377	11.151628	–273.511375	118.725351	–154.786024
		7.0	0.56244	219.588104	–41125.525210	17852.743400	–23272.781810
25a	BrH	89.9	0.55028	0.129446	–0.165702	0.077727	–0.087975
		24.6	0.57368	12.871053	–347.221259	150.831234	–196.390024
		6.8	0.56094	243.495600	–48924.537010	21338.330580	–27586.206430

26a	$KrH^{\oplus}$	82.0 23.6 6.6	0.53145 0.57438 0.56166	0.184994 14.910916 270.126191	–0.317978 –444.594109 –58114.155080	0.152038 192.191470 25293.494340	–0.165939 –252.402639 –32820.660740

[a]The upper values refer to the outer electron shell, the lower values refer to the inner electron shell. [b]The upper values refer to the outer electron shell, the middle values refer to the first inner electron shell, the lower values refer to the second (closest to the atomic nucleus) inner electron shell.

5. Table S3. The values of the calculated parameters for the (3,–3) critical point in the LOL space topology related to the electron shell of element hydrides and methyls **1a; 2a; 3a,b; 4a,b; 5a–c; 6a–d; 7a–d; 8a–c; 9a,b; 10a; 11a–d; 12a,b; 13a–c; 14a–c; 15a–d; 16a–c; 17a,b; 18a; 19a–d; 20a–c; 21a–c; 22a–d; 23a–d; 24a–d; 25a,b; 26a,b**: the distance between the (3,–3) LOL critical point and the element nucleus (r(LOL–shell) in pm), the value of LOL at the (3,–3) LOL–shell critical point, the value of ρ electron density at the (3,–3) LOL–shell critical point (ρ(LOL–shell), in a.u., 1 a.u. = 6.7483 eÅ^{-3}), the value of potential V electron energy density at the (3,–3) LOL–shell critical point (V(LOL–shell), in a.u., 1 a.u. = 1 Hartree), the value of kinetic K electron energy density at the (3,–3) LOL–shell critical point (K(LOL–shell), in a.u., 1 a.u. = 1 Hartree) and the value of total H electron energy density at the (3,–3) LOL–shell critical point (H(LOL–shell), in a.u., 1 a.u. = 1 Hartree).

No	structure	r(LOL–shell)	LOL–shell	ρ(LOL–shell)	V(LOL–shell)	K(LOL–shell)	H(LOL–shell)
			1st period				
1a	H	8.6	0.77361	0.235706	–1.379736	0.119961	–1.259776
2a	HeH⊕	4.2	0.77110	2.637644	–61.044998	4.291500	–56.753499
			2nd period				
3a	LiH●⊖	159.7	0.83583	0.003370	–0.000588	0.000068	–0.000521
3b	$LiCH_3$②⊖	158.3	0.56442	0.002053	–0.000423	0.000074	–0.000350
4a	BeH●	90.9	0.79328	0.031525	–0.019778	0.003702	–0.016076
4b	BeH⊖	92.9	0.73905	0.031668	–0.015534	0.003214	–0.012320
5a	BH_2●	71.4	0.70851	0.079912	–0.095575	0.025826	–0.069750
5b	BH_2⊖	71.1	0.68453	0.091047	–0.094083	0.024383	–0.069701
5c	BH	65.4	0.75401	0.125089	–0.141752	0.029308	–0.112444
6a	CH_3●	59.9	0.58975	0.143062	–0.283892	0.111020	–0.172871
6b	CH_3⊖	59.4	0.58820	0.175716	–0.306553	0.110810	–0.195743
6c	CH_2	54.0	0.70109	0.263786	–0.501404	0.132820	–0.368584
6d	$CH_2$②⊖	60.7	0.60409	0.174082	–0.279714	0.102132	–0.177583
7a	NH_3	47.1	0.62301	0.433379	–1.246359	0.431206	–0.815153
7b	NH_3●⊕	47.1	0.62301	0.433379	–1.246359	0.431206	–0.815152
7c	NH_2⊖	48.3	0.59048	0.378762	–1.065874	0.394843	–0.671031
7d	NH_2⊕	44.0	0.69470	0.555357	–1.698246	0.473459	–1.224787
8a	OH_2	40.5	0.59972	0.737219	–3.080308	1.152935	–1.927373
8b	OH⊕	38.0	0.68080	0.964238	–4.222897	1.266951	–2.955945
8c	$OH_2$②⊕	37.4	0.68452	0.992681	–4.417230	1.307202	–3.110028
9a	FH	35.8	0.57947	1.153258	–6.593179	2.642722	–3.950457
9b	FH_2⊕	33.1	0.66476	1.548121	–9.328061	2.999893	–6.328168
10a	NeH⊕	31.4	0.57783	1.825768	–13.979907	5.721411	–8.258497
			3rd period[a]				
11a	NaH●⊖	216.9	0.74142	0.002036	–0.000225	0.000050	–0.000175
		28.2	0.56889	2.648198	–26.020247	11.029371	–14.990877
11b	$NaCH_3$②⊖	255.7	0.58340	0.000951	–0.000088	0.000019	–0.000069
		28.2	0.56819	2.636347	–25.854581	10.978544	–14.876036
11c	NaH②⊖	239.2	0.61671	0.001147	–0.000112	0.000022	–0.000090
		28.2	0.56844	2.639395	–25.892888	10.988480	–14.904408
11d	$NaCH_3$●⊖	218.2	0.72088	0.001901	–0.000199	0.000490	–0.000149
		28.2	0.56776	2.655960	–26.258947	11.134436	–15.124512
12a	MgH●	141.2	0.65696	0.010438	–0.003528	0.001103	–0.002426
		25.0	0.57309	3.956147	–50.431881	21.168405	–29.263476
12b	MgH⊖	144.5	0.63660	0.011007	–0.002838	0.000893	–0.001945
		25.0	0.57411	3.982646	–50.909024	21.313665	–29.595359
13a	AlH_2●	117.2	0.71808	0.026050	–0.014256	0.003752	–0.010504
		22.6	0.57484	5.568760	–87.721242	37.154764	–50.566478
13b	AlH_2⊖	118.1	0.69213	0.028794	–0.012291	0.003455	–0.008836
		22.5	0.57535	5.606019	–88.668740	37.491259	–51.177481
13c	AlH	113.6	0.64574	0.029378	–0.013549	0.004406	–0.009143
		22.5	0.57803	5.675715	–90.105529	37.853383	–52.252146
14a	SiH_3●	101.4	0.69177	0.046218	–0.037801	0.010872	–0.026929
		20.5	0.57459	7.572301	–146.578010	62.073158	–84.504852
14b	SiH_3⊖	100.1	0.69599	0.057434	–0.039153	0.010722	–0.028430
		20.4	0.57560	7.693785	–150.465611	63.477324	–86.988287
14c	SiH_2	96.9	0.69155	0.062244	–0.044723	0.012519	–0.032203
		20.4	0.57822	7.802601	–153.378057	64.286600	–89.091457

15a	PH_3	85.3	0.69053	0.105765	−0.108668	0.030438	−0.078230
		18.6	0.57700	10.361623	−246.822943	103.658739	−143.164204
15b	PH_3●	86.7	0.65610	0.079675	−0.096310	0.030750	−0.065560
		18.8	0.57535	10.120470	−237.616915	100.348032	−137.268882
15c	PH_2⊖	87.6	0.65299	0.094451	−0.095877	0.029889	−0.065988
		18.7	0.57592	10.238845	−242.279418	103.658739	−140.206776
15d	PH_2⊕	83.2	0.68384	0.109464	−0.117273	0.033251	−0.084022
		18.6	0.57971	10.500920	−251.302499	104.820347	−146.482152
16a	SH_2	76.5	0.65976	0.162196	−0.231199	0.071427	−0.159772
		17.2	0.57642	13.412808	−379.575770	159.757841	−219.817929
16b	SH⊕	74.4	0.70121	0.187032	−0.276473	0.074837	−0.201637
		17.1	0.57946	13.683332	−390.740323	163.119764	−227.620559
16c	$SH_2$②⊕	73.3	0.67546	0.175051	−0.263265	0.075567	−0.187698
		17.1	0.58046	13.724548	−391.922601	163.264690	−228.657912
17a	ClH	69.2	0.62076	0.231341	−0.441498	0.152927	−0.288571
		15.9	0.57510	17.047062	−567.917354	239.534994	−328.382360
17b	ClH_2⊕	66.3	0.68978	0.281769	−0.560191	0.156379	−0.403812
		15.8	0.57954	17.596629	−595.172446	247.990107	−347.182340
18a	ArH⊕	62.2	0.61675	0.340758	−0.854533	0.296605	−0.557928
		14.9	0.57473	21.293736	−818.364883	347.551464	−470.813419
4th period[b]							
19a	$KCH_3$②⊖	268.2	0.30933	0.000665	−0.000075	0.000033	−0.000043
		57.1	0.59914	0.468889	−1.511413	0.543639	−0.967774
		14.0	0.57248	25.960089	−1137.546925	488.019500	−649.527425
19b	KH●⊖	299.5	0.73886	0.000945	−0.000047	0.000014	−0.000033
		56.8	0.59728	0.468301	−1.521794	0.546733	−0.975061
		14.0	0.57234	25.943903	−1136.692971	487.803784	−648.889187
19c	K–*i*–Pr②⊖	272.8	0.35460	0.000723	−0.000081	0.000030	−0.000051
		57.0	0.59914	0.468923	−1.512204	0.543722	−0.968483
		14.0	0.57243	25.949909	−1136.921133	487.814902	−649.106428
19d	KCH_3●⊖	296.7	0.67710	0.000901	−0.000052	0.000017	−0.000035
		57.0	0.59980	0.471032	−1.523502	0.546326	−0.977177
		14.0	0.57241	25.952433	−1137.148413	487.915944	−649.232469
20a	CaH⊖	218.2	0.60399	0.003596	−0.000372	0.000159	−0.000213
		51.6	0.60558	0.669117	−2.728220	0.957251	−1.770969
		13.1	0.57183	31.966382	−1613.925010	692.210787	−921.714223
20b	CaH●	203.4	0.51056	0.003501	−0.000654	0.000307	−0.000346
		51.8	0.60578	0.663462	−2.695604	0.943708	−1.751896
		13.1	0.57216	31.596505	−1580.177739	677.995499	−902.182240
20c	$CaCH_3$⊖	218.3	0.56414	0.003089	−0.000365	0.000145	−0.000219
		51.9	0.63175	0.698982	−2.788345	0.921401	−1.866944
		13.0	0.57489	32.151522	−1635.097587	690.207259	−944.890328
21a	GaH_2●	133.5	0.48415	0.020488	−0.010958	0.006398	−0.004560
		29.6	0.56866	6.773438	−119.595316	52.812283	−66.783033
		7.8	0.56469	157.974324	−23736.946580	10218.022490	−13518.749780
21b	GaH_2⊖	134.8	0.48461	0.023907	−0.009877	0.006059	−0.003818
		29.6	0.56871	6.791828	−120.171058	53.039081	−67.131977
		7.8	0.56476	158.000619	−23739.853930	10218.022490	−13521.831440
21c	GaH	127.2	0.44342	0.027206	−0.013186	0.008870	−0.004317
		29.6	0.56831	6.772597	−119.673835	52.873867	−66.799969
		7.8	0.56449	157.577084	−23641.008650	10183.576050	−13457.432600
22a	GeH_3●	123.0	0.53633	0.029948	−0.019234	0.009926	−0.009308
		28.2	0.57051	8.029421	−158.945125	69.595124	−89.350001
		7.6	0.56348	175.946670	−28311.995730	12288.304150	−16023.691580
22b	GeH_3⊖	120.7	0.54977	0.039708	−0.021222	0.010867	−0.010355
		28.1	0.57226	8.133695	−161.977999	70.598729	−91.379270
		7.6	0.56345	175.922818	−28306.822980	12287.135700	−16019.687280
22c	GeH_2	115.4	0.52451	0.045060	−0.027320	0.014852	−0.012469

		28.1	0.57216	8.149474	−162.630378	70.855685	−91.774692
		7.6	0.56330	175.426170	−28175.752550	12236.617190	−15939.135360
22d	$GeH_2$②⊖	118.1	0.50482	0.039471	−0.022965	0.012887	−0.010078
		28.1	0.57177	8.112678	−161.422266	70.437875	−90.984392
		7.6	0.56324	175.558414	−28216.417670	12255.309380	−15961.108290
23a	AsH_3	105.4	0.54625	0.067020	−0.052902	0.026374	−0.026528
		26.8	0.57358	9.591482	−212.901362	92.423042	−120.478320
		7.3	0.56281	196.953579	−34204.711870	14870.374390	−19334.337480
23b	AsH_3●	107.7	0.52818	0.048400	−0.042703	0.022311	−0.020392
		26.9	0.57152	9.446270	−208.158337	90.873248	−117.285089
		7.3	0.56278	196.888088	−34187.107870	14863.581000	−19323.526870
23c	AsH_2⊖	108.8	0.55829	0.060237	−0.043677	0.021027	−0.022649
		26.9	0.57273	9.534142	−210.941689	91.822613	−119.119076
		7.3	0.56268	196.871189	−34188.698730	14867.394780	−19321.303950
23d	AsH_2⊕	102.2	0.51891	0.071204	−0.062312	0.032562	−0.029750
		26.8	0.57334	9.607931	−213.695841	92.779764	−120.916077
		7.3	0.56304	197.433182	−34335.345800	14916.797610	−19418.548190
24a	SeH_2	97.3	0.57123	0.097376	−0.096929	0.044418	−0.052511
		25.7	0.57377	11.151628	−273.511375	118.725351	−154.786024
		7.0	0.56244	219.588104	−41125.525210	17852.743400	−23272.781810
24b	SeH⊖	98.9	0.54170	0.086756	−0.084839	0.041301	−0.043538
		25.7	0.57288	11.082408	−270.962387	117.927866	−153.034521
		7.1	0.56238	219.472347	−41092.968370	17841.985460	−23250.982910
24c	SeH⊕	95.0	0.59400	0.110130	−0.114436	0.049658	−0.064778
		25.6	0.57468	11.252724	−277.197651	120.077123	−157.120529
		7.0	0.56264	220.381413	−41369.730580	17945.915290	−23423.815290
24d	$SeH_2$②⊕	92.3	0.51887	0.104874	−0.123060	0.062095	−0.060965
		25.6	0.57427	11.225393	−276.542875	119.791393	−156.751481
		7.0	0.56315	220.389317	−41330.153610	17909.673410	−23420.480200
25a	BrH	89.9	0.55028	0.129446	−0.165702	0.077727	−0.087975
		24.6	0.57368	12.871053	−347.221259	150.831234	−196.390024
		6.8	0.56094	243.495600	−48924.537010	21338.330580	−27586.206430
25b	BrH_2⊕	86.4	0.58510	0.155630	−0.212625	0.091679	−0.120946
		24.5	0.57555	13.077563	−355.572975	153.704322	−201.868653
		6.8	0.56129	244.635223	−49293.031310	21474.722440	−27818.308870
26a	KrH⊕	82.0	0.53145	0.184994	−0.317978	0.152038	−0.165939
		23.6	0.57438	14.910916	−444.594109	192.191470	−252.402639
		6.6	0.56166	270.126191	−58114.155080	25293.494340	−32820.660740
26b	$KrCH_3$⊕	82.4	0.52755	0.182179	−0.311870	0.150543	−0.161327
		23.6	0.57414	14.887451	−443.581397	191.878323	−251.703074
		6.6	0.56144	270.056671	−58116.153710	25306.238710	−32809.915000

[a]The upper values refer to the outer electron shell, the lower values refer to the inner electron shell. [b]The upper values refer to the outer electron shell, the middle values refer to the first inner electron shell, the lower values refer to the second (closest to the atomic nucleus) inner electron shell.

6. Table S4. Filled and empty ranges for the r(LOL–shell), ρ(LOL–shell), V(LOL–shell), K(LOL–shell) and H(LOL–shell) parameters of the (3,–3) LOL–shell critical point for the elements of 2nd period of periodic table.

E	**Li**		**filled range**	**empty range**	**Be**		**filled range**	**empty range**	**B**			**filled range**
E–X	**3a.** LiH●⊖	**3b.** $LiCH_3$②⊖	**Li**	**Li – Be**	**4a.** BeH●	**4b.** BeH⊖	**Be**	**Be – B**	**5a.** BH_2●	**5a.** BH_2⊖	**5c.** BH	**B**
r(LOL–shell)	159.7	158.3	158.3 – 159.7	93.0 – 158.2	90.9	92.9	90.9 – 92.9	71.5 – 90.8	71.4	71.1	65.4	65.4 – 71.4
ρ(LOL–shell)	0.00337	0.00205	0.00205 – 0.00337	0.00338 – 0.03151	0.03152	0.03167	0.03152 – 0.03167	0.03168 – 0.07990	0.07991	0.09105	0.12509	0.07991 – 0.12509
V(LOL–shell)	–0.000588	–0.000423	–0.000588 ÷ –0.000423	–0.015533 ÷ –0.000589	–0.019778	–0.015534	–0.019778 ÷ –0.015534	–0.094082 ÷ –0.019779	–0.095575	–0.094083	–0.141752	–0.141752 ÷ –0.094083
K(LOL–shell).	0.000068	0.000074	0.000068 – 0.000074	0.000075 – 0.003213	0.003702	0.003214	0.003214 – 0 .003702	0.003703 – 0.024382	0.025826	0.024383	0.029308	0.024383 – 0.029308
H(LOL–shell)	–0.000521	–0.000350	–0.000521 ÷ –0.000350	–0.012319 ÷ –0.000522	–0.016076	–0.012320	–0.016076 ÷ –0.012320	–0.069700 ÷ –0.016077	–0.069750	–0.069701	–0.112444	–0.112444 ÷ –0.069701

E	**empty range**	**C**				**filled range**	**empty range**	**N**				**filled range**
E–X	**B – C**	**6a.** CH_3●	**6b.** CH_3⊖	**6c.** CH_2	**6d.** $CH_2$②⊖	**C**	**C – N**	**7a.** NH_3	**7b.** NH_3●⊕	**7c.** NH_2⊖	**7d.** NH_2⊕	**N**
r(LOL–shell)	60.8 – 65.3	59.9	59.4	54.0	60.7	54.0 – 60.7	48.4 – 53.9	47.1	47.1	48.3	44.0	44.0 – 48.3
ρ(LOL–shell)	0.12510 –0.14305	0.14306	0.17572	0.26379	0.17408	0.14306 – 0.26379	0.26380 – 0.37875	0.43338	0.43338	0.37876	0.55536	0.37876 – 0.55536
V(LOL–shell)	–0.279713 ÷ –0.141753	–0.283892	–0.306553	–0.501404	–0.279714	–0.501404 ÷ –0.279714	–1.065873 ÷ –0.501405	–1.246359	–1.246359	–1.065874	–1.698246	–1.698246 ÷ –1.065874
K(LOL–shell)	0.029309 – 0.102131	0.111020	0.110810	0.132820	0.102132	0.102132 – 0.132820	0.132821 – 0.394842	0.431206	0.431206	0.394843	0.473459	0.394843 – 0.473459
H(LOL–shell)	–0.172870 ÷ –0.112445	–0.172871	–0.195743	–0.368584	–0.177583	–0.368584 ÷ –0.172871	–0.671030 ÷ –0.368585	–0.815153	–0.815152	–0.671031	–1.224787	–1.224787 ÷ –0.671031

E	**empty range**	**O**			**filled range**	**empty range**	**F**		**filled range**	**empty range**	**Ne**
E–X	**N – O**	**8a.** OH_2	**8b.** OH⊕	**8c.** $OH_2$②⊕	**O**	**O – F**	**9a.** FH	**9b.** FH_2⊕	**F**	**F – Ne**	**10a.** NeH⊕
r(LOL–shell)	40.6 – 43.9	40.5	38.0	37.4	37.4 – 40.5	35.9 – 37.3	35.8	33.1	33.1 – 35.8	31.5 – 33.0	31.4
ρ(LOL–shell)	0.55537 – 0.73721	0.73722	0.96424	0.99268	0.73722 – 0.99268	0.99269 – 1.15325	1.15326	1.54812	1.15326 – 1.54812	1.54813 – 1.82576	1.82577
V(LOL–shell)	–3.080307 ÷ –1.698247	–3.080308	–4.222897	–4.417230	–4.417230 ÷ –3.080308	–6.593178 ÷ –4.417231	–6.593179	–9.328061	–9.328061 ÷ –6.593179	–13.979906 ÷ –9.328062	–13.979907
K(LOL–shell)	0.473460 – 1.152934	1.152935	1.266951	1.307202	1.152935 – 1.307202	1.307203 – 2.642721	2.642722	2.999893	2.642722 – 2.999893	2.999894 – 5.721410	5.721411
H(LOL–shell)	–1.927372 ÷ –1.224788	–1.927373	–2.955945	–3.110028	–3.110028 ÷ –1.927373	–3.950456 ÷ –3.110029	–3.950457	–6.328168	–6.328168 ÷ –3.950457	–8.258496 ÷ –6.328169	–8.258497

7. Table S5. Filled and empty ranges for the r(LOL–shell), ρ(LOL–shell), V(LOL–shell), K(LOL–shell) and H(LOL–shell) parameters of the (3,–3) LOL–shell critical point for the elements of 3rd period of periodic table.

E	**Na**				**filled range**	**empty range**	**Mg**		**filled range**	**empty range**
E–X	**11a.** NaH●⊖	**11b.** $NaCH_3$②⊖	**11c.** NaH②⊖	**11d.** $NaCH_3$●⊖	**Na**	**Na – Mg**	**12a.** MgH●	**12b.** MgH⊖	**Mg**	**Mg – Al**
r(LOL–shell)[a]	216.9	255.7	239.2	218.2	216.9 – 255.7	144.6 – 216.8	141.2	144.5	141.2 – 144.5	118.2 – 141.1
r(LOL–shell)[b]	28.2	28.2	28.2	28.2	28.2	25.1 – 28.1	25.0	25.0	25.0	22.7 – 24.9
ρ(LOL–shell)[a]	0.00203	0.00095	0.00114	0.00190	0.00095 – 0.00203	0.00204 – 0.01043	0.01044	0.01101	0.01044 – 0.01101	0.01102 – 0.02604
ρ(LOL–shell)[b]	2.64820	2.63635	2.63939	2.65596	2.63635 – 2.65596	2.65597 – 3.95614	3.95615	3.98265	3.95615 – 3.98265	3.98266 – 5.56875
V(LOL–shell)[a]	–0.000225	–0.000088	–0.000112	–0.000199	–0.000225 ÷ –0.000088	–0.002837 ÷ –0.000226	–0.003528	–0.002838	–0.003528 ÷ –0.002838	–0.012290 ÷ –0.003529
V(LOL–shell)[b]	–26.020247	–25.854581	–25.892888	–26.258947	–26.258947 ÷ –25.854581	–50.431880 ÷ –26.258948	–50.909024	–50.431881	–50.909024 ÷ –50.431881	–87.721243 ÷ –50.909025
K(LOL–shell)[a]	0.000050	0.000018	0.000022	0.000490	0.000018 – 0.00050	0.000051 – 0.000893	0.001103	0.000893	0.000894 – 0.001103	0.001104 – 0.003454
K(LOL–shell)	11.029371	10.978544	10.988480	11.134436	10.978544 – 11.134436	11.134437 – 21.168404	21.168405	21.313665	21.168405 – 21.313665	21.313666 – 37.154763
H(LOL–shell)[a]	–0.000174	–0.000069	–0.000090	–0.000149	–0.000174 ÷ –0.000069	–0.001944 ÷ –0.000175	–0.002426	–0.001945	–0.002426 ÷ –0.001945	–0.008835 ÷ –0.002427
H(LOL–shell)[b]	–14.990876	–14.876036	–14.904408	–15.124511	–15.124511 ÷ –14.876036	–29.263475 ÷ –15.124512	–29.263476	–29.595359	–29.595359 ÷ –29.263476	–50.566477 ÷ –29.595360

E	**Al**			**filled range**	**empty range**	**Si**			**filled range**	**empty range**
E–X	**13a.** AlH_2●	**13b.** AlH_2⊖	**13c.** AlH	**Al**	**Al – Si**	**14a.** SiH_3●	**14b.** SiH_3⊖	**14c.** SiH_2	**Si**	**Si – P**
r(LOL–shell)[a]	117.2	118.1	113.6	113.6 – 118.1	101.5 – 113.5	101.4	100.1	96.9	96.9 – 101.4	87.7 – 96.8
r(LOL–shell)[b]	22.6	22.5	22.5	22.5 – 22.6	20.6 – 22.4	20.5	20.4	20.4	20.4 – 20.5	18.9 – 20.3
ρ(LOL–shell)[a]	0.02605	0.02879	0.02938	0.02605 – 0.02938	0.02939 – 0.04621	0.04622	0.05743	0.06224	0.04622 – 0.06224	0.06225 – 0.07967
ρ(LOL–shell)[b]	5.56876	5.60602	5.67572	5.56876 – 5.67572	5.67573 – 7.57229	7.57230	7.69378	7.80260	7.57230 – 7.80260	7.80261 – 10.12046
V(LOL–shell)[a]	–0.014256	–0.012291	–0.013549	–0.014256 ÷ –0.012291	–0.037800 ÷ –0.014257	–0.037801	–0.039153	–0.044723	–0.044723 ÷ –0.037801	–0.095876 ÷ –0.044724
V(LOL–shell)[b]	–87.721242	–88.668740	–90.105529	–90.105529 ÷ –87.721242	–146.578009 ÷ –90.105530	–146.578010	–150.465611	–153.378057	–153.378057 ÷ –146.578010	–237.616914 ÷ –153.378058
K(LOL–shell)[a]	0.003752	0.003455	0.004406	0.003455 – 0.004406	0.004407 – 0.010721	0.010872	0.010722	0.012519	0.010722 – 0.012519	0.012520 – 0.029888
K(LOL–shell)[b]	37.154764	37.491259	37.853383	37.154764 – 37.853383	37.853384 – 62.073157	62.073158	63.477324	64.286600	62.073158 – 64.286600	64.286601 – 100.348031
H(LOL–shell)[a]	–0.010504	–0.008836	–0.009143	–0.010504 ÷ –0.008836	–0.026930 ÷ –0.010505	–0.026929	–0.028430	–0.032203	–0.032203 ÷ –0.026931	–0.065559 ÷ –0.032204
H(LOL–shell)[b]	–50.566478	–51.177481	–52.252146	–52.252146 ÷ –50.566478	–84.504851 ÷ –52.252147	–84.504852	–86.988287	–89.091457	–89.091457 ÷ –84.504852	–137.268881 ÷ –89.091458

E	**P**				**filled range**	**empty range**	**S**			**filled range**	**empty range**
E–X	**15a.** PH_3	**15b.** PH_3●	**15c.** PH_2⊖	**15d.** PH_2⊕	**P**	**P – S**	**16a.** SH_2	**16b.** SH⊕	**16c.** $SH_2$②⊕	**S**	**S – Cl**
r(LOL–shell)[a]	85.3	86.7	87.6	83.2	83.2 – 87.6	76.6 – 83.1	76.5	74.4	73.3	73.3 – 76.5	69.3 – 73.2
r(LOL–shell)[b]	18.6	18.8	18.7	18.6	18.6 – 18.8	17.3 – 18.5	17.2	17.1	17.1	17.1 – 17.2	16.0 – 17.0
ρ(LOL–shell)[a]	0.10577	0.07968	0.09445	0.10946	0.07968 – 0.10946	0.10947 – 0.16219	0.16220	0.18703	0.17505	0.16220 – 0.18703	0.18704 – 0.23134
ρ(LOL–shell)[b]	10.36162	10.12047	10.23885	10.50092	10.12047 – 10.50092	10.50093 – 13.41280	13.41281	13.68333	13.72454	13.41281 – 13.72454	13.72455 – 17.04705
V(LOL–shell)[a]	–0.108668	–0.096310	–0.095877	–0.117273	–0.117273 ÷ –0.095877	–0.231198 ÷ –0.117274	–0.231199	–0.276473	–0.263265	–0.276473 ÷ –0.231199	–0.441497 ÷ –0.276474
V(LOL–shell)[b]	–246.822943	–237.616915	–242.279418	–251.302499	–251.302499 ÷ –237.616915	–379.575769 ÷ –251.302500	–379.575770	–390.740323	–391.922601	–391.922601 ÷ –379.575770	–567.917353 ÷ –391.922602
K(LOL–shell)[a]	0.030438	0.030750	0.029889	0.033251	0.029889 – 0.033251	0.033252 – 0.071426	0.071427	0.074837	0.075567	0.071427 – 0.075567	0.075568 – 0.152926
K(LOL–shell)	103.658739	100.348032	103.658739	104.820347	100.348032 – 104.820347	104.820348 – 159.757840	159.757841	163.119764	163.264690	159.757841 – 163.264690	163.264691 – 239.534993
H(LOL–shell)[a]	–0.078230	–0.065560	–0.065988	–0.084022	–0.084022 ÷ –0.065560	–0.159771 ÷ –0.084023	–0.159772	–0.201637	–0.187698	–0.201637 ÷ –0.159772	–0.288570 ÷ –0.201638
H(LOL–shell)[b]	–143.164204	–137.268882	–140.206776	–146.482152	–146.482152 ÷ –137.268882	–219.817928 ÷ –146.482153	–219.817929	–227.620559	–228.657912	–228.657912 ÷ –219.817929	–328.382359 ÷ –228.657913

E	**Cl**		**filled range**	**empty range**	**Ar**
E–X	**17a.** ClH	**17b.** ClH_2⊕	**Cl**	**Cl – Ar**	**18a.** ArH⊕
r(LOL–shell)[a]	69.2	66.3	66.3 – 69.2	62.3 – 66.2	62.2
r(LOL–shell)[b]	15.9	15.8	15.8 – 15.9	15.0 – 15.7	14.9
ρ(LOL–shell)[a]	0.23134	0.28177	0.23135 – 0.28177	0.28178 – 0.34075	0.34076
ρ(LOL–shell)[b]	17.04706	17.59663	17.04706 – 17.59663	17.59664 – 21.29373	21.29374
V(LOL–shell)[a]	–0.441498	–0.560191	–0.560191 ÷ –0.441498	–0.854532 ÷ –0.560192	–0.854533
V(LOL–shell)[b]	–567.917354	–595.172446	–595.172446 ÷ –567.917354	–818.364882 ÷ –595.172447	–818.364883
K(LOL–shell)[a]	0.152927	0.156379	0.152927 – 0.156379	0.156380 – 0.296604	0.296605
K(LOL–shell)[b]	239.534994	247.990107	239.534994 – 247.990107	247.990108 – 347.551463	347.551464
H(LOL–shell)[a]	–0.288571	–0.403812	–0.403812 ÷ –0.288571	–0.557927 ÷ –0.403813	–0.557928
H(LOL–shell)[b]	–328.382360	–347.182340	–347.182340 ÷ –328.382360	–470.813418 ÷ –347.182341	–470.813419

[a]The values refer to the outer electron shell; [b]the values refer to the inner electron shell.

8. Table S6. Filled and empty ranges for the r(LOL–shell), ρ(LOL–shell), V(LOL–shell), K(LOL–shell) and H(LOL–shell) parameters of the (3,–3) LOL–shell critical point for the elements of 4th period of periodic table.

E	**K**				**filled range**	**empty range**	**Ca**			**filled range**
E–X	**19a.** $KCH_3$②⊖	**19b.** KH●⊖	**19c.** K–*i*–Pr②⊖	**19d.** KCH_3●⊖	**K**	**K – Ca**	**20a.** CaH⊖	**20b.** CaH●	**20c.** $CaCH_3$⊖	**Ca**
r(LOL–shell)[a]	268.2	299.5	272.8	296.7	268.2 – 299.5	218.4 – 268.1	218.2	203.4	218.3	203.4 – 218.3
r(LOL–shell)[b]	57.1	56.8	57.0	57.0	56.8 – 57.1	52.0 – 56.7	51.6	51.8	51.9	51.6 – 51.9
r(LOL–shell)[c]	14.0	14.0	14.0	14.0	14.0	13.2 – 13.9	13.1	13.1	13.0	13.0 – 13.1
ρ(LOL–shell)[a]	0.00067	0.00095	0.00072	0.00090	0.00067 – 0.00095	0.00096 – 0.00308	0.00360	0.003501	0.00309	0.00309 – 0.00360
ρ(LOL–shell)[b]	0.46889	0.46830	0.46892	0.47103	0.46830 – 0.47103	0.47104 – 0.663461	0.66912	0.663462	0.69898	0.663462 – 0.69898
ρ(LOL–shell)[c]	25.96009	25.94390	25.94990	25.95243	25.94390 – 25.96009	25.96010 – 31.59649	31.96638	31.59650	32.15152	31.59650 – 32.15152
V(LOL–shell)[a]	–0.000075	–0.000047	–0.000081	–0.000052	–0.000081 ÷ –0.000047	–0.000364÷ –0.000082	–0.000372	–0.000654	–0.000365	–0.000654 ÷ –0.000365
V(LOL–shell)[b]	–1.511413	–1.521794	–1.512204	–1.523502	–1.523502 ÷ –1.511413	–2.695603 ÷ –1.523503	–2.728220	–2.695604	–2.788345	–2.788345 ÷ –2.695604
V(LOL–shell)[c]	–1137.546925	–1136.692971	–1136.921133	–1137.148413	–1137.546925 ÷ –1136.692971	–1580.177738 ÷ –1137.546926	–1613.925010	–1580.177739	–1635.097587	–1635.097587 ÷ –1580.177739
K(LOL–shell)[a]	0.000033	0.000014	0.000030	0.000017	0.000014 – 0.000033	0.000034 – 0.000144	0.000159	0.000307	0.000145	0.000145 – 0.000307
K(LOL–shell)[b]	0.543639	0.546733	0.543722	0.546326	0.543639 – 0.546733	0.546734 – 0.921400	0.957251	0.943708	0.921401	0.921401 – 0.957251
K(LOL–shell)[c]	488.019500	487.803784	487.814902	487.915944	487.803784 – 488.019500	488.019501 – 677.995498	692.210787	677.995499	690.207259	677.995499 – 692.210787
H(LOL–shell)[a]	–0.000043	–0.000033	–0.000050	–0.000035	–0.000050 ÷ –0.000033	–0.000212 ÷ –0.000051	–0.000213	–0.000346	–0.000219	–0.000346 ÷ –0.000213
H(LOL–shell)[b]	–0.967774	–0.975061	–0.968483	–0.977177	–0.977177 ÷ –0.967774	–1.751895 ÷ –0.977178	–1.770969	–1.751896	–1.866944	–1.866944 ÷ –1.751896
H(LOL–shell)[c]	–649.527425	–648.889187	–649.106428	–649.232469	–649.527425 ÷ –649.106428	–902.182239 ÷ –649.527426	–921.714223	–902.182240	–944.890328	–944.890328 ÷ –902.182240

E	**empty range**	**Ga**			**filled range**	**empty range**	**Ge**			
E–X	**Ca – Ga**	**21a.** GaH_2●	**21b.** GaH_2⊖	**21c.** GaH	**Ga**	**Ga – Ge**	**22a.** GeH_3●	**22b.** GeH_3⊖	**22c.** GeH_2	**22d.** $GeH_2$②⊖
r(LOL–shell)[a]	134.9 – 203.3	133.5	134.8	127.2	127.2 – 134.8	123.1 – 127.1	123.0	120.7	115.4	118.1
r(LOL–shell)[b]	29.7 – 51.5	29.6	29.6	29.6	29.6	28.3 – 29.5	28.2	28.1	28.1	28.1
r(LOL–shell)[c]	7.9 – 12.9	7.8	7.8	7.8	7.8	<0.1	7.6	7.7	7.6	7.6
ρ(LOL–shell)[a]	0.00361 – 0.02048	0.02049	0.02391	0.02721	0.02049 – 0.02721	0.02722 – 0.02994	0.02995	0.03971	0.04506	0.03947
ρ(LOL–shell)[b]	0.69899 – 6.77259	6.77344	6.79183	6.77260	6.77260 – 6.79183	6.79184 – 8.02941	8.02942	8.13370	8.14947	8.11268
ρ(LOL–shell)[c]	32.15153 – 157.57707	157.97432	158.00062	157.57708	157.57708 – 158.00062	158.00063 – 175.42616	175.94667	175.92282	175.42617	175.55841
V(LOL–shell)[a]	–0.009876 ÷ –0.000655	–0.010958	–0.009877	–0.013186	–0.013186 ÷ –0.009877	–0.019233 ÷ –0.013187	–0.019234	–0.021222	–0.027320	–0.022965
V(LOL–shell)[b]	–119.595315 ÷ –2.788346	–119.595316	–120.171058	–119.673835	–120.171058 ÷ –119.595316	–158.945124 ÷ –120.171059	–158.945125	–161.977999	–162.630378	–161.422266
V(LOL–shell)[c]	–23641.00864 ÷ –1635.097588	–23736.94658	–23739.85393	–23641.00865	–23739.85393 ÷ –23641.00865	–28175.75254 ÷ –23739.85394	–28311.99573	–28306.82298	–28175.75255	–28216.41767
K(LOL–shell)[a]	0.000308 – 0.006058	0.006398	0.006059	0.008870	0.006059 – 0.008870	0.008871– 0.009925	0.009926	0.010867	0.014852	0.012887
K(LOL–shell)[b]	0.957252 – 52.812282	52.812283	53.039081	52.873867	52.812283 – 53.039081	53.039082 – 69.595120	69.595121	70.598729	70.855685	70.437875
K(LOL–shell)[c]	692.210788 – 10183.57604	10218.02249	10218.02249	10183.57605	10183.57605 – 10218.02249	10218.02250 – 12236.6178	12288.30415	12287.1357	12236.61719	12255.30938
H(LOL–shell)[a]	–0.003817 ÷ –0.000347	–0.004560	–0.003818	–0.004317	–0.004560 ÷ –0.003818	–0.009307 ÷ –0.004561	–0.009308	–0.010355	–0.012469	–0.010078
H(LOL–shell)[b]	–66.783032 ÷ –1.866945	–66.783033	–67.131977	–66.799969	–67.131977 ÷ –66.783033	–89.349990 ÷ —67.131978	–89.35000	–91.379270	–91.774693	–90.984392
H(LOL–shell)[c]	–13518.74977 ÷ –944.890329	–13518.74978	–13521.83144	–13457.43260	–13457.43260 ÷ –13518.74978	–15939.13535 ÷ –13457.43261	–16023.69158	–16019.68728	–15939.13536	–15961.10829

E	**filled range**	**empty range**	**As**				**filled range**	**empty range**
E–X	**Ge**	**Ge – As**	**23a.** AsH_3	**23b.** AsH_3●	**23c.** AsH_2⊖	**23d.** AsH_2⊕	**As**	**As – Se**
r(LOL–shell)[a]	115.4 – 123.0	108.9 – 115.3	105.4	107.7	108.8	102.2	102.2 – 108.8	99.0 – 102.1
r(LOL–shell)[b]	28.1 – 28.2	27.0 – 28.0	26.8	26.9	26.9	26.8	26.8 – 26.9	25.7 – 26.7
r(LOL–shell)[c]	7.6 – 7.7	7.4 – 7.5	7.3	7.3	7.3	7.3	7.3	<0.2
ρ(LOL–shell)[a]	0.02995 – 0.04506	0.04507 – 0.04839	0.06702	0.04840	0.06024	0.07120	0.04840 – 0.07120	0.07121 – 0.08675
ρ(LOL–shell)[b]	8.02942 – 8.14947	8.14948 – 9.44626	9.59148	9.44627	9.53414	9.60793	9.44627 – 9.60793	9.60794 – 11.08240
ρ(LOL–shell)[c]	175.42617 – 175.94667	175.94668 – 196.87118	196.95358	196.88809	196.87119	197.43318	196.87119 – 197.43318	197.43319 – 219.47234
V(LOL–shell)[a]	–0.027320 ÷ –0.019234	–0.042702 ÷ –0.027321	–0.052902	–0.042703	–0.043677	–0.062312	–0.062312 ÷ –0.042703	–0.084838 ÷ –0.062313
V(LOL–shell)[b]	–162.630378 ÷ –158.945125	–208.158336 ÷ –162.630379	–212.901362	–208.158337	–210.941689	–213.695841	–213.695841 ÷ –208.158337	–270.962386 ÷ –213.695842
V(LOL–shell)[c]	–28306.82298 ÷ –28175.75255	–34187.10786 ÷ –28306.82299	–34204.71187	–34187.10787	–34188.69873	–34335.3458	–34335.3458 ÷ –34187.10787	–41092.96836 ÷ –34335.3459
K(LOL–shell)[a]	0.009926 – 0.012887	0.012888 – 0.021026	0.026374	0.022311	0.021027	0.032562	0.021027 – 0.032562	0.032563 – 0.041300
K(LOL–shell)[b]	69.595121 – 70.855685	70.855686 – 90.873247	92.423042	90.873248	91.822613	92.779764	90.873248 – 92.779764	92.779765 – 117.927865

K(LOL–shell)[c]	12236.61719 – 12288.30415	12288.30416 – 14863.580	14870.37439	14863.581	14867.39478	14916.79761	14863.581 – 14916.79761	14916.79762 – 17841.98545
H(LOL–shell)[a]	–0.012469 ÷ –0.009308	–0.020391 ÷ –0.012470	–0.026528	–0.020392	–0.022649	–0.029750	–0.029750 ÷ –0.020392	–0.043537 ÷ –0.029751
H(LOL–shell)[b]	–91.774693 ÷–89.35000	–117.285088 ÷ –91.774694	–120.478320	–117.285089	–119.119076	–120.916077	–120.916077 ÷ –117.285089	–153.034520 ÷ –120.916078
H(LOL–shell)[c]	–16023.69158 ÷ –15939.13536	–19321.30394 ÷ –16023.69159	–19334.33748	–19323.52687	–19321.30395	–19418.54819	–19418.54819 ÷ –19321.30395	–23250.98290 ÷ –19418.54820

E	**Se**				**filled range Se**	**empty range Se – Br**	**Br**		**filled range Br**
E–X	**24a.** SeH_2	**24b.** SeH⊖	**24c.** SeH⊕	**24d.** $SeH_2$②⊕			**25a.** BrH	**25b.** BrH_2⊕	
r(LOL–shell)[a]	97.3	98.9	95.0	92.3	92.3 – 98.9	90.0 – 92.4	89.9	86.4	86.4 – 89.9
r(LOL–shell)[b]	25.7	25.7	25.6	25.6	25.6 – 25.7	24.7 – 25.5	24.6	24.5	24.5 – 24.6
r(LOL–shell)[c]	7.0	7.1	7.0	7.0	7.0 – 7.1	<0.2	6.8	6.8	6.8
ρ(LOL–shell)[a]	0.09738	0.08676	0.11013	0.10487	0.08676 – 0.11013	0.11014 – 0.12944	0.12945	0.15563	0.12945 – 0.15563
ρ(LOL–shell)[b]	11.15163	11.08241	11.25272	11.22539	11.08241 – 11.25272	11.25273 – 12.87104	12.87105	13.07756	12.87105 – 13.07756
ρ(LOL–shell)[c]	219.58810	219.47235	220.38141	220.38932	219.47235 – 220.38932	220.38933 – 243.49559	243.49560	244.63522	243.49560 – 244.63522
V(LOL–shell)[a]	–0.096929	–0.084839	–0.114436	–0.123060	–0.123060 ÷ –0.084839	–0.165701 ÷ –0.123061	–0.165702	–0.212625	–0.212625 ÷ –0.165702
V(LOL–shell)[b]	–273.511375	–270.962387	–277.197651	–276.542875	–277.197651 ÷ –270.962387	–347.221258 ÷ –277.197652	–347.221259	–355.572975	–355.572975 ÷ –347.221259
V(LOL–shell)[c]	–41125.52521	–41092.96837	–41369.73058	–41330.15361	–41369.73058 ÷ –41092.96837	—48924.53700 ÷ –41369.73059	–48924.53701	–49293.03131	–49293.03131 ÷ –48924.53701
K(LOL–shell)[a]	0.044418	0.041301	0.049658	0.062095	0.041301 – 0.062095	0.062096 – 0.077726	0.077727	0.091679	0.077727 – 0.091679
K(LOL–shell)[b]	118.725351	117.927866	120.077123	119.791393	117.927866 – 120.077123	120.077124 – 150.831233	150.831234	153.704322	150.831234 – 153.704322
K(LOL–shell)[c]	17852.7434	17841.98546	17945.91529	17909.67341	17841.98546 – 17945.91529	17945.91530 – 21338.33057	21338.33058	21474.72244	21338.33058 – 21474.72244
H(LOL–shell)[a]	–0.052511	–0.043538	–0.064778	–0.060965	–0.064778 ÷ –0.043538	–0.087974 ÷ –0.064779	–0.087975	–0.120946	–0.120946 ÷ –0.087975
H(LOL–shell)[b]	–154.786024	–153.034521	–157.120529	–156.751481	–157.120529 ÷ –153.034521	–196.390023 ÷ –157.120530	–196.390024	–201.868653	–201.868653 ÷ –196.390024
H(LOL–shell)[c]	–23272.78181	–23250.98291	–23423.81529	–23420.48020	–23423.81529 ÷ –23250.98291	–27586.20642 ÷ –23423.81530	–27586.20643	–27818.30887	–27818.30887 ÷ –27586.20643

E	**empty range Br – Kr**	**Kr**	
E–X		**26a.** KrH⊕	**26b.** $KrCH_3$⊕
r(LOL–shell)[a]	82.5 – 86.3	82.0	82.4
r(LOL–shell)[b]	23.7 – 24.4	23.6	23.6
r(LOL–shell)[c]	<0.2	6.6	6.6
ρ(LOL–shell)[a]	0.15564 – 0.18217	0.18499	0.18218
ρ(LOL–shell)[b]	13.07757 – 14.88744	14.91092	14.88745
ρ(LOL–shell)[c]	244.63523 – 270.05666	270.12619	270.05667
V(LOL–shell)[a]	–0.311869 ÷ –0.212626	–0.317978	–0.311870
V(LOL–shell)[b]	–443.581396 ÷ –355.572976	–444.594109	–443.581397
V(LOL–shell)[c]	–58114.15507 ÷ –49293.03132	–58114.15508	–58116.15371
K(LOL–shell)[a]	0.091680 – 0.150542	0.152038	0.150543
K(LOL–shell)[b]	153.704323 – 191.878322	192.19147	191.878323
K(LOL–shell)[c]	21474.72245 – 25293.49433	25293.49434	25306.23871
H(LOL–shell)[a]	–0.161326 ÷ –0.120947	–0.165939	–0.161327
H(LOL–shell)[b]	–251.703073 ÷ –201.868654	–252.402639	–251.703074
H(LOL–shell)[c]	–32809.914990 ÷ –27818.30888	–32820.66074	–32809.91500

[a]The values refer to the outer electron shell; [b]the values refer to the first inner electron shell;
[c]the lower values refer to the second (closest to the atomic nucleus) inner electron shell.

9. Table S7. The value of electronegativity, atomic, covalent, van der Waals radii and energy of ionization for elements of 1st, 2nd, 3rd and 4th periods of periodic table.

№	element	electronegativity χ, Pauling	r(LOL), pm	radii, pm			energy of ionization[4], eV
				atomic[1]	covalent[2]	van der Waals[3]	
1	H	2.20	8.6	53	32	120	13.60
2	He	–	4.2	32	46	143	24.59
3	Li	0.98	159.7	167	133	212	5.39
4	Be	1.57	90.9	112	102	198	9.32
5	B	2.04	71.4	87	85	191	8.30
6	C	2.55	59.9	67	75	177	11.26
7	N	3.04	47.1	56	71	166	14.53
8	O	3.44	40.5	48	63	150	13.62
9	F	3.98	35.8	42	64	146	17.42
10	Ne	–	31.4	38	67	158	21.56
11	Na	0.93	216.9	190	155	250	5.14
12	Mg	1.31	141.2	145	139	251	7.65
13	Al	1.61	117.2	118	126	225	5.99
14	Si	1.90	101.4	111	116	219	8.15
15	P	2.19	85.3	98	111	190	10.49
16	S	2.58	76.5	88	103	189	10.36
17	Cl	3.16	69.2	79	99	182	12.97
18	Ar	–	62.2	71	96	183	15.76
19	K	0.82	268.2	243	196	273	4.34
20	Ca	1.00	218.2	194	171	262	6.11
31	Ga	1.81	133.5	136	124	232	6.00
32	Ge	2.01	123.0	125	121	229	7.90
33	As	2.18	105.4	114	121	188	9.79
34	Se	2.55	97.3	103	116	182	9.75
35	Br	2.96	89.9	94	114	186	11.81
36	Kr	–	82.0	88	117	225	14.0

1. E. Clementi, D. L. Raimondi and W. P. Reinhardt, *J. Chem. Phys.* 1967, **47**, 1300 – 1307.

2. P. Pyykkö and M. Atsumi, *Chem. Eur. J.* 2009, **15**, 186 – 197.

3. S. Alvarez, *Dalton Trans.*, 2013, **42**, 8617.

4. J. E. Sansonetti, W.C. Martin and S. L. Yong, *Handbook of Basic Atomic Spectroscopic Data*. 2004, National Institute of Standards and Technology, Gaithersburg, USA.

10. Table S8. The values of the calculated parameters for the (3,–3) LOL and ELF critical points related to the electron shells of element hydrides and methyls **3a–26a**[a]: the distance between the (3,–3) CPs LOL, ELF and the element nucleus (r(LOL-shell) and r(ELF-shell) in pm), the value of LOL and ELF at the (3,–3) LOL-shell and ELF-shell critical points, the value of ρ electron density at the (3,–3) LOL and ELF critical points (ρ(LOL-shell) and ρ(ELF-shell), in a.u.), the value of total H electron energy density at the (3,–3) LOL and ELF critical points (H(LOL-shell) and H(ELF-shell), in a.u).

No	structure	shell number	r(LOL–shell)	r(ELF–shell)	LOL–shell	ELF–shell	ρ(LOL–shell)	ρ(ELF–shell)	H(LOL–shell)	H(ELF–shell)
1st period										
1a	H		8.6		0.77361		0.235706		–1.259776	
2a	HeH⊕		4.2		0.77110		2.637644		–56.753499	
2nd period										
3a	LiH●⊖	1[b]	159.7	187.2	0.83583	0.99772	0.003370	0.002758	–0.000521	–0.000309
4a	BeH●	1	90.9	134.8	0.79328	0.99998	0.031525	0.013465	–0.016076	–0.002713
5a	BH_2●	1	71.4	128.6	0.70851	0.99096	0.079912	0.017221	–0.069750	–0.002992
6a	CH_3●	1	59.9	93.3	0.58975	0.91592	0.143062	0.046673	–0.172871	–0.017107
7a	NH_3	1	47.1	77.6	0.62301	0.95373	0.433379	0.126944	–0.815153	–0.055146
8a	OH_2	1	40.5	59.5	0.59972	0.91895	0.737219	0.300631	–1.927373	–0.253280
9a	FH	1	35.8	50.6	0.57947	0.88686	1.153258	0.511776	–3.950457	–0.634354
10a	NeH⊕	1	31.4	44.2	0.57783	0.88170	1.825768	0.809814	–8.258497	–1.373279
3rd period										
11a	NaH●⊖	1[b]	216.9	233.2	0.74142	0.98629	0.002036	0.001804	–0.000175	–0.000135
		2[c]	28.2	39.4	0.56889	0.86410	2.648198	1.201658	–14.990877	–2.864951
12a	MgH●	1	141.2	182.9	0.65696	0.99895	0.010438	0.005135	–0.002426	–0.000546
		2	25.0	34.3	0.57309	0.86750	3.956147	1.872124	–29.263476	–6.081514
13a	AlH_2●	1	117.2	162.8	0.71808	0.99773	0.026050	0.010556	–0.010504	–0.001682
		2	22.6	30.5	0.57484	0.86876	5.568760	2.706365	–50.566478	–11.493671
14a	SiH_3●	1	101.4	141.4	0.69177	0.98628	0.046218	0.018412	–0.026929	–0.004150
		2	20.5	27.7	0.57459	0.86862	7.572301	3.684395	–84.504852	–19.305191
15a	PH_3	1	85.3	118.8	0.69053	0.98975	0.105765	0.043576	–0.078230	–0.011326
		2	18.6	25.0	0.57700	0.86725	10.361623	5.104863	–143.164204	–34.040473
16a	SH_2	1	76.5	99.5	0.65976	0.96289	0.162196	0.084397	–0.159772	–0.038789
		2	17.2	22.7	0.57642	0.86531	13.412808	6.853390	–219.817929	–56.826740
17a	ClH	1	69.2	87.0	0.62076	0.91950	0.231341	0.132297	–0.288571	–0.086352
		2	15.9	20.9	0.57510	0.86320	17.047062	8.961013	–328.382360	–90.347600

18a	ArH⊕	1	62.2	77.8	0.61675	0.91627	0.340758	0.194675	–0.557928	–0.161556
		2	14.9	19.2	0.57473	0.86083	21.293736	11.600451	–470.813419	–142.912160
4th period										
19a	$KCH_3$②⊖	1[b]	268.2	277.4	0.30933	0.37121	0.000665	0.000606	–0.000043	–0.000035
		2[c]	57.1	70.1	0.59914	0.88222	0.468889	0.283535	–0.967774	–0.305399
		3[d]	14.0	17.8	0.57248	0.85580	25.960089	14.722280	–649.527425	–215.780357
20a	CaH⊖	1	218.2	246.1	0.60399	0.98055	0.003596	0.002618	–0.000213	–0.000158
		2	51.6	61.8	0.60558	0.88581	0.669117	0.432462	–1.770969	–0.679772
		3	13.1	16.5	0.57183	0.85350	31.966382	18.533133	–921.714223	–321.797323
21a	GaH_2●	1	133.5	170.8	0.48415	0.96622	0.020488	0.007941	–0.004560	–0.000607
		2	29.6	34.4	0.56866	0.77580	6.773438	4.642486	66.783033	–31.511063
		3	7.8	9.0	0.56469	0.80150	157.974324	116.853307	–13518.749780	–7464.670300
22a	GeH_3●	1	123.0	158.7	0.53633	0.96531	0.029948	0.011826	–0.009308	–0.001562
		2	28.2	32.9	0.57051	0.77751	8.029421	5.477499	–89.350001	–41.793248
		3	7.6	8.7	0.56348	0.79705	175.946670	131.619374	–16023.691580	–9093.975953
23a	AsH_3	1	105.4	133.9	0.54625	0.97716	0.067020	0.029063	–0.026528	–0.004202
		2	26.8	31.1	0.57358	0.78120	9.591482	6.644906	–120.478320	–58.080467
		3	7.3	8.4	0.56281	0.79267	196.953579	148.697903	–19334.337480	–11187.429620
24a	SeH_2	1	97.3	117.8	0.57123	0.95581	0.097376	0.052955	–0.052511	–0.015292
		2	25.7	29.7	0.57377	0.78162	11.151628	7.721873	–154.786024	–74.506297
		3	7.0	8.0	0.56244	0.78978	219.588104	167.809988	–23272.781810	–13751.515260
25a	BrH	1	89.9	105.3	0.55028	0.91034	0.129446	0.079553	–0.087975	–0.033208
		2	24.6	28.5	0.57368	0.78167	12.871053	8.911306	–196.390024	–94.459803
		3	6.8	7.8	0.56094	0.78518	243.495600	187.168019	–27586.206430	–16514.267640
26b[a]	$KrCH_3$⊕	1	82.4	99.6	0.52755	0.88133	0.182179	0.097759	–0.161327	–0.045283
		2	23.6	27.2	0.57414	0.78245	14.887451	10.358985	–251.703074	–122.505984
		3	6.6	7.5	0.56144	0.78297	270.056671	209.706874	–32809.915000	–20016.812560

[a] No (3,–3) ELF critical points were found for compounds **1a**, **2a** and **26a**.

[b]The values refer to the outer electron shell.

[c]The values refer to the first inner electron shell;

[d]The lower values refer to the second (closest to the atomic nucleus) inner electron shell.

11. Cartesian coordinates (in Å) of studied compounds, optimized at the (u)B3LYP/AQZP//ATZP level in gas phase.

Compound: **1a** H●
H 0.000000000 0.000000000 0.000000000

Compound: **2a** HeH⊕
He –0.697000000 –0.071967000 –0.003000000
H –0.697000000 0.715967000 –0.003000000

Compound: **3a** LiH●⊖
Li 0.183000000 –0.254858000 0.000000000
H 0.183000000 1.410858000 0.000000000

Compound: **3b** $LiCH_3$②⊖
Li 0.891001000 –1.726416000 –0.000000000
C 0.890971000 0.274684000 0.000000000
H 1.906030000 0.692921000 0.000000000
H 0.383446000 0.692891000 –0.879073000
H 0.383446000 0.692891000 0.879073000

Compound: **4a** BeH●
Be 0.183000000 –0.091757000 0.000000000
H 0.183000000 1.247757000 0.000000000

Compound: **4b** BeH⊖
Be –0.691000000 0.366301000 0.000000000
H –0.691000000 –1.044301000 0.000000000

Compound: **5a** BH_2●
B –0.690690000 0.122837000 –0.000000000
H 0.381705000 –0.380835000 –0.000000000
H –1.763014000 –0.381002000 –0.000000000

Compound: **5b** BH_2⊖
B –0.690706000 0.277527000 0.000000000
H 0.296721000 –0.458166000 0.000000000
H –1.678015000 –0.458361000 0.000000000

Compound: **5c** BH
B –0.730103000 0.189559000 0.000000000
H 0.336103000 –0.425559000 –0.000000000

Compound: **6a** CH_3●
C –0.000134000 0.000090000 –0.121020000
H –1.002468000 –0.226847000 0.242197000
H 0.305208000 0.980973000 0.242105000
H 0.698067000 –0.754666000 0.241818000

Compound: **6b** CH_3⊖
C –0.690691000 0.077416000 –0.000000000
H 0.349148000 –0.275402000 0.000000000
H –1.210147000 –0.275520000 0.900544000

H –1.210147000 –0.275520000 –0.900544000

Compound: **6c** CH_2
C –0.709271000 0.111078000 –0.032100000
H 0.321503000 –0.290986000 0.030191000
H –1.170231000 –0.291092000 0.891909000

Compound: **6d** $CH_2$②⊖
C –0.725597000 0.134108000 –0.060341000
H 0.347324000 –0.302489000 0.034091000
H –1.179727000 –0.302620000 0.916249000

Compound: **7a** NH_3
N –0.731443000 –0.008448000 –0.070499000
H –0.713322000 1.002770000 –0.038709000
H 0.228058000 –0.328350000 –0.038497000
H –1.183293000 –0.327972000 0.776704000

Compound: **7b** NH_3●⊕
N 0.000023000 –0.000077000 –0.111561000
H 0.838199000 –0.427861000 0.260410000
H –0.790017000 –0.511471000 0.260349000
H –0.048345000 0.939869000 0.260165000

Compound: **7c** NH_2⊖
N –0.750471000 –0.022075000 –0.049000000
H –0.689886000 1.002021000 –0.049000000
H 0.235358000 –0.305946000 –0.049000000

Compound: **7d** NH_2⊕
N –0.741830000 –0.015958000 –0.049000000
H –0.721770000 1.037935000 –0.049000000
H 0.258600000 –0.347977000 –0.049000000

Compound: **8a** OH_2
O –0.758998000 –0.086272000 –0.003000000
H –0.722748000 0.873285000 –0.003000000
H 0.157746000 –0.372013000 –0.003000000

Compound: **8b** OH⊕
O –0.743000000 –0.114272000 –0.003000000
H –0.743000000 0.924272000 –0.003000000

Compound: **8c** $OH_2$②⊕
O –0.755877000 –0.084063000 –0.003000000
H –0.895044000 1.113665000 –0.003000000
H 0.326921000 –0.614602000 –0.003000000

Compound: **9a** FH
F –0.697000000 –0.138994000 –0.003000000
H –0.697000000 0.782994000 –0.003000000

Compound: **9b** FH_2⊕

F 0.000000000 0.000000000 0.140000000
H 0.000000000 0.000000000 –1.260000000

Compound: **10a** $NeH^{\oplus}$
Ne –0.697000000 –0.180888000 –0.003000000
H –0.697000000 0.824888000 –0.003000000

Compound: **11a** $NaH^{\bullet\ominus}$
Na 0.183000000 –0.424966000 0.000000000
H 0.183000000 1.580966000 0.000000000

Compound: **11b** $NaCH_3^{(2)\ominus}$
Na 0.891016000 –1.989738000 0.000000000
C 0.891619000 0.375814000 0.000000000
H 1.921953000 0.746804000 0.000000000
H 0.376664000 0.747427000 –0.892163000
H 0.376664000 0.747427000 0.892163000

Compound: **11c** $NaH^{(2)\ominus}$
Na 0.183000000 –0.404551000 0.000000000
H 0.183000000 1.560551000 0.000000000

Compound: **11d** $NaCH_3^{\bullet\ominus}$
Na 0.890771000 –2.037025000 0.000000000
C 0.890822000 0.371088000 0.000000000
H 1.916417000 0.764867000 0.000000000
H 0.378043000 0.763909000 –0.888432000
H 0.378043000 0.763909000 0.888432000

Compound: **12a** $MgH^{\bullet}$
Mg 0.183000000 –0.292190000 0.000000000
H 0.183000000 1.448190000 0.000000000

Compound: **12b** $MgH^{\ominus}$
Mg –0.691000000 0.596610000 0.000000000
H –0.691000000 –1.274610000 0.000000000

Compound: **13a** $AlH_2^{\bullet}$
Al –0.690733000 0.335618000 0.000000000
H 0.680382000 –0.487198000 0.000000000
H –2.061649000 –0.487420000 0.000000000

Compound: **13b** $AlH_2^{\ominus}$
Al –0.690717000 0.546882000 0.000000000
H 0.556208000 –0.592817000 0.000000000
H –1.937491000 –0.593065000 0.000000000

Compound: **13c** AlH
Al –0.916731000 0.297230000 0.000000000
H 0.522731000 –0.533230000 –0.000000000

Compound: **14a** $SiH_3^{\bullet}$
Si –0.126757000 0.029483000 –0.054973000

H	–0.148681000	1.512033000	–0.092257000
H	1.263413000	–0.486057000	–0.092747000
H	–0.854975000	–0.485459000	1.129977000

Compound: **14b** $SiH_3\ominus$

Si	–0.697139000	0.415567000	0.000000000
H	0.615198000	–0.392711000	–0.000000000
H	–1.359035000	–0.382924000	1.140708000
H	–1.359035000	–0.382924000	–1.140708000

Compound: **14c** SiH_2

Si	–0.808681000	0.251362000	–0.204133000
H	0.571365000	–0.361108000	0.000574000
H	–1.320684000	–0.361254000	1.093559000

Compound: **15a** PH_3

P	–0.869638000	–0.106259000	–0.313705000
H	–0.708927000	1.274539000	–0.028969000
H	0.485786000	–0.414729000	–0.028727000
H	–1.307221000	–0.415551000	1.000401000

Compound: **15b** $PH_3\bullet$

P	–0.731907000	–0.008819000	–0.074418000
H	–0.781151000	1.391594000	–0.153608000
H	0.572090000	–0.521864000	–0.153352000
H	–1.459031000	–0.522912000	1.010376000

Compound: **15c** $PH_2\ominus$

P	–0.942117000	–0.157662000	–0.049000000
H	–0.728738000	1.260192000	–0.049000000
H	0.465855000	–0.428530000	–0.049000000

Compound: **15d** $PH_2\oplus$

P	–0.941852000	–0.157484000	–0.049000000
H	–0.725335000	1.255103000	–0.049000000
H	0.462188000	–0.423618000	–0.049000000

Compound: **16a** SH_2

S	–0.946363000	–0.218756000	–0.003000000
H	–0.749801000	1.110286000	–0.003000000
H	0.372164000	–0.476530000	–0.003000000

Compound: **16b** $SH\oplus$

S	–0.743000000	–0.281010000	–0.003000000
H	–0.743000000	1.091010000	–0.003000000

Compound: **16c** $SH_2②\oplus$

S	–0.970789000	–0.236023000	–0.003000000
H	–0.785849000	1.187171000	–0.003000000
H	0.432638000	–0.536148000	–0.003000000

Compound: **17a** ClH

Cl	–0.697000000	–0.319288000	–0.003000000

H –0.697000000 0.963288000 –0.003000000

Compound: **17b** $ClH_2\oplus$
Cl –0.697000000 –0.421425000 –0.003000000
H –0.697000000 1.065425000 –0.003000000

Compound: **18a** $ArH\oplus$
Ar –0.697000000 –0.324755000 –0.003000000
H –0.697000000 0.968755000 –0.003000000

Compound: **19a** $KCH_3②\ominus$
K 0.892616000 –2.316315000 –0.000000000
C 0.893768000 0.437370000 –0.000000000
H 1.918029000 0.833266000 –0.000000000
H 0.383205000 0.837416000 –0.886025000
H 0.383205000 0.837416000 0.886025000

Compound: **19b** $KH\bullet\ominus$
K 0.183000000 –0.618926000 0.000000000
H 0.183000000 1.774926000 0.000000000

Compound: **19c** K–*i*–Pr②⊖
K –0.386803000 –1.679364000 0.326543000
C –0.295510000 1.127302000 0.168398000
C 1.110017000 1.710276000 0.235690000
C –1.056628000 1.710323000 –1.015097000
H –0.826981000 1.410634000 1.089030000
H 1.134772000 2.824630000 0.212454000
H 1.643259000 1.408834000 1.143517000
H 1.731144000 1.391362000 –0.611059000
H –1.048780000 2.824677000 –1.048185000
H –0.634012000 1.391347000 –1.976416000
H –2.109479000 1.408979000 –1.022875000

Compound: **19d** $KCH_3\bullet\ominus$
K 0.893214000 –2.349856000 0.000000000
C 0.893273000 0.441854000 0.000000000
H 1.916568000 0.842432000 0.000000000
H 0.383768000 0.847367000 –0.884880000
H 0.383768000 0.847367000 0.884880000

Compound: **20a** $CaH\ominus$
Ca –0.691000000 0.772960000 0.000000000
H –0.691000000 –1.450960000 0.000000000

Compound: **20b** $CaH\bullet$
Ca 0.183000000 –0.460176000 0.000000000
H 0.183000000 1.616176000 0.000000000

Compound: **20c** $CaCH_3\ominus$
Ca 0.890492000 –2.062774000 0.000000000
C 0.890983000 0.352446000 0.000000000
H 1.907776000 0.780170000 0.000000000

H	0.382138000	0.778379000	–0.881059000
H	0.382138000	0.778379000	0.881059000

Compound: **21a** GaH_2●

Ga	–0.690726000	0.316848000	0.000000000
H	0.688647000	–0.477827000	0.000000000
H	–2.069921000	–0.478021000	0.000000000

Compound: **21b** $GaH_2\ominus$

Ga	–0.690697000	0.563195000	0.000000000
H	0.558387000	–0.600996000	0.000000000
H	–1.939690000	–0.601199000	0.000000000

Compound: **21c** GaH

Ga	–0.924271000	0.301579000	0.000000000
H	0.530271000	–0.537579000	–0.000000000

Compound: **22a** GeH_3●

Ge	–0.119492000	0.034614000	–0.042229000
H	–0.154738000	1.531678000	–0.103039000
H	1.279934000	–0.498317000	–0.103551000
H	–0.872703000	–0.497975000	1.138819000

Compound: **22b** $GeH_3\ominus$

Ge	–0.698616000	0.414497000	–0.000000000
H	0.630856000	–0.392771000	0.000000000
H	–1.369694000	–0.381755000	1.155441000
H	–1.369694000	–0.381755000	–1.155441000

Compound: **22c** GeH_2

Ge	–0.807296000	0.249406000	–0.201734000
H	0.573936000	–0.360135000	–0.002503000
H	–1.324640000	–0.360271000	1.094237000

Compound: **22d** $GeH_2\textcircled{2}\ominus$

Ge	–0.806594000	0.248423000	–0.200534000
H	0.595331000	–0.359629000	–0.015687000
H	–1.346737000	–0.359795000	1.106220000

Compound: **23a** AsH_3

As	–0.897464000	–0.125939000	–0.363199000
H	–0.709175000	1.336645000	–0.028960000
H	0.544269000	–0.435655000	–0.028711000
H	–1.337630000	–0.437051000	1.049870000

Compound: **23b** AsH_3●

As	–0.743377000	–0.016934000	–0.093533000
H	–0.787285000	1.461503000	–0.167037000
H	0.635962000	–0.550942000	–0.166766000
H	–1.505300000	–0.555628000	1.056335000

Compound: **23c** $AsH_2\ominus$

As	–0.983250000	–0.186740000	–0.049000000

H –0.737508000 1.316210000 –0.049000000
H 0.515758000 –0.455469000 –0.049000000

Compound: **23d** $AsH_2\oplus$
As –0.982406000 –0.186148000 –0.049000000
H –0.732502000 1.308232000 –0.049000000
H 0.509907000 –0.448084000 –0.049000000

Compound: **24a** SeH_2
Se –1.001140000 –0.257482000 –0.003000000
H –0.757240000 1.178904000 –0.003000000
H 0.434379000 –0.506422000 –0.003000000

Compound: **24b** $SeH\ominus$
Se –0.743000000 –0.325004000 –0.003000000
H –0.743000000 1.135004000 –0.003000000

Compound: **24c** $SeH\oplus$
Se –0.743000000 –0.333544000 –0.003000000
H –0.743000000 1.143544000 –0.003000000

Compound: **24d** $SeH_2②\oplus$
Se –1.025468000 –0.274680000 –0.003000000
H –0.782757000 1.240796000 –0.003000000
H 0.484225000 –0.551116000 –0.003000000

Compound: **25a** BrH
Br –0.697000000 –0.385078000 –0.003000000
H –0.697000000 1.029078000 –0.003000000

Compound: **25b** $BrH_2\oplus$
Br –0.697000000 –0.450276000 –0.003000000
H –0.697000000 1.094276000 –0.003000000

Compound: **26a** $KrH\oplus$
Kr –0.697000000 –0.394797000 –0.003000000
H –0.697000000 1.038797000 –0.003000000

Compound: **26b** $KrCH_3\oplus$
Kr 0.891042000 –1.690437000 0.000000000
C 0.891864000 0.441634000 –0.000000000
H 1.958219000 0.625253000 0.000000000
H 0.359027000 0.625905000 –0.923515000
H 0.359027000 0.625905000 0.923515000