Supporting Information
Theoretical Study of Complexes of *Closo* Borane, Alane and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [A₁₂H₁₂²⁻] (A = B, Al, and Ga)
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Table S1. Calculated^a geometrical parameters, distances *R* (Å) and angles φ (degrees) of *closo*-boranes, alanes, and gallanes Lⁿ⁺·A₁₂H₁₂²⁻ (L, C_{3v}(I)).

L ⁿ⁺ ·B ₁₂ H ₁₂ ²⁻										
L ⁿ⁺	Li ⁺	Be ²⁺	Na ⁺	Mg ²⁺	Al ⁺	Cu ⁺	Zn ²⁺	Ga ⁺	Al ³⁺	
R(L ₁ A ₂)	2.137	1.797	2.518	2.217	2.417	2.179	2.158	2.498	2.158	
R(A ₂ A ₃)	1.789	1.808	1.794	1.813	1.781	1.812	1.836	1.788	1.817	
R(L ₁ H ₁₄)	1.900	1.545	2.203	1.956	2.107	1.973	1.973	2.197	1.889	
R(A ₂ H ₁₄)	1.226	1.288	1.223	1.260	1.220	1.243	1.257	1.221	1.269	
R(A ₂ A ₇)	1.779	1.776	1.779	1.772	1.779	1.777	1.765	1.779	1.750	
R(A ₂ A ₈)	1.761	1.730	1.766	1.742	1.768	1.760	1.748	1.771	1.744	
R(A ₇ A ₈)	1.796	1.813	1.794	1.811	1.798	1.801	1.822	1.798	1.837	
R(A ₇ A ₁₃)	1.779	1.773	1.783	1.780	1.778	1.780	1.786	1.779	1.787	
R(A ₈ A ₁₃)	1.788	1.791	1.786	1.786	1.784	1.785	1.780	1.783	1.781	
R(A ₁₂ A ₁₃)	1.792	1.802	1.790	1.802	1.795	1.795	1.821	1.795	1.915	
φ(H ₁₄ L ₁ H ₁₅)	101.8 ^b	117.1 ^b	88.0 ^b	100.4 ^b	91.1 ^b	101.1 ^b	102.8 ^b	88.5 ^b	103.3 ^b	
φ(L ₁ H ₁₄ A ₂)	83.3	78.2	89.9	84.0	89.1	81.9	80.5	89.2	83.8	
φ(A ₂ A ₇ A ₃)	60.4	61.2	60.5	61.5	60.1	61.3	62.7	60.3	62.6	

a)

b)

$L^{n+} \cdot Al_{12}H_{12}^{2-}$								
L^{n+}	Li^+	Be^{2+}	Na^+	Mg^{2+}	Al^{3+}	Cu^+	Ga^+	
$R(L_1A_2)$	2.654	2.299	2.985	2.689	2.546	2.322	2.977	
$R(A_2A_3)$	2.695	2.730	2.706	2.746	2.822	2.797	2.727	
$R(L_1H_{14})$	1.984	1.471	2.538	1.904	1.659	1.723	2.547	
$R(A_2H_{14})$	1.648	1.756	1.746	1.726	1.932	1.719	1.619	
$R(A_2A_7)$	2.677	2.679	2.681	2.673	2.688	2.672	2.693	
$R(A_2A_8)$	2.630	2.611	2.640	2.609	2.610	2.608	2.670	
$R(A_7A_8)$	2.753	2.802	2.742	2.793	2.845	2.768	2.732	
$R(A_7A_{13})$	2.706	2.696	2.702	2.699	2.694	2.665	2.685	
$R(A_8A_{13})$	2.673	2.672	2.678	2.677	2.692	2.707	2.690	
$R(A_{12}A_{13})$	2.718	2.742	2.711	2.730	2.756	2.729	2.721	
$\varphi(H_{14}L_1H_{15})$	112.9 ^b	119.7 ^c	103.3 ^b	114.2 ^b	120.0	120.0	103.2 ^b	
$\varphi(L_1H_{14}A_2)$	93.5	90.4	94.5	95.5	90.0	84.9	88.3	
$\varphi(A_2A_7A_3)$	59.6	59.2	59.7	59.2	63.3	61.6	60.8	

c)

$L^{n+} \cdot Ga_{12}H_{12}^{2-}$											
L^{n+}	Li^+	$Be^{2+}(b)$	$Be^{2+}(s)^d$	Na^+	Mg^{2+}	Ga^+	$Ga^{3+}(b)$	$Ga^{3+}(s)$	$Al^{3+}(s)$		
$R(L_1A_2)$	2.601	2.254	2.176	2.928	2.643	2.828	2.829	2.430	2.474		
$R(A_2A_3)$	2.592	2.644	3.757	2.606	2.633	2.615	2.757	4.055	4.037		
$R(L_1H_{14})$	2.038	1.476	3.202	2.391	1.931	2.501	2.480	3.530	3.536		
$R(A_2H_{14})$	1.617	1.746	1.542	1.608	1.708	1.580	1.575	1.540	1.540		
$R(A_2A_7)$	2.567	2.557	2.612	2.566	2.556	2.569	2.488	2.750	2.726		
$R(A_2A_8)$	2.505	2.484	2.444	2.515	2.479	2.533	2.567	2.492	2.501		
$R(A_7A_8)$	2.646	2.719	2.663	2.634	2.703	2.620	2.766	2.650	2.649		
$R(A_7A_{13})$	2.538	2.536	2.581	2.547	2.534	2.555	2.594	2.605	2.610		
$R(A_8A_{13})$	2.578	2.558	2.561	2.576	2.569	2.565	2.523	2.556	2.555		
$R(A_{12}A_{13})$	2.594	2.627	2.597	2.589	2.611	2.596	2.988	2.546	2.548		
$\phi(H_{14}L_1H_{13})^c$	112.3 ^b	119.7 ^c	108.3 ^c	102.5 ^b	113.8 ^b	104.7 ^b	106.8 ^b	119.0 ^c	119.9 ^c		
$\phi(L_1H_{14}A_2)$	90.0	68.4	36.9	92.0	93.0	84.5	25.4	34.9	36.5		
$\phi(A_2A_7A_3)$	60.7	62.3	92.0	61.0	62.0	61.2	67.3	95.2	95.5		
$\phi(A_{12}A_8A_{13})$	60.4	61.8	60.9	60.3	61.1	60.8	72.6	59.7	59.8		

^aData for B3LYP calculations with the 6-311+G* basis set for boranes and alanes and 6-311G* for gallanes. Extension of the basis set to 6-311+G** does not affect the results significantly.

^bAtom L is located above hydrogen atoms H_{14} , H_{15} , and H_{16} .

^cAtom L is located below hydrogen atoms H_{14} , H_{15} , and H_{16} .

^d $N_m=2$.

Table S2. Calculated^a geometrical parameters, distances R (Å) and angles φ (degrees) of *cislo*- boranes, alanes, and gallanes $L^{n+}A_{12}H_{12}^{2-}$ (2 C₂(b)).

a)

		$L^{n+}B_{12}H_{12}^{2-}$							
L^{n+}	Li^+	Be^{2+}	Na^+	Mg^{2+}	Al^+	Cu^+	Zn^{2+}	Ga^+	
RL_1A_2	2.109	1.729	2.460	2.166	2.354	1.984	2.056	2.365	
RA_2A_3	1.805	1.892	1.809	1.855	1.778	1.823	1.854	1.788	
RL_1H_{12}	1.784	1.456	2.057	1.882	1.967	1.692	1.855	2.046	
RA_2H_{12}	1.233	1.315	1.230	1.267	1.223	1.295	1.271	1.220	
$RA_{12}A_{13}$	1.788	1.796	1.786	1.798	1.793	1.794	1.813	1.792	
$RA_{12}H_{22}$	1.198	1.189	1.199	1.190	1.196	1.197	1.189	1.196	
$\varphi(A_2L_1A_3)$	50.7	66.4	43.1	50.7	44.4	54.7	53.6	44.4	
$\varphi(H_{14}L_1H_{15})^b$	122.1	162.0	103.0	122.0	106.9	135.3	128.6	106.6	
$\varphi(H_{14}A_2A_3)$	122.3	112.0	125.0	124.5	124.4	120.3	125.8	127.7	
$\varphi(H_{24}A_{12}A_{13})$	121.8	121.4	122.0	121.4	122.2	121.6	121.0	122.3	

b)

L^{n+}	$L^{n+}Al_{12}H_{12}^{2-}$						
	Li^+	Be^{2+}	Na^+	Mg^{2+}	Al^{3+}	Cu^+	Ga^+
$R(L_1A_2)$	2.586	2.164	2.900	2.578	2.427	2.412	2.820
$R(A_2A_3)$	2.724	2.994	2.731	2.907	3.950	2.764	2.753
$R(L_1H_{14})$	1.856	1.420	2.193	1.896	1.749	1.672	2.338
$R(A_2H_{14})$	1.663	1.813	1.654	1.731	1.795	1.761	1.621
$R(A_{12}A_{13})$	2.708	2.722	2.702	2.716	2.728	2.708	2.705
$R(A_{12}H_2)$	1.597	1.585	1.598	1.586	1.578	1.594	1.595
$\varphi(A_2L_1A_3)$	63.6	87.6	56.2	68.5	108.9	69.9	58.4
$\varphi(H_{14}L_1H_{13})^b$	143.4	200.1	125.1	153.0	204.1	163.8	128.6
$\varphi(H_{14}A_2A_3)$	103.9	86.9	110.6	103.0	81.5	98.9	116.8
$\varphi(H_{14}A_{12}A_{13})$	121.2	120.5	121.5	121.7	121.3	121.5	122.4

c)

L^{n+}	$L^{n+}, Ga_{12}H_{12}^{2-}$					
	Li^+	Na^+	$Be^{2+}(b)^c$	$Be^{2+}(s)^c$	Mg^{2+}	Ga^+
$R(L_1A_2)$	2.483	2.841	2.148	2.182	2.544	2.742
$R(A_2A_3)$	2.630	2.640	2.771	4.149	2.744	2.586
$R(L_1H_{14})$	1.876	2.216	1.416	3.042	1.902	2.307
$R(A_2H_{14})$	1.628	1.620	1.853	1.549	1.720	1.586
$R(L_1A_4)$	3.480	3.823	3.023	2.222	3.142	3.766
$R(A_4A_5)$	4.240	4.223	4.312	3.874	4.268	4.270
$R(A_{12}A_{13})$	2.574	2.570	2.597	2.482	2.580	2.582
$R(A_{12}H_{26})$	1.555	1.556	1.545	1.544	1.547	1.555
$\varphi(A_2L_1A_3)$	64.0	55.4	80.3	143.8	65.3	56.3
$\varphi(H_{14}L_1H_{15})^b$	145.9	124.6	197.2	201.8	150.3	126.9
$\varphi(H_{14}A_2A_3)$	107.1	113.4	90.4	126.1	105.7	119.1
$\varphi(H_{24}A_{12}A_{13})$	121.2	121.3	119.3	130.0	121.0	122.2
$\theta(A_4A_3A_2A_3)^d$	127.2	126.1	141.9	157.7	138.5	124.2

^aData of B3LYP/6-31G* calculations.^bThe values larger 180° indicate that atom L is located below hydrogen atoms H_{14} and H_{15} .^cIn this cases “bridged” and “skeletal” $Be^{2+}Ga_{12}H_{12}^{2-}$ are local minima.^d $\theta(A_4A_3A_2A_3)$ in icosahedron is 116.6°.

Table S3. Calculated^a vibrational frequencies ν_i (cm⁻¹) of *closo*-boranes, alanes, and gallanes $L^{n+}A_{12}H_{12}^{2-}$ ($L = \text{Li, Be, Na, Mg, Al, Cu, Zn, Ga, Al}^{3+}$).

L ⁿ⁺ .B ₁₂ H ₁₂ ²⁻									
L ⁿ⁺	Li ⁺	Be ²⁺	Na ⁺	Mg ²⁺	Al ⁺	Cu ⁺	Zn ²⁺	Ga ⁺	Al ³⁺
1e	258 (27)	409 (15)	153 (12)	227 (18)	157 (5)	113 (1)	170 (6)	123 (4)	218 (3)
7e	727 (9)	726 (1)	724 (8)	723 (6)	727 (12)	720 (4)	705 (3)	724 (8)	655 (1)
11e	804 (2)	861 (2)	798 (1)	832 (3)	800 (12)	793 (1)	813 (3)	801 (9)	742 (12)
17e	969 (0)	992 (17)	967 (0)	958 (2)	968 (3)	964 (1)	949 (0)	965 (1)	931 (0)
18e	1029 (13)	1040 (0)	1032 (14)	1026 (7)	992 (0)	992 (10)	978 (0)	1006 (0)	972 (1)
19e	1120 (22)	1241 (11)	1119 (28)	1172 (5)	1087 (22)	1102 (19)	1076 (7)	1080 (22)	1083 (2)
20e	2338 (116)	2047 (17)	2341 (166)	2109 (67)	2394 (1)	2169 (86)	2201 (12)	2400 (1)	2136 (3)
21e	2598 (54)	2681 (29)	2584 (106)	2662 (60)	2618 (1)	2607 (2)	2667 (45)	2614 (1)	2685 (1)
22e	2602 (12)	2686 (0)	2594 (0)	2672 (13)	2624 (46)	2613 (47)	2685 (2)	2621 (35)	2702 (14)
23e	2615 (564)	2693 (222)	2605 (584)	2680 (255)	2636 (499)	2625 (538)	2692 (256)	2632 (529)	2738 (6)
1a ₁	480 (112)	545 (16)	262 (56)	369 (33)	286 (133)	269 (16)	261 (1)	186 (76)	258 (136)
2a ₁	612 (21)	633 (2)	595 (1)	602 (0)	583 (3)	591 (8)	545 (28)	586 (3)	428 (121)
3a ₁	658 (1)	684 (33)	660 (0)	632 (17)	650 (0)	653 (0)	597 (23)	649 (0)	606 (13)
4a ₁	713 (4)	700 (0)	713 (5)	696 (5)	694 (6)	681 (17)	659 (22)	690 (2)	611 (20)
5a ₁	747 (5)	734 (13)	744 (4)	729 (14)	736 (6)	730 (3)	714 (14)	736 (11)	688 (10)
8a ₁	837 (34)	914 (0)	820 (4)	872 (1)	810 (66)	823 (36)	812 (5)	818 (34)	756 (531)
10a ₁	947 (0)	1013 (13)	949 (0)	939 (9)	944 (0)	940 (1)	902 (25)	937 (0)	902 (12)
11a ₁	1002 (3)	1047 (9)	1002 (0)	993 (26)	984 (0)	949 (20)	935 (6)	997 (2)	925 (2)
12a ₁	1093 (90)	1223 (259)	1097 (651)	1075 (0)	1087 (87)	1067 (65)	1019 (32)	1081 (71)	991 (139)
13a ₁	2380 (831)	2117 (395)	2383 (927)	2165 (378)	2439 (4)	2207 (623)	2222 (59)	2436 (71)	2145 (92)
14a ₁	2597 (51)	2680 (20)	2582 (70)	2662 (16)	2621 (19)	2609 (25)	2678 (15)	2618 (10)	2694 (0)
15a ₁	2607 (195)	2688 (82)	2597 (171)	2674 (66)	2625 (195)	2615 (195)	2686 (80)	2622 (203)	2706 (7)
16a ₁	2636 (161)	2705 (104)	2627 (197)	2693 (239)	2652 (180)	2643 (201)	2705 (234)	2649 (196)	2756 (58)

b)

$L^{n+} \cdot Al_2H_{12}^{2-}$							
L^{n+}	Li^+	Be^{2+}	Na^+	Mg^{2+}	Al^{3+}	Cu^+	Ga^+
1e	159 (2)	147 (1)	97 (4)	135 (3)	125 (1)	126 (0)	38 (4)
9e	317 (8)	318 (8)	314 (8)	315 (12)	309 (15)	317 (6)	312 (22)
11e	362 (4)	396 (2)	344 (1)	380 (5)	371 (0)	374 (4)	334 (0)
15e	464 (3)	446 (0)	464 (2)	447 (4)	409 (3)	463 (4)	451 (1)
17e	499 (36)	514 (103)	488 (12)	487 (59)	456 (52)	510 (103)	460 (4)
18e	570 (101)	719 (45)	546 (87)	575 (128)	546 (54)	627 (99)	471 (1)
19e	662 (153)	1152 (0)	639 (190)	1016 (40)	655 (32)	948 (14)	564 (264)
20e	1618 (120)	1510 (85)	1638 (177)	1314 (107)	1602 (68)	1427 (48)	1753 (62)
21e	1867 (49)	1924 (29)	1860 (163)	1920 (2)	1963 (22)	1867 (25)	1874 (28)
22e	1869 (146)	1932 (183)	1865 (67)	1923 (223)	1971 (49)	1874 (271)	1875 (0)
23e	1875 (873)	1938 (438)	1870 (905)	1931 (482)	1975 (274)	1880 (742)	1880 (993)
2a ₁	239 (1)	226 (1)	207 (0)	224 (11)	204 (6)	215 (2)	193 (10)
5a ₁	307 (3)	295 (2)	299 (5)	292 (5)	274 (0)	292 (3)	287 (0)
6a ₁	309 (0)	311 (3)	304 (0)	297 (12)	288 (18)	299 (3)	303 (12)
7a ₁	326 (6)	321 (0)	320 (1)	319 (1)	308 (0)	304 (0)	316 (1)
8a ₁	407 (11)	419 (0)	347 (8)	386 (30)	391 (11)	412 (2)	338 (5)
10a ₁	446 (5)	514 (160)	449 (0)	434 (1)	414 (1)	453 (1)	441 (2)
11a ₁	540 (113)	548 (36)	523 (65)	531 (159)	497 (178)	548 (217)	484 (20)
12a ₁	652 (167)	1368 (630)	605 (200)	965 (38)	901 (535)	1011 (135)	566 (263)
13a ₁	1660 (1408)	1437 (46)	1669 (1397)	1388 (1089)	1526 (26)	1472 (678)	1776 (434)
14a ₁	1867 (82)	1928 (305)	1862 (72)	1923 (142)	1966 (161)	1872 (438)	1872 (14)
15a ₁	1871 (321)	1931 (15)	1867 (234)	1924 (147)	1971 (24)	1873 (22)	1877 (346)
16a ₁	1888 (233)	1944 (76)	1884 (280)	1937 (144)	1978 (27)	1891 (213)	1893 (294)

c)

$L^{n+} \cdot Ga_{12}H_{12}^{2-}$							
L^{n+}	Li^+	Be^{2+}	Na^+	Mg^{2+}	Ga^{+b}	$Ga^{3+}(b)$	$Ga^{3+}(s)$
12e	388 (0)	411 (1)	396 (0)	384 (0)	343 (17)	306 (9)	372 (12)
15e	478 (0)	459 (0)	478 (0)	472 (0)	448 (4)	403 (29)	447 (1)
17e	500 (6)	512 (88)	506 (0)	499 (22)	476 (3)	435 (0)	516 (29)
18e	552 (64)	710 (39)	537 (58)	568 (113)	506 (5)	452 (1)	521 (20)
19e	644 (136)	1032 (0)	623 (150)	945 (18)	567 (173)	514 (117)	573 (70)
20e	1613 (145)	1508 (74)	1643 (209)	1287 (123)	1794 (69)	1838 (26)	2039 (88)
21e	1965 (4)	2018 (68)	1959 (405)	2019 (62)	1969 (360)	2053 (24)	2057 (87)
22e	1970 (667)	2042 (296)	1964 (94)	2934 (348)	1974 (117)	2056 (162)	2087 (145)
23e	1973 (338)	2047 (195)	1967 (549)	2039 (208)	1979 (470)	2074 (116)	2096 (52)
4a ₁	205 (1)	194 (2)	194 (10)	196 (3)		138 (7)	131 (0)
6a ₁	214 (0)	209 (0)	207 (1)	207 (2)		186 (0)	197 (4)
8a ₁	393 (116)	409 (2)	253 (30)	308 (30)		213 (0)	230 (1)
10a ₁	475 (1)	506 (67)	479 (4)	470 (2)	473 (13)	447 (17)	456 (4)
11a ₁	543 (45)	532 (39)	531 (4)	536 (86)	487 (1)	482 (26)	472 (17)
12a ₁	619 (220)	1275 (726)	588 (209)	905 (105)	567 (208)	560 (12)	568 (112)
13a ₁	1651 (1413)	1438 (19)	1672 (1369)	1340 (948)	1816 (456)	1849 (138)	2041 (33)
14a ₁	1965 (44)	2023 (304)	1956 (86)	2023 (304)	1967 (6)	2054 (3)	2057 (6)
15a ₁	1969 (402)	2038 (26)	1965 (258)	2031 (39)	1977 (386)	2058 (228)	2088 (97)
16a ₁	1985 (154)	2050 (11)	1979 (272)	2041 (32)	1989 (206)	2073 (0)	2096 (89)

^aData of B3LYP/6-31G* calculations. Intensities of ν_{in} vibrations active in IR spectra (KM/mol) are given in parentheses.

^bSymmetry C_{3v} . The frequencies corresponding to 4a₁, 6a₁, and 8a₁ in C_{3v} symmetry could not be assigned.

Table S4. Calculated^a geometrical parameters (Å) of *closo*-boranes, alanes, and gallanes $L^+ @ A_{12}H_{12}^{2-}$ (3, 1_h) with L ions at the center of the [A₁₂] icosahedron.

L	empty ^b	Li ⁺	Na ⁺	Be ²⁺	Mg ²⁺	Al ³⁺	Ga ³⁺
Borane							
R(B-L)	(1.700)	1.784	1.922	1.780	1.923	1.912	1.961
R(B-B)	1.787	1.876	2.021	1.872	2.022	2.010	2.062
R(B-H)	1.205	1.186	1.186	1.177	1.176	1.172	1.179
Alane							
R(Al-L)	(2.571)	2.612	2.671	-	2.665	2.656	-
R(Al-Al)	2.703	2.746	2.809	-	2.803	2.793	-
R(Al-H)	1.605	1.586	1.587	-	1.574	1.598	-
Gallane							
R(Ga-L)	(2.453)	2.489	2.530	-	2.579	-	2.498
R(Ga-Ga)	2.579	2.616	2.659	-	2.712	-	2.626
R(Ga-H)	1.568	1.554	1.552	-	1.542	-	1.531

^aData of B3LYP calculations with the 6-311+G* basis set for boranes and alanes and 6-31G* for gallanes.

^bData for isolated $A_{12}H_{12}^{2-}$ (calculations at the same level of theory, in parentheses: the distance from the center of icosahedron $A_{12}H_{12}^{2-}$ to vertex A).

Table S5. Calculated^a vibrational frequencies ν_i (cm⁻¹) of *closo*-boranes, alanes and gallanes $L@A_{12}H_{12}^{2-}$ (3, 1b) with L atoms at the center of the [A₁₂] icosahedron.

	B							Al							Ga						
	L	empty ^b	Li ⁺	Na ⁺	Be ²⁺	Mg ²⁺	Al ³⁺	Ga ³⁺	empty ^b	Li ⁺	Na ⁺	Al ³⁺	Mg ²⁺	empty ^b	Li ⁺	Na ⁺	Mg ²⁺				
<i>h_u</i> 1	521	414	254	410	234	232	249	174	155	135	138	133	92	87	78	85					
2	959	911	870	884	857	818	943	486	457	459	453	426	488	527	547	501					
<i>h_g</i> 1	575	541	328	497	309	307	289	185	173	186	176	133	114	110	115	108					
2	765	714	712	701	705	670	755	328	316	303	302	305	219	210	203	218					
3	962	898	869	871	861	840	933	450	418	437	358	386	450	475	518	457					
4	2517	2681	2688	2766	2788	2829	2840	1880	1894	1893	1848	1954	1883	1987	2011	2057					
<i>g_u</i> 1	747	583	292	585	290	318	482	307	273	246	260	181	200	185	168	170					
2	879	817	802	759	774	720	1012	426	382	405	493	315	426	479	517	435					
<i>g_g</i> 1	662	548	376	553	372	390	415	246	227	206	195	206	148	138	129	141					
2	946	879	844	848	823	781	983	450	403	414	331	363	433	475	503	441					
<i>t_{1u}</i> 1	710	528	274	487	259	250	148	309	251	214	149	194	212	194	164	177					
	(7)	(7)	(2)	(32)	(9)	(18)	(10)	(5)	(9)	(5)	(19)	(10)	(0)	(0)	(0)	(2)					
2	–	933	915	801	880	802	835	–	383	382	336	364	–	412	300	408					
	–	(9)	(37)	(3)	(13)	(2)	(8)	–	(10)	(13)	(6)	(22)	–	(1)	(4)	(4)					
3	1089	1190	1033	1128	1059	1054	994	578	563	544	509	528	567	581	600	571					
	(64)	(25)	(9)	(38)	(3)	(0)	(0)	(288)	(230)	(232)	(59)	(164)	(218)	(158)	(172)	(106)					
4	2535	2692	2697	2771	2793	2831	2832	1810	1898	1897	1850	1956	1883	1986	2010	2057					
	(1149)	(502)	(590)	(109)	(165)	(3)	(1)	(1656)	(1040)	(1102)	(1540)	(524)	(1656)	(1035)	(1041)	(483)					
<i>t_{2u}</i> 1	765	801	801	775	811	790	813	253	276	288	261	292	155	162	164	189					
2	2510	2679	2684	2767	2787	2829	2842	1800	1891	1890	1839	1952	1876	1979	2005	2052					
<i>t_{1g}</i> 1	961	922	883	892	864	824	857	420	379	378	385	333	387	396	437	359					
<i>a_g</i> 1	744	705	651	720	659	678	723	299	296	291	297	299	208	199	198	211					
2	2572	2708	2714	2775	2798	2830	2829	1834	1913	1912	1877	1964	1910	2007	2030	2067					

^aData of B3LYP/6-31G* calculations. Intensities of *t_{1u}* vibrations active in IR spectra (KM/mol) are given in parentheses.

^bData for isolated A₁₂H₁₂²⁻ (calculations at the same level of theory).