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Quantum-Chemical Estimation of the Relaxation of Equilibrium Structure upon Radiochemical Reactions of Iodine-Containing Molecules and Ions

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Abstract—Energy of vibrational relaxation E_r upon nuclear β-decay of the Ph_2I^+, C_2F_3I, (C_{4v})- and (C_{2v})-$C_2B_4H_5I$, (D_{5d})-$C_2B_{10}H_{10}I_2$ iodine-containing compounds as well as undecafluorinated and hexachlorinated anions of iodocarba-*closo*-dodecaborane has been determined using the PBE0/SDD and MP2full/SDD quantum-chemical methods. Diphenyliodonium Ph_2I^+ is directly converted into $PhXe^+$ and Ph^+ cations pair. The $PhXe^+$ cation can be stabilized via *ortho*-fluorination of the phenyl substituent.

Keywords: nuclear β-decay, organoxenon compound, *closo*-carborane, xenon–boron bond, DFT, MP2

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Radiochemical methods taking advantage of the β-decay of metastable isotopes sometimes yield the compounds that cannot be prepared via conventional chemical reactions [1]. For example, aromatic compound containing a xenon–carbon bond ($PhXe^+$) have been obtained from diphenyliodonium Ph_2I^+ containing iodine-131 [2]. Organoelemental synthetic methods to prepare more stable fluorine-containing derivatives of phenylxenonium have been developed 21 year later by Naumann et al. [3] and Frohn et al. [4].

The unexpected syntheses of the $AuXe_4^{2+}(Sb_2F_{11}^-)_2$ [5], *cis*-$AuXe_2^{2+}(Sb_2F_{11}^-)_2$, *trans*-$AuXe_2^{2+}(SbF_6^-)_2$, $FAuXe_2FSbF_5^+Sb_2F_{11}^-$ [6], $F_3AsAuXe^+Sb_2F_{11}^-$, and $HgXe^{2+}SbF_6^-Sb_2F_{11}^-$ [7] salts calls for the search for new chemical compounds containing bonds between the inert gas atom and an atom of an element of a low electronegativity. β-Decay of the parent compounds containing radioactive iodine isotopes, ^{131}I (half-life period τ_S = 8 d), ^{133}I (τ_S = 20.5 h), or ^{135}I (τ_S = 6.7 h) [1], can serve as a universal method of preparation of such compounds. The radiochemical synthesis is favored by the heavy xenon nucleus in combination with the low energy of the emitted β-particles and the existence of several chains of transformation of radioactive iodine isotopes into radioactive xenon ones with suitable nuclear-physical parameters [1]. The target product yield is affected by the recoil momentum and the preservation of the energy of the nuclei configuration after iodine transformation into the xenon cation.

The recoil momentum is exactly opposite to the vector sum of the impulses of the emitted antineutrino and electron. The corresponding recoil energy is a random value ranging between zero and certain maximum value. The average recoil energy is a function of the molecule mass; for instance, the value for $Me^{131}I$ is higher than that for $Et^{131}I$ (60 and 55 kcal/mol, respectively, [8]).

The energy of the vibrational relaxation E_r is determined by the difference of the structural parameter of the parent and the daughter compounds and, similarly to "deformational" energy of the cation upon the β-decay of tritium compounds (cf. review [9]), it can be estimated using modern quantum-chemical methods. This work provides such estimation for a series of iodine-containing organic and organoboron compounds.

Quantum-chemical simulations were performed using the DFT PBE0/SDD and MP2full/SDD methods

implemented in GAUSSIAN-09 software [10]. The SDD basis contained the Gaussian orbitals of the valence and outer subvalence electron shells of the atoms. The electron shells located closer to the nuclei of xenon and iodine were not explicitly considered in the DFT and MP2full methods; they were accounted for using the SDD pseudo potentials [11–13]. Atomic charges were determined via the natural population analysis of the atomic orbitals (NPA [14, 15]).

According to the simulation, the $PhXe^+$ and Ph^+ cations were the primary products of β-decay of diphenyliodonium Ph_2I^+ (Fig. 1). The equilibrium nuclei configuration corresponding to the Ph_2Xe^{2+} intermediate was not found in the decay route of the dication into the two singly-charged cations. The energy of the vibrational relaxation E_r of 58 kcal/mol was calculated via subtraction of a sum of energies of the equilibrium configurations of the $PhXe^+$ and Ph^+ free cations from the energy of non-equilibrium Ph_2Xe^{2+} configuration identical to the equilibrium Ph_2I^+ configuration. The relaxation energy E_r was transformed into the kinetic energy of the single-charged cations.

The Xe–C internuclear distance of 221 pm in the free $PhXe^+$ cation was by 5 pm longer than the I–C distance in the starting symmetrical (C_{2v}) Ph_2I^+ cation but sufficiently narrow to confirm the existence of a chemical bond between the xenon and carbon atoms. The charge was distributed between the xenon atom (+0.71 a. u.) and the phenyl group (+0.29 a. u.).

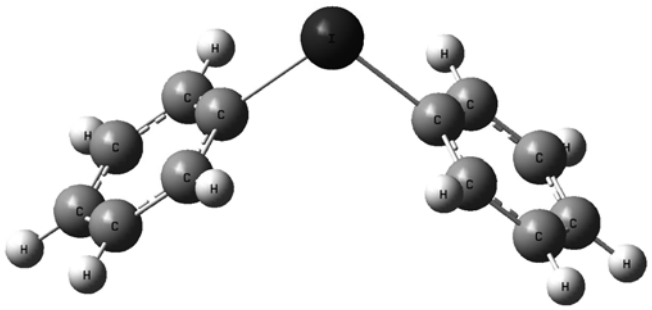

Fig. 1. Structure of diphenyliodonium Ph_2I^+.

The Xe–C bond was strengthened upon substitution of hydrogen atoms in the phenyl group with fluorine atoms. The strongest stabilizing effect of the fluorination was observed in the case of the *ortho*-substitution, whereas the *meta*-substitution caused the weakest stabilization. The Xe–C bond was shortened, and the charge on the xenon atom and its bond energy were increased in the following series of the related cations: $C_6H_5Xe^+$, 3-$C_6H_4FXe^+$, 4-$C_6H_4FXe^+$, 3,4-$C_6H_3F_2Xe^+$, 3,4,5-$C_6H_2F_3Xe^+$, 2-$C_6H_4FXe^+$, 2,6-$C_6H_3F_2Xe^+$, 2,4,6-$C_6H_2F_3Xe^+$, and $C_6F_5Xe^+$. The perfluorination of the phenyl group decreased the Xe–C distance by 12 pm and increased the charge at xenon atom by 0.21 a. u. (Table 1).

The energy of vibrational relaxation E_r during β-decay of iodine in trifluoroiodoethylene $F_2C{=}CFI$ was determined as the energy of deformed xenon-containing cation (with the structure of the parent iodine-containing molecule) relative to the minimum without

Table 1. The Xe–C bond length, charge at xenon, bond energy, and experimental decomposition temperature of fluorinated derivatives of phenilxenonium cation

Cation	Xe–C, pm[a]	q, a. u.	E_b, kcal/mol	T_{decomp}, °C
$C_6H_5Xe^+$	220.9	0.710	21.4	–
3-$C_6H_4FXe^+$	218.8	0.745	25.8	–
4-$C_6H_4FXe^+$	218.1	0.748	27.1	–14[b]
3,5-$C_6H_3F_2Xe^+$	217.0	0.778	31.7	–
3,4,5-$C_6H_2F_3Xe^+$	215.8	0.798	35.7	–
2-$C_6H_4FXe^+$	214.7	0.801	36.3	36[b]
2,6-$C_6H_3F_2Xe^+$	210.5 (209 [16])	0.869	51.3	130[b]
2,4,6-$C_6H_2F_3Xe^+$	209.7	0.886	56.5	128[b]
$C_6F_5Xe^+$	209.1 (208–210 [17, 18])	0.915	56.2	125–180[c]

[a] Data of the PBE0/SDD are given; the X-ray diffraction data are given in parentheses. The RHF/LANL2DZ simulation gave the bond lengths of 255 ($C_6H_5Xe^+$) and 219 ($C_6F_5Xe^+$) pm [17]; the B3LYP/[6-311G(3df,p)&Xe 3-111G(d)] simulation gave the bond length of 213 pm ($C_6F_5Xe^+$) [19]. [b] Crystalline tetrafluoroborates [20]. [c] Slight decomposition after melting of the crystalline hexafluoroarsenate [17].

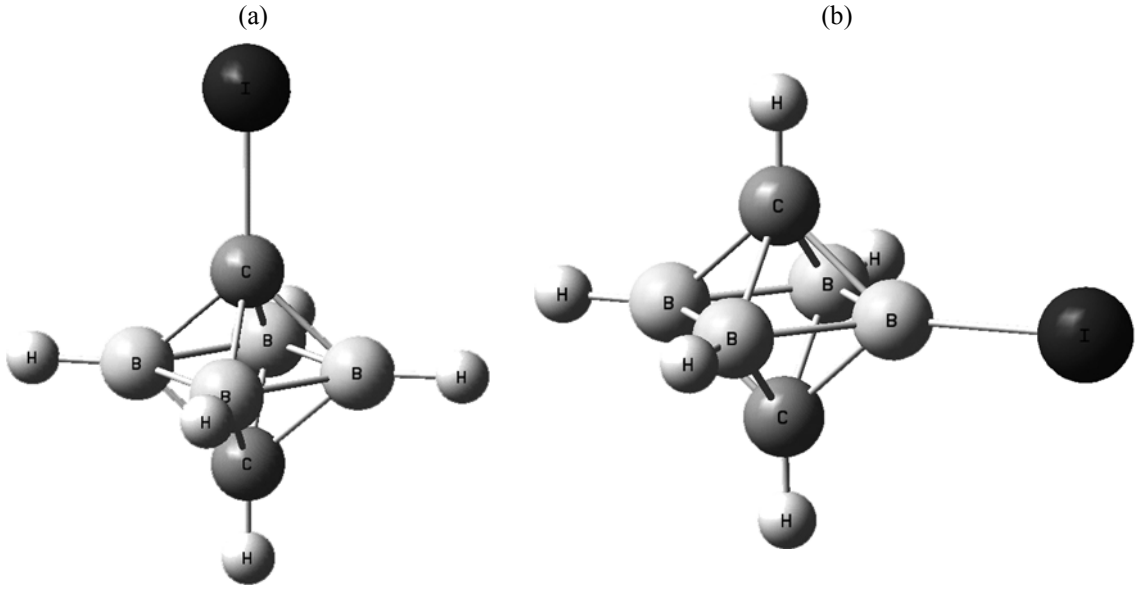

Fig. 2. Structures of 1- and 2-iodo-1,6-dicarba-*closo*-hexaboranes (a) (C_{4v})-$C_2B_4H_5I$ and (b) (C_{2v})-$C_2B_4H_5I$.

taking into account the zero vibrations energy. The relaxation resulted in both lengthening of the bond between the carbon atom and the heavy nucleus by 1 pm and shortening of the C–F bonds by 2–5 pm (Table 2). The simulated energy of the bond formed by the xenon atom E_b in the $F_2C{=}CFXe^+$ cation, 49.7 kcal/mol (PBE0) or 43.5 kcal/mol (MP2full), was more than an order of magnitude larger than the energy of vibrational relaxation E_r, 2.9 kcal/mol (PBE0) or 3.9 kcal/mol (MP2full).

The preparation of the $F_2C{=}CFXe^+BF_4^-$ salt, decomposing at temperature above 0°C, was possible by organic synthesis [21].

The simulated length of the bond between xenon and 5-coordinated carbon in the hypothetic (1,6-dicarba-*closo*-hexaboran-1-yl)xenonium (C_{4v})-$C_2B_4H_5Xe^+$ cation (210 pm) was smaller than the simulated Xe–C bonds length in the $F_2C{=}CFXe^+$ and $PhXe^+$ cations. The energy of relaxation of the equilibrium configuration of the (C_{4v})-$C_2B_4H_5I$ molecule (Fig. 2a) into the equilibrium configuration of the (C_{4v})-$C_2B_4H_5Xe^+$ cation was small (1.8 kcal/mol). The transformation of the iodine nucleus into the xenon one shortened its bond with carbon atom by 0.9 pm.

In the (1,6-dicarba-*closo*-hexaboran-2-yl)xenonium (C_{2v})-$C_2B_4H_5Xe^+$ cation formed from 2-iodo-1,6-dicarba-*closo*-hexaborane (C_{2v})-$C_2B_4H_5I$ (Fig. 2b) the simulated bond length of the xenon with 5-coordinated boron equaled 216 pm and the relaxation energy, 1.6 kcal/mol. The energy of the (C_{2v})-$C_2B_4H_5I$ molecule was by 26 kcal/mol lower than that of the isomeric (C_{4v})-$C_2B_4H_5I$ molecule; the energy of the free (C_{2v})-$C_2B_4H_5Xe^+$ cation was by 37 kcal/mol lower than that of the isomeric (C_{4v})-$C_2B_4H_5Xe^+$ cation.

The simulated length of the bond between the xenon atom and the 6-coordinated carbon atom in the hypothetic (12-iodo-1,12-dicarba-*closo*-dodecaboran-1-yl)xenonium (C_{5v})-$IC(BH)_{10}CXe^+$ cation was equal to that in the simulated Xe–C bond length in the phenylxenonium cation, the charge on the xenon atom being by 0.13 a. u. higher in the former case. The energy of relaxation of the equilibrium configuration of molecule **1** (Fig. 3) into the equilibrium configuration of the (C_{5v})-$IC(BH)_{10}CXe^+$ cation was small (1.8 kcal/mol). The transformation of the iodine atom of the 1,12-diiodo-1,12-dicarba-*closo*-dodecaborane

Table 2. Bond lengths (pm) in the molecule of trifluoroiodoethylene and in the trifluorovinylxenonium cation

Compound	(I, Xe)–C^1	C^1–F	C^2–F_{cis}	C^2–F_{trans}	$C^1{=}C^2$
PBE0/SDD					
$F_2C^2{=}C^1FI$	209.9	138.0	135.9	135.9	133.5
$F_2C^2{=}C^1FXe^+$	211.1	134.1	134.4	133.0	134.0
MP2full/SDD					
$F_2C^2{=}C^1FI$	211.0	142.1	139.0	138.8	135.6
$F_2C^2{=}C^1FXe^+$	211.9	137.3	137.4	135.8	136.1

molecule into xenon increased the length of the bond with the corresponding carbon atom by 6.6 pm and decreased the equilibrium length of the adjacent carbon–boron bonds by 1.0 pm.

The prepared organoxenon compounds were either salts containing the positively charged 1-, 2-, or 3-coordinated xenon in the RXe^+, $[RXeHalXeR]^+$, or $[RXeF_2]^+$ cation or the RXeR' molecules with the 2-coordinated xenon forming two coaxial bonds. The electrically neutral xenon-containing carba-*closo*-dodecaboranes RXe that could be formed via β-decay of iodine in the undecafluorinated and hexachlorinated carba-*closo*-borane anions **2**–**4** (Fig. 4) belonged to the fifth group of organoxenon compounds, unknown so far.[1] In the three studied hypothetic compounds, the 1-coordinated xenon atom and the 6-coordinated carbon atom formed the Xe–C bonds possessing a relatively small equilibrium length of 212–226 pm, positive charge at the xenon atom, and the energy of the vibrational relaxation no higher than 3.3 kcal/mol (Table 3). The high dipole moments of those molecules suggested that they could be regarded as zwitter ions.

β-Decay of iodine in the isomeric anions **5**–**7** containing the I−B bonds yielded the corresponding xenon-containing carba-*closo*-dodecaboranes with the short Xe–B bonds (220–229 pm), the charge of the xenon atoms no lower than +0.58 a. u., and high dipole moments. The simulated energy of their vibrational relaxation (Table 3) suggested that those compounds could be isolated in the low-temperature matrix.

The only compound containing the xenon–boron chemical bond prepared so far ($FXeBF_2$) decomposes at heating above 243 K [22]. Our simulations via the PBE0/SDD and MP2full/SDD methods revealed the local energy minimum of the metastable $FXeBF_2$ molecule at the equilibrium Xe–B bond length of 220.1 pm (PBE0) or 220.4 pm (MP2full). The exothermic effect of its isomerization into the $Xe{\cdot}BF_3$ van der Waals' complex[2] with accounting for the zero vibrations was 101 kcal/mol (PBE0) or 111 kcal/mol (MP2full). The Xe–B bond was stabilized by the electrostatic interaction of the directly linked xenon and boron atoms: Xe +0.71 and B +1.00 a. u. (PBE0) or Xe +0.76 and B +1.21 a. u. (MP2full). The Xe–B bond of close length (222.7 pm) has been earlier simulated for the xenon adduct with pentafluoroborabenzene [23][3]. The xenon–boron bond length in the hypothetic (C_{5v})-$CB_{10}F_{11}BXe$ zwitter ion was shorter than that in the $FXeBF_2$ and C_5F_5BXe molecules.

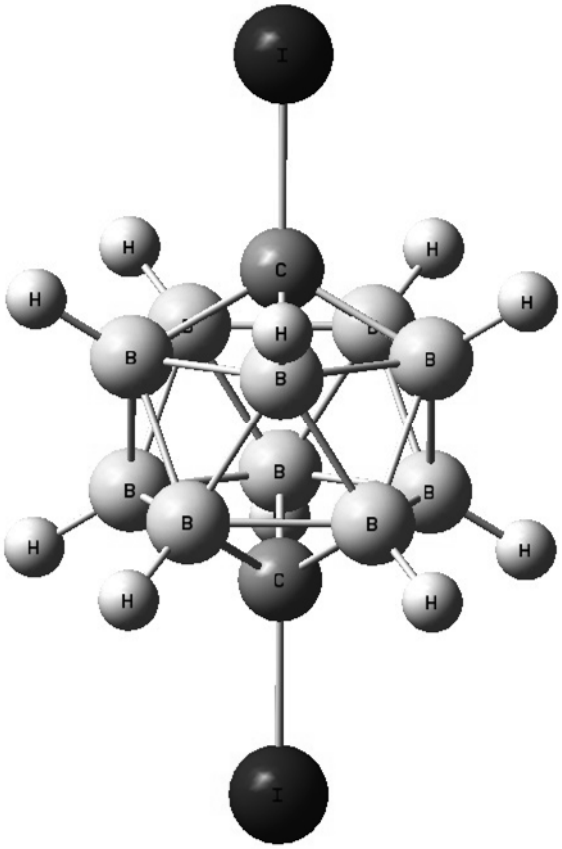

Fig. 3. Structure of 1,12-diiodo-1,12-dicarba-*closo*-dodecaborane **1**.

Synthesis of saturated organoxenon compounds (molecules or ionic crystals) containing xenon atom linked to the 4-coordinated carbon atoms has remained an important challenge. The problem has been approached, for example, in the quantum-chemical study of β-decay of iodocubane C_8H_7I [24]. The simulation of the daughter cation $C_8H_7Xe^+$ using the PBE0/SDD and MP2/SDD methods with accounting

[1] The same group includes the $HOC_6H_2I(Xe^+)CH_2CH(NH_2)CO_2^-$, $HOC_6H_2I(Xe^+)OC_6H_2I_2CH_2CH(NH_2)CO_2^-$, and $HOC_6H_2I_2OC_6H_2I{\cdot}(Xe^+)CH_2CH(NH_2)CO_2^-$ zwitter ions formed via β-decay of radioactive iodine in the anions of 3,5-diiodotyrosine $HOC_6H_2I_2{\cdot}CH_2CH(NH_2)CO_2H$ and tiroxine $HOC_6H_2I_2OC_6H_2I_2CH_2CH{\cdot}(NH_2)CO_2H$ generated by thyroid gland.

[2] Equilibrium structure of the $Xe{\cdot}BF_3$ complex: the internuclear distances Xe–B 358–369 pm and B–F 135–137 pm, a planar BF_3 fragment (PBE0 – MP2full simulation).

[3] Possibility of the C_5F_5BXe molecule generation via positron β-decay of the $C_6F_5Xe^+$ cation enriched with the ^{11}C isotope has been suggested in [23].

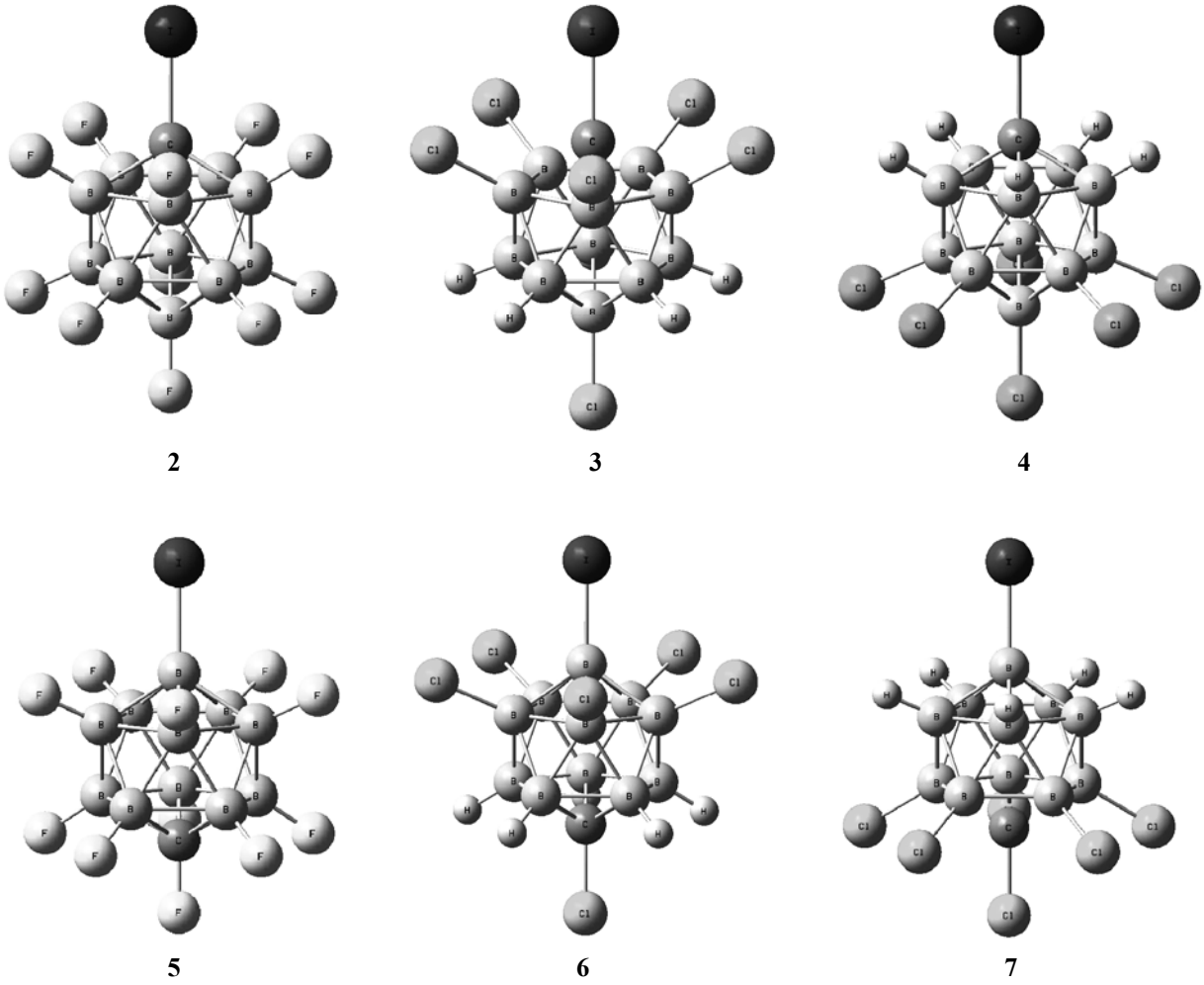

Fig. 4. Structures of anions of the iodine-containing carba-*closo*-dodecaboranes **2–7**.

for the zero vibrations energy has revealed the low energy of the bond formed by xenon atom: 6.4 kcal/mol (PBE0) and 7.6 kcal/mol (MP2) [24]; the MP2full method gave the simulated bond energy of 7.5 kcal/mol. Comparison of that values with the relaxation energy E_r obtained in this work, 6.0 kcal/mol (PBE0) and 5.8 kcal/mol (MP2full), corresponding to the increase in the equilibrium length of the exopolyhedral bond

Table 3. The Xe–R bond length, charge at xenon, dipole moment, relaxation energy, and decline of the zero vibrations energy due to the β-decay of iodine in derivatives of carba-*closo*-dodecaborane (the PBE0/SDD simulation)

Parent compound	Xe–R, pm	q, a. u.	μ, D	E_r, kcal/mol	δ_0, kcal/mol
Compounds with the Xe–C bond					
1	221	+0.84	–	1.76	1.02
2	212	+0.96	12.9	3.29	1.03
3	215	+0.91	8.0	2.78	0.81
4	226	+0.74	15.6	2.55	1.55
Compounds with the Xe–B bond					
5	220	+0.69	8.9	3.75	0.08
6	222	+0.67	2.7	3.79	–0.06
7	229	+0.58	10.9	3.49	0.17

C–I → C–Xe^+ by 37 pm (PBE0) or 38 pm (MP2full) evidenced that the product of β-decay of iodocubane should be the cubyl cation $C_8H_7^+$ rather than cubylxenonium cation $C_8H_7Xe^+$.

To conclude, the quantum-chemical simulations revealed the small difference between the energy of zero vibrations of the parent iodine-containing and the daughter xenon-containing compounds. The PBE0/SDD-simulated change in the energy of zero vibrations of 2-iodo-1,6-dicarba-*closo*-hexaborane (C_{2v})-$C_2B_4H_5I$ and the carba-*closo*-dodecaborane anions **5**–**7** containing the B–I bond as well as of trifluoroiodoethylene transforming into the trifluorovinylxenonium cation was below 0.2 kcal/mol. The energy of zero vibrations of iodocubane C_8H_7I, 1-iodo-1,6-dicarba-*closo*-hexaborane (C_{4v})-HCB_4H_4CI, 1,12-diiodo-1,12-dicarba-*closo*-dodecaborane **1**, and carba-*closo*-dodecaborane anions **2**–**4** containing the C–I bond was 1.3, 0.6, 1.0, and 0.8–1.6 kcal/mol, respectively, higher than that of the daughter xenon-containing compounds.

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