Electronic Supplementary Material (ESI) for RSC Advances.

Are noble gas molecules able to exhibit a superhalogen nature?

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SUPPLEMENTARY INFORMATION

Table ESI.1. The MP2/6-311++G(3df,3pd)+ECPs geometrical parameters and corresponding harmonic vibrational frequencies (in cm^{-1}) for the transition state connecting the KrF_7^- anion and its fragmentation products.

Species *(Symmetry)*	Geometrical parameters		Vibrational frequencies [cm^{-1}]		
KrF_7^- TS (C_{2v})	r(Kr–$F_{1\text{-}4}$)=1.953 r(Kr–F_5)=1.988 r(Kr–$F_{6,7}$)=1.989 α(F_1KrF_2)=81.63 α(F_1KrF_3)=94.75 α(F_1KrF_4)=159.58	α(F_1KrF_5)=79.79 α(F_1XeF_6)=75.92 α(F_1XeF_7)=121.96 ω($F_1KrF_2F_6$)=67.56 ω($F_1KrF_2F_7$)=126.05 ω($F_2KrF_3F_4$)=81.05	υ_1=-82 (a_2) υ_2=34 (b_2) υ_3=210 (a_1) υ_4=224 (b_1) υ_5=262 (b_2) υ_6=274 (a_1)	υ_7=281 (a_2) υ_8=296 (a_2) υ_9=297 (b_2) υ_{10}=300 (b_1) υ_{11}=310 (b_1) υ_{12}=330 (a_1)	υ_{13}=353 (a_1) υ_{14}=355 (a_1) υ_{15}=362 (b_2) υ_{16}=543 (a_1) υ_{17}=552 (b_1) υ_{18}=568 (b_2)

Bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

Table ESI.2. The MP2/6-311++G(3df,3pd)+ECPs geometrical parameters and corresponding harmonic vibrational frequencies (in cm^{-1}) for the $Xe_2F_{13}^-$ and $Rn_7F_{13}^-$ anions. The E_R values (in kcal/mol) stand for the relative energies estimated for the $Xe_2F_{13}^-$ isomers with respect to its corresponding global minimum.

Species *(Symmetry)*	Geometrical parameters	Vibrational frequencies [cm^{-1}]				
$Xe_2F_{13}^-$ (C_2) E_R=0.0	$r(Xe_{1,2}–F_1)$=2.269 $r(Xe_1–F_2)$=2.025 $r(Xe_1–F_3)$=3.010 $r(Xe_{1,2}–F_4)$=1.996 $r(Xe_{1,2}–F_5)$=1.946 $r(Xe_{1,2}–F_6)$=1.947 $r(Xe_{1,2}–F_7)$=1.950 $r(Xe_{1,2}–F_8)$=1.979 $\alpha(F_1XeF_2)$=71.52	$\alpha(F_1XeF_4)$=73.48 $\alpha(F_4XeF_5)$=84.88 $\alpha(F_4XeF_6)$=76.93 $\alpha(F_5XeF_7)$=76.81 $\alpha(F_4XeF_8)$=101.18 $\omega(F_4XeF_6F_7)$=172.32 $\omega(F_8XeF_1F_5)$=176.01 $\omega(F_8XeF_6F_4)$=103.63 $\omega(F_8XeF_7F_4)$=99.54	υ_1=29 (b) υ_2=35 (a) υ_3=40 (a) υ_4=66 (b) υ_5=87 (a) υ_6=90 (b) υ_7=107 (a) υ_8=116 (b) υ_9=141 (a) υ_{10}=161 (a)	υ_{11}=195 (a) υ_{12}=198 (b) υ_{13}=208 (a) υ_{14}=211 (b) υ_{15}=226 (b) υ_{16}=238 (b) υ_{17}=246 (a) υ_{18}=252 (b) υ_{19}=258 (a) υ_{20}=263 (b)	υ_{21}=287 (a) υ_{22}=302 (a) υ_{23}=307 (b) υ_{24}=324 (b) υ_{25}=335 (a) υ_{26}=355 (b) υ_{27}=369 (a) υ_{28}=470 (a) υ_{29}=473 (b) υ_{30}=478 (a)	υ_{31}=479 (b) υ_{32}=511 (b) υ_{33}=523 (a) υ_{34}=541 (b) υ_{35}=544 (a) υ_{36}=550 (a) υ_{37}=550 (b) υ_{38}=570 (b) υ_{39}=575 (a)
$Xe_2F_{13}^-$ (C_{2v}) E_R=0.3	$r(Xe_1–F_1)$=2.547 $r(Xe_1–F_2)$=2.006 $r(Xe_1–F_3)$=1.946 $r(Xe_1–F_4)$=1.932 $r(Xe_2–F_1)$=2.093 $r(Xe_2–F_5)$=1.968 $r(Xe_2–F_6)$=1.996 $r(Xe_2–F_7)$=1.985 $\alpha(F_1Xe_1F_1)$=56.11	$\alpha(F_1Xe_2F_1)$=69.83 $\alpha(F_1Xe_1F_2)$=70.62 $\alpha(F_1Xe_1F_3)$=71.41 $\alpha(F_3Xe_1F_4)$=82.48 $\alpha(F_1Xe_2F_5)$=90.89 $\alpha(F_5Xe_2F_6)$=89.69 $\alpha(F_5Xe_2F_7)$=88.91 $\omega(F_1Xe_1F_3F_4)$=142.32 $\omega(F_1Xe_2F_6F_5)$=91.04	υ_1=18 (b_2) υ_2=26 (b_2) υ_3=47 (b_2) υ_4=72 (b_2) υ_5=84 (b_2) υ_6=89 (b_2) υ_7=95 (b_2) υ_8=123 (b_2) υ_9=128 (b_2)	υ_{10}=146 (b_2) υ_{11}=160 (b_2) υ_{12}=168 (b_2) υ_{13}=173 (b_2) $\upsilon_{14,15}$=204 (b_2) υ_{16}=206 (b_2) υ_{17}=222 (b_2) υ_{18}=233 (a) υ_{19}=253 (a)	υ_{20}=285 (b) υ_{21}=290 (b) υ_{22}=304 (b) υ_{23}=331 (b_1) υ_{24}=373 (b_2) υ_{25}=384 (a_1) υ_{26}=397 (c) υ_{27}=401 (c) υ_{28}=444 (a_1)	υ_{29}=462 (a_1) υ_{30}=481 (b_1) υ_{31}=482 (a_1) υ_{32}=500 (d) υ_{33}=527 (d) υ_{34}=528 (d) υ_{35}=535 (a_1) $\upsilon_{36,37}$=559 (d) υ_{38}=575 (d) υ_{39}=585 (d)
$Xe_2F_{13}^-$ (D_{5d}) E_R=18.7	$r(Xe–F_1)$=2.308 $r(Xe–F_2)$=1.981 $r(Xe–F_3)$=1.865 $\alpha(F_1XeF_2)$=95.44 $\alpha(F_2XeF_2)$=71.62 $\omega(F_1XeF_2F_2)$=93.94	υ_1=3 (a_{1u}) $\upsilon_{2,3}$=18 (e_{1u}) $\upsilon_{4,5}$=32 (e_{1g}) $\upsilon_{6,7}$=71 (e_{2u}) $\upsilon_{8,9}$=72 (e_{2g})	υ_{10}=73 (a_{2u}) υ_{11}=77 (a_{1g}) $\upsilon_{12,13}$=95 (e_{1u}) $\upsilon_{14,15}$=264 (e_{1g}) $\upsilon_{16,17}$=265 (e_{1u})	υ_{18}=285 (a_{1g}) υ_{19}=320 (a_{2u}) $\upsilon_{20,21}$=340 (e_{1g}) $\upsilon_{22,23}$=340 (e_{1u}) $\upsilon_{24,25}$=423 (e_{2u})	$\upsilon_{26,27}$=424 (e_{2g}) $\upsilon_{28,29}$=474 (e_{2u}) $\upsilon_{30,31}$=474 (e_{2g}) υ_{32}=529 (a_{1g}) υ_{33}=538 (a_{2u})	$\upsilon_{34,35}$=540 (e_{1g}) $\upsilon_{36,37}$=553 (e_{1u}) υ_{38}=606 (a_{2u}) υ_{39}=618 (a_{1g})
$Xe_2F_{13}^-$ (D_{5h}) E_R=18.7	$r(Xe–F_1)$=2.308 $r(Xe–F_2)$=1.981 $r(Xe–F_3)$=1.865 $\alpha(F_1XeF_2)$=95.44 $\alpha(F_2XeF_2)$=71.62 $\omega(F_1XeF_2F_2)$=93.94	υ_1=5 (a) $\upsilon_{2,3}$=18 (b) $\upsilon_{4,5}$=32 (b) $\upsilon_{6,7}$=70 (c) $\upsilon_{8,9}$=73 (a)	υ_{10}=73 (a) υ_{11}=77 (d) $\upsilon_{12,13}$=94 (b) $\upsilon_{14,15}$=264 (b) $\upsilon_{16,17}$=265 (b)	υ_{18}=285 (d) υ_{19}=320 (a) $\upsilon_{20,21}$=340 (b) $\upsilon_{22,23}$=340 (b) $\upsilon_{24,25}$=423 (c)	$\upsilon_{26,27}$=424 (e_{2g}) $\upsilon_{28,29}$=474 (c) $\upsilon_{30,31}$=475 (a) υ_{32}=529 (d) υ_{33}=538 (a)	$\upsilon_{34,35}$=540 (b) $\upsilon_{36,37}$=553 (b) υ_{38}=606 (a_{2u}) υ_{39}=618 (a_{1g})

Species *(Symmetry)*	Geometrical parameters	Vibrational frequencies [cm^{-1}]				
$Rn_2F_{13}^-$ (C_2)	$r(Rn_{1,2}–F_1)$= 2.305 $r(Rn_1–F_2)$= 2.202 $r(Rn_1–F_3)$= 2.460 $r(Rn_{1,2}–F_4)$= 2.039 $r(Rn_{1,2}–F_5)$= 2.034 $r(Rn_{1,2}–F_6)$= 2.016 $r(Rn_{1,2}–F_7)$= 2.038 $r(Rn_{1,2}–F_8)$= 2.049 $\alpha(F_1RnF_4)$=132.28	$\alpha(F_2RnF_4)$=87.72 $\alpha(F_4RnF_5)$=84.17 $\alpha(F_4RnF_6)$=78.71 $\alpha(F_4RnF_7)$=94.86 $\alpha(F_4RnF_8)$=155.66 $\omega(F_4RnF_2F_8)$=159.66 $\omega(F_4RnF_5F_8)$=160.71 $\omega(F_8RnF_6F_4)$=169.42 $\omega(F_8RnF_7F_4)$=156.16 $\omega(F_8RnF_1F_4)$=179.79	υ_1=7 (b) υ_2=27 (a) υ_3=72 (a) υ_4=80 (b) υ_5=95 (a) υ_6=119 (a) υ_7=127 (b) υ_8=144 (a) υ_9=146 (b)	υ_{10}=165 (b) υ_{11}=165 (a) υ_{12}=190 (a) υ_{13}=193 (b) υ_{14}=224 (a) υ_{15}=228 (b) υ_{16}=246 (b) υ_{17}=248 (a) υ_{18}=260 (a)	υ_{19}=260 (b) υ_{20}=277 (b) υ_{21}=285 (a) υ_{22}=301 (a) υ_{23}=312 (b) υ_{24}=324 (b) υ_{25}=333 (a) υ_{26}=351 (b) υ_{27}=393 (a)	υ_{28}=439 (b) υ_{29}=456 (a) $\upsilon_{30,31}$=518 (a) υ_{32}=531 (a) υ_{33}=534 (b) υ_{34}=545 (a) $\upsilon_{35,36}$=547 (b) υ_{37}=560 (a) υ_{38}=560 (b) υ_{39}=563 (a)

Bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.