

Figure S1. $1,3\Delta$ adiabatic potential energy curves.

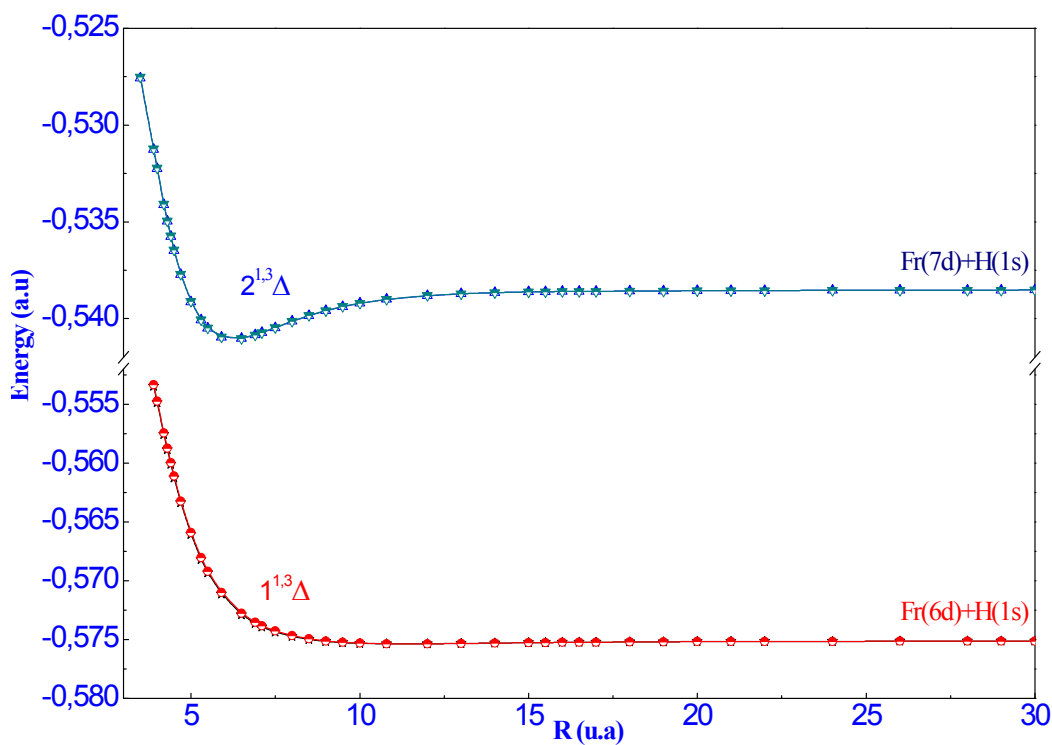


Figure.S2. Diabatic $1,3\Delta$ potential energy curves dissociating below the ionic limit Fr^+H^- .

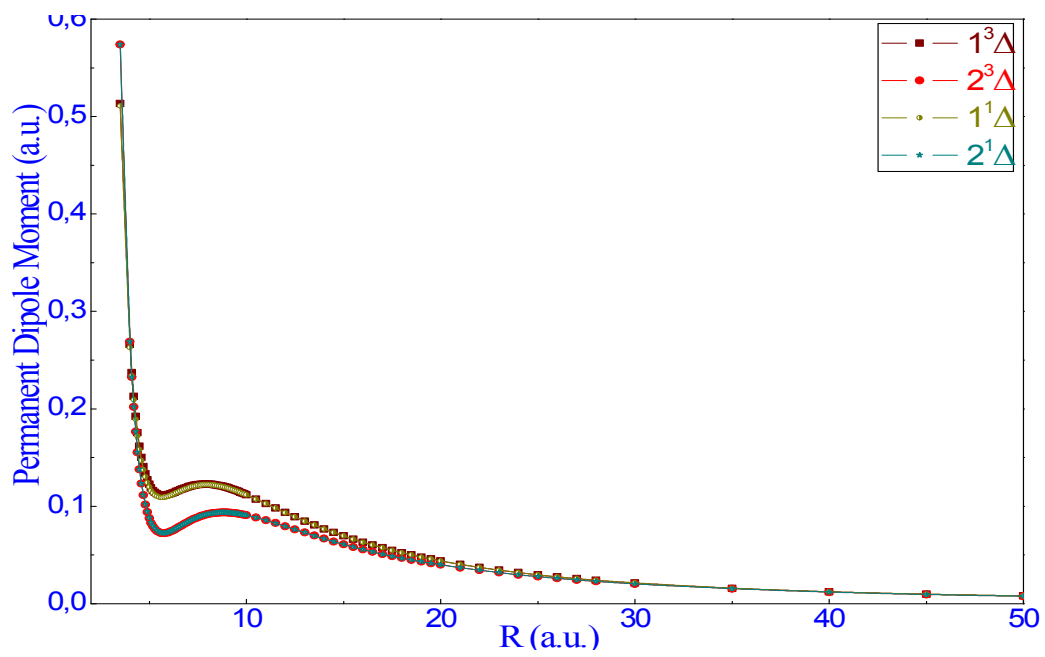


Figure S3. Adiabatic permanent dipole moment for the states of $1,3\Delta$ for the FrH.

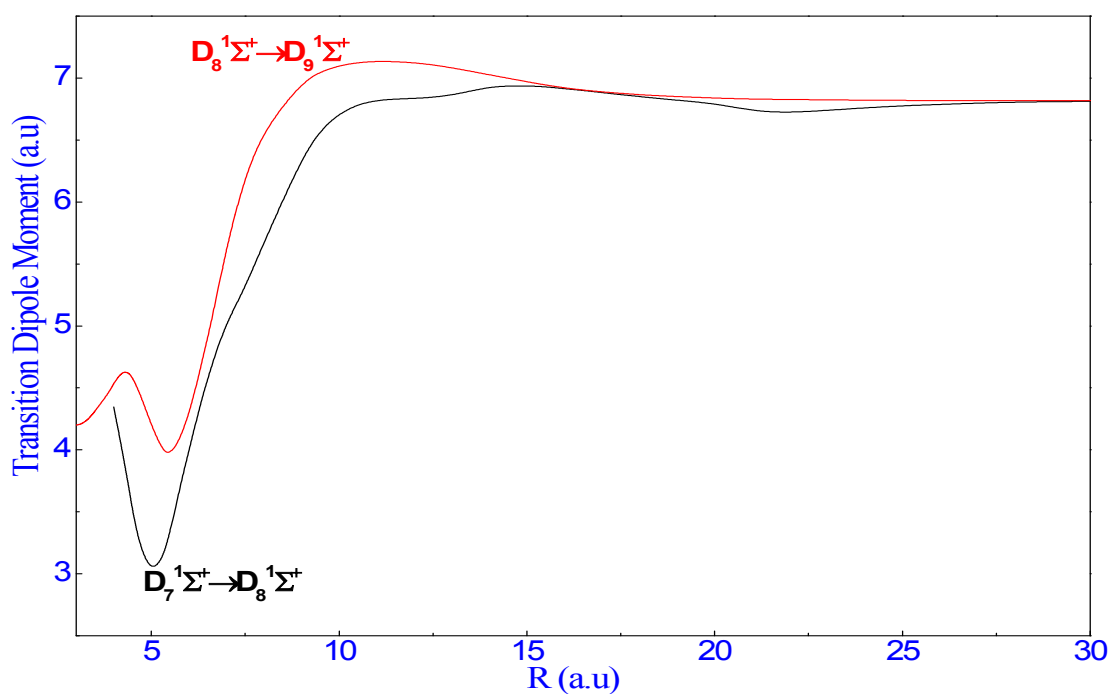
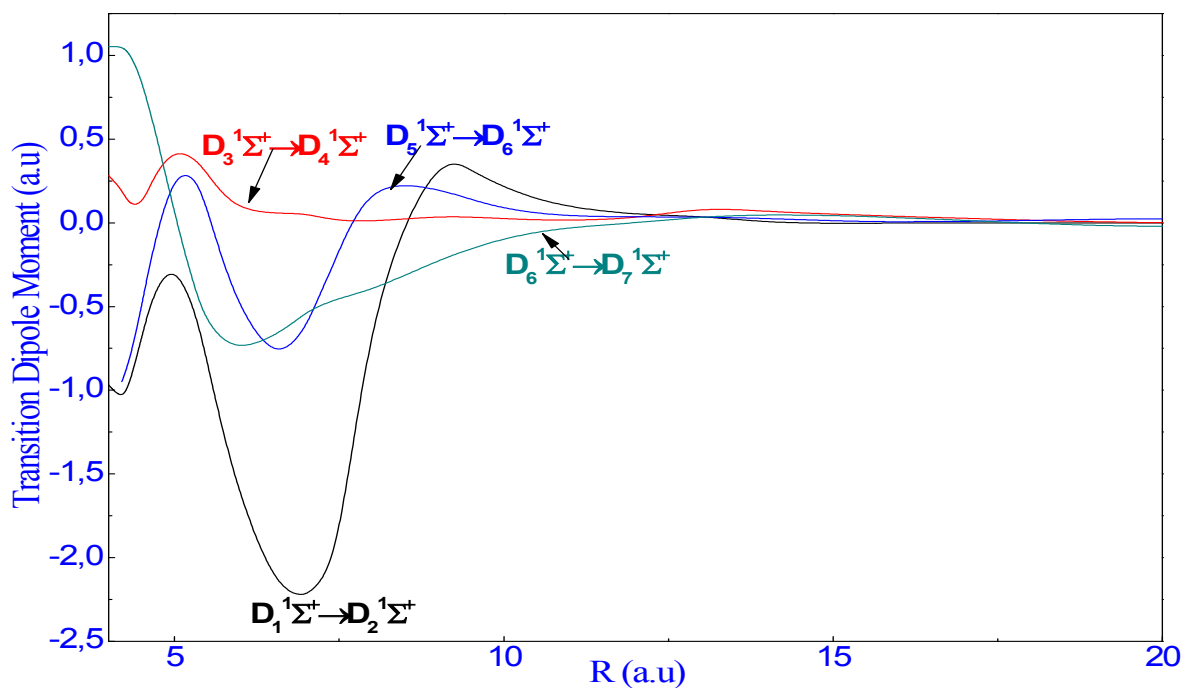


Figure.S4. Transition dipole moment between selected $1\Sigma^+$ diabatic states.

Table S1. Basis set for francium.

	Exponents
s	1.3
	0.650
	0.28
	0.109
	0.0400
	0.01980
	0.00620
	0.00208
p	0.330
	0.1090
	0.0310
	0.0150
	0.0047
	0.0020
d	0.90
	0.208
	0.0634
	0.0196
	0.0057

Table S2. Theoretical ionization energies (in cm^{-1}) of hydrogen atom compared with the experimental ones⁸³.

Atomic levels	Expt. ⁸³	This work	$\Delta E(\text{cm}^{-1})$
1s	-109678	-109725	47
2s	-27419	-27371	48
2p	-27419	-27369	50
3s	-12186	-12189	3

ΔE : Energy difference between the experimental values and theoretical work in cm^{-1} .

Table S3. Theoretical ionization energies (in cm^{-1}) of francium atom compared with the experimental energies⁸³.

Atomic levels	Expt. ⁸³	This work	ΔE	M. Aymar et al. ⁴⁹	ΔE
7s	-32848	-32848	0	-32 848	0
7p	-19487	-19487	0	-19 486	1
6d	-16499	-16499	0	-16 470	29
8s	-13108	-13176	68	-13 161	53
8p	-9372	-9425	53	-9448	76
7d	-8551	-8463	88	-8394	157
9s	-7177	-7192	15	-7161	16
9p	-5565	-5580	15	-5619	54

ΔE : Energy difference between the experimental values and theoretical work in cm^{-1} .

Table S4. Various molecular states of FrH below the ionic limit ($\text{Fr}^+ + \text{H}^-$).

Asymptotic limits	Molecular states	Exp ⁸³ (cm^{-1})	This work (cm^{-1})	Δ
Fr (7s) +H (1s)	$1,3\Sigma^+$	-142527	-142574	0.033
Fr (7p) +H (1s)	$1,3\Sigma^+, 1,3\Pi$	-129165	-129212	0.036
Fr (6d) +H (1s)	$1,3\Sigma^+, 1,3\Pi, 1,3\Delta$	-126177	-126225	0.038
Fr (8s) +H (1s)	$1,3\Sigma^+$	-122787	-122902	0.094
Fr (8p) +H (1s)	$1,3\Sigma^+, 1,3\Pi$	-119051	-119151	0.084
Fr (7d) +H (1s)	$1,3\Sigma^+, 1,3\Pi, 1,3\Delta$	-118230	-118189	0.035
Fr (9s) +H (1s)	$1,3\Sigma^+$	-116856	-116918	0.053
Fr (9p) +H (1s)	$1,3\Sigma^+, 1,3\Pi$	-115244	-115306	0.054
$\text{Fr}^+ + \text{H}^-$		-115761		

Δ : Relative errors between the experimental and theoretical energy values ($\Delta = ((\text{Exp} - \text{this work}/E) * 100)$) (in %).