Electronic Supplementary Information

Stable copernicium hexafluoride (CnF_6) with an oxidation state of +VI

Computational details

Basis functions of Cn used in the X2C-AU/PBE0 calculations

Cn: (32s29p20d13f3g1h)/[28s24p16d10f3g1h]

S

5.2838921E+07 0.6094847011E-01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.4052181E+07 0.1246189615E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.7818084E+06 0.2068473915E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.7994843E+06 0.3147706366E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4188602E+05 0.4649291068E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.2382387E+05 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.4919768E+05 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.1554389E+04 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.5610846E+04 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.8252319E+04 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.6124347E+03 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.1812551E+03 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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1.6067219E+03 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.2685750E+02 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.5041539E+02 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.3675766E+02 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.1031410E+02 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.3165655E+02 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.2006316E+01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
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1.0801119E+01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0
6.2356361E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
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P

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8.2556172E+06 0.7042031628E-01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

3.1140912E+06 0.1500978605E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.2178111E+06 0.3067590648E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.9112174E+05 0.6190988080E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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1.6815031E+04 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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4.6359849E+02 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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1.3354890E+02 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4458648E+01 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0
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2.3594039E+01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0
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7.4766155E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
4.0745243E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0
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1.0779145E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0
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1.9532125E-01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0
7.3226404E-02 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0
2.6615576E-02 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0
D
2.3667019E+05 0.1917081348E-02 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.4508363E+04 0.1062880618E-01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.7089094E+04 0.4958447204E-01 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.3873362E+03 0.2103238087E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.6994303E+03 0.8154571425E+00 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.2476450E+03 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.1547151E+02 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
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9.4318316E+01 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0
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2.9204773E+01 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
1.6442916E+01 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0
9.1635830E+00 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0
4.9682649E+00 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0
2.6263205E+00 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0
1.2986248E+00 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0

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  6.1079932E-01  0                    0 0 0 0 0 0 0 0 0 0 0 0 1 0 0
  2.6714924E-01  0                    0 0 0 0 0 0 0 0 0 0 0 0 0 1 0
  1.0675309E-01  0                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
F
  3.4400792E+03  0.3787122722E-02 0 0 0 0 0 0 0 0 0
  1.1249902E+03  0.3488135826E-01 0 0 0 0 0 0 0 0 0
  4.6967988E+02  0.2053349102E+00 0 0 0 0 0 0 0 0 0
  2.2245189E+02  0.8258429538E+00 0 0 0 0 0 0 0 0 0
  1.1278088E+02  0                    1 0 0 0 0 0 0 0 0
  5.9810059E+01  0                    0 1 0 0 0 0 0 0 0
  3.2337736E+01  0                    0 0 1 0 0 0 0 0 0
  1.7715413E+01  0                    0 0 0 1 0 0 0 0 0
  9.6421473E+00  0                    0 0 0 0 1 0 0 0 0
  5.0879257E+00  0                    0 0 0 0 0 1 0 0 0
  2.5803052E+00  0                    0 0 0 0 0 0 1 0 0
  1.2008221E+00  0                    0 0 0 0 0 0 0 1 0
  4.3021888E-01  0                    0 0 0 0 0 0 0 0 1
G
  8.6351253E+00  1  0  0
  3.2652063E+00  0  1  0
  9.7673453E-01  0  0  1
H
  6.0979820E+00  1
```

In the contact density calculations, the s- and p-functions are decontracted and are supplemented by two steep s-functions (α=424285762.33, 200225782.68) and two steep p-functions (α=193370401.96, 111623241.44).

Active spinors (orbitals) in coupled-cluster calculations

SOECP/CCSD(T) by CFour
Spinors from Cn 6s6p6d7s and F 2s2p are correlated.

SOECP/FS-CCSD by DIRAC
The active spinors are taken from O 2s2p (O^{2-} and O_2^{2-}), F 2s2p (F^- and CnF^-) and Cn 6d7s (Cn).

The complete basis set (CBS) limit

The SOECP/CCSD(T)/CBS energies were estimated by SOECP/CCSD(T)/VTZ and SOECP/CCSD(T)/VQZ energies through

$$E_{CBS} = \frac{E_X X^3 - E_Y Y^3}{X^3 - Y^3}$$

with X, Y = 3, 4.

LOBA

The formal oxidation states of Cn in CnF_n (n = 1, 2, 4, and 6) were estimated by localized orbital bonding analysis (LOBA) at the spin-free X2C-AU/PBE0 level. In the orbital localization, some missing parameters of Cn were taken from Hg. The default threshold of 50% was taken for LOBA. The computed oxidation states are +n for Cn and -1 for F.

Optimized Cartesian coordinates

SOECP/PBE0

O_2

O	0.0000000000	0.0000000000	0.5971657532
O	0.0000000000	0.0000000000	-0.5971657532

F_2

F	0.0000000000	0.0000000000	0.6864919594
F	0.0000000000	0.0000000000	-0.6864919594

CnF

Cn	0.0000000000	0.0000000000	-0.0362783766
F	0.0000000000	0.0000000000	2.0716783766

CnF_2

Cn	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.9257831739
F	0.0000000000	0.0000000000	-1.9257831739

CnF_4

Cn	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	1.9288437143	0.0000000000
F	0.0000000000	-1.9288437143	0.0000000000
F	1.9288437143	0.0000000000	0.0000000000
F	-1.9288437143	0.0000000000	0.0000000000

CnF_6

Cn	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.9324926753
F	0.0000000000	0.0000000000	-1.9324926753
F	0.0000000000	1.9324926753	0.0000000000
F	0.0000000000	-1.9324926753	0.0000000000
F	1.9324926753	0.0000000000	0.0000000000
F	-1.9324926753	0.0000000000	0.0000000000

CnO

Cn	0.0000000000	0.0000000000	-0.0100346381
O	0.0000000000	0.0000000000	1.8525346381

CnO_2

Cn	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.8298334709
O	0.0000000000	0.0000000000	-1.8298334709

CnO_3

Cn	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	1.8349244513	0.0000000000
O	1.5890973790	-0.9174631615	0.0000000000
O	-1.5890973790	-0.9174631615	0.0000000000

$CnOF_2$

Cn	0.0000000000	0.0000000000	0.2526577871
O	0.0000000000	0.0000000000	-1.6975065666
F	0.0000000000	1.9299167556	0.3327750398
F	0.0000000000	-1.9299167556	0.3327750398

CnO_2F_2

Cn	0.0000000000	0.0000000000	-0.0913874709
O	0.0000000000	1.4101669664	-1.2754198229
O	0.0000000000	-1.4101669664	-1.2754198229
F	0.0000000000	1.3004008893	1.3752169433
F	0.0000000000	-1.3004008893	1.3752169433

X2C-AU/PBE0

F_2

F	0.00000000	0.00000000	-0.68795154
F	0.00000000	0.00000000	0.68795154

CnF

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	2. 0692118

CnF_2

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.91964368
F	0.00000000	0.00000000	-1.91964368

CnF_4

Cn	0.00000000	0.00000000	0.00000000
F	1.92679331	0.00000000	0.00000000
F	0.00000000	-1.92679331	0.00000000

F	-1.92679331	0.00000000	0.00000000
F	0.00000000	1.92679331	0.00000000

CnF_6

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.93250318
F	1.93250318	0.00000000	0.00000000
F	0.00000000	-1.93250318	0.00000000
F	-1.93250318	0.00000000	0.00000000
F	0.00000000	1.93250318	0.00000000
F	0.00000000	0.00000000	-1.93250318

CnF_6 (TS_1)

Cn	0.00104621	0.17705208	-0.01224303
F	1.09187438	-1.79489701	0.10678514
F	-1.03294280	-1.83715977	0.09805537
F	-1.89733939	0.47488709	-0.02748258
F	1.88437439	0.55707801	-0.03582623
F	-0.00338130	0.13549196	-1.94047814
F	0.00127897	0.30898164	1.91086286

CnF_6 (TS_2)

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	2.75118019
F	1.92569808	0.00000000	0.00000000
F	0.00000000	-1.92569808	0.00000000
F	-1.92569808	-0.00000000	0.00000000
F	-0.00000000	1.92569808	0.00000000
F	0.00000000	-0.00000000	-2.75118019

SOECP/CCSD(T)

F_2

F	0.00000000	0.00000000	-0.70986737
F	0.00000000	0.00000000	0.70986737

CnF_2

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	-1.95750382
F	0.00000000	0.00000000	1.95750382

CnF_4

Cn	0.00000000	0.00000000	0.00000000

F	0.00000000	1.94797437	0.00000000
F	1.94797437	0.00000000	0.00000000
F	0.00000000	-1.94797437	0.00000000
F	-1.94797437	0.00000000	0.00000000

CnF_6

Cn	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.95137055
F	0.00000000	1.95137055	0.00000000
F	1.95137055	0.00000000	0.00000000
F	0.00000000	-1.95137055	0.00000000
F	-1.95137055	0.00000000	0.00000000
F	0.00000000	0.00000000	-1.95137055

Harmonic vibrational frequencies at the X2C-AU/PBE0 level

Species	Symm.	ZPE (kcal/mol)	Harmonic frequencies (cm^{-1})
F_2	$D_{\infty h}$	1.57	1100 (σ^+_g)
$^{285}CnF_6$ (TS_1)	C_1 (C_{2v})	6.79	380i, 67, 93, 170, 210, 220, 240, 244, 253, 259, 376, 615, 641, 669, 691
$^{285}CnF_6$ (TS_2)	D_{4h}	5.68	57i(a_{1g}), 23(e_u), 40(e_g), 57(a_{2u}), 167(b_{1g}), 212(b_{1u}), 242(a_{2u}), 248(e_u), 640(b_{2g}), 659(a_{1g}), 687(e_u)

See Table 3 in the text about harmonic vibrational frequencies of ^{285}CnF, $^{285}CnF_2$, $^{285}CnF_4$ and $^{285}CnF_6$.

Effective contact densities of Cn in fluorides

The effective contact densities are computed at the optimized geometries by X2C-AU/PBE0, and a root-mean-square charge radius of 6.07 fm is used for the Cn nucleus. For sf-X2C-AU/CCSD(T), only valence electrons in Cn 6d7s and F 2s2p are correlated. The total density is given for the Cn atom and the density differences for molecules. Unit: $bohr^{-3}$.

	xf-X2C-AU/PBE0	X2C-AU/PBE0	sf-X2C-AU/CCSD(T)
Cn	28657175	29879227	28999920
CnF	-124	-34	-144
CnF_2	-414	-304	-421
CnF_4	-760	-604	-753
CnF_6	-970	-782	-933