

**On the chemical identification of E112:  
is E112 a relatively inert element?  
Precise calculations of E112 compounds.**

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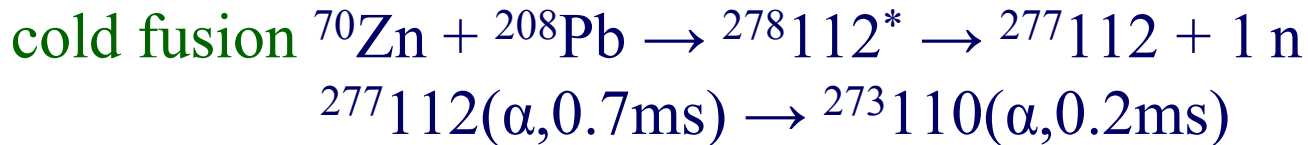
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1. Importance of chemical identification of E112.
2. Historical review of calculations on E112 compounds.
3. Our calculations of E112H, E112H<sup>+</sup>, E112<sub>2</sub>, E112Au.

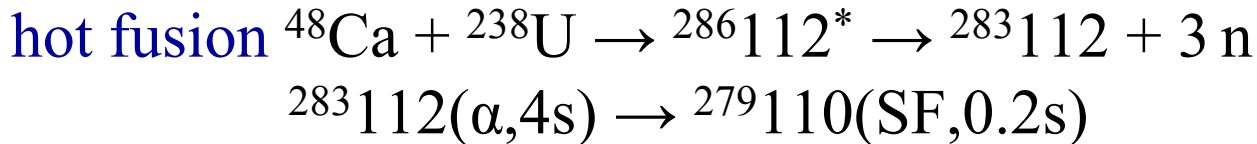
# Synthesis of E112

1996, GSI (Darmstadt) [Hofmann:96]:



It was confirmed at RIKEN (Japan) [Morita:04].

JINR (Dubna) [Oganessian:99, Oganessian:04]:



JINR result was not confirmed at LBNL (Berkeley)  
[Loveland:02, Gregorich:05].

Chemical identification is required [Yakushev:03, Soverna:05].

# Semiempirical estimations for properties of E112

E112 has the closed shell  $6d^{10}7s^2$  configuration in the ground state (Hg:  $5d^{10}6s^2$ , Rn:  $6s^26p^6$ ).

In [Pitzer:75], extreme **volatility and inertness** of E112 was suggested.

Atom	Transition	Promotion energy (HFD)
Hg	$5d^{10}6s^2 \rightarrow 5d^{10}6s^16p^1$	5.2 eV
E112	$6d^{10}7s^2 \rightarrow 6d^{10}7s^17p^1$	8.6 eV
Rn	$6s^26p^6 \rightarrow 6s^26p^57s^1$	9.2 eV

Discussion was initiated on the question: *will E112 behave like noble gas Rn rather than Hg.*

## First *ab initio* calculations

In [Eliav:95], accurate relativistic **correlation** (DCB/RCCSD) calculations on Hg and E112 atoms were first carried out.

The ground state of E112<sup>+</sup> ion will be  $6d_{3/2}^4 6d_{5/2}^5 7s_{1/2}^2$  unlike Hg<sup>+</sup>  $5d_{3/2}^4 5d_{5/2}^6 6s_{1/2}^1$ .

In [Seth:97], correlation (CCSD(T), MRCI) calculations on the E112H<sup>+</sup>, E112F<sub>2</sub> and E112F<sub>4</sub> **molecules** were carried out with the help of the pseudopotential (adjusted in the **LS-coupling** scheme) method.

However, the XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub> molecules *also exist*, so these calculations do not answer the question about Hg- or Rn-like behaviour.

Table 1. Transition Energies (TE) for E112 (in cm<sup>-1</sup>).

	HFDB	GRECP	RECP Nash 1997	PP Seth 1997	PP Seth 2003
Configuration	TE	Absolute errors			
$6d_{3/2}^4 6d_{5/2}^6 7s_{1/2}^2 \rightarrow$					
$6d_{3/2}^4 6d_{5/2}^6 7s_{1/2}^1 7p_{1/2}^1$	46406	-17	3198	-14254	153
$6d_{3/2}^4 6d_{5/2}^6 7s_{1/2}^1 7p_{3/2}^1$	64559	-29	5480	-3754	27
$6d_{3/2}^4 6d_{5/2}^6 7s_{1/2}^2 \rightarrow$					
$6d_{3/2}^4 6d_{5/2}^5 7s_{1/2}^2 7p_{1/2}^1$	28701	305 <sup>a</sup>	-3723	-15073	380
$6d_{3/2}^4 6d_{5/2}^5 7s_{1/2}^2 7p_{1/2}^1 \rightarrow$					
$6d_{3/2}^4 6d_{5/2}^5 7s_{1/2}^2 7p_{3/2}^1$	23894	-28	2469	12876	-192
$6d_{3/2}^4 6d_{5/2}^5 7s_{1/2}^2$	55747	17	2192	16855	-73

<sup>a</sup>This error can be removed by self-consistent GRECP correction.

## Calculations of other groups

In [Nakajima:00], scalar-relativistic correlation (DK3/CCSD(T)) calculations on E112H, E112H<sup>+</sup> and E112H<sup>-</sup> were carried out. However, they neglect the *large spin-orbit interactions*.

In [Nash:05], correlation (RCCSD(T)) calculations on E112H<sup>+</sup> and E112<sub>2</sub> with the help of the RECP method were carried out. However, Hg<sub>2</sub>, E112<sub>2</sub> and Xe<sub>2</sub> are *Van der Waals systems* with a small dissociation energy.

**Semiempirical** (RDFT) calculations on E112X (X=Au,Ag,Cu,Pd) [Pershina:02], E112Au [Tudoran:03] and E112<sub>2</sub> [Anton:05] were carried out. However, the **point nuclear model** was used in [Tudoran:03] and [Anton:05]. The errors of using the point nuclear model and neglecting Breit interactions attain several tenths and several hundredths of eV for the transition energies of E112.

## Our calculations

**Our** correlation (RCCSD+HOCA) calculations on E112H and E112H<sup>+</sup> with the help of the GRECP method.

The ground state RnH and XeH molecules are not observed in the gas phase, whereas HgH can be obtained by *radiofrequency discharge* in hydrogen and metal vapor (see, e.g., Ref. [Dufayard:88]).

**Our** *ab initio correlation* (CCSD(T)) calculations on E112<sub>2</sub> and *semiempirical* (SO-DFT) calculations on E112H, E112Au with the help of the GRECP method.

Table 2. Spectroscopic constants for E112H and HgH.

Method	$R_e(\text{\AA})$	$w_e(\text{cm}^{-1})$	$D_e(\text{eV})$
The HgH molecule			
GRECP/13e-RCCSD-1	1.709	1575	0.35
GRECP/13e-RCCSD(T)-1	1.738	1395	0.41
Experiment	1.738±0.003	1403±18	0.46
VGRECP/21e-SO-DFT (becke98)	1.742	1353	0.45
The E112H molecule			
GRECP/13e-RCCSD-1	1.638	1859	0.36
GRECP/13e-RCCSD-1 + HOCA	1.662	1800	0.42
GRECP/13e-CCSD-1	1.746	1402	-0.03
DK3/19e-CCSD(T) [Nakajima:00]	1.829	1007	0.06
VGRECP/21e-SO-DFT (becke98)	1.651	1766	0.62



# Dispersion interactions between atoms

$$E_{\text{disp}} = -1.5 \alpha_A \alpha_B I_A I_B / (I_A + I_B) R_{AB}^6 \quad \text{for } R_{AB} \gg r_A + r_B$$

X	HFDB	Experiment. for H, Hg and Xe, [Seth:97] and [Eliav:95] for E112		For XH and $R_{AB} = r_A + r_B$
Hg	$\langle r \rangle_{6s} = 2.85$ a.u.	$\alpha = 34.$ a.u.	$I = 0.384$ a.u.	$E_{\text{disp}} = 0.20$ eV
E112	$\langle r \rangle_{7s} = 2.50$ a.u.	$\alpha = 26.$ a.u.	$I = 0.440$ a.u.	$E_{\text{disp}} = 0.27$ eV
Xe	$\langle r \rangle_{5p} = 2.35$ a.u.	$\alpha = 27.$ a.u.	$I = 0.446$ a.u.	$E_{\text{disp}} = 0.36$ eV
H	$\langle r \rangle_{1s} = 1.50$ a.u.	$\alpha = 4.5$ a.u.	$I = 0.500$ a.u.	

Table 3. Spectroscopic constants for Hg<sub>2</sub> and E112<sub>2</sub>.

Method	R <sub>e</sub> (Å)	w <sub>e</sub> (cm <sup>-1</sup> )	D <sub>e</sub> (eV)
The Hg <sub>2</sub> molecule			
RDFT (B88/P86) [Anton:05]	3.63	14	0.009
GRECP/36e-CCSD(T)+SO	3.74	18.5	0.043
Experiment	3.66±0.03	19.65±0.05	0.045±0.002
RDFT (PW91) [Anton:05]	3.55	24	0.048
RECP/RCCSD(T) [Nash:05]	3.60		0.072
The E112 <sub>2</sub> molecule			
RDFT (B88/P86) [Anton:05]	3.45	25	0.039
GRECP/36e-CCSD(T)+SO	3.65	23.5	0.053
RDFT (PW91) [Anton:05]	3.39	30	0.080
RECP/RCCSD(T) [Nash:05]	3.07		0.187

Table 4. Spectroscopic constants for HgAu and E112Au.

Method	$R_e(\text{\AA})$	$w_e(\text{cm}^{-1})$	$D_e(\text{eV})$
The HgAu molecule			
VGRECP/39e-SO-DFT (becke98)	2.71	104	0.51
RDFT (RLDA/RGGA) [Persina:02]	2.67	100	0.50
RDFT (RLDA) [Tudoran:03]	2.6		1.03
RDFT (GGA) [Tudoran:03]			0.55
The E112Au molecule			
VGRECP/39e-SO-DFT (becke98)	2.77	83	0.36
RDFT (RLDA/RGGA) [Persina:02]	2.73	74	0.27
RDFT (RLDA) [Tudoran:03]	2.6		0.93
RDFT (GGA) [Tudoran:03]			0.41

## *Conclusions:*

1. Accounting not only for scalar-relativistic but also for spin-dependent effects is mandatory in calculations of SHE compounds even for  $\Sigma$ -states (where the spin-orbit contribution is suppressed in the leading order).
2. Our *ab initio* precise GRECP calculations on E112H and E112H<sup>+</sup> can be used for calibration of other more approximate methods (DFT, semiempirical, etc.) to study more complicated systems (interactions with surfaces, etc.).
3. **E112 demonstrate *more complicated behaviour* than just Hg-like or Rn-like one in opposite to that suggested earlier.**

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