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Materials Considerations for UF_6 Gas-Core Reactor
Interim Report for Preliminary Design Study

by

Paul Wagner

los alamos
scientific laboratory

of the University of California

LOS ALAMOS, NEW MEXICO 87545

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MATERIALS CONSIDERATIONS FOR UF_6 GAS-CORE REACTOR.

INTERIM REPORT FOR PRELIMINARY DESIGN STUDY

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ABSTRACT

The limiting materials problem in a high-temperature UF_6 core reactor is the corrosion of the core containment vessel. The UF_6 , the lower fluorides of uranium, and the fluorine that exist at the anticipated reactor operating conditions (1000 K and about one atmosphere UF_6) are all corrosive. Because of this, the materials evaluation effort for this reactor design study has concentrated on the identification of a viable system for the containment vessel that meets both the materials and neutronic requirements. A study of the literature has revealed that the most promising corrosion-resistant candidates are Ni or Ni-Al alloys. One of the conclusions of this work is that the containment vessel use a nickel liner or clad since the use of Ni as a structural member is precluded by its relative blackness to thermal neutrons.

Estimates of corrosion rates of Ni and Ni-Al alloys, the effects of the pressure and temperature of F_2 on the corrosion rates, calculated equilibrium gas compositions at reactor core operating conditions, suggested methods of fabrication, and recommendations for future research and development are included.

I. INTRODUCTION

Examination of the UF_6 gas-core reactor concept and preliminary design shows that the limiting materials problem is the containment of the hot UF_6 in the reactor core. UF_6 is itself a good fluorinating agent as are F_2 , F , and some of the lower fluorides which can be present from thermal dissociation of UF_6 . Therefore, at the design temperature of 1000 K the corrosion of the containment vessel could limit, or even dictate, the core operating conditions. Other materials considerations are certainly as important as the corrosion problem, but all other recognizable potential problems (i.e., those associated with the Molten Salt Reactor, engineering materials problems, radiation effects, etc.) probably have solutions either from existing science and technology or from straightforward research and development projects directed towards appropriate specific goals. Nickel and a nickel-aluminum alloy are the most promising containment materials for the extremely corrosive gases in the core; however, nickel has an undesirably high capture cross-section for thermal neutrons which further complicates the overall problem. Thus, in the time allotted to this feasibility study, it was felt that the effort would be optimized by concentrating on an in-depth study of the containment vessel corrosion problem and its ramifications.

The materials that are most compatible with UF_6 at temperatures of interest to us include pure nickel and some of the nickel alloys.¹ Other materials, such as Au or CaF_2 may be even more corrosion-resistant, but suffer from the other disadvantages of cost, difficulty of fabrication, and neutronic penalties. At the anticipated reactor operating conditions, thermodynamic equilibrium calculations for the system Ni-UF_6 show that NiF_2 , UF_5 , $\text{UF}_{4.5}$, UF_4 , F_2 , and F can also be present, indicating the possibility of reaction of fluorine and the various fluorides with the nickel. Some laboratory experiments, however, show that little UF_6 is consumed at 1030 K¹ in the presence of Ni pre-coated with NiF_2 (reaction time ~ 6 days)! Michallet reported² that UF_6 does not react with the metallic difluorides, but no temperature region was specified. In general, little quantitative experimental data for the Ni-UF_6 system has been found in the literature. In the absence of detailed information, we have adopted the viewpoint that a discussion of the corrosion problem by considering the most reactive species present (F and F_2) will be beneficial. In this manner the effects of temperature and pressure

on corrosion rates can be considered in some detail. It is also possible that this approach will actually describe the high-temperature corrosion behavior.

II. REACTIONS OF F_2 WITH NICKEL

A. General Observations

The corrosion of nickel by fluorine has been very widely studied. Rather than review the work in the literature in detail, this is a summary of the work of interest to this study. All the original information is obtainable from the materials listed in the bibliography.

For high-temperature applications, Ni has been demonstrated to be the metal most resistant to attack by F_2 and HF.³ The F_2 will be present in a UF_6 gas-core reactor at the reactor operating conditions as a result of the normal thermal dissociative process and also as a consequence of the interaction of the UF_6 with the various high-energy species in the fission field. The HF will be present as a result of the reaction of the UF_6 with the unavoidable H_2O contamination.

We have not found experimental data for the effect of F_2 on the core containment material for the exact conditions of temperature and pressure to be present in the reactor core. Furthermore, most of the data on F_2 have been generated at P_{F_2} in the vicinity of one atmosphere -- we anticipate* pressures much lower, of the order of one percent of an atmosphere for the F_2 . This will ameliorate the deleterious effects of temperature to some degree. Table I (taken from Ref. 3) is a compilation of data from several sources showing the influence of temperature on the corrosion of Ni by F_2 . Some of the rate constants for the longest time tests available⁴ (~ 32 hr.) are plotted in Figure 1.

In general, at temperatures of interest, the reactions between the F_2 and Ni seem to follow the relation,

$$\begin{aligned} y^n &= kt \\ \text{where } y &= \text{fluoride film thickness} \\ t &= \text{time} \\ k, n &= \text{constants} \end{aligned}$$

* See section V.

TABLE I

DATA FOR NICKEL-FLUORINE REACTIONS

T(°C)	P _{F₂} (atm)	Test duration (min)	$\Delta y(\mu)^a$ for t = 1 yr
-196	Liquid	5.26 x 10 ⁵ (1 yr)	0.25
-80	0.26-0.92	240	0.17
27	1.0	250	0.0012
30	0.26-0.92	210	0.00055
84	0.26-0.92	210	0.21
300	0.92	480	5.0
300	0.92	1900	0.73
400	0.92	34	15
400	0.92	1700	1.2
500	0.92	14	18
500	0.92	1800	3.0
540	1.0	120	25
550	1.0	120	36
600	0.92	14	74
600	0.92	1900	17
600	1.0	120	80
640	1.0	150	140
660	1.0	90	150
710	1.0	150	190
720	1.0	120	210
770	1.0	100	240
810	1.0	100	310
816	0.2-0.9		

^aEstimated loss of metallic nickel after a 1-yr-long exposure. Above 700°C, grain boundary attack may penetrate 5-8 times deeper than uniform surface NiF₂ scale formation.

The temperature dependence is of the form,

$$k \propto e^{-Q/RT},$$

where Q is the activation energy. For the data shown in Figure 1, n = 3.3, Q = 22 kcal/mole. The dependence of the reaction rate on the F₂ pressure has the form,

$$k_p \propto P_{F_2}^{1/m},$$

where m has been reported³ to have values from 1.15-2.7. It is a fact that the fluorination rate of nickel also seems to be sensitive to small amounts of impurities; for example, the pressure dependence for the fluorination of A-nickel (99.4% pure) is $P_F^{0.87}$ while for higher purity Ni it is $P_F^{0.56}$.

The mechanism² of the corrosion resistance of Ni to F_2 is one of passivation of the Ni surface by NiF_2 . However, as the temperature increases, the mobility of the fluorine anions increases whereupon they diffuse into the unreacted substrate to form NiF_2 .⁵ The Ni-rich surface layer then reacts with the gaseous species to maintain the NiF_2 stoichiometry. The rate of the diffusion of the fluorine anions is also influenced by the nature of the alloying agents or impurities in the substrate.

Figure 1. Rate constants for the Ni- F_2 reaction from reference 2.

TABLE II

PURE NICKEL IMPURITY ANALYSIS FROM INCO, (Ni > 99.97%)

<u>Element</u>	<u>Content (ppm)</u>
Ag	< 20
Al	< 100
As	20
Bi	< 20
C	< 10000
Cd	50
Co	50
Cu	100
Fe	1500
H	100-200
P	< 50
Pb	50
S	300
Sb	50
Se	20
Si	< 500
Sn	50
Te	20
Tl	50
Zn	50

In the vicinity of 1000 K, the vapor pressure of NiF_2 is

$$\log_{10} P_{\text{NiF}_2} \text{ (atm)} = 10.7 - \frac{16900}{T} .$$

The evaporation rate of the NiF_2 may also depend on the P_F in gas phase. Above ca. 1300 K, vaporization of the NiF_2 from pure Ni is² sufficiently rapid that no further protection is afforded and the exothermic Ni- F_2 reaction bootstraps itself to ignition.

Most impurities or alloying materials used with Ni degrade the corrosion resistance to F_2 . Materials to be avoided in this regard are Cr, Ti, Si, S, C, Sb, Nb, Cd, Pb, V, and P.⁶ Other impurities such as ThO_2 can lower the resistance of Ni to F_2 corrosion.³ For purposes of reference, an impurity analysis of pure nickel is included in Table II. This information was supplied to LASL by the International Nickel Co. Inc., New York, NY and is for their highest purity Ni.

B. The Ni-Al Alloys

Studies on the resistance of Ni-Al alloys to F_2 corrosion⁷ have shown that for high-temperature application the Ni-10 atomic percent Al alloy is significantly superior to pure Ni. A summary of some of the lower temperature work is shown in Figure 2. In the original report the authors claim that this improvement in protectivity extends to at least 1100 K. Conversations with persons currently active in fluorine corrosion studies at the Goodyear Atomic Co. have confirmed that the Ni-Al system is the best material identified to date for high-temperature F_2 application. It would appear that this material is the best candidate for use as the containment vessel in light of what is now known.

Based on the observations made on the Ni-Al alloys, it is speculated that a good candidate for investigation would be the Ni-Mg system. Russian work⁶ with Fe-Mg alloys showed improvement over pure Fe in behavior in halogen environments. By analogy, the Ni-Mg system, although not yet investigated, should be a strong candidate for a possible F_2 -resistant material.

III. OTHER CONSIDERATIONS CONCERNING THE USE OF NICKEL

From a purely materials viewpoint, Ni or an appropriate Ni alloy is the best candidate with which to build the UF_6 containment vessel. For the reactor design being considered⁸ Ni has some severe disadvantages. The mean free path of the thermal neutrons in Ni is sufficiently short that the use of enough Ni in the core to make it a structural material could prevent the reactor from going critical. However, it may be possible to tolerate small amounts of Ni if used in a suitable geometry. For example, if the structural part of the containment vessel is made of the Be reflector and the cavity that is exposed to the hot UF_6 is protected by a thin nickel cladding, a workable compromise of the neutronic and materials requirements can be made. Since the thermal expansion coefficients for Ni and Be are almost identical, the thermo-mechanical stresses induced by temperature changes would be minimized. The Ni cladding can be applied in several different ways⁹ (e.g., Ni electroplating on a Be substrate is a demonstrated technology), and if desired, the Ni-Al alloy described in the previous section may be made by plasma-spraying the Al on the Ni cladding and heat treating.⁷ This example is one of several possibilities and is cited to help bring into focus the components that might go into designing and engineering a Ni-containing core for the high-temperature UF_6 reactor.

Figure 2. Influence of composition on resistance to fluorine corrosion.

IV. OTHER MATERIALS AND THEIR REACTIONS WITH FLUORINE

Nickel is not the only material that has good resistance to fluorine corrosion.^{3,10-17} Al, Mg, and Al-Mg alloys have excellent F_2 corrosion resistance; however, since both metals melt at < 1000 K they could not be used at the intended reactor operating conditions. Zr is another metal that forms a passive fluoride layer (ZrF_4). While this protects the Zr from further fluorine attack at low temperatures, ZrF_4 sublimates at ~ 975 K and would not be suitable for high-temperature use. Zircaloy-2 (Zr + 1.5% Sn + 0.3% (Fe+Cr+Ni)), a much used reactor component, would be expected to be less resistant to F_2 attack^{3,15} than the pure Zr because of the alloying materials used, but thus far no specific experimental data have been found in the literature.

Since there is a possibility of using a Ni clad directly on the Be, it is possible that the Be could be exposed through cracks, pinholes, etc. The BeF_2 that forms when Be reacts with F_2 is reported¹⁶ to passivate the surface. However, BeF_2 melts at 1076 K and may be a problem if this temperature is exceeded. Table III shows the kinetic data reported for the Be- F_2 reaction as compiled in Ref. 1.

V. POSSIBLE ADVANTAGEOUS PRESSURE EFFECTS

The work reported on fluorine corrosion of various materials has been done at F_2 pressures considerably higher than those expected in the reactor core. Lower pressures of F_2 would be expected to decrease the rate of F_2 attack on the materials being discussed. Quantitative estimates of the effect of pressure on the thermal dissociation of UF_6 have been made by computing the F_2 pressure from existing thermodynamic data^{*6}. If indeed the NiF_2 layer inhibits the reaction of the gaseous components with the Ni substrate, then calculation of F_2 and F pressures from UF_6 alone (no NiF_2 in the system) should be a reasonable approximation. Free energy functions and heats of formation for the uranium fluorides were taken from Hildenbrand's recent work.¹⁷ The calculations were performed using the SENECA complex equilibrium computing code. The pressures of F_2 and F were calculated for total initial pressures of one and two

*These calculations were performed by Dr. R. C. Feber of LASL.

TABLE III

KINETIC DATA FOR BERYLLIUM-FLUORINE REACTIONS

<u>T (°C)</u>	<u>P_{F₂}^a (atm)</u>	<u>Δy(μm)^b</u> <u>for t = 1.0 yr</u>
125	0.263	4.9
225	0.263	4.7
525	0.079	2.2
	0.263	4.0
	0.829	9.3
	0.921	11.5
575	0.263	8.7
625	0.263	20
	0.829	31
675	0.026	9.7
	0.053	15
	0.079	19
	0.263	40
775	0.079	55
	0.263	80

^aTests were in static rather than flowing fluorine.

^bEstimated metal loss after 1-yr-long exposure to fluorine attack.

atmospheres of UF₆ and temperatures 800-1200 K at 100 K intervals. The results are summarized in Table IV. The complete computational results are appended to this report. Since the SENECA code can handle complex heterogeneous equilibria, provision was made to identify formation of non-gaseous UF₄, UF₅, and U₂F₉. None of these appeared for the calculational conditions assuming that only thermal dissociation of UF₆ was occurring. This is equivalent to the assumption that only F₂ is diffusing through the protective layer.

Using the data in Table IV, estimates of the corrosion rates of the nickel used in the reactor cavity may be made. Relative rates can be obtained by estimating an m in $k \propto P^{1/m}$ and using the data in Figure 1. For example, if we choose m to be some mean of the reported values (1.15-2.7),

$$k \propto P^{0.52}$$

TABLE IV
EQUILIBRIUM F AND F₂ PRESSURES FOR THERMAL DISSOCIATION OF UF₆

Temperature	1 atmosphere UF ₆		2 atmospheres UF ₆	
	P _F	P _{F₂}	P _F	P _{F₂}
K	mm	mm	mm	mm
800	.0073	.00084	.0099	.0016
900	.084	.0074	.11	.014
1000	.58	.040	.76	.076
1100	2.8	.16	3.9	.30
1200	10.6	.49	14.4	.99

If we now take the pressures of F and F₂ at 1000 K to be (0.58 + 0.04) mm, the ratio of rates in the cavity to the 1 atmosphere corrosion test should go as;

$$\frac{k_{\text{cavity}}}{k} \propto \left(\frac{0.62}{760} \right)^{0.52} = 7.87 \times 10^{-4} ,$$

or the rate will decrease by approximately three orders of magnitude which would correspond to Ni corrosion by F₂ at 600 K (see Fig. 1). From Table I it is seen that at 600 K one would expect corrosion rates of the order of micrometres per year. If the Ni-Al alloy is as good as the preliminary evidence indicates, such a clad should corrode at the rate of a fraction of a micrometre per year.

It is to be emphasized that such a calculation -- extrapolating from 32 hours to one year and assuming no diffusion of uranium fluorides through the protective layer -- is tenuous at best. However, it is clear that the high stability of the UF₆ at planned reactor operating conditions will result in very low F-F₂ pressures by thermal dissociation and thus beneficially low Ni corrosion rates.

TABLE V
MATERIALS R AND D OUTLINE

<u>Data Needed</u>	<u>Under These Conditions</u>	<u>For These Materials</u>
Accurate corrosion rate data for high-temperature UF_6 under realistic operating conditions	Proper UF_6 or F_2 T and P Dynamic conditions In-pile if proven necessary On test samples fabricated in a realistic manner	Ni and Ni-Al Ni and its alloys deposited on candidate substrates using realistic fabrication methods Experimental materials such as Ni-Mg, Al, Mg, Al-Mg
Gaseous species present in UF_6	At core T and P Possibly at core T, P, and nv	UF_6 and possibly F_2

VI. RECOMMENDATIONS FOR FUTURE WORK

In the event the actual construction of the UF_6 cavity reactor were to be initiated, it is felt that the data contained in this report could be used for the basic design of the containment vessel. However, it is recommended that experimental work, designed to simulate realistic core operating conditions, on the reactions of hot UF_6 (i.e., F_2 and F) with the cavity materials be pursued in parallel with any design and construction. Table V is an outline of the core materials research and development work that would be carried out as an adjunct to the effort.

Accurate corrosion rate data for the systems being considered would be obtained initially using UF_6 at 1000 K and one atmosphere in a reactor test. With experience, it might be possible to demonstrate that in-pile experimental results are the same as those obtained out-of-pile and that duplicating the required T and P conditions in the laboratory would suffice. This has been the case in the past; for example, the amoeba effect in the HTGR fuel is the same in- and out-of-pile. Additionally, accurate knowledge of the gaseous species present in UF_6 at core operating conditions could well allow us to perform simulated experiments with a degree of control and rapidity not possible in an in-pile experiment. LASL's capabilities in computing reaction rates using results from equilibrium calculations in conjunction with diffusion rate data

would lend themselves admirably to modelling the Ni-UF₆ system. Once this point is reached, efforts to look for even more satisfactory or new materials could be carried out in a methodical and efficient manner.

VII. CONCLUDING REMARKS

The corrosive action of the hot gases in a UF₆ gas-core reactor is the most serious of the recognizable materials problems. Unfortunately, the material most likely to contain the UF₆ at one atmosphere and 1000 K is nickel and nickel is relatively black to thermal neutrons. An exhaustive literature study plus considerations based on the equilibrium gas composition of UF₆ for the described conditions and the neutronic requirements have resulted in the recommendation that a workable containment vessel can be made using nickel as a cladding material. Examples of fabrication methods that can be used and estimates of corrosion rates of the Ni clad are included. A brief outline of a recommended R and D effort on this problem is also included.

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APPENDIX

Results of the equilibrium composition calculations for UF_6 . (All calculations done by R. C. Feber.)

1 ATM OF UF6 INITIALLY

TEMPERATURE = .8000E+03 DEG K

INITIAL PRESSURE = .1000E+01 ATM

FINAL PRESSURE = .1000E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.1000E+01	.1000E+01	.1000E+01
F2(G)	1	.1131E-05	.1131E-05	.1131E-05
F(G)	1	.9552E-05	.9552E-05	.9552E-05
UF5(G)	1	.1181E-04	.1181E-04	.1181E-04
.1000E+01				

2 ATM OF UF6 INITIALLY

TEMPERATURE = .8000E+03 DEG K

INITIAL PRESSURE = .2000E+01 ATM

FINAL PRESSURE = .2000E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.1000E+01	.1000E+01	.2000E+01
UF5(G)	1	.8642E-05	.8642E-05	.1728E-04
F(G)	1	.6529E-05	.6529E-05	.1306E-04
F2(G)	1	.1057E-05	.1057E-05	.2113E-05
.1000E+01				

1 ATM OF UF₆ INITIALLY

TEMPERATURE = .9000E+03 DEG K

INITIAL PRESSURE = .1000E+01 ATM

FINAL PRESSURE = .1000E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF ₆ (G)	1	.9999E+00	.9998E+00	.9999E+00
F(G)	1	.1088E-03	.1088E-03	.1088E-03
F ₂ (G)	1	.9685E-05	.9684E-05	.9685E-05
UF ₅ (G) .1000E+01	1	.1282E-03	.1282E-03	.1282E-03

2 ATM OF UF₆ INITIALLY

TEMPERATURE = .9000E+03 DEG K

INITIAL PRESSURE = .2000E+01 ATM

FINAL PRESSURE = .2000E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF ₆ (G)	1	.9999E+00	.9998E+00	.2000E+01
F ₂ (G)	1	.9165E-05	.9164E-05	.1833E-04
F(G)	1	.7484E-04	.7483E-04	.1497E-03
UF ₅ (G) .1000E+01	1	.9317E-04	.9316E-04	.1863E-03

1 ATM OF UF6 INITIALLY

TEMPERATURE = .1000E+04 DEG K

INITIAL PRESSURE = .1000E+01 ATM

FINAL PRESSURE = .1001E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9991E+00	.9983E+00	.9991E+00
F(G)	1	.7581E-03	.7575E-03	.7581E-03
UF5(G)	1	.8638E-03	.8631E-03	.8638E-03
F2(G) .1001E+01	1	.5288E-04	.5284E-04	.5288E-04

2 ATM OF UF6 INITIALLY

TEMPERATURE = .1000E+04 DEG K

INITIAL PRESSURE = .2000E+01 ATM

FINAL PRESSURE = .2001E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9945E+00	.9988E+00	.1999E+01
UF5(G)	1	.6251E-03	.6247E-03	.1250E-02
F(G)	1	.5240E-03	.5237E-03	.1048E-02
F2(G) .1001E+01	1	.5053E-04	.5050E-04	.1011E-03

1 ATM OF UF6 INITIALLY

TEMPERATURE = .1100E+04 DEG K

INITIAL PRESSURE = .1000E+01 ATM

FINAL PRESSURE = .1004E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9959E+00	.9920E+00	.9959E+00
UF5(G)	1	.4107E-02	.4091E-02	.4107E-02
F(G)	1	.3690E-02	.3676E-02	.3690E-02
F2(G)	1	.2088E-03	.2080E-03	.2088E-03
.1004E+01				

2 ATM OF UF6 INITIALLY

TEMPERATURE = .1100E+04 DEG K

INITIAL PRESSURE = .2000E+01 ATM

FINAL PRESSURE = .2006E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9970E+00	.9943E+00	.1994E+01
UF5(G)	1	.2963E-02	.2955E-02	.5926E-02
F(G)	1	.2561E-02	.2554E-02	.5121E-02
F2(G)	1	.2011E-03	.2005E-03	.4021E-03
.1003E+01				

1 ATM OF UF6 INITIALLY

TEMPERATURE = .1200E+04 DEG K

INITIAL PRESSURE = .1000E+01 ATM

FINAL PRESSURE = .1014E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9850E+00	.9711E+00	.9850E+00
UF5(G)	1	.1500E-01	.1479E-01	.1500E-01
F(G)	1	.1371E-01	.1352E-01	.1371E-01
F2(G)	1	.6440E-03	.6340E-03	.6440E-03
.1014E+01				

2 ATM OF UF6 INITIALLY

TEMPERATURE = .1200E+04 DEG K

INITIAL PRESSURE = .2000E+01 ATM

FINAL PRESSURE = .2020E+01 ATM

SPECIES	PHASE NUMBER	AMOUNT	MOLE FRACTION	PARTIAL PRESSURE
UF6(G)	1	.9892E+00	.9792E+00	.1978E+01
F(G)	1	.9557E-02	.9460E-02	.1911E-01
UF5(G)	1	.1001E-01	.1070E-01	.2162E-01
F2(G)	1	.6255E-03	.6192E-03	.1251E-02
.1010E+01				