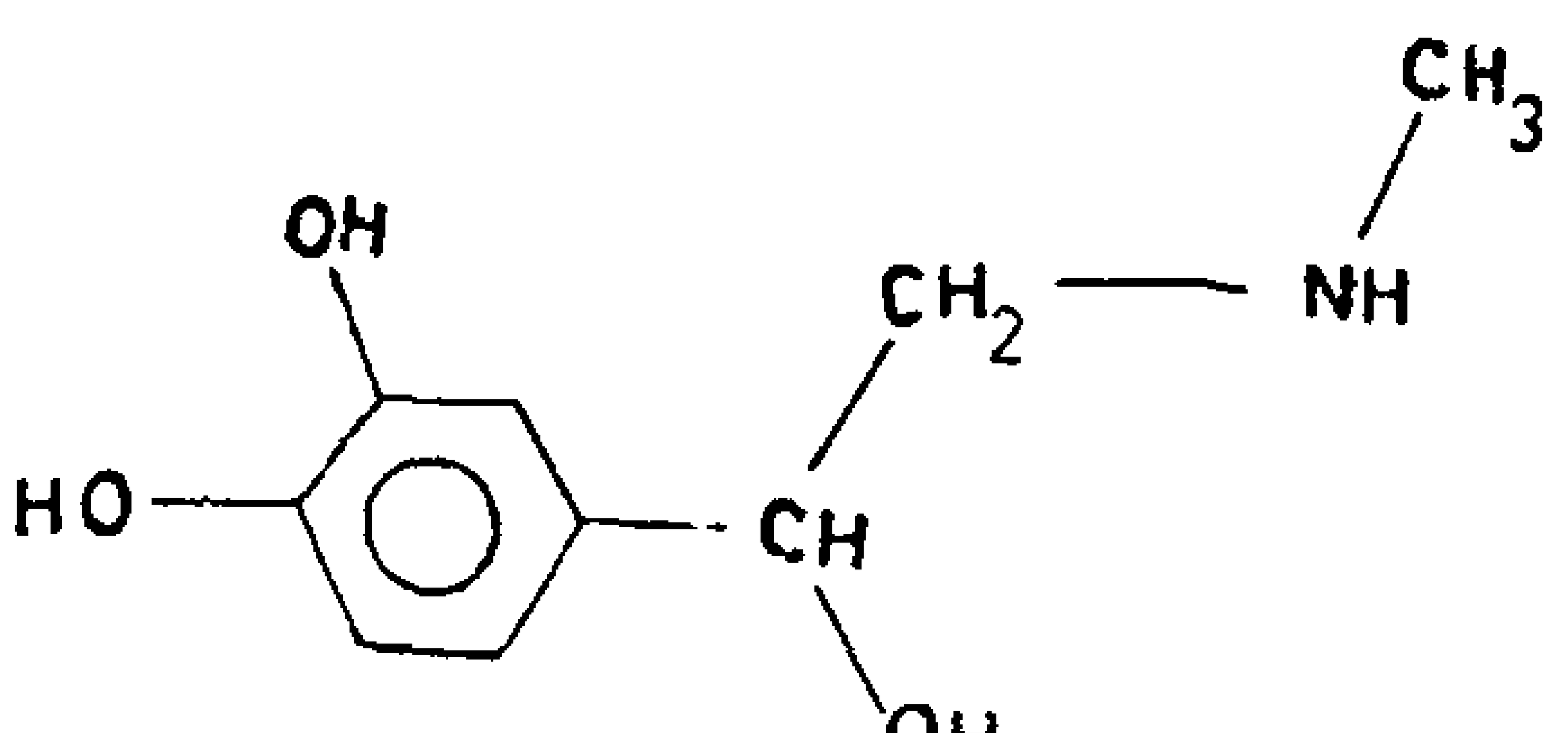
# LETTERS TO THE EDITOR

## CRYSTAL DATA ON L-EPINEPHRINE HYDROCHLORIDE MONOHYDRATE

B. M. Vedavathi, A. Mani and Kalyani Vijayan
Materials Science Division, National Aeronautical Laboratory, Bangalore 560 017, India.

Epinephrine (or adrenaline) (I), is known to possess protective action against ionizing radiation[1]. As part of a series[2,3] of x-ray investigations on chemical radioprotectants, preliminary crystal data have been collected on L-epinephrine hydrochloride monohydrate. Commercially obtained L-epinephrine was dissolved in dilute hydrochloric acid and needle-shaped brownish crystals of the title compound were obtained by slow evaporation. Unit cell dimensions and space group were determined from oscillation and Weissenberg photographs. Presence of the chloride ion was verified by conducting the 'chloride test' and the presence of the adrenaline moiety was confirmed from an ultraviolet absorption spectrum. The preliminary crystal data have been listed in table 1.




(I)

Table 1
*Crystal data on L-epinephrine HCl. H₂O*

| | |
|---|---|
| Formula | $C_8H_{13}NO_3.HCl.H_2O$ |
| Molecular weight | 219.6 |
| Crystal system | Triclinic |
| $a$ | = 10.59 ± 0.02 Å |
| $b$ | = 10.61 ± 0.02 |
| $c$ | = 11.12 ± 0.01 |
| $\alpha$ | = 112.6 ± 0.3° |
| $\beta$ | = 90 ± 0.2 |
| $\gamma$ | = 100.6 ± 0.3 |
| Space group | P1 or P$\bar{1}$ |
| Density (Calc) | 1.40 gcm$^{-3}$ |
| Density (Expt) (Flotation in acetone and $CCl_4$) | 1.40 gcm$^{-3}$ |
| Z | = 4 |

12 January 1982

1. Gray, J. L., Moulden, E. J., Tew, J. T., and Jensen, H., *Proc. Soc. Exp. Biol.*, 1952, **79**, 384.
2. Vedavathi, B. M., and Vijayan, K., *Acta. Crystallogr.*, 1981, **B37**, 475 and the references therein.
3. Mani, A., Vedavathi, B. M., and Vijayan, K., *Curr. Sci.*, 1982, (In press).

## (n, α) AND (n, p) CROSS SECTIONS IN SOME Se AND Zn ISOTOPES AT 14 MeV

C. V. Srinivasa Rao†, N. Lakshmana Das, B. V. Thirumala Rao and J. Rama Rao*
Laboratories for Nuclear Research, Andhra University, Waltair, Visakhapatnam 530 003, India.
† Department of Physics, Indian Institute of Technology, Kanpur 208 016, India.
* Department of Physics, Banaras Hindu University, Varanasi 221 005, India.

The cross sections reported in literature[1] for some $(n, \alpha)$ and $(n, p)$ reactions at 14 MeV in some selenium and zinc isotopes show a wide discrepency. Thus, in the case of $^{80}Se(n, \alpha)^{77m}$ Ge, the cross-section values vary between 6 mb to 134 mb[2-5]. Even the Ge(Li) measurement[4] gave only the limits to this cross-section as 2–9 mb. In $^{78}Se(n, \alpha)^{75}$Ge reaction, the reported cross-section values range from 6 mb to 38 mb[2,4-6]. Only one value is reported on the cross-section of the reaction $^{68}Zn(n,p)^{68m}$ Cu giving a value of 4.5 ± 0.08 mb which is not verified so far. These lacunae prompted the present work. Along with the above three, we also measured the cross-section for $^{66}Zn(n,p)^{66}$Cu. The mixed powder technique[4] and high resolution Ge(Li) detection have been employed in the present measurement.

Mixed powders of the specpure ( > 99.9% pure) sample and aluminium serving as the monitor, were irradiated at an incident neutron energy of 14.2 ± 0.2 MeV at the 600 keV Cockcroft-Walton accelerator of Andhra University. The gamma activities produced in the irradiated samples were measured with a 35 c.c coaxial Ge(Li) detector (FWHM: 4.6 at 1332 keV) coupled to a ND512 channel analyser system. The method of evaluating the cross-section and the error is given in our earlier paper[8]. The cross-sections measured in the present work along with those reported in the literature, are presented in table 1, besides the half-life ($T_{1/2}$), energy ($E_r$) and absolute abundance in photons per disintegration ($\theta$) of the measured gamma ray. Also presented in the same table are the theoretical estimates[9-11].

TABLE 1

*$(n, \alpha)$ and $(n, p)$ cross-sections at $14.2 \pm 0.2$ MeV*

| Reaction | Decay data of the product nuclide[12] | | | $\sigma$ expt (mb) | Literature values | | | Theoretical cross sections* (mb) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | $T_{1/2}$ | $E_\gamma$ (kev) | | | $\sigma$ | detector employed | Ref | Levkovskii[9] | Lu & Fink[10] | Pearlstein[11] |
| $^{80}Se(n, \alpha)^{77m}Ge$ | 53.6 s | 160 | 0.21 | $4.6 \pm 0.5$ | $37.7 \pm 15.4$ | GM | 3 | 3.58 | 3.13 | 2 |
| | | | | | $6 \pm 2$ | GM | 2 | | | |
| | | | | | $134 \pm 25$ | GM | 5 | | | |
| | | | | | 2–9 | Ge(Li) | 4 | | | |
| $^{78}Se(n, \alpha)^{75}Ge$ | 82.8 m | 265 | 0.1 | $2.7 \pm 0.3$ | $6 \pm 1$ | Ge(Li) | 4 | 7.20 | 0.99 | 5.5 |
| | | | | | $7 \pm 1$ | NaI(Tl) | 6 | | | |
| | | | | | $19 \pm 2$ | NaI(Tl) | 2 | | | |
| | | | | | $38 \pm 16$ | NaI(Tl) | 5 | | | |
| $^{68}Zn(n, p)^{68m}Cu$ | 3.8 m | 84 | 0.68 | $7.3 \pm 1.6$ | $4.5 \pm 0.08$ | Ge(Li) | 7 | 24.05 | 13.3 | 26 |
| $^{66}Zn(n, p)^{66}Cu$ | 5.1 m | 1039 | 0.09 | $54 \pm 9$ | $77 \pm 10$ | NaI(Tl) | 14 | 57.2 | 48.8 | 68 |
| | | | | | $100 \pm 15$ | GM | 15 | | | |
| | | | | | $65 \pm 6$ | Ge(Li) | 13 | | | |
| | | | | | $62 \pm 15$ | NaI(Tl) | 16 | | | |
| | | | | | $72 \pm 8$ | Ge(Li) | 17 | | | |
| | | | | | 60–78 | Various detectors | 1 | | | |

*Total cross-section

In the case of $^{80}Se(n,\alpha)^{77m}Ge$ reaction cross-section, the present work offers first Ge(Li) measurement with a definite value. Though Venugopala Rao and Fink[4] tried this reaction with a Ge(Li) detector, they gave only a limit to the cross-section as 2-9 mb. The present value of the cross-section for the reaction $^{78}Se(n,\alpha)^{75}Ge$ is smaller than the only Ge(Li) value reported earlier[4], while for the reaction $^{68}Zn(n,p)^{68m}Cu$, the present value is more than that of the only earlier measurement[7]. In the latter case, the difference might be due to the self absorption of 84 keV gamma ray within the sample. In our measurement, the relative efficiency of the detector, corrected for self absorption and scattering within the sample, was calibrated using the simulation technique. In the case of $^{66}Zn(n,p)^{66}Cu$, the present cross-section value is in agreement, within the limits of error, with the earlier measurement[13] using Ge(Li) detector giving a value of 65 ± 6 mb.

NLD is thankful to the University Grants Commission for fellowship.

16 February 1982

1. CINDA 78: *An index to the literature on microscopic neutron data*, IAEA, Vienna, 1978.
2. Minette, B. and Pasquerelli, A., *Nucl. Phys.*, 1967, **100**, 186.
3. Paul, E. B., and Clarke, R. L., *Can. J. Phys.*, 1953, **31**, 267.
4. Venugopala Rao, P., and Fink, R. W., *Phys. Rev.*, 1967, **154**, 1023.
5. Ivanenka, V. V., and Petrazhak, K. A., *Sov. J. Nucl. Phys.*, 1969, **9**, 152.
6. Vinitskaya, G. P., Levkovskii, V. N., and Sokolskii, V. V., *Sov. J. Nucl Phys.*, 1967, **6**, 174.
7. Tikku, V. K., Singh, H., and Sethi, B., *Proc. Nucl. Phys. and Solid State Physics* (India), Chandigarh, 1972, **15**, 115.
8. Lakshmana Das, N., Srinivasa Rao, C. V., Thirumala Rao, B. V. and Rama Rao, J., *IL Nuovo Cim.*, 1978, **A48**, 500.
9. Levkovskii, V. N., *Sov. J. Nucl. Phys.*, 1974, **18**, 361.
10. Lu, W. D. and Fink, R. W., *Phys. Rev.*, 1971, **C4**, 1173.
11. Pearlstein, S., *J. Nucl. Energy*, 1973, **27**, 81.
12. Bowman, W. W., and MacMurdo, K. W., *Atomic and Nuclear Data Tables*, 1974, **13**, 89.
13. Ranakumar, N., Kondaiah, E., and Fink, R. W., *Nucl. Phys.*, 1960, **122**, 679.
14. Priess, I. L., and Fink, R. W., *Nucl. Phys.*, 1960, **15**, 326.
15. Gardner, D. G., and Rosenblum, S., *Nucl. Phys.*, 1967, **A96**, 121.
16. Prasad, R., and Sarkar, D. C., *Nuovo Cim.*, 1971, **A3**, 467.
17. Qaim, S. M., and Molla, N. I., *Nucl. Phys.*, 1977, **A283**, 269.

## STUDY OF ESCA AND AUGER CHEMICAL SHIFTS IN SOME GALLIUM COMPOUNDS

P. S. Murty, S. V. N. Bhaskara Rao, S. K. Sharma* and S. V. Grampurohit
Spectroscopy Division, Bhabha Atomic Research Centre, Trombay, Bombay 400 085, India.
*Metallurgy Division

The pioneering work of Siegbahn and his co-workers[1] in the field of x-ray photoelectron spectroscopy (XPS) has resulted in a technique having a variety of applications. One of the most important applications of this technique, widely referred to as ESCA (electron spectroscopy for chemical analysis), is the determination of the so-called chemical shift in the core electron binding energy (BE). The BE of a core electron of free atom is different from that when it is a part of a molecule. Thus ESCA not only provides a rapid elemental analysis of a specimen, but also tells in what chemical form a particular element is present.

### *ESCA Chemical shift in GaP*

The ESCA chemical shift of $Ga2p_{3/2}$ core level in gallium phosphide with reference to $Ga_2O_3$ is not listed in literature. Therefore, we have attempted the present study. A small piece of GaP specimen, approximately 5 mm × 5 mm and 1 mm thick, was exposed to atmosphere for a few hours so that a layer of $Ga_2O_3$ was formed on GaP surface. The electron spectrometer employed is the Physical Electronics Industries Model 550 ESCA/Auger spectrometer. It has a double pass cylindrical mirror analyser for the energy analysis of the electrons. Using Mg $K\alpha$ ($h\nu = 1253.6$ eV) x-rays (power = 400 W) the photoelectron spectrum in the BE range, 1110-1130 eV was scanned. Two peaks were seen corresponding to $Ga2p_{3/2}$ core electrons. On the basis of electronegativity, we could assign the peak at higher BE to $Ga2p_{3/2}$ core level from $Ga_2O_3$ while the peak at lower BE to the same core level from GaP. The electronegativity of oxygen is more than that of phosphorus. Further confirmation was obtained by running the ESCA spectrum of a pure $Ga_2O_3$ specimen. The BE's of the two peaks are 1124.1 eV and 1121.4 eV and the difference which is equal to 2.7 eV is the chemical shift of $Ga2p_{3/2}$ from GaP w.r.t. $Ga_2O_3$.

### *Auger Chemical Shift in $Ga_2O_3$*

Auger lines also show chemical shift corresponding to different species of an element[1,2]. Often the chemi-