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# Transition probability parameters for certain band systems of astrophysical molecule GeO

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**Abstract**

The transition probability parameters, Franck–Condon factors and *r*-centroids, have been evaluated using the most reliable numerical integration procedure for the bands of $E^1\Sigma^+$, $F^1\Sigma^+$, $G\Sigma$, $H\Pi$, $J\Sigma$–$X^1\Sigma^+$ systems of astrophysical molecule GeO, using a suitable potential.


## 1. Introduction

The transition probability parameters such as Franck–Condon (FC) factors and *r*-centroids are required for diagnostic applications in astronomy, astrophysics and related subjects. Accurate values of FC factors and *r*-centroids are essential to understand and to evaluate the radiative life time, variation of electronic transition moment with internuclear separation, vibrational temperature of the source and relative band strengths. The FC factors are useful in studies of radiative transfer in the atmospheres of stellar and other astronomical objects, which contain molecular species [1].

GeO belongs to the homologous monoxides with CO, SiO, SnO and PbO [2]. Hence the spectra and molecular structure are similar, specially for GeO, CO and SiO [3]. For instance, the triplet to singlet intercombination bands of SiO and GeO are analogous to Cameron and Hopfield–Birge systems of CO [4,5]. The molecular states of SiO, GeO and SnO give rise to absorption in the Schumann region, below 2000 Å [6]. Further CO and SiO are well known and extensively studied molecules of astrophysical interest. For instance CO and SiO are observed and studied in supernova 1987 a [7]. CO is observed in cool evolved star, star-forming galaxies [8–10]. SiO is observed in a variety of sources including young globular cluster [11], Sagittarious B2 [12] and interstellar medium [13]. These sources have a wide range of effective temperature including very low temperature in the case of SiO.

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The UV spectra of GeO are particularly difficult to observe in the laboratory due to interaction of $GeO_2$ with quartz windows and presence of isotope shifts [3,5]. The source temperature is in the range 700–1200 °C.

The presence of Ge II lines has been identified in the diffuse halo clouds in milkyway [14]. Model atmosphere calculations for red giant star of solar composition show a significant elemental abundance for Ge. Further, oxides are among the most readily formed diatoms in a variety of astrophysical contexts [15]. Fegley and Prinn [16] have noted the presence of GeO molecule in the deep atmosphere of Uranus. Observation from space with the International Ultraviolet Explorer (IUE) has produced vast archives of UV spectra of various astrophysical sources including region below 2000 Å. These archives are used in studying UV spectra of variety of stars [17,18]. In view of the above facts and arguments it turns out that GeO is a strong case, specially in UV region as an astrophysically important diatomic molecule to be looked for in supernovae, ISM, gallactic halos, star-forming regions and various other such astrophysical sources. Besides, the presence of isotopic shifts makes GeO spectroscopically of special interest.

There has been no report on the FC factors and *r*-centroids for the band systems $E^1\Sigma^+$, $F^1\Sigma^+$, $G\Sigma$, $H\Pi$, $J\Sigma$–$X^1\Sigma^+$ of GeO molecule, to our best knowledge, in the literature. Therefore the reliable values of FC factors and *r*-centroids for these band systems of astrophysical molecule GeO have been determined by the most accurate numerical integration procedure using a suitable potential.

## 2. Franck–Condon factors and *r*-centroids

One of the parameters which controls the intensity distribution in the molecular bands is the FC factor. The square of the overlap integral is termed as FC factor [19]

$$q_{v'v''} = |\langle \psi_{v'} | \psi_{v''} \rangle|^2 \tag{1}$$

where $\psi_{v'}$ and $\psi_{v''}$, are the vibrational wave functions for the upper and lower states, respectively. The *r*-centroid is a unique value of internuclear separation, which may be associated with a $v'$–$v''$ band and defined as

$$\bar{r}_{v'v''} = \frac{\langle \psi_{v'} | r | \psi_{v''} \rangle}{\langle \psi_{v'} | \psi_{v''} \rangle} \tag{2}$$

The Morse [20] potential yields accurate FC factors especially for vibrational transition involving low quantum numbers [21–23]. The computation of the FC factor is made using Bates's [24] method of numerical integration according to the detailed procedure provided by Rajamanickam et al. [25]. Morse wave functions were calculated at intervals of 0.01 Å for the range of *r* respectively from 1.49 to 2.39 Å, from 1.49 to 1.90 Å, from 1.56 to 2.01 Å, from 1.56 to 2.04 Å and from 1.56 to 1.99 Å for every observed vibrational level of each state of E–X, F–X, G–X, H–X and J–X systems, respectively. Once the appropriate wave functions are obtained, the FC factors can be evaluated by integrating the expression (1). The definition of *r*-centroids offers a method of computing *r*-centroids directly. Integrals in Eqs. (1) and (2) for the FC factors ($q_{v'v''}$) and *r*-centroids ($\bar{r}_{v'v''}$) were computed numerically and the results are presented respectively in Tables 1–5 for the bands of E–X, F–X, G–X, H–X and J–X systems of GeO molecule. The wavelengths ($\lambda_{v'v''}$) data [12,13] are also included. The molecular constants used in the present study

Table 1
$q_{v'v''}$ and $\bar{r}_{v'v''}$ for E–X system of GeO

| $v', v''$ | $\lambda_{v'v''}$ (Å) | $q_{v'v''}$ | $\bar{r}_{v'v''}$ (Å) |
|---|---|---|---|
| 0, 2 | 2107.4 | 0.002 | 1.774 |
| 0, 3 | 2151.0 | 0.007 | 1.792 |
| 1, 1 | 2044.5 | 0.002 | 1.748 |
| 2, 0 | 1984.9 | 0.001 | 1.721 |
| 2, 1 | 2024.4 | 0.009 | 1.738 |
| 3, 0 | 1966.6 | 0.003 | 1.712 |
| 4, 0 | 1948.7 | 0.008 | 1.703 |
| 5, 0 | 1931.5 | 0.016 | 1.694 |
| 6, 0 | 1914.9 | 0.028 | 1.686 |
| 7, 0 | 1899.0 | 0.041 | 1.677 |
| 8, 0 | 1883.6 | 0.056 | 1.669 |
| 9, 0 | 1869.1 | 0.070 | 1.661 |
| 9, 1 | 1904.0 | 0.056 | 1.678 |
| 10, 0 | 1854.9 | 0.081 | 1.652 |
| 12, 0 | 1828.5 | 0.089 | 1.636 |

Table 2
$q_{v'v''}$ and $\bar{r}_{v'v''}$ for F–X system of GeO

| $v', v''$ | $\lambda_{v'v''}$ (Å) | $q_{v'v''}$ | $\bar{r}_{v'v''}$ (Å) |
|---|---|---|---|
| 0, 0 | 1483.9 | 0.670 | 1.651 |
| 0, 1 | 1505.8 | 0.264 | 1.717 |
| 0, 2 | 1528.2 | 0.058 | 1.771 |
| 1, 0 | 1466.6 | 0.270 | 1.597 |
| 1, 1 | 1487.9 | 0.232 | 1.656 |
| 1, 2 | 1509.7 | 0.333 | 1.726 |
| 1, 3 | 1532.0 | 0.133 | 1.779 |
| 2, 0 | 1449.9 | 0.054 | 1.535 |
| 2, 1 | 1470.8 | 0.348 | 1.607 |
| 2, 2 | 1492.0 | 0.040 | 1.650 |
| 3, 0 | 1433.9 | 0.007 | 1.459 |
| 3, 1 | 1454.2 | 0.129 | 1.549 |
| 3, 2 | 1475.0 | 0.309 | 1.616 |
| 4, 1 | 1438.1 | 0.025 | 1.478 |
| 4, 2 | 1458.5 | 0.196 | 1.561 |

Table 3
$q_{v'v''}$ and $\bar{r}_{v'v''}$ for G–X system of GeO

| $v', v''$ | $\lambda_{v'v''}$ (Å) | $q_{v'v''}$ | $\bar{r}_{v'v''}$ (Å) |
|---|---|---|---|
| 1, 0 | 1533.4 | 0.062 | 1.684 |
| 3, 0 | 1501.3 | 0.153 | 1.653 |
| 4, 0 | 1486.0 | 0.162 | 1.638 |

Table 4
$q_{v'v''}$ and $\bar{r}_{v'v''}$ for H–X system of GeO

| $v', v''$ | $\lambda_{v'v''}$ (Å) | $q_{v'v''}$ | $\bar{r}_{v'v''}$ (Å) |
|---|---|---|---|
| 1, 0 | 1530.2 | 0.078 | 1.680 |
| 2, 0 | 1513.4 | 0.140 | 1.664 |
| 3, 0 | 1497.3 | 0.176 | 1.647 |
| 4, 0 | 1481.9 | 0.174 | 1.631 |
| 5, 0 | 1466.4 | 0.144 | 1.616 |

Table 5
$q_{v'v''}$ and $\bar{r}_{v'v''}$ for J–X system of GeO

| $v', v''$ | $\lambda_{v'v''}$ (Å) | $q_{v'v''}$ | $\bar{r}_{v'v''}$ (Å) |
|---|---|---|---|
| 0, 0 | 1376.5 | 0.011 | 1.705 |
| 1, 0 | 1363.1 | 0.044 | 1.689 |
| 2, 0 | 1349.6 | 0.092 | 1.673 |
| 3, 0 | 1336.9 | 0.136 | 1.658 |

are collected from the analysis of Appelblad et al. [26].

## 3. Results and discussion

The FC factors of GeO molecule indicate that the most intense bands are the $(10, 0)$ and $(12, 0)$ for the E–X system; the $(0, 0)$, $(0, 1)$, $(1, 0)$, $(1, 1)$, $(1, 2)$, $(1, 3)$, $(2, 1)$, $(3, 1)$, $(3, 2)$ and $(4, 2)$ for the F–X system; the $(3, 0)$ and $(4, 0)$ for the G–X system. In the case of H–X system all bands are intense except $(1, 0)$. For the J–X system the $(3, 0)$ band is intense while all other bands are weak.

For all these band systems of GeO molecule, it is found that $r'_e > r''_e$ and hence the $r$-centroid values increase with increasing wavelength, which is expected in the red degraded band system.

The sequence differences for the E–X and F–X band systems are found to be a constant and is about 0.01 Å which suggests that the potentials are not so wide.

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