CHAPTER IV

Measurements and Calculations.
Part I of this chapter presents the decay curves of the BaS:Cu (Borax) phosphors, calculation of the decay constants and their analysis. Thermoluminescence studies of the phosphors are included in Part II of the chapter.

The main purpose of the analysis of the decay curves is to calculate the rate of decay of phosphorescence, and, if possible to ascertain the nature of the decay viz. whether it is monomolecular or hyperbolic. Randall and Wilkins (1), Garlick and Wilkins (2) showed that the bimolecular theory of phosphorescence is unsatisfactory in most of the cases and tried to explain the results on the basis of trap distribution, assuming that the decay process is basically monomolecular in nature. The complex shape of the decay curve is then attributed to the contribution from traps of varying depths to the phosphorescence. The form of the decay curve was derived theoretically by them assuming a single trap depth, and a distribution of trap depths such as, uniform, quasi-uniform, and exponential. The usual practice is to fit afterwards the decay curve data into one of these theoretical formulae. A second approach, which has also been used extensively, consists in breaking off the complex curves into a series of exponential curves. Each exponential is then
supposed to correspond to one trap of a certain depth. Starting
with the exponential responsible for the long decay time,
successive subtractions yield a set of exponentials. Normally,
a decay curve reduces to two or three exponentials. Bube (3) has used this method to analyze the decay curves of
hex. ZnS: Cu (0.01) : [Zn] phosphor. He has also pointed
out that the successive subtractions involve increasingly large
errors and the only result that may be used safely is that with
the minimum number of exponentials.

The decay of phosphorescence and the
thermoluminescence are the two aspects of the same phenomena,
viz. release of electrons from the traps. In the former, the
temperature is kept constant, while in the latter the temperature
rises at a predetermined linear rate. Decay curves can be
recorded at various temperatures and then correlated with the
thermoluminescence data. Such a procedure can help in
interpreting the experimental data. This method was first used
by Randall and Wilkins (4). They computed the mathematical
formulae for the correlation and applied them to the analysis of
a KCl: Tl phosphor. Bube (3) has measured the decay of
hex. ZnS: Cu (0.01) : [Zn] phosphor at a number of
temperatures between 135° and 163° C. At 151° C the decay was
found to be exponential. The decay curve at 146° C was split up
into two exponentials. A graph plotted between the decay
constant and the temperature at seven decay temperatures between 135° and 168°C showed that the log. of decay constant varies inversely as the temperature. It was concluded from this that retrapping is negligible for the deepest traps in the hex. ZnS: Cu (0.01): [Zn] phosphor.

Emigh and Megill (5) have observed the decay of Tl-activated NaI phosphor crystal at a number of temperatures. The decay curves have been analysed into exponentials. Each trap is found to decay independently of the others according to a monomolecular process. The decay of KI-TlI phosphor has been recorded by Smaller and Avery (6) at several temperatures between -20° and 100°C. The resulting decay curves were analysed into exponentials and the decay time assigned to each exponential. The frequency factor 's' and the trap depth E was calculated from the variation of the various decay times with temperature. Complete analysis of the curves permitted the decay curves to be divided into a long-lived and a short-lived set. Each set was found to contain four trap depths.

Honing (7) has shown how the trap distributions can be computed theoretically from the decay curves. The decay curve is expressed as a Laplace transform of the distribution density function for activation energies. The trap
distribution is then calculated by the inversion of the transform. Nazarian (8) has pointed out that the usual practice of expressing the intensity of phosphorescence $I(t)$ in terms of $N(E)$, the trap distribution, and calculating the trap distribution by a trial and error method can be avoided by a new mathematical process devised by him. By this method the expression for $N(E)$ can be solved directly in terms of $I(t)$. The method was applied by him for the analysis of the trap distribution of a ZnS phosphor. A continuous trap distribution was obtained.

2. **Rise of fluorescence with time**:

When a phosphor, in which all the centres are filled and all the traps are empty, is excited by a constant source of light, the electrons excited from the centres are captured by the empty traps. This results in the emptying of the luminescent centres which will then capture electrons and produce fluorescence. This fluorescence builds itself till an equilibrium state is reached when all the traps are full. The area under the fluorescence rise curve and the saturation level gives the total energy stored in the phosphor. Strictly speaking, this area should be equal to the area under the decay or thermoluminescence curve.

In order to determine the saturation time of the phosphor and to fix the time of excitation, the phosphor was
kept in dark for a very long period to empty all the filled traps and then excited at room temperature. The apparatus used for this purpose was exactly the same as described in the previous chapter. The brightest sample in the series prepared, $K_3S_{45}$, was selected. The phosphor was excited by a constant exciting source for 5 secs. The exciting source was then cut off and the maximum reading of the galvanometer noted. Subsequently, the phosphor was allowed to decay completely in dark, and again excited for 10 secs. The galvanometer reading was again noted as in the previous case. Such a process was continued for the successive excitation times of 15, 20, 25, 30, 45, 60, 75 secs. respectively. Further increase in the excitation time did not result in the increase of the maximum galvanometer deflection. A graph was plotted between the excitation time as the abscissa and the maximum intensity as the ordinate. The resulting fluorescence rise curve is shown in Fig. 1. It is obvious from the graph that the intensity initially rises very rapidly. It reaches to about 75% of the equilibrium value in about 15 secs., and thereafter rises slowly until the saturation value is attained at about 1 minute exposure. The time of excitation was therefore fixed at 4 minutes, that is, nearly four times the time taken to attain the saturation value. This was done so as to make sure that the phosphor was always excited to the saturation value.
Fig. 1. Fluorescence intensity vs. time of excitation.
The total amount of energy stored in a phosphor is affected by the intensity of excitation. The electrons in the shallow traps of the phosphor leave the traps at an appreciable rate. The number of shallow traps filled will therefore increase with the increase in the intensity of excitation (4). In the decay and thermoluminescence measurements described below, the intensity of the exciting source was maintained constant as far as possible.

3. Decay Curves of the Phosphors:

The decay curves of the phosphors KS$_{39}$ to KS$_{68}$ prepared (flux varied from 0 to 40% of the BaS content) are presented in Fig. 2. The abscissa indicates the time in minutes and the ordinate intensity of phosphorescence in arbitrary units. To start with, the brightest sample in the series, KS$_{45}$, was taken. The phosphor was excited for the predetermined time of 4 mins. and the galvanometer reading noted 10 secs. after the cessation of excitation. By repeated observations the sensitivity knobs of the photo-multiplier were so adjusted that the galvanometer indicated a full scale deflection 10 secs. after the removal of the exciting radiation. This preliminary calibration of the galvanometer scale facilitated the recording of the decay of the phosphorescent emission of all the samples.
Fig. 2. Decay curves of phosphors: $KS_{39} \rightarrow KS_{46}$. 
FIG. 2 (cont'd). DECAY CURVES OF PHOSPHORS:

KS 47. → KS 58.
Fig. 2. (Contd). Decay curves of phosphors:

KS 59 $\rightarrow$ KS 68.
The first curve in the graph represents the decay of the phosphorescence of the $\text{K}_3\text{S}_9$ phosphor. This phosphor was prepared without adding any flux. The intensity of the phosphor, as the graph shows, was very weak. Proceeding further from this phosphor, the maximum intensity of phosphorescence increases with increasing quantity of the flux up to the phosphor $\text{K}_3\text{S}_{45}$, and thereafter shows a continuous decline. A general look at the figure does not reveal any marked change in the shape of the decay curves. All the curves were then replotted on a semi-log. graph paper. Fig. 3 shows the plot, in which X-axis denotes the time of decay and Y-axis, the log. (intensity) of phosphorescence in arbitrary units. An exponential decay will produce a straight line on this plot. From the figure it is clear that except the first ($\text{K}_3\text{S}_{39}$) and the last few decay curves, which are almost straight lines, all others are markedly curved.

To ascertain the true form of the decay curves, a log.-log. plot of them also was made. A truly hyperbolic decay curve will yield a straight line on this plot. Fig. 4 is the plot, with abscissa as the log. (time) and ordinate log. (intensity). Here also, excepting the first and the last few decay curves, which are almost straight lines, all others are significantly curved. The curvature of all the curves is convex upwards. Since none of the curves is a straight
Fig. 3. Log. of decay intensity vs. decay time.
Fig. 3 (contd). Log. of Decay Intensity

Vs. Decay Time.
Fig. 4. Log. of Decay Intensity Vs. Log. Decay Time.
FIG. 4 (Contd). LOG. OF DECAY INTENSITY VS. LOG. DECAY TIME.
Fig. 4 (Cont’d). Log. Decay Intensity Vs. Log. Decay Time.
line, all the decay curves can be classified as 'power-law' decay curves.

4. Variation of the intensity of phosphors with flux:

The mode of change of the intensity of the phosphors $\text{KS}_{39}$ to $\text{KS}_{68}$ prepared with increasing percentage of flux (Borax) is shown in Fig. 5. The $X$-axis denotes the flux percentage, varied from 0 to 40% at steps of 1.37% of the $\text{BaS}$ content in the phosphor. The intensity of phosphorescence of the phosphors plotted along the $Y$-axis, was taken 30 secs. after the cessation of excitation. The intensity increases almost from 0 ($\text{KS}_{39}$, flux 0%) to a maximum at the phosphor $\text{KS}_{45}$ (flux ~9%). Further addition of the flux decreases the intensity continuously till the last phosphor prepared $\text{KS}_{68}$ (40% flux) is reached, when the phosphorescence is hardly perceptible. The ratio of the intensity of the brightest and the dullest sample, as plotted in the graph, is approximately 1:100. Although the intensity does not increase in a strictly regular fashion, it shows a definite increase up to about 9% of flux material and then decreases till at 40% it is very feeble.

5. Calculation of the decay constants:

An attempt was made to fit the decay curve
**Fig. 5. Relative Intensity**  
Vs. % of Flux.
data into a suitable mathematical equation and to determine the constants of the equation. From the previous figures (2, 3, 4) it is clear that the shape of the decay curves is neither exponential nor strictly hyperbolic. Hence a 'power-law' type equation was considered. The equation was:

\[ I = Kt^{-n} \]

where \( I \) is the intensity of phosphorescence at a time \( t \) after the cessation of excitation and \( K, n \), the constants to be determined. The constant \( n \) was calculated by drawing tangents to the decay curves (Fig. 4). Two tangents were drawn in order to obtain a better fit of the curves. Knowing the values of the slopes \( n_1 \) and \( n_2 \) of the tangents of the decay curves and substituting the values of \( I, t \), the values of \( K_1 \) and \( K_2 \) corresponding to the values of \( n_1 \) and \( n_2 \) could be determined. The values of \( K_1 \) and \( K_2 \) were calculated for all the intensity observations taken at intervals of 10 secs. The probable errors of \( K_1 \) and \( K_2 \) were calculated for each decay curve. The values of \( n_1 \) and \( n_2 \), \( K_1 \) and \( K_2 \) are shown in Table I. Probable errors are included along with the \( K_1 \) and \( K_2 \) values.

6. Variation of the decay constants with flux:

The decay constants \( n_1 \) and \( n_2 \), \( K_1 \) and \( K_2 \)
<table>
<thead>
<tr>
<th>S.No.</th>
<th>Phosphor No.</th>
<th>% of flux (Borax)</th>
<th>n</th>
<th>n₁</th>
<th>n₂</th>
<th>K₁ (with probable error)</th>
<th>K₂ (with probable error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>KS 39</td>
<td>0.00 %</td>
<td>1.29</td>
<td>1.29</td>
<td></td>
<td>131.74 ± 4.26</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>KS 40</td>
<td>1.377 %</td>
<td>1.42</td>
<td>1.42</td>
<td></td>
<td>925.7 ± 37.53</td>
<td></td>
</tr>
<tr>
<td>3.</td>
<td>KS 41</td>
<td>2.75 %</td>
<td>1.37</td>
<td>1.35</td>
<td>1.49</td>
<td>3365.7 ± 105.2</td>
<td>7088.6 ± 215.9</td>
</tr>
<tr>
<td>4.</td>
<td>KS 42</td>
<td>4.13 %</td>
<td>1.31</td>
<td>1.26</td>
<td>1.56</td>
<td>4171.2 ± 104.0</td>
<td>19510.0 ± 378.2</td>
</tr>
<tr>
<td>5.</td>
<td>KS 43</td>
<td>5.51 %</td>
<td>1.20</td>
<td>1.13</td>
<td>1.33</td>
<td>1292.8 ± 28.71</td>
<td>3324.0 ± 114.9</td>
</tr>
<tr>
<td>6.</td>
<td>KS 44</td>
<td>6.89 %</td>
<td>1.34</td>
<td>1.10</td>
<td>1.60</td>
<td>2049.0 ± 36.40</td>
<td>21258.0 ± 703.6</td>
</tr>
<tr>
<td>7.</td>
<td>KS 45</td>
<td>8.27 %</td>
<td>1.32</td>
<td>1.17</td>
<td>1.51</td>
<td>4039.6 ± 25.65</td>
<td>21802.7 ± 603.4</td>
</tr>
<tr>
<td>8.</td>
<td>KS 46</td>
<td>9.64 %</td>
<td>1.30</td>
<td>1.14</td>
<td>1.49</td>
<td>2496.3 ± 44.78</td>
<td>12662.7 ± 305.9</td>
</tr>
<tr>
<td>9.</td>
<td>KS 47</td>
<td>11.02 %</td>
<td>1.12</td>
<td>1.17</td>
<td>1.51</td>
<td>1985.4 ± 54.09</td>
<td>10490.4 ± 282.0</td>
</tr>
<tr>
<td>10.</td>
<td>KS 48</td>
<td>12.40 %</td>
<td>1.44</td>
<td>1.15</td>
<td>1.53</td>
<td>2278.6 ± 56.56</td>
<td>12506.6 ± 283.5</td>
</tr>
<tr>
<td>11.</td>
<td>KS 49</td>
<td>13.78 %</td>
<td>1.18</td>
<td>1.15</td>
<td>1.28</td>
<td>1644.1 ± 54.95</td>
<td>3030.6 ± 35.54</td>
</tr>
<tr>
<td>S.No.</td>
<td>Phosphor No.</td>
<td>% of flux (Borax)</td>
<td>n</td>
<td>n₁</td>
<td>n₂</td>
<td>$K_1$ (with probable error)</td>
<td>$K_2$ (with probable error)</td>
</tr>
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<td>-------</td>
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</tr>
<tr>
<td>12.</td>
<td>KS 50</td>
<td>15.15 %</td>
<td>1.28</td>
<td>1.12</td>
<td>1.30</td>
<td>1114.1 ± 69.29</td>
<td>2213.0 ± 68.93</td>
</tr>
<tr>
<td>13.</td>
<td>KS 51</td>
<td>16.53 %</td>
<td>1.26</td>
<td>1.20</td>
<td>1.36</td>
<td>1034.0 ± 72.18</td>
<td>2263.0 ± 47.51</td>
</tr>
<tr>
<td>14.</td>
<td>KS 52</td>
<td>17.91 %</td>
<td>1.24</td>
<td>1.25</td>
<td>1.38</td>
<td>707.1 ± 17.78</td>
<td>1271.0 ± 33.69</td>
</tr>
<tr>
<td>15.</td>
<td>KS 53</td>
<td>19.29 %</td>
<td>1.29</td>
<td>1.20</td>
<td>1.35</td>
<td>964.2 ± 36.32</td>
<td>1726.1 ± 23.70</td>
</tr>
<tr>
<td>16.</td>
<td>KS 54</td>
<td>20.66 %</td>
<td>1.26</td>
<td>1.23</td>
<td>1.60</td>
<td>645.0 ± 17.59</td>
<td>3229.1 ± 103.4</td>
</tr>
<tr>
<td>17.</td>
<td>KS 55</td>
<td>22.04 %</td>
<td>1.28</td>
<td>1.22</td>
<td>1.38</td>
<td>531.3 ± 12.39</td>
<td>970.2 ± 21.69</td>
</tr>
<tr>
<td>18.</td>
<td>KS 56</td>
<td>23.42 %</td>
<td>1.37</td>
<td>1.27</td>
<td>1.51</td>
<td>677.3 ± 18.20</td>
<td>1802.0 ± 88.80</td>
</tr>
<tr>
<td>19.</td>
<td>KS 57</td>
<td>24.80 %</td>
<td>1.42</td>
<td>1.13</td>
<td>1.60</td>
<td>131.4 ± 2.0</td>
<td>817.9 ± 8.80</td>
</tr>
<tr>
<td>20.</td>
<td>KS 58</td>
<td>26.18 %</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
<td>277.9 ± 8.15</td>
<td>75.35 ± 3.0</td>
</tr>
<tr>
<td>21.</td>
<td>KS 59</td>
<td>27.55 %</td>
<td>1.20</td>
<td>1.20</td>
<td>1.20</td>
<td>75.35 ± 3.0</td>
<td>75.35 ± 3.0</td>
</tr>
<tr>
<td>S.No.</td>
<td>Phosphor No.</td>
<td>% of flux (borax)</td>
<td>$n_1$</td>
<td>$n_2$</td>
<td>$K_1$ (with probable error)</td>
<td>$K_2$ (with probable error)</td>
<td></td>
</tr>
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<td></td>
</tr>
<tr>
<td>22.</td>
<td>KS 60</td>
<td>23.93 %</td>
<td>1.35</td>
<td>1.35</td>
<td>157.25 ± 8.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>23.</td>
<td>KS 61</td>
<td>30.30 %</td>
<td>1.16</td>
<td>1.16</td>
<td>101.80 ± 2.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24.</td>
<td>KS 62</td>
<td>31.69 %</td>
<td>1.20</td>
<td>1.20</td>
<td>47.52 ± 1.53</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25.</td>
<td>KS 63</td>
<td>33.06 %</td>
<td>1.20</td>
<td>1.20</td>
<td>47.52 ± 1.53</td>
<td></td>
<td></td>
</tr>
<tr>
<td>26.</td>
<td>KS 64</td>
<td>34.44 %</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27.</td>
<td>KS 65</td>
<td>35.82 %</td>
<td>1.23</td>
<td>1.23</td>
<td>55.53 ± 4.40</td>
<td></td>
<td></td>
</tr>
<tr>
<td>28.</td>
<td>KS 66</td>
<td>37.20 %</td>
<td>1.23</td>
<td>1.23</td>
<td>56.68 ± 6.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>29.</td>
<td>KS 67</td>
<td>38.57 %</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30.</td>
<td>KS 68</td>
<td>39.95 %</td>
<td>1.23</td>
<td>1.23</td>
<td>75.93 ± 2.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
calculated above are plotted against the percentage of flux in Figs. 6 and 7. The decay constants \( n_1 \) and \( n_2 \), which represent the rate of decay, show two peaks each. The second peak, in both the cases is lower than the first. The value of constant \( n_1 \) varies between the limits 1.1 and 1.42, while that of \( n_2 \) varies between 1.28 and 1.6, that is, the limits of \( n_2 \) are higher than that of \( n_1 \). \( n_1 \) represents the rate of decay of the initial part of the curve (Fig. 4), that is, the decay of short-time phosphorescence and \( n_2 \) that of long-time phosphorescence. \( K_1 \) and \( K_2 \) each show a peak. In reality, \( K_1 \) and \( K_2 \) represent the change of the phosphorescent intensity with flux, a better idea of which is furnished by the Fig. 5. As a matter of fact, none of the constants shows a very satisfactory plot, but taken statistically, the general shape of the curves may be taken as true.
Fig. 6. \( n_1 \) vs. \( \% \) of flux.
\( n_2 \) vs. \( \% \) of flux.

Fig. 7. \( k_1 \) vs. \( \% \) of flux.
\( k_2 \) vs. \( \% \) of flux.
1. Introduction:

Thermoluminescence provides an easier and a better method of calculating the trap depths and their distribution in the phosphor, than the analysis of decay curves. The phosphor, after being excited at a low temperature, is heated at a uniform linear rate. The thermally released electrons from the traps produce enhanced glow. For traps, of one depth only, the glow curve is given by:

\[ I = C \frac{dn}{dt} = C n_0 s \exp\left(-\frac{S}{kT}\right) \exp\left[-\int_0^T \frac{S}{\beta} \exp\left(-\frac{E}{kT}\right) dt\right] \]

where \( I \) is the intensity of glow, \( \beta \) the rate of heating, \( E \), the trap depth, \( s \) the frequency factor and \( C \) and \( n_0 \) are constants. The temperature of the maximum glow is found to be less than the temperature at which the escape probability of electrons is \( 1/\text{sec} \). Equation (1) yields,

\[ E = T_G \left\{ 1 + \left( \frac{s}{\epsilon} \right) \right\} \approx \log s \]

\( T_G \) being the temperature of maximum glow, and \( \left( \frac{s}{\epsilon} \right) \) has a value small compared to \( 1 \). Trap depths are then calculated from the approximate formula,

\[ E = K T_G \log s \]

2. Calibration Curve of the heater:

The calibration curve of the heater used in
the thermoluminescence experiments is shown in Fig. 8. The rate of heating used was 0.16°C/sec. (calculated for the time of the glow curve). The comparatively slow rate of heating found out by preliminary experiments, provided a good resolution of the peaks. Since the traps of the phosphors studied are rather shallow, the glow curve was completed within 4 mins. of the starting of heating.

3. Thermoluminescence Curves of the phosphors:

The thermoluminescence curves of the phosphors studied are shown in Fig. 9. The X-axis denotes the time in minutes and the Y-axis, the intensity of thermoluminescence in arbitrary units. Since no automatic intensity recording system was available, it was not possible to record both the temperature and the intensity at the same time. Therefore, an indirect procedure was adopted. The intensity was plotted against the time and then from the previously plotted graph of temperature of the heater Vs. time, the temperature corresponding to the peak of the glow curve could be determined. This procedure was checked by independent experiments and was found to be sufficiently accurate for the present work. The measurements were started from the room temperature i.e. 302°C.
Fig. 8. Calibration Curve of the Thermoluminescence Apparatus.
Fig. 9. Thermoluminescence Curves of Phosphors: KS₃₉ → KS₄₀.
Fig. 9 (Contd.). Thermoluminescence curves of phosphors: $KS_{50} \rightarrow KS_{55}$. 
Fig. 9 shows in general that there is only one peak above the room temperature. In one or two brightest samples there was some indication of a second peak at higher temperature but its intensity was too feeble to be detected. No efforts were made to record the glow curve below the room temperature, since the author was primarily interested in the behaviour of the traps above the room temperature.

The glow curve of the first phosphor $^{39}$KS is very small, with the peak just above the room temperature. The maximum glow intensity thereafter increases from sample to sample up to the phosphor $^{45}$KS. After this the glow curve continuously diminishes. Also, the thermoluminescence peak shifts towards higher temperature up to the phosphor $^{44}$KS and then recedes again to low temperature side. The maximum shift of the peak from the phosphor $^{39}$KS to $^{44}$KS is of 7.2°C.

Another observation may be made about the shape of the glow curves. In the first eleven phosphors ($^{39}$KS to $^{49}$KS), the peak of the glow curve is quite sharp and well defined. From the phosphor $^{50}$KS onwards the peak becomes broadened and is no longer sharp. The thermoluminescence curves of the first fifteen samples are shown in the figure attached. The glow intensity of the phosphors after $^{57}$KS is extremely weak and very difficult to record.
4. Variation of the trap depth of the phosphors with flux:

The trap depths of the phosphors were calculated from the above glow curves. The relation used for this purpose was:

\[ E = K T_G \log \, s \]

where \( E \) is the trap depth, \( K \) the Boltzmann constant, \( s \) the frequency factor and \( T_G \) the temperature corresponding to the peak of the glow curve. Using the values of \( K \) and \( s = 10^{8.1 \text{sec}^{-1}} \), the equation simplifies to:

\[ E = 18.4 K T_G \]

The values of the trap depths of the phosphors are shown in Table II.
### Table II

| S.No. | Phosphor No. | Percentage of flux (Borax) | Temperature (°K) corresponding to peak (T<sub>G</sub>) | Trap depth E ≤ 18.4 KT<sub>G</sub> |
|-------|--------------|---------------------------|------------------------------------------------------|___________________________________|
| 1.    | KS 39        | 0.00 %                    | 303.0                                                | 0.4803 eV.                          |
| 2.    | KS 41        | 2.75 %                    | 304.6                                                | 0.4829 eV.                          |
| 3.    | KS 42        | 4.13 %                    | 306.5                                                | 0.4859 eV.                          |
| 4.    | KS 43        | 5.51 %                    | 307.8                                                | 0.4878 eV.                          |
| 5.    | KS 44        | 6.89 %                    | 310.2                                                | 0.4918 eV.                          |
| 6.    | KS 45        | 8.27 %                    | 309.4                                                | 0.4906 eV.                          |
| 7.    | KS 46        | 9.64 %                    | 309.4                                                | 0.4906 eV.                          |
| 8.    | KS 48        | 12.40 %                   | 308.6                                                | 0.4894 eV.                          |
| 9.    | KS 49        | 13.78 %                   | 307.0                                                | 0.4866 eV.                          |
| 10.   | KS 50        | 15.15 %                   | 309.4                                                | 0.4906 eV.                          |
| 11.   | KS 51        | 16.53 %                   | 306.5                                                | 0.4859 eV.                          |
| 12.   | KS 52        | 17.91 %                   | 306.5                                                | 0.4859 eV.                          |
| 13.   | KS 53        | 19.29 %                   | 307.8                                                | 0.4878 eV.                          |
| 14.   | KS 54        | 20.66 %                   | 305.4                                                | 0.4842 eV.                          |
| 15.   | KS 55        | 22.04 %                   | 305.4                                                | 0.4842 eV.                          |
REFERENCES