

**Table 1.** Results of linear combination of theoretical spectra obtained using the *differential evolution* routine (see text for details)

<b>Sample</b>	<b>model</b>	<b>weight</b>
<b>ZnO</b> $R_f=0.027, \sigma^2=0.035$	ZnO + 1V <sub>Zn</sub> ( <i>out-of-plane</i> )	0.28
	ZnO + 1V <sub>O</sub>	0.00
	ZnO + 1Zn <sub>oct</sub>	0.38
	ZnO + (1V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.26
	ZnO + (1V <sub>Zn</sub> +2V <sub>O</sub> – complex)	0.00
	ZnO+(4V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.07
<b>5e14</b> $R_f=0.022, \sigma^2=0.028$	ZnO + 1V <sub>Zn</sub> ( <i>out-of-plane</i> )	0.00
	ZnO + 1V <sub>O</sub>	0.20
	ZnO + 1Zn <sub>oct</sub>	0.34
	ZnO + (1V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.31
	ZnO + (1V <sub>Zn</sub> +2V <sub>O</sub> – complex)	0.00
	ZnO + (4V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.15
<b>5e15</b> $R_f=0.018, \sigma^2=0.022$	ZnO + 1V <sub>Zn</sub> ( <i>out-of-plane</i> )	0.00
	ZnO + 1V <sub>O</sub>	0.15
	ZnO + 1Zn <sub>oct</sub>	0.31
	ZnO + (1V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.33
	ZnO + (1V <sub>Zn</sub> +2V <sub>O</sub> – complex)	0.08
	ZnO + (4V <sub>Zn</sub> +1V <sub>O</sub> – complex)	0.13