

List of AIOMFAC-web Error and Warning Codes and Messages

Error or Warning Code	Message
01	AIOMFAC ERROR 1: mixture related. An organic main group <-> cation interaction parameter is not defined for the requested mixture. Please check your mixture components for available parameters stated in the AIOMFAC interaction matrix.
02	AIOMFAC ERROR 2: mixture related. An organic main group <-> anion interaction parameter is not defined for the requested mixture. Please check your mixture components for available parameters stated in the AIOMFAC interaction matrix.
03	AIOMFAC ERROR 3: Mixture composition related. Composition data for this point is missing or incorrect! The sum of the mole or mass fractions of all components has to be equal to 1.0 and individual mole or mass fractions have to be positive values ≤ 1.0 ! Composition point no.: <i>pointi</i>
04, 05	AIOMFAC ERROR 4: Mixture composition related. Composition data for this point is incorrect! The sum of the mole or mass fractions of all components has to be equal to 1.0 and individual mole or mass fractions have to be positive values ≤ 1.0 ! Composition point no.: <i>pointi</i>
06, 07	AIOMFAC ERROR 6: Numerical issue. A numerical issue occurred during computation of the data points flagged in the output tables. This error was possibly caused due to input of very high electrolyte concentrations. Composition point no.: <i>pointi</i>
08	AIOMFAC ERROR 8: Mixture composition related. At least one neutral component must be present in the system! Composition point no.: <i>pointi</i>
09	AIOMFAC ERROR 9: mixture related. At least one cation <-> anion interaction parameter is not defined for the requested mixture. Please check all ion combinations for available parameters stated in the AIOMFAC interaction matrix.
10	AIOMFAC WARNING 10: Temperature range related. At least one data point has a set temperature outside of the recommended range for model calculations of electrolyte-containing mixtures. This may be intended, but caution is advised as AIOMFAC is not designed to perform well at this temperature. Data point no.: <i>pointi</i>

Error or Warning Code	Message
11	<p>AIOMFAC WARNING 11: Temperature range related.</p> <p>At least one data point has a set temperature outside of the recommended range for model calculations of electrolyte-free organic mixtures. This may be intended, but caution is advised as AIOMFAC is not designed to perform well at this temperature.</p> <p>Data point no.: <i>pointi</i></p>
12	<p>AIOMFAC ERROR 12: Charge neutrality violated.</p> <p>The mixture violates the electrical charge neutrality condition ($\text{moles cation} \times [\text{cation charge}] = \text{moles anion} \times [\text{anion charge}]$).</p> <p>Make sure that selected integer amounts of cation and anion 'subgroups' fulfill the charge balance (in the inorganic component definition of the input file).</p> <p>Composition point no.: <i>pointi</i></p>
13	<p>AIOMFAC ERROR 13: Incorrect hydroxyl group assignment.</p> <p>At least one component containing (CH_n[(OH)]) groups has been assigned an incorrect number of (OH) groups. Note that the notation of a CH_n group bonded to an OH group does not include the OH group; rather the hydroxyl groups have to be defined separately.</p>
14	<p>AIOMFAC ERROR 14: Missing short-range ARR parameter.</p> <p>A neutral main group <-> main group interaction coeff. of this particular mixture is not available in the SR part of the model. Check your organic components and their subgroups in comparison to available subgroups in the AIOMFAC matrix.</p>
15	<p>AIOMFAC ERROR 15: Missing short-range BRR parameter.</p> <p>A neutral main group <-> main group interaction coeff. of this particular mixture is not available in the SR part of the model for 3-parameter temperature dependence. Check your organic components and their subgroups in comparison to available subgroups in the AIOMFAC matrix.</p>
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31	<p>AIOMFAC WARNING 31: Invalid composition input.</p> <p>At least one data point contains invalid, non-numeric data that cannot be processed.</p>
32	<p>MESSAGE from AIOMFAC: input file did not pass full validation and may be a spam file.</p> <p>MESSAGE from AIOMFAC: the input file will be deleted to prevent spam files and malicious code from occupying the server.</p>
33	<p>MESSAGE from AIOMFAC: no composition points have been entered in the text field. There is nothing to calculate.</p>