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# The energetics of $La_4LiAuO_8$

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(Received 14 January 2011; accepted 11 March 2011)

$La_4LiAuO_8$ is a stable $Au^{3+}$ oxide that was recently examined as a possible model compound for the role of $Au^{3+}$ in heterogeneous catalysis. Due to the paucity of thermodynamic data, the energetics of $La_4LiAuO_8$ and its likely decomposition product, $LiLaO_2$, were investigated. The $\Delta H_{f-ox}$, of $La_4LiAuO_8$ and $LaLiO_2$ are both exothermic at $-187.7 \pm 5.8$ and $-41.4 \pm 9.6$ kJ/mol, respectively. From the thermodynamic data, the decomposition temperature of $La_4LiAuO_8$ was calculated as either $979 \pm 95$ or $1331 \pm 43$ °C for the formation of $LiLaO_2$ or $Li_2O$, respectively. Thus, $LiLaO_2$ is the expected decomposition product.

Gold is an interesting and unique catalyst that is relatively inert in the bulk state, but catalytically active when its particle size is reduced to the nanoscale regime.[1] Excellent catalytic activities are observed for highly dispersed gold nanoparticles on metal oxide supports, particularly for CO oxidation.[2] The catalytic activity of gold nanoparticles is strongly dependent on particle size, but the composition and structure of the supporting oxide also play a role.[2]

The exact nature of the catalytically active species within metal oxide support systems is still unclear.[1] Several studies have suggested that $Au^0$ is the active species, but mechanisms involving cationic gold ($Au^{3+}$, $Au^+$, or both) have also been proposed.[3] The low concentration and fine dispersion of gold particles on metal oxide supports hamper experimental investigations of the catalytic species.[1] Modeling the system is also a challenge as a wide array of interactions between the gold nanoparticles and oxide supports are possible.[3]

To investigate the importance of $Au^{3+}$ as a catalytic species, Kurzman et al.[4] have studied CO oxidation in the presence of $La_4LiAuO_8$. Originally reported by Abbattista et al.,[5] $La_4LiAuO_8$ crystallizes in an ordered variant of the $Nd_2CuO_4$ structure, containing layers of corner-connected $LiO_4$ and $AuO_4$ square planes separated by two fluorite-type layers of La and O. Each $AuO_4$ moiety is isolated, which makes $La_4LiAuO_8$ an interesting model compound to investigate heterogeneous catalysis by square planar $Au^{3+}$ ions. Although not an effective catalyst for the oxidation of CO, the compound is remarkably stable toward thermal decomposition, which occurs near 935 °C.[4] The observed weight loss upon decomposition has been reported as 2.7%, corresponding to the formation of metallic Au and either 2 $La_2O_3$ + ½ $Li_2O$ or 1.5 $La_2O_3$ + $LiLaO_2$.[4] $LiLaO_2$ is more likely to form than $Li_2O$, but the results are ambiguous as only one small diffraction peak could be indexed to $LaLiO_2$ in the decomposed material.

$LiLaO_2$ is the only binary compound in the $La_2O_3$–$Li_2O$ system that forms between 750 and 1000 °C.[6] It is believed to be isomorphous to $LiEuO_2$, but the detailed crystal structures of $LiEuO_2$ and $LiLaO_2$ are not known. $LiLaO_2$ was observed as a decomposition product of $Li_3La(C_2O_4)_3 \cdot 9\ H_2O$,[7] and it has been reported as an effective catalyst for methane oxidation.[8]

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DOI: 10.1557/jmr.2011.87

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https://doi.org/10.1557/jmr.2011.87 Published online by Cambridge University Press

The thermal stability of $La_4LiAuO_8$, along with the paucity of thermochemical data for trivalent gold oxide compounds, led us to investigate the energetics of $La_4LiAuO_8$ and its decomposition product $LiLaO_2$. Here, we present the enthalpies of formation for $La_4LiAuO_8$ and $LiLaO_2$ obtained by high-temperature oxide melt solution calorimetry and investigate the energetics of the $La_4LiAuO_8$ decomposition.

The $La_4LiAuO_8$ powder was synthesized according to previously reported methods by Kurzman et al.[4] $LiLaO_2$ was synthesized following the procedure by Abbattista and Vallino.[6] $LiOH{\cdot}H_2O$ (Aldrich Chemical 131066-3, Aldrich, St. Louis, MO) was heated for 16 h at 250 °C to form LiOH. An excess of LiOH (2:1 ratio) was ground with $La_2O_3$ (Aldrich Chemical 131281-8), pelletized, and wrapped in silver foil. The sample was heated at 775 °C for 10 h.

The samples were characterized by powder x-ray diffraction using a Bruker D8 Advance diffractometer (Cu Kα radiation; Bruker, Madison, WI) equipped with a LynxEye solid state detector. Rietveld refinements were performed using the XND code; the GSAS/EXPGUI suite was used for simultaneous Lebail fitting and Rietveld refinement; and the JADE 8.0 software was used for particle size estimation from Scherrer broadening. Thermogravimetric analysis (TGA)/differential scanning calorimetry (DSC) analysis was performed on a LABSYS Evo (Setaram Instruments, Caluire, France) from 30 to 1200 °C in air with heating rate of 10 °C/min.

High-temperature oxide melt solution calorimetry was performed using a specially built twin calorimeter of the Tian–Calvet type operating at 800 °C that has been previously described.[9] Pelletized samples (~5 mg) were dropped into a platinum crucible containing 30 g of a lead borate, $2PbO{\cdot}B_2O_3$, solvent. The drop solution experiments were performed with air bubbling through the melt to sweep out evolved gases. The calorimeter was calibrated using ~5 mg pellets of α-$Al_2O_3$ (99.997 wt% metal basis; Alfa Aesar, Ward Hill, MA). The drop solution enthalpy value for $Li_2O$ is necessary component of the thermochemical cycle. Lithium oxide absorbs water to form $LiOH{\cdot}H_2O$, and it is difficult to accurately measure the $\Delta H_{dsol}$ directly. However, the $\Delta H_{dsol}$ has been calculated from the $\Delta H_{dsol}$ of the more stable $Li_2CO_3$ compound and related thermodynamic parameters.

The powder x-ray diffraction pattern of $La_4LiAuO_8$ confirmed that the sample was nearly phase-pure with small amounts of $La_2O_3$ and metallic gold. Quantitative analysis by multiphase Rietveld refinement indicated the sample contained 0.5 wt% face-centered cubic (fcc) Au and 2.8 wt% $La_2O_3$. The x-ray diffraction pattern of the $LaLiO_2$ sample agreed with that obtained by Abbatista and Vallino[6] and also indicated a small amount of $La_2O_3$. Because phase fractions cannot be estimated from diffraction data of a multiphase mixture when one (or more) of the phases lacks a structural model, quantification of the impurity amounts was determined by thermogravimetry, described in the following section. Preparing pure $LaLiO_2$ is problematic because it is a very reactive material; the absence of any high quality structural work in the literature reflects the difficulty in obtaining the phase. Despite numerous attempts, it was not possible to prepare better samples of $LiLaO_2$. The major impurity phases were lithium hydroxide and lanthanum oxide and have been corrected for in the thermochemical calculations.

The TGA of $La_4LiAuO_8$ indicates that the material persists up to 931 °C [Fig. 1(a)]. The DSC curve contains two endothermic peaks, one accounting for the decomposition of $La_4LiAuO_8$ and the second corresponding to the melting of gold (1064 °C). Kurzman et al.[4] previously reported the decomposition temperature for $La_4LiAuO_8$ in air as 935 °C, in good agreement with our results. The weight loss after decomposition of $La_4LiAuO_8$ is 2.6 wt%, which correlates with the final products: Au + 2 $La_2O_3$+ 1/2 $Li_2O$ or Au + 1.5 $La_2O_3$ + $LiLaO_2$. The diffraction pattern of the decomposition products contains peaks of metallic gold and lanthanum oxide. An additional broad peak at 29° 2θ may be associated with a major peak of $LiLaO_2$, though this assignment is unclear given the absence of intensity at 35° 2θ, which is claimed to be the strongest reflection associated with $LiLaO_2$.[6]

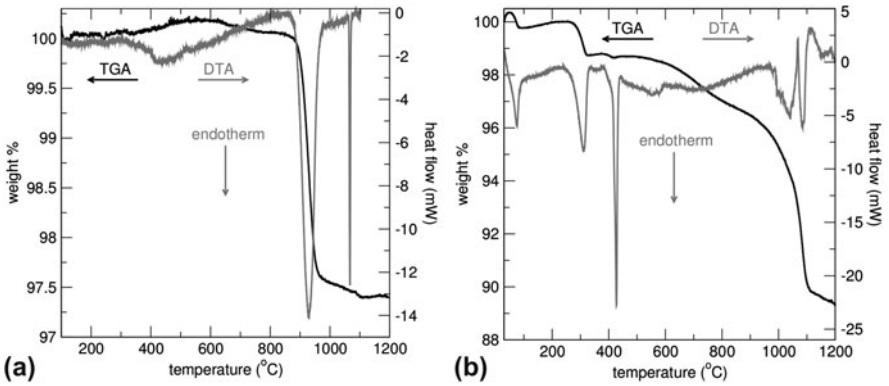



FIG. 1. The thermogravimetric analysis/differential scanning calorimetry (TGA/DSC) curves for (a) $La_4LiAuO_8$ indicate that the compound is stable until 931 °C. The weight changes observed in (b) $LaLiO_2$ indicates that a small amount of the initial starting materials are still present in the final sample.



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The TGA/DSC curve of $LiLaO_2$ is more complex, with weight changes occurring at several temperatures [Fig. 1(b)]. Initially, a weight gain occurs followed immediately by a weight loss from 50 to 110 °C, indicating the presence of a small amount of the initial LiOH starting material. Additional evidence for the presence of LiOH includes the sharp endothermic peak in the DSC curve at 425 °C that corresponds to the melting temperature of LiOH. Decomposition of LiOH to $Li_2O$ is also evident with the weight loss and broad exothermic peak from 450 to 825 °C. From the weight loss in the TGA curve, the amount of LiOH in the sample was estimated to be 1.8 wt%. The weight loss at 300 °C corresponds to the decomposition of $La(OH)_3$ to $La_2O_3$. Lanthanum oxide readily transforms to a hydroxide phase in the presence of a base (LiOH). The weight loss associated with the decomposition of $La(OH)_3$ indicates that $La_2O_3$ is present as 12 wt% in the sample.

$La_4LiAuO_8$ and $LiLaO_2$ dissolved completely in the lead borate melt, which was evidenced by a stable baseline during the calorimetric experiments, consistent measured enthalpies, and visual inspection of the solidified melt. The heat effects observed for both samples were endothermic. The average $\Delta H_{dsol}$ (in kJ/mol) for the $La_4LiAuO_8$, $LiLaO_2$, and $Li_2CO_3$ and two standard deviations of the mean were calculated from a total of eight to ten measurements for each and are summarized in Table I.

TABLE I. Enthalpy of drop solution $\Delta H_{dsol}$ (kJ/mol) for $Li_2CO_3$, $La_4LiAuO_8$, and $LiLaO_2$ in lead borate at 800 °C.

| $Li_2CO_3$ (kJ/mol) | $La_4LiAuO_8$ (kJ/mol) | $LaLiO_2$ (kJ/mol) |
|---|---|---|
| 243.855 | 166.101 | 47.979 |
| 228.848 | 157.847 | 47.965 |
| 227.631 | 151.599 | 45.869 |
| 244.843 | 156.995 | 42.655 |
| 237.533 | 157.468 | 48.403 |
| 242.895 | 160.341 | 44.898 |
| 237.293 | 157.557 | 42.510 |
| 236.233 | 160.980 | 43.961 |
| | | 42.054 |
| | | 46.319 |
| | | 46.515 |
| 237.39 ± 4.61[a] | 158.61 ± 1.84[a] | 45.38 ± 1.40[a] |

[a]Error is two standard deviations of the mean.

The thermochemical cycle used to calculate the enthalpy of drop solution for $Li_2O$ is given in Table II. The formation enthalpy of $Li_2CO_3$ was calculated from $Li_2O$ and $CO_2$ gas[10] and the heat capacity of $CO_2$ gas from 25 to 800 °C.[12] Using the enthalpy of drop solution for $Li_2CO_3$, the $\Delta H_{drp-sol}$ for $Li_2O$ was calculated to be $-23.83 \pm 5.06$ kJ/mol.

The enthalpy of drop solution for $La_4LiAuO_8$ was corrected for the 7.16 mol% $La_2O_3$ and 2.1 mol% Au resulting in $\Delta H_{dsol-corr}$ of $160.16 \pm 1.84$ kJ/mol. The thermochemical cycles used in the calculations for the heats of formation from the oxides for $La_4LiAuO_8$ are summarized in Table II. The $\Delta H_{corr-dsol}$ for $La_4LiAuO_8$ ($\Delta H_5$), the $\Delta H_{dsol}$ for $LaO_{1.5}$ ($\Delta H_6$),[12] $\Delta H_{dsol}$ of $Li_2O$ ($\Delta H_4$) and the integrated heat capacity from 298 to 800 °C for Au metal ($\Delta H_7$) and $O_2$ gas ($\Delta H_8$)[12] were used to calculate the enthalpy of formation from the oxides for $La_4LiAuO_8$, $-187.66 \pm 5.84$ kJ/mol.

The residue from the thermal analysis experiment was analyzed by powder x-ray diffraction. The diffraction peaks matched those of fcc Au and $La_2O_3$. $Li_2O$ was not observed in the x-ray diffraction pattern. The three peaks associated with Au metal were fit, and the average particle size was calculated based on the Scherrer[11] equation to be $39 \pm 2$ nm.

The effect of the Au particle size on the heat of formation of $La_4LiAuO_8$ was estimated using the following relationship

TABLE II. Thermochemical cycles used to determine $\Delta H_{f-ox}$ for $La_4LiAuO_8$.

Enthalpy of drop solution for $Li_2O$

| | |
|---|---|
| $Li_2CO_3$ (xl, 25 °C) → $Li_2O$ (sln, 800 °C) + $CO_2$ (g, 800 °C) | $\Delta H_1 = 237.39 \pm 4.61$ kJ/mol |
| $Li_2O$ (xl, 25 °C) + $CO_2$ (g, 25 °C) → $Li_2CO_3$ (xl, 25 °C) | |
| $H_2 = (-1216.038 \pm 0.17) - (-598.73 \pm 2.1) - (-393.522 \pm 0.05)$ | $\Delta H_2 = -233.786 \pm 2.107$ kJ/mol[10] |
| $CO_2$ (g, 800 °C) → $CO_2$ (g, 25 °C) | $\Delta H_3 = -37.437$ kJ/mol[12] |
| $Li_2O$ (xl, 25 °C) → $Li_2O$ (sln, 800 °C) | $\Delta H_4 = \Delta H_{dsol\text{-}Li2O,800°C}$ |

$$\Delta H_4 = \Delta H_1 + \Delta H_2 + \Delta H_3 = -23.83 \pm 5.06 \text{ kJ/mol}$$

Enthalpy of formation for $La_4LiAuO_8$

| | |
|---|---|
| $La_4LiAuO_8$ (xl, 25 °C) → 4 $LaO_{1.5}$ (sln, 800 °C) + 0.5 $Li_2O$ (sln, 800 °C) + Au (sln, 800 °C) + 0.75 $O_2$ (g, 800 °C) | $\Delta H_5 = 160.16 \pm 2.92$ kJ/mol |
| $LaO_{1.5}$ (xl, 25 °C) → $LaO_{1.5}$ (sln, 800 °C) | $\Delta H_6 = -13.88 \pm 0.09$ kJ/mol[13] |
| $Li_2O$ (xl, 25 °C) → $Li_2O$ (sln, 800 °C) | $\Delta H_4 = -23.83 \pm 5.06$ kJ/mol |
| Au (xl, 25 °C) → Au (sln, 800 °C) | $\Delta H_7 = 20.97$ kJ/mol[12] |
| $O_2$ (g, 25 °C) → $O_2$ (g, 800 °C) | $\Delta H_8 = 25.29$ kJ/mol[12] |

4 $LaO_{1.5}$ (xl, 25 °C) + Au (xl, 25 °C) + 0.5 $Li_2O$ (xl, 25 °C) + 0.75 $O_2$ (g, 25 °C) → $La_4AuLiO_8$ (xl, 25 °C) $\Delta H_9 = \Delta H_f$

$$\Delta H_9 = -\Delta H_5 + 4\,\Delta H_6 + \Delta H_7 + 0.5\,\Delta H_4 + 0.75\,\Delta H_8 = -187.66 \pm 5.84 \text{ kJ/mol}$$

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$$SA^{*}\gamma = \Delta H_{dsol-bulk} - \Delta H_{dsol-nano}$$

where SA is the surface area of the particle in $m^2$/mol and $\gamma$ is the surface energy ($J/m^2$). The surface energy of gold nanoparticles is in the range of 1.2–1.5 $J/m^2$.[14] The value used for these calculations, 1.46 $J/m^2$, was taken from size-dependent evaporation data reported by Nanda.[15] Using this value, the difference in the $\Delta H_{dsol-nano}$ from the $\Delta H_{dsol-bulk}$ is 1.12 kJ/mol. Therefore, the $\Delta H_7$ value decreases from 20.97 to 19.85 kJ/mol. This change results in a $\Delta H_{f-corr}$ value for $La_4LiAuO_8$ of $-188.77 \pm 5.1$ kJ/mol. The correction, however, is within the experimental error of the enthalpy of formation.

Few studies on the energetics of trivalent gold oxides have been reported. The enthalpy of formation for $Au_2O_3$ has been determined using several different techniques, including DSC.[15] The experimental values for the $\Delta H_f$ of $Au_2O_3$ range from $-3.5$ to $-13$ kJ/mol.[16] DFT calculations[17] estimate $\Delta H_f$ of $Au_2O_3$ to be $-50.1$ kJ/mol. Thus, $La_4LiAuO_8$ is energetically more stable than $Au_2O_3$ when compared on a per mol basis. The heats of formation for other trivalent gold oxides have not been reported.

The average $\Delta H_{dsol}$ for $LiLaO_2$ was based upon 10 drops, resulting in a value of $45.38 \pm 1.40$ kJ/mol (Fig. 1). The value was corrected for the presence of 12.6 mol% LiOH and 6.2 mol% $La_2O_3$. The drop solution value for LiOH has not been measured, but a thermochemical cycle can be written from $\Delta H_{drp-sol}$ ($\Delta H_1$) and $\Delta H_{f-ox}$ ($\Delta H_8$) of $Li_2CO_3$,[10] the integrated heat capacity of $H_2O$ ($\Delta H_{10}$) and $CO_2$ ($\Delta H_3$) gas from 800 to 25 °C,[12] and the formation enthalpy ($\Delta H_{11}$) of LiOH (Table III).[10] The corrected enthalpy of drop solution ($\Delta H_{13} = \Delta H_{dsol-corr}$) for $LiLaO_2$ is $15.62 \pm 8.18$ kJ/mol.

The enthalpy of formation for $LiLaO_2$ was calculated from the $\Delta H_{dsol-corr}$ for $LiLaO_2$ ($\Delta H_{13}$), the measured enthalpy of drop solution for $La_2O_3$ ($\Delta H_6$), and the calculated drop solution value for $Li_2O$ ($\Delta H_4$), resulting in a value of $-41.4 \pm 9.6$ kJ/mol. The large error associated with the $\Delta H_{f-ox}$ for $LaLiO_2$ is due to the presence of LiOH and the error of the $\Delta H_{f-ox}$ of LiOH.

The thermal stability of $La_4LiAuO_8$ is interesting given the oxophobic nature of gold. Kurzman et al.[4] suggest that the stability can be attributed to the presence of covalent Au–O bonding due to the presence of highly electropositive counter cations. To provide insight into the decomposition of $La_4LiAuO_8$, the decomposition temperature was calculated from the experimentally derived thermodynamic data for $La_4LiAuO_8$ and $LiLaO_2$.

The enthalpy of decomposition based upon the formation of $LaLiO_2$ can be determined from the following thermochemical cycle

$$La_4LiAuO_8\,(xl, 25\,^{\circ}C) \rightarrow 0.5\,Li_2O\,(xl, 25\,^{\circ}C) + 2\,La_2O_3\,(xl, 25\,^{\circ}C) + 0.75\,O_2\,(g, 25\,^{\circ}C)$$

$$\Delta H_{15} = -\Delta H_{f-ox} = 188.77 \pm 5.12\ kJ/mol$$

$$0.5\,La_2O_3\,(xl, 25\,^{\circ}C) + 0.5\,Li_2O\,(xl, 25\,^{\circ}C) \rightarrow LiLaO_2\,(xl, 25\,^{\circ}C)$$

$$\Delta H_{16} = \Delta H_{f-ox} = -41.4 \pm 9.6\ kJ/mol$$

$$La_4LiAuO_8\,(xl, 25\,^{\circ}C) \rightarrow LiLaO_2\,(xl, 25\,^{\circ}C) + 1.5\,La_2O_3\,(xl, 25\,^{\circ}C) + Au\,(xl, 25\,^{\circ}C) + 0.75\,O_2\,(g, 25\,^{\circ}C)$$

$$\Delta H_{17} = \Delta H_{decomp} = \Delta H_1 + \Delta H_2 = 147.35 \pm 11.26\ kJ/mol$$

The Ellingham diagram for oxidation reactions involving solid phases plots $\Delta G^{o}$ versus temperature.[18] As $\Delta G^{o} = \Delta H^{o} - T\Delta S^{o}$, the slope of the line is equal to $-\Delta S^{o}$ and the lines are generally parallel to one another for most oxides. For the decomposition of $La_4LiAuO_8$, the oxygen is released rather than consumed so the entropy change is

TABLE III. Thermochemical cycles used to determine $\Delta H_{f\text{-}ox}$ for $LiLaO_2$.

| | |
|---|---|
| Enthalpy of drop solution for LiOH | |
| $Li_2CO_3$ (xl, 25 °C) → $Li_2O$ (sln, 800 °C) + $CO_2$ (g, 800 °C) | $\Delta H_1 = 237.39 \pm 4.61$ kJ/mol |
| $Li_2O$ (xl, 25 °C) + $CO_2$ (g, 25 °C) → $Li_2CO_3$ (xl, 25 °C) | $\Delta H_2 = -233.786 \pm 2.107$ kJ/mol[10] |
| $CO_2$ (g, 800 °C) → $CO_2$ (g, 25 °C) | $\Delta H_3 = -37.437$ kJ/mol[12] |
| $H_2O$ (l, 25 °C) → $H_2O$ (g, 800 °C) | $\Delta H_{10} = 67.4$ kJ/mol[12] |
| 0.5 $Li_2O$ (xl, 25 °C) + 0.5 $H_2O$ (l, 25 °C) → LiOH (xl, 25 °C) | $\Delta H_{11} = -234.30 \pm 6.27$ kJ/mol[10] |
| LiOH (xl, 25 °C) → 0.5 $Li_2O$ (sln, 800 °C) + 0.5 $H_2O$ (g, 800 °C) | $\Delta H_{12} = H_{dsol}$ |
| $\Delta H_{12} = -\Delta H_{11} + 0.5\,\Delta H_1 + 0.5\,\Delta H_2 + 0.5\,\Delta H_3 + 0.5\,\Delta H_{10} = 249.73 \pm 8.06$ kJ/mol | |
| Enthalpy of formation for $LiLaO_2$ | |
| $LiLaO_2$ (xl, 25 °C) → $LaO_{1.5}$ (sln, 800 °C) + 0.5 $Li_2O$ (sln, 800 °C) | $\Delta H_{13} = H_{dsol-corr} = 15.62 \pm 8.19$ kJ/mol |
| $LaO_{1.5}$ (xl, 25 °C) → $LaO_{1.5}$ (sln, 800 °C) | $\Delta H_6 = -13.88 \pm 0.09$ kJ/mol[13] |
| $Li_2O$ (xl, 25 °C) → $Li_2O$ (sln, 800 °C) | $\Delta H_4 = -23.83 \pm 5.06$ kJ/mol |
| LaO1.5 (xl, 25 °C) + $Li_2O$ (xl, 25 °C) → $LiLaO_2$ (xl, 25 °C) | $\Delta H_{14} = \Delta H_{f-ox}$ |
| $\Delta H_{14} = -\Delta H_{13} + \Delta H_6 + 0.5\,\Delta H_4 = -41.41 \pm 9.62$ kJ/mol | |

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positive. The entropy value used for these calculations, per mole of $O_2$ gas, (145 J/mol K) was taken from the average value for metal oxides.[19]

$$\Delta S^{\circ}_{\text{decomp}} = 0.75\,(145\,\text{J/mol K}) = 108\,\text{J/mol K}$$

At a given temperature and $pO_2$

$$\Delta G_{\text{decomp}} = \Delta H_{\text{decomp}} - T\Delta S_{\text{decomp}} + \text{RT}0.75\ln(pO_2)$$

for air, $pO_2 = 0.21\text{atm}$,

so

$$\Delta G_{\text{decomp}} = 147356 - 108\text{T} - 9.7\text{T for}$$

$$\Delta G_{\text{decomp}} = 0, \text{T} = 147356/117.7 = 1234\,\text{K} = 979 \pm 95\,^{\circ}\text{C}$$

The calculated decomposition temperature is within error of the experimental value.

Considering the formation of $Li_2O$ as a decomposition product of $La_4LiAuO_8$ involves the following reaction

$$\text{La}_4\text{AuLiO}_8\,(\text{s}, 25\,^{\circ}\text{C}) \rightarrow 4\text{LaO}_{1.5}\,(\text{s}, 25\,^{\circ}\text{C}) + \text{Au}\,(\text{s}, 25\,^{\circ}\text{C}) + 0.5\text{Li}_2\text{O}\,(\text{s}, 25\,^{\circ}\text{C}) + 0.75\,\text{O}_2\,(\text{g}, 25\,^{\circ}\text{C}) = \Delta H_{\text{decomp}} = \Delta H_{18} = 188.77 \pm 5.12$$

Inserting this $\Delta H_{\text{decomp}}$ value into the equation for $\Delta G_{\text{decomp}}$ results in a decomposition temperature of 1331 ± 43 °C, which is 396 °C higher than the experimental value. Therefore, the thermodynamics of the decomposition reaction of $La_4AuLiO_8$ indicate that $LaLiO_2$ is the likely product.

The results from the oxide melt solution calorimetry of $La_4LiAuO_8$ indicate that the compound is thermodynamically stable with respect to the constituent oxides and is more stable than binary trivalent gold oxide, $Au_2O_3$. The enthalpy of formation for $LaLiO_2$ with respect to the oxides is small and exothermic. The decomposition of $La_4LiAuO_8$ occurs at 931 °C and results in metallic gold, lanthanum oxide, and lanthanum lithium oxide. The formation of $LaLiO_2$ as a decomposition product for $La_4LiAuO_8$ was confirmed by calculating the decomposition temperature from measured thermodynamic parameters. The calculated value (979 ± 95 °C) agrees well with the experimental results.

## ACKNOWLEDGMENTS

The authors thank the U.S. Department of Energy, Office of Basic Energy Sciences for supporting this work through Grants DE-FG02-03ER46053 and DE-FG02-10ER16081. J.A. Kurzman thanks the ConvEne Integrative Graduate Education and Research Traineeship (IGERT) Program (NSF-DGE0801627) for an Associateship.

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https://doi.org/10.1557/jmr.2011.87 Published online by Cambridge University Press