

AD-A172 203 APPLICATION OF COMPUTER METHODS FOR CALCULATION OF
MULTICOMPONENT PHASE D. (U) MANLABS INC CAMBRIDGE MASS
L KAUFMAN 28 FEB 86 AFOSR-TR-86-0693 F49620-84-C-0078

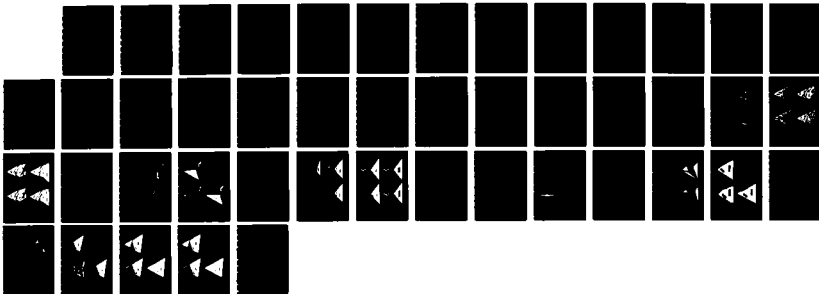
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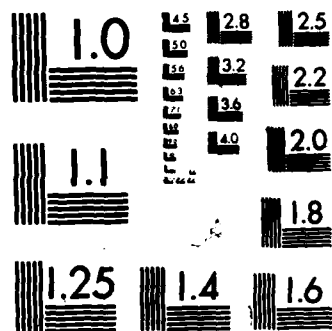
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Annual Report

on

CONTRACT F49620-84-C-0078

APPLICATION OF COMPUTER METHODS FOR CALCULATION
OF MULTICOMPONENT PHASE DIAGRAMS OF HIGH TEMPERATURE
STRUCTURAL CERAMICS

1 October 1984 to 28 February 1986

Air Force of Scientific Research (AFSC)

Bolling Air Force Base, D.C. 20332

28 February 1986

by

Larry Kaufman

ManLabs, Inc.

21 Erie Street

Cambridge, Massachusetts 02139

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20. ABSTRACT (Continue on reverse side if necessary, and identify by block number) Computer Coupled Phase Diagrams and Thermochemical Data have been used to calculate the $\text{GeO}_2\text{-MgO}$, $\text{GeO}_2\text{-HfO}_2$, $\text{GeO}_2\text{-TiO}_2$, $\text{GeO}_2\text{-Al}_2\text{O}_3$, $\text{GeO}_2\text{-CaO}$, $\text{GeO}_2\text{-SiO}_2$, $\text{TiO}_2\text{-MgO}$, $\text{HfO}_2\text{-SiO}_2$, $\text{HfO}_2\text{-MgO}$, $\text{HfO}_2\text{-CaO}$, $\text{Al}_2\text{O}_3\text{-HfO}_2$, $\text{HfO}_2\text{-Y}_2\text{O}_3$, $\text{HfO}_2\text{-TiO}_2$, $\text{Ce}_2\text{O}_3\text{-Al}_2\text{O}_3$, $\text{ZrO}_2\text{-HfO}_2$, $\text{ZrO}_2\text{-SiO}_2$, $\text{ZrO}_2\text{-CaO}$, $\text{Y}_2\text{O}_3\text{-MgO}$ and $\text{Y}_2\text{O}_3\text{-CaO}$ binary systems as well as isothermal sections in the $\text{MgO-TiO}_2\text{-SiO}_2$, $\text{MgO-SiO}_2\text{-GeO}_2$, $\text{GeO}_2\text{-MgO-CaO}$, $\text{HfO}_2\text{-CaO-MgO}$, $\text{HfO}_2\text{-SiO}_2\text{-ZrO}_2$ and $\text{HfO}_2\text{-CaO-Y}_2\text{O}_3$ at temperatures between 700K and 3000K.		

I. PROGRESS DURING THE CURRENT YEAR

The methods developed under the previous Contract F49620-80-C-0020 and described in the final report on that contract dated 30 November 1983 entitled "Computer Based Methods for Thermodynamics Analysis of Materials Processing" by Larry Kaufman are to be employed to carry out the following tasks during the first year of the current program:

1. A combined thermochemical and phase diagram analysis was performed for the $\text{GeO}_2\text{-HfO}_2$, $\text{GeO}_2\text{-TiO}_2$, $\text{GeO}_2\text{-Al}_2\text{O}_3$, $\text{GeO}_2\text{-MgO}$, $\text{GeO}_2\text{-SiO}_2$, $\text{GeO}_2\text{-CaO}$, and $\text{TiO}_2\text{-MgO}$, quasi-binary systems in order to define the lattice stability, solution and compound phase parameters and expand the current data base.
2. Isothermal section in the $\text{GeO}_2\text{-MgO-SiO}_2$, $\text{GeO}_2\text{-MgO-TiO}_2$, $\text{GeO}_2\text{-CaO-MgO}$ systems were calculated between 700K and 2700K. The calculated phase diagrams were compared with available experimental phase diagrams to test the data base.
3. A combined Thermochemical and phase diagram analysis was performed for the $\text{HfO}_2\text{-SiO}_2$, $\text{HfO}_2\text{-MgO}$, $\text{HfO}_2\text{-CaO}$, $\text{Al}_2\text{O}_3\text{-HfO}_2$, $\text{HfO}_2\text{-Y}_2\text{O}_3$, $\text{HfO}_2\text{-TiO}_2$, $\text{Ce}_2\text{O}_3\text{-Al}_2\text{O}_3$, $\text{ZrO}_2\text{-HfO}_2$, $\text{ZrO}_2\text{-SiO}_2$, $\text{ZrO}_2\text{-CaO}$, $\text{Y}_2\text{O}_3\text{-CaO}$ and $\text{Y}_2\text{O}_3\text{-MgO}$ quasibinary systems in order to define the lattice stability, solution and compound phase parameters and expand the current data base.
4. Isothermal sections in the $\text{MgO-TiO}_2\text{-SiO}_2$, $\text{MgO-SiO}_2\text{-GeO}_2$, $\text{GeO}_2\text{-MgO-CaO}$, $\text{HfO}_2\text{-CaO-MgO}$, $\text{HfO}_2\text{-SiO}_2\text{-ZrO}_2$ and $\text{HfO}_2\text{-CaO-Y}_2\text{O}_3$ have been calculated between 700K and 3000K.
5. It is expected that the remaining ternary systems defined under the current option II work statement; $\text{HfO}_2\text{-Y}_2\text{O}_3\text{-CaO}$, $\text{HfO}_2\text{-Y}_2\text{O}_3\text{-MgO}$, $\text{HfO}_2\text{-SiO}_2\text{-Y}_2\text{O}_3$ and $\text{HfO}_2\text{-SiO}_2\text{-MgO}$ will be completed on time during the present contract.

Figures 1-19 show the calculated quasibinary systems listed in items 1 and 3 above while Figures 20-39 show the isothermal sections for the quasiternary systems listed in items 2 and 4 above.

During the year the following personnel have been active in the program: L. Kaufman, D. Birnie, V. Farber, E. P. Warekois, P. Neshe, J. Smith and D. Ray. The following technical lectures and papers were presented in connection with work performed under this contract.

1. "Calculation of Quasibinary and Quasiternary Ceramic Systems" CALPHAD XIV, M.I.T. Cambridge, MA June 1985.
2. "Calculation of Ternary Isothermal Sections in the Ni-Cr-Al and Ni-Cr-Si Systems" CALPHAD XIV, M.I.T. Cambridge, MA June 1985.
3. "Binary Common Ion Alkali Halide Mixtures - Solid/Liquid Equilibria in Systems Showing Isodimorphism" CALPHAD (1986) vol. 10, No.2 pp 163-174.
4. "CALPHAD Generated Multicomponent Phase Diagrams for Elements II Through VI" Annual Meeting TMS-ASM, New Orleans, LA March 1986.



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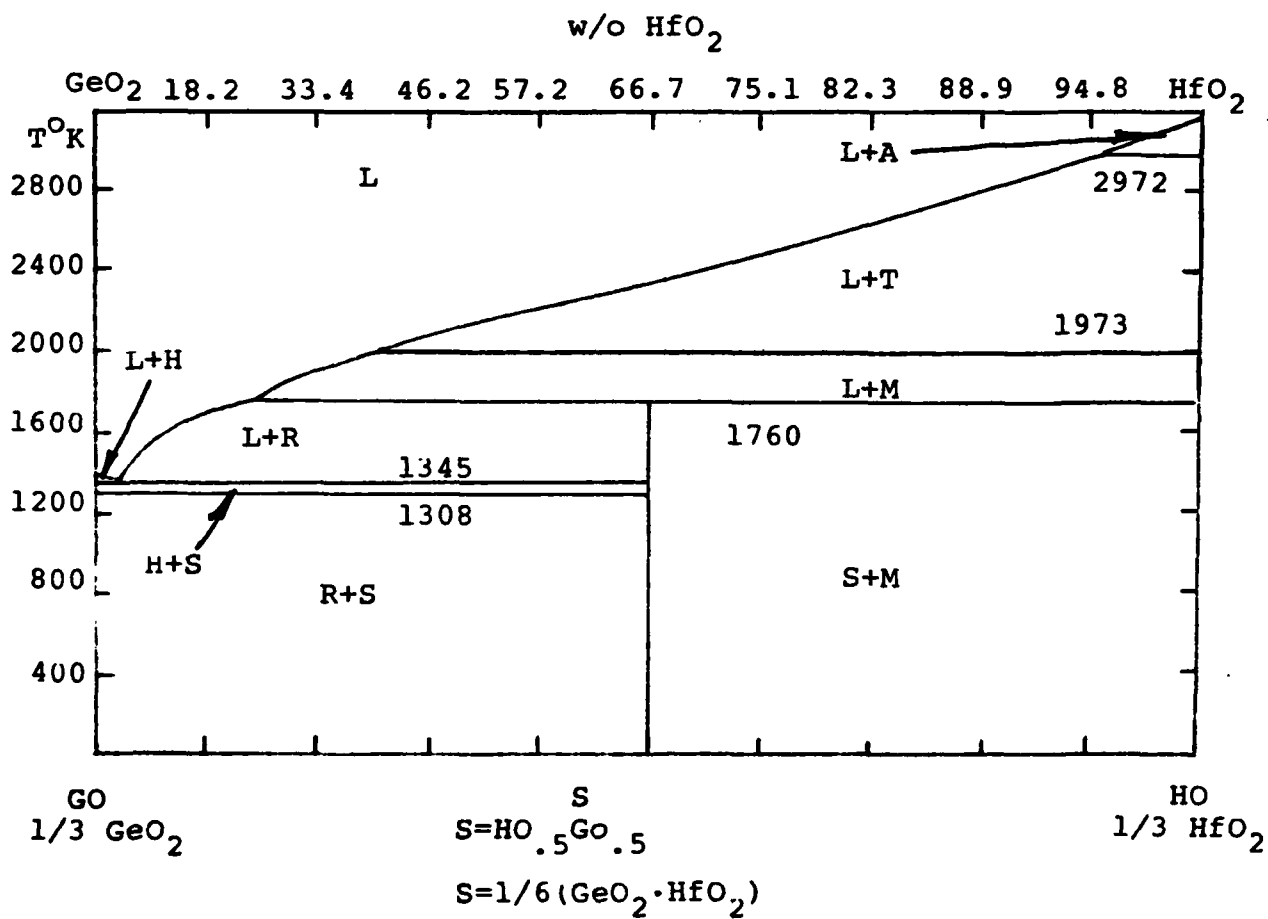


Figure 1. Calculated GeO_2 - HfO_2 Phase Diagram.

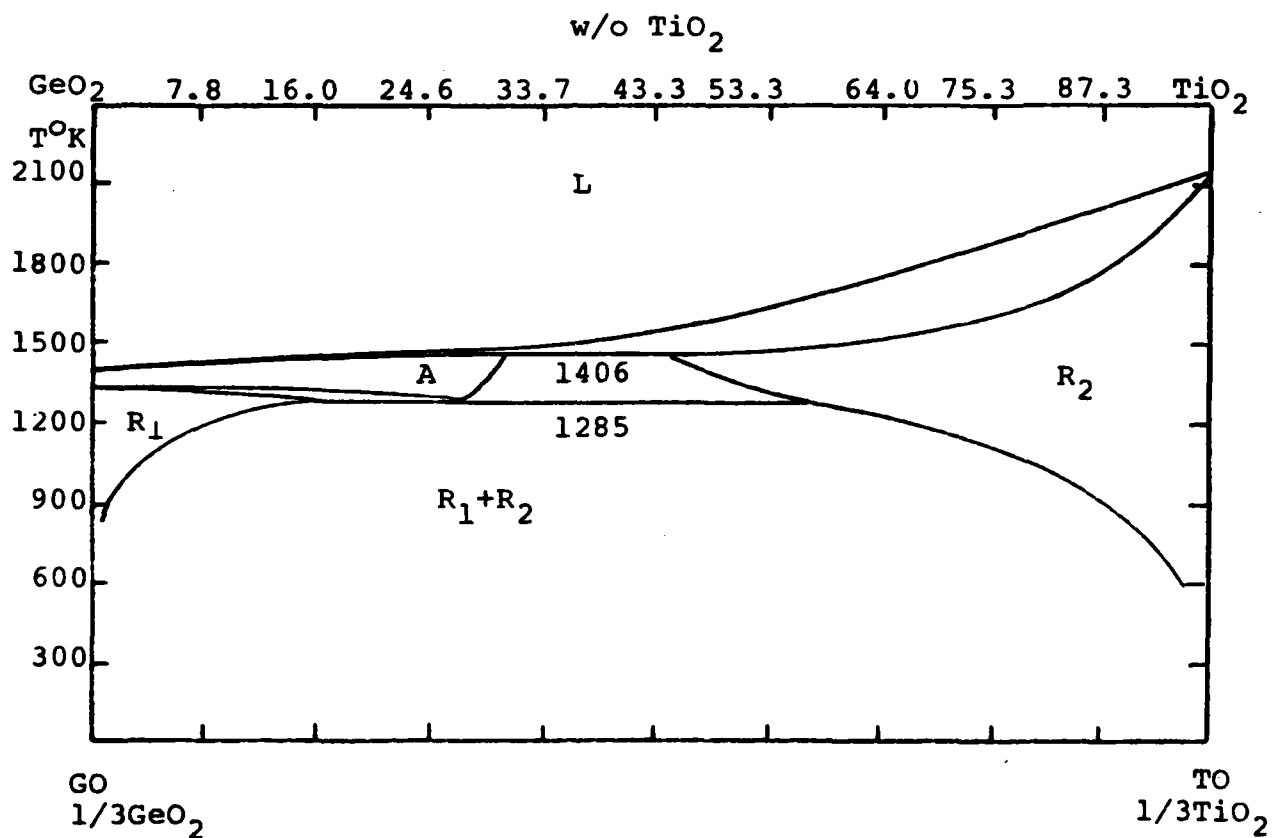


Figure 2. Calculated GeO_2 - TiO_2 Phase Diagram.

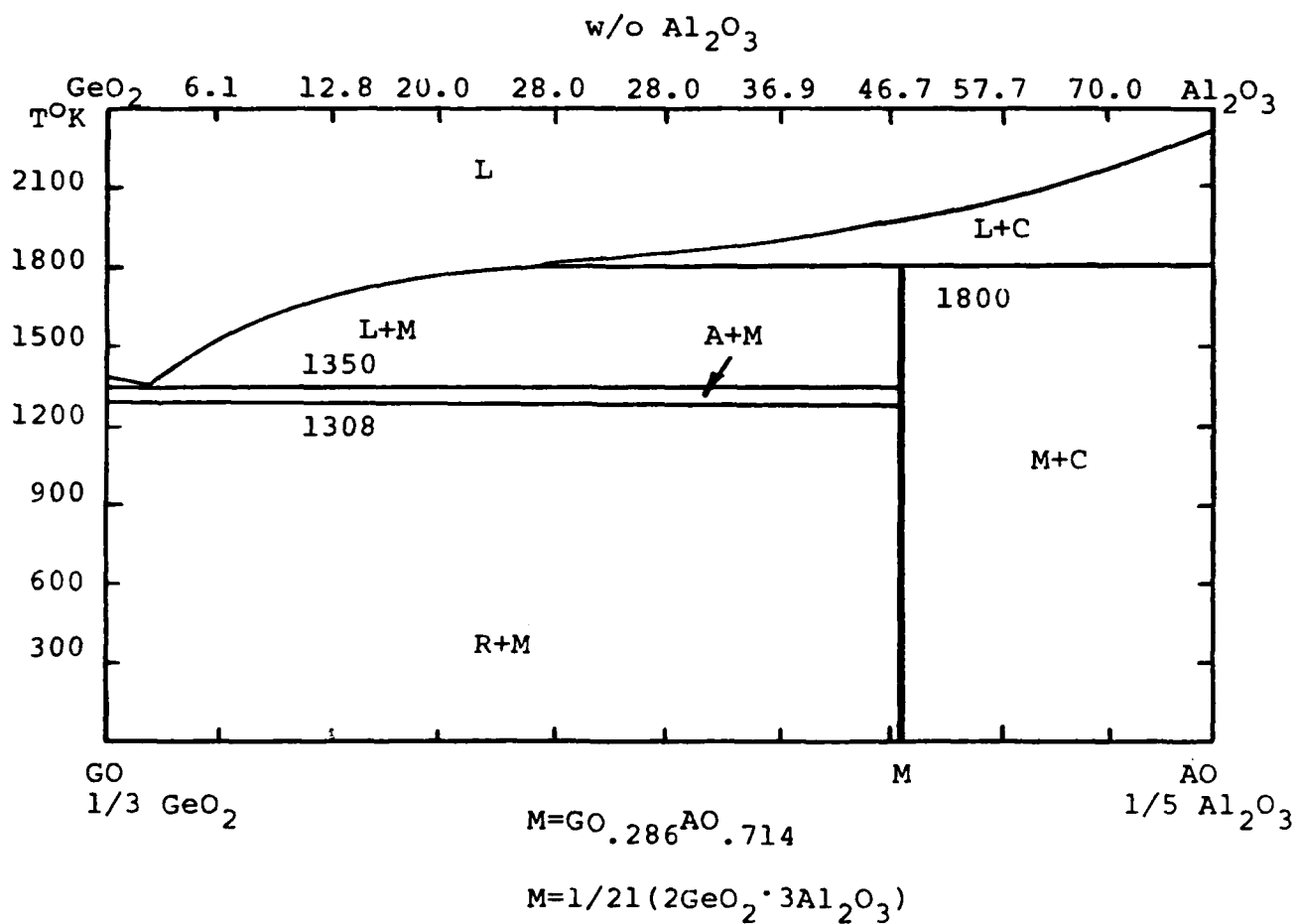


Figure 3. Calculated GeO_2 - Al_2O_3 Phase Diagram.

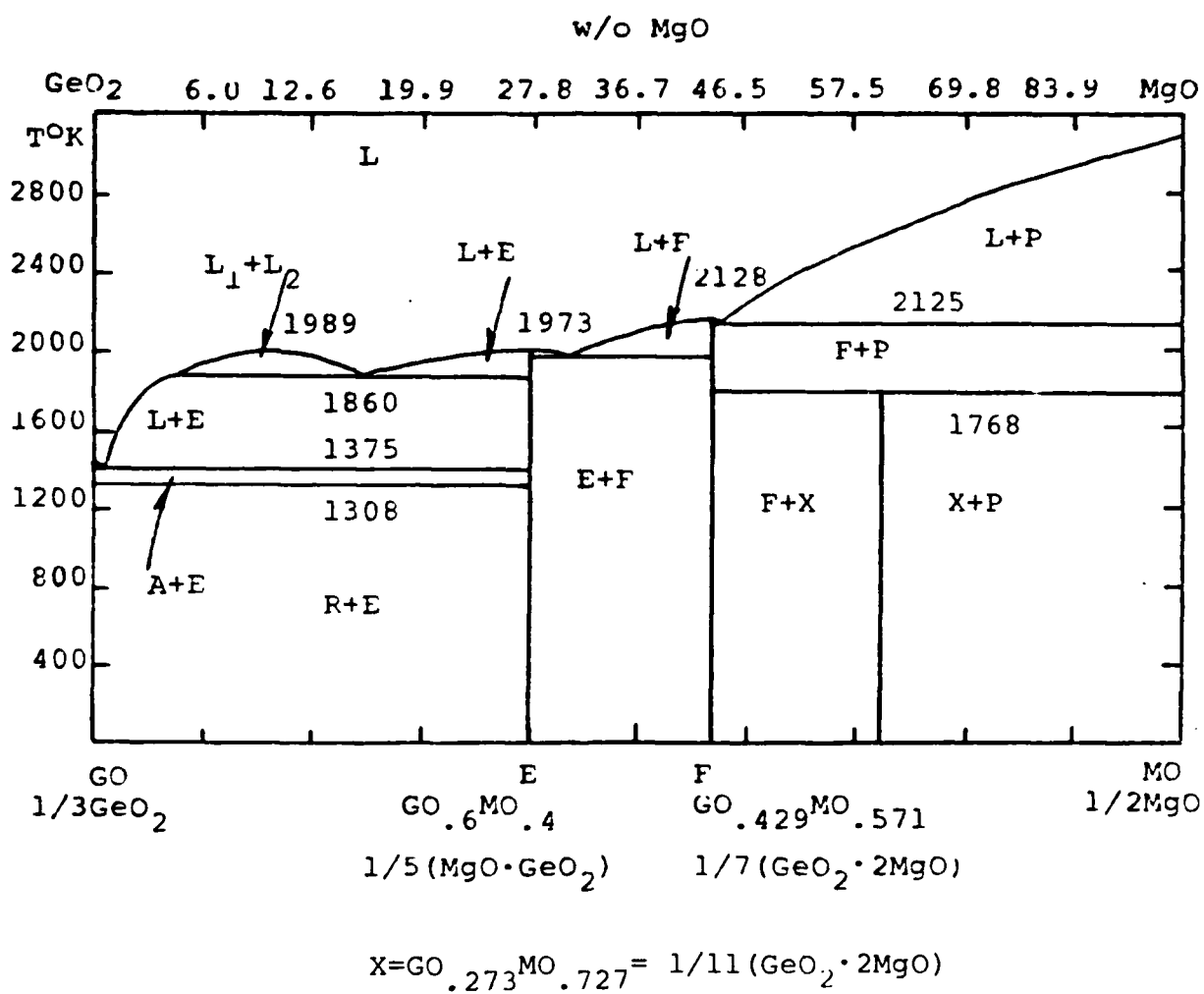


Figure 4. Calculated GeO₂-MgO Phase Diagram.

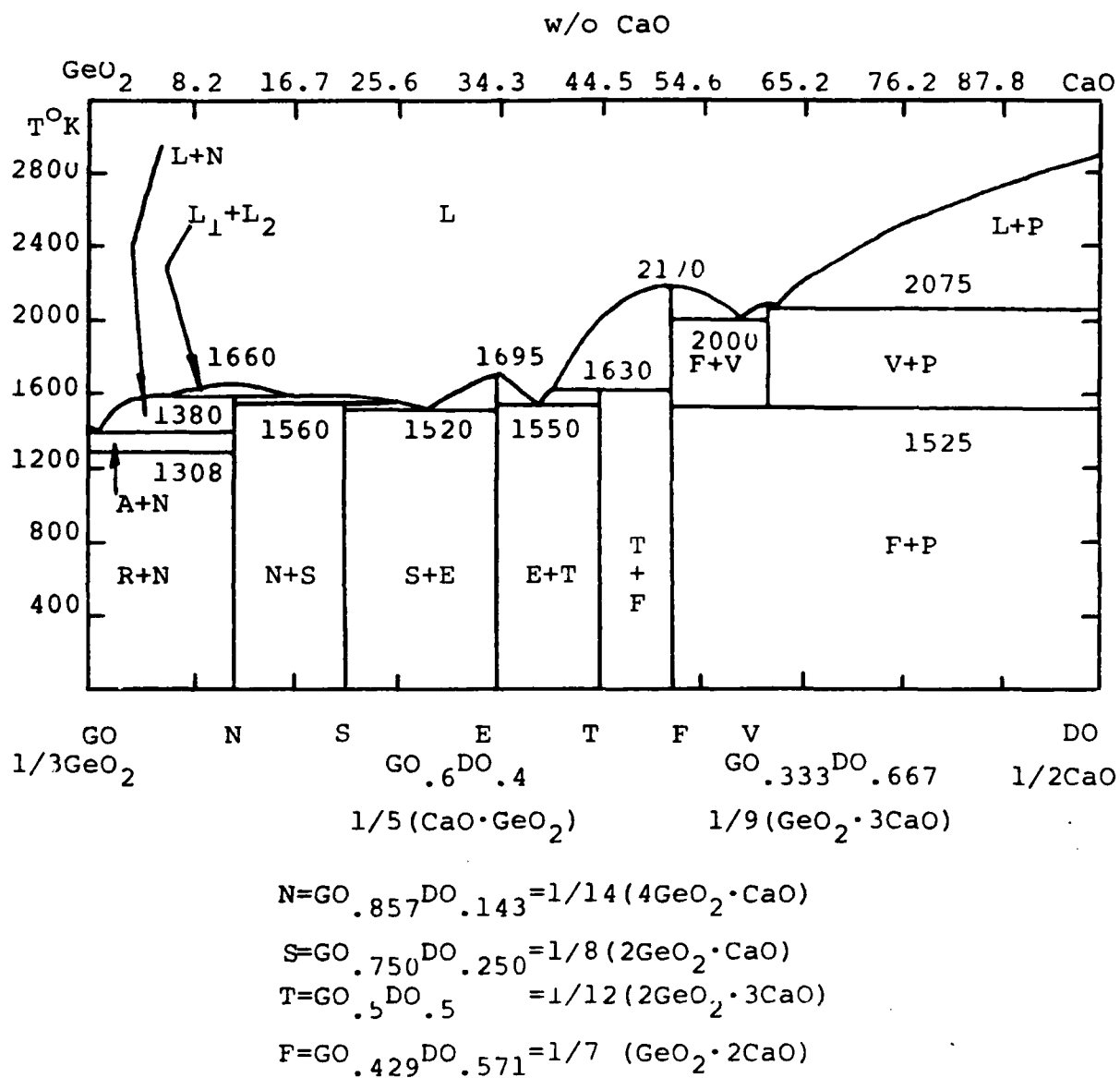


Figure 5. Calculated GeO_2 -CaO Phase Diagram.

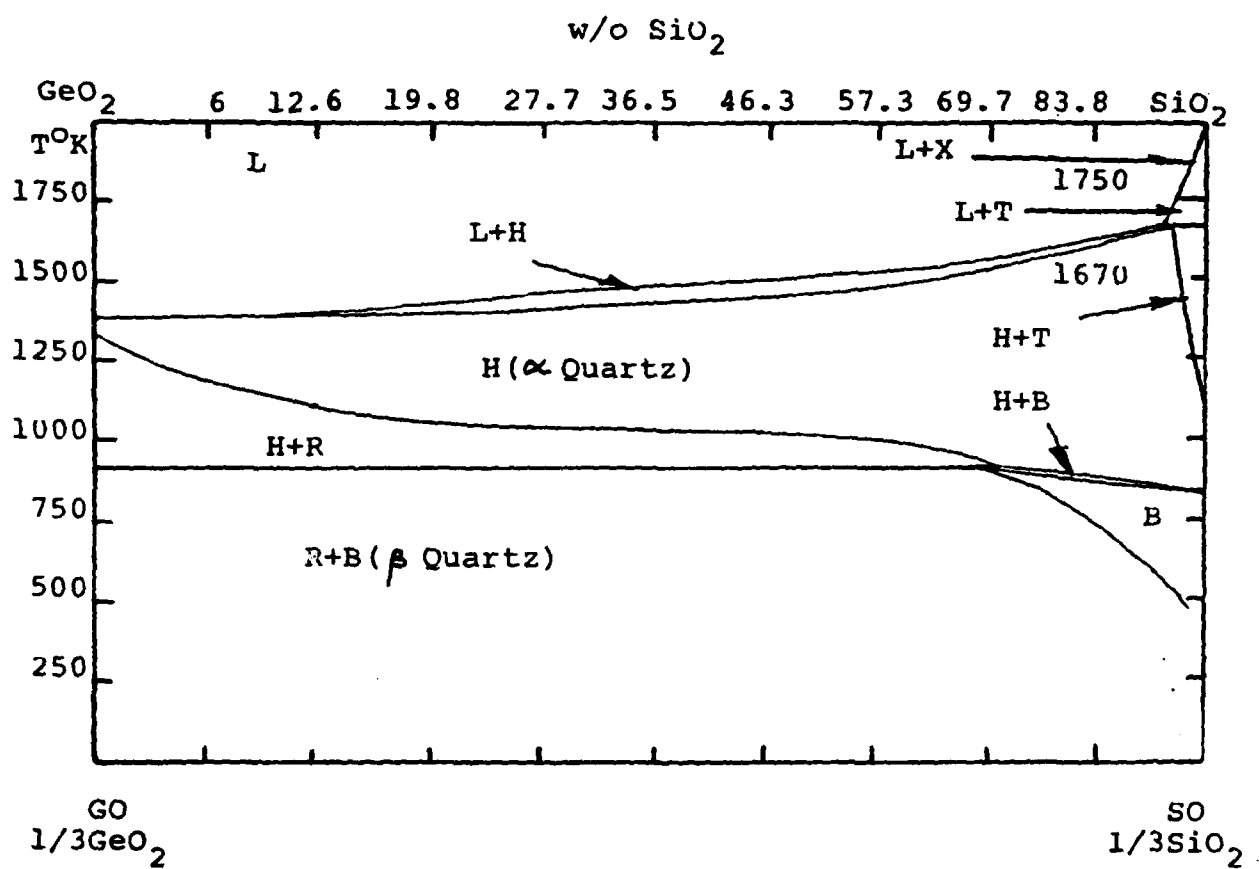


Figure 6. Calculated GeO_2 - SiO_2 Phase Diagram.

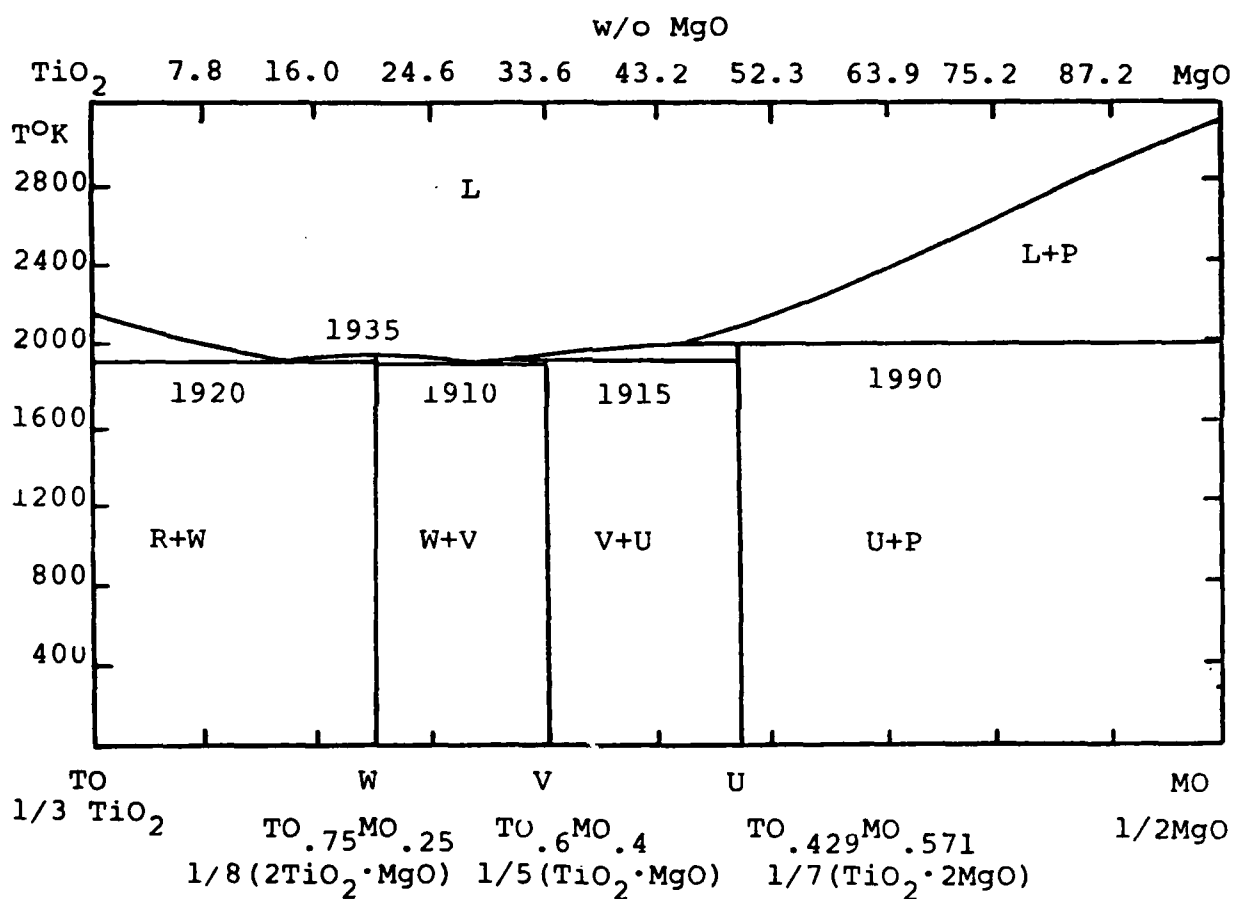


Figure 7. Calculated TiO_2 - MgO Phase Diagram.

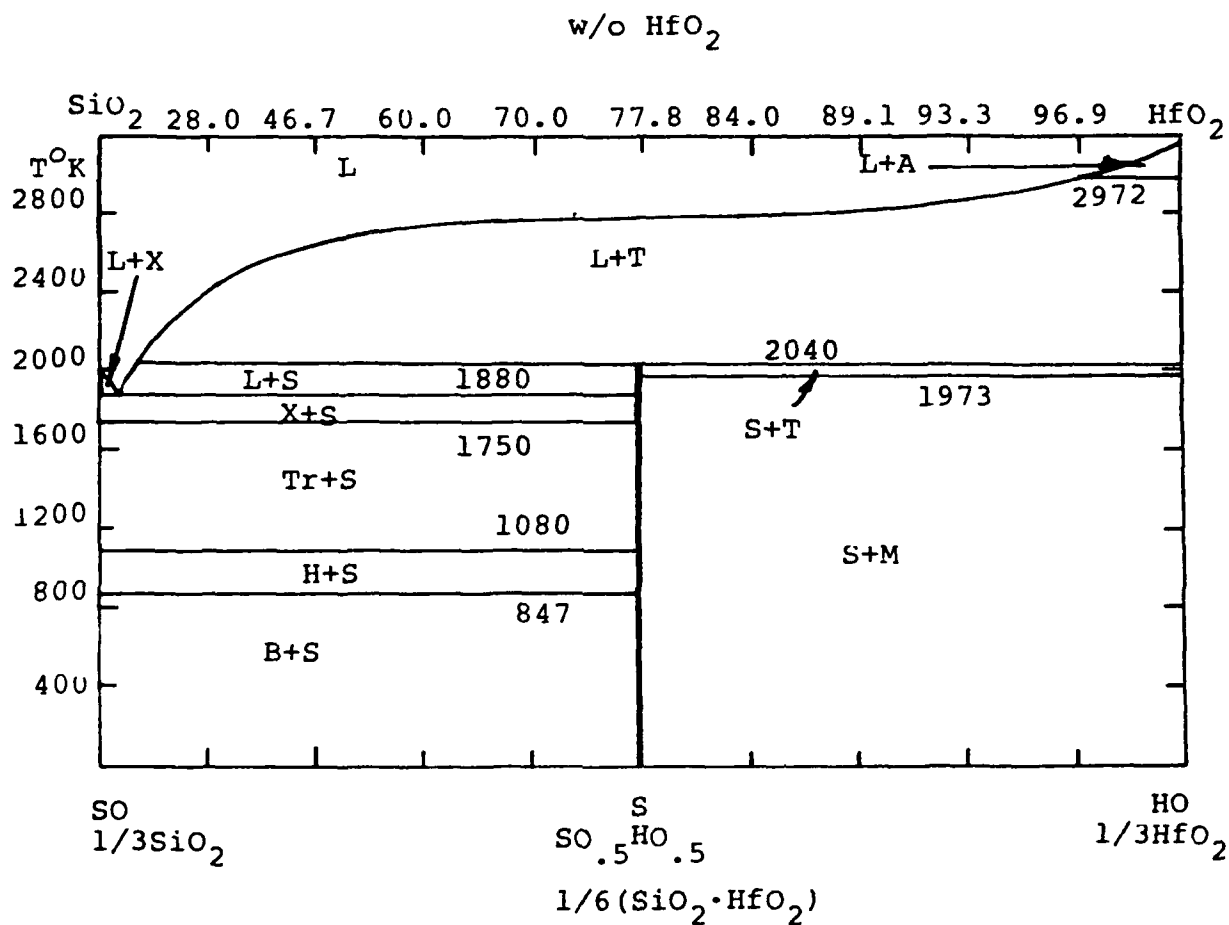


Figure 8. Calculated SiO_2 - HfO_2 Phase Diagram.

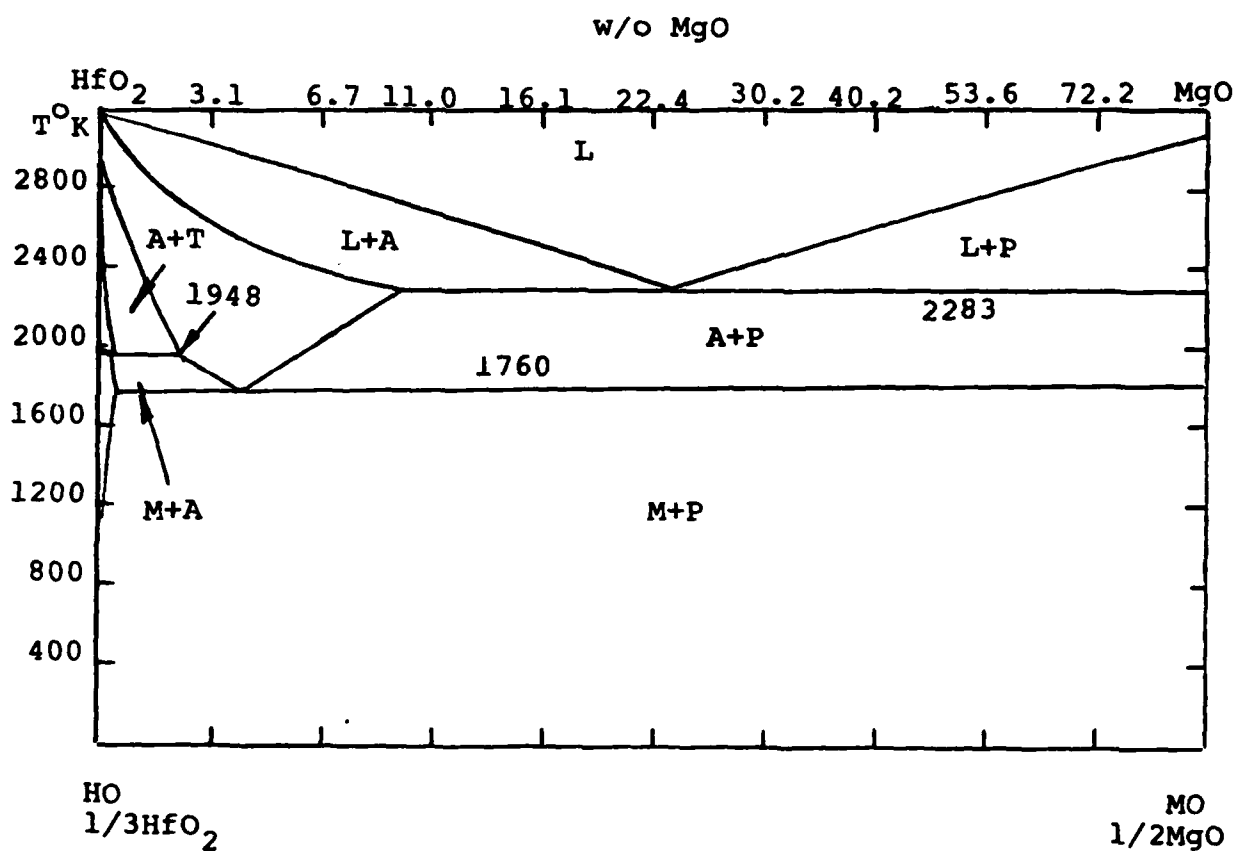


Figure 9. Calculated HfO₂-MgO Phase Diagram.

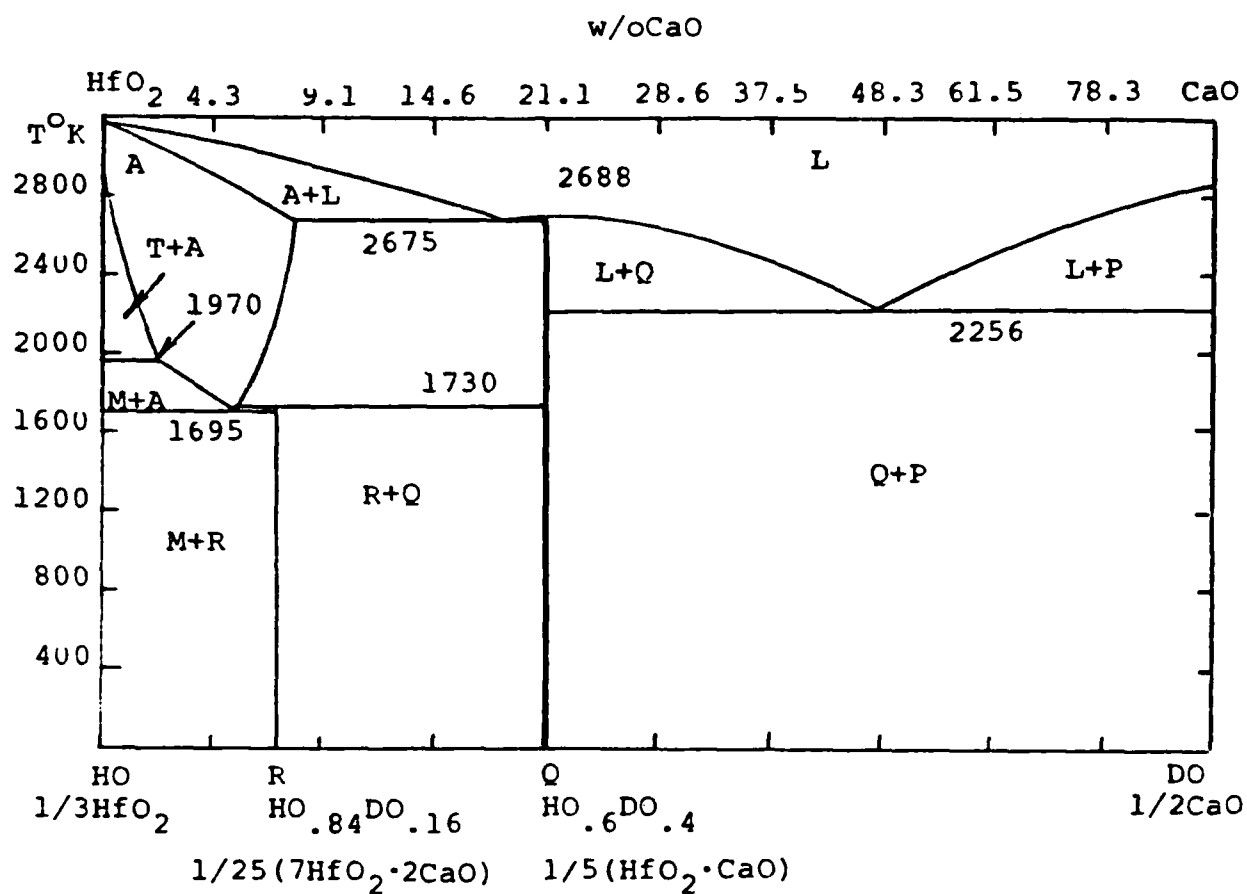


Figure 10. Calculated HfO₂-CaO Phase Diagram.

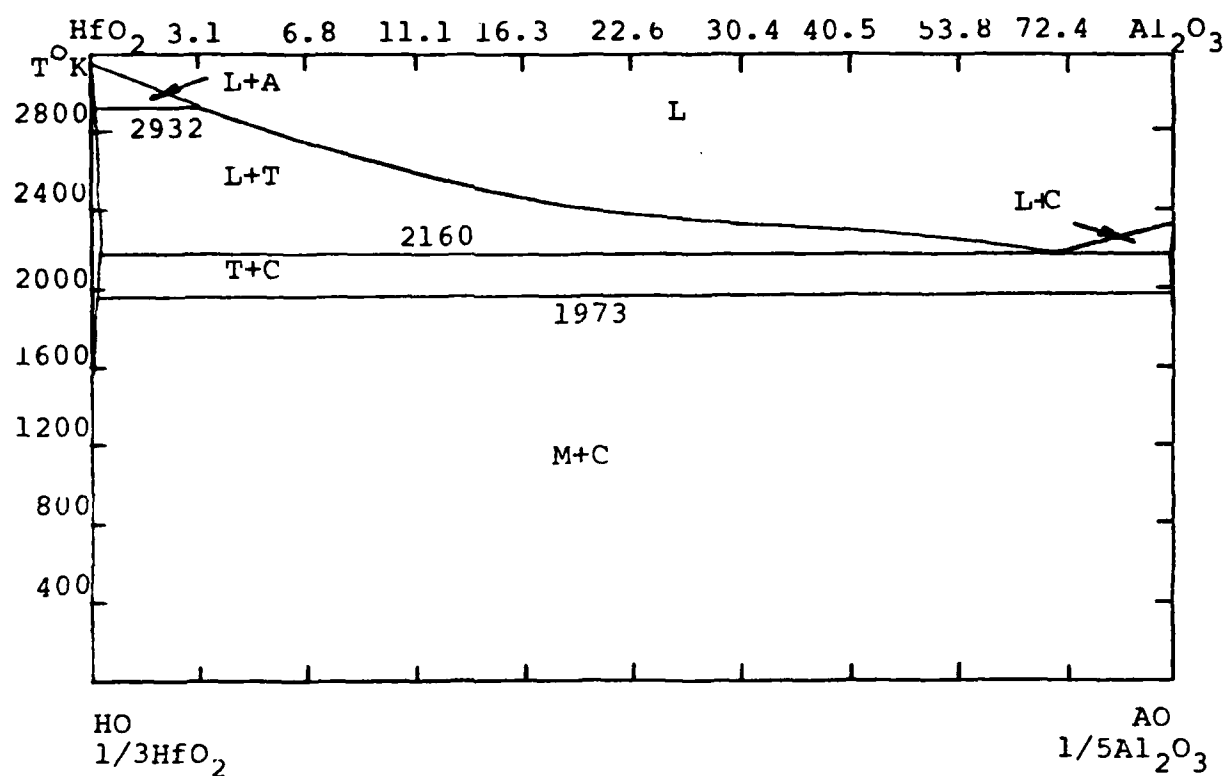


Figure 11. Calculated HfO_2 - Al_2O_3 Phase Diagram.

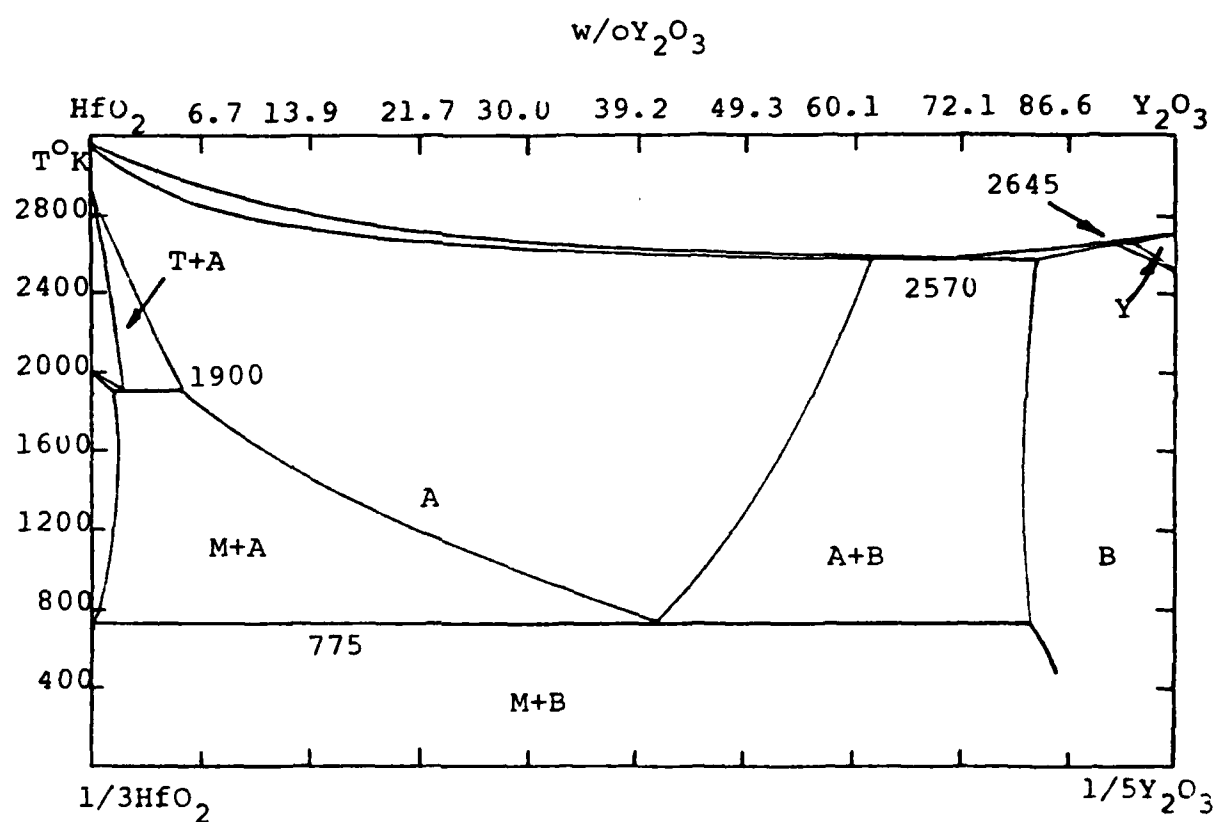


Figure 12. Calculated HfO_2 - Y_2O_3 Phase Diagram.

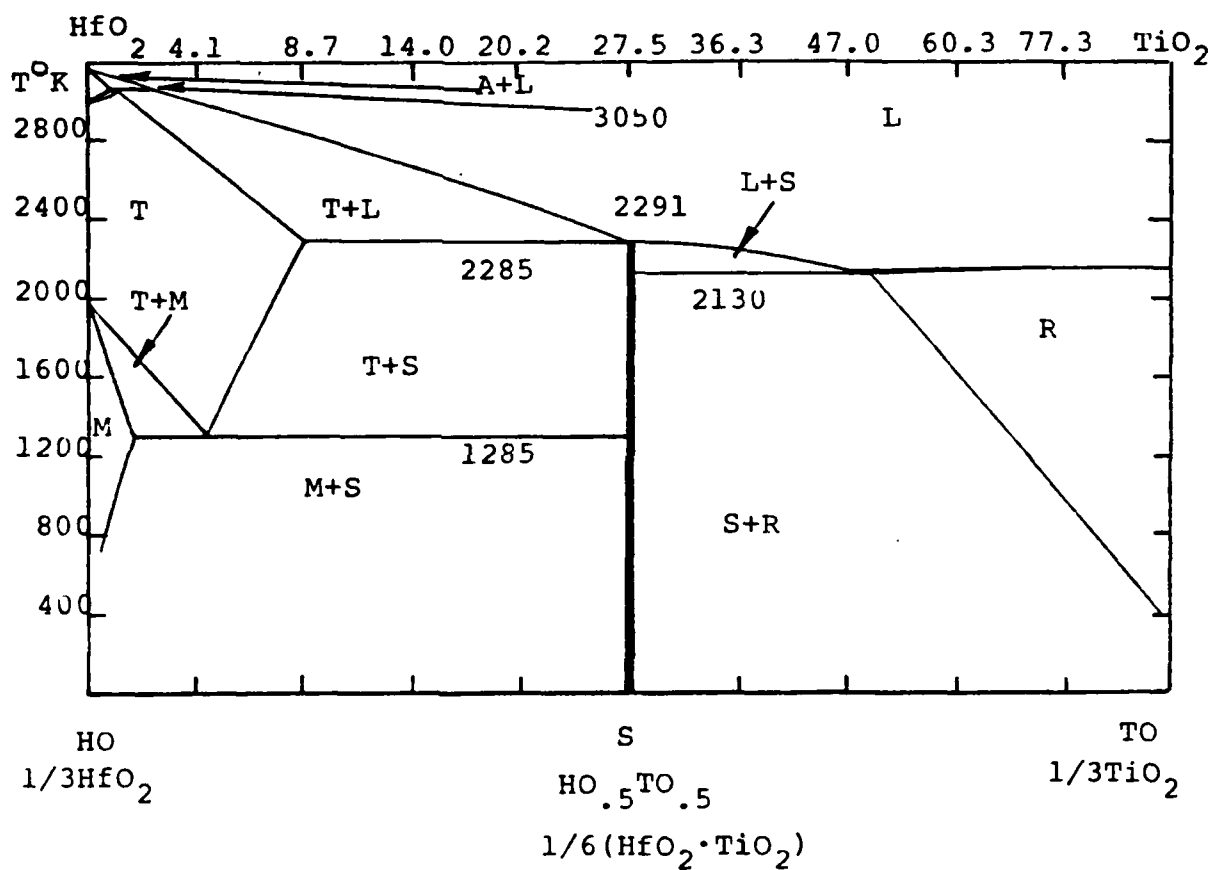


Figure 13 Calculated HfO₂-TiO₂ Phase Diagram.

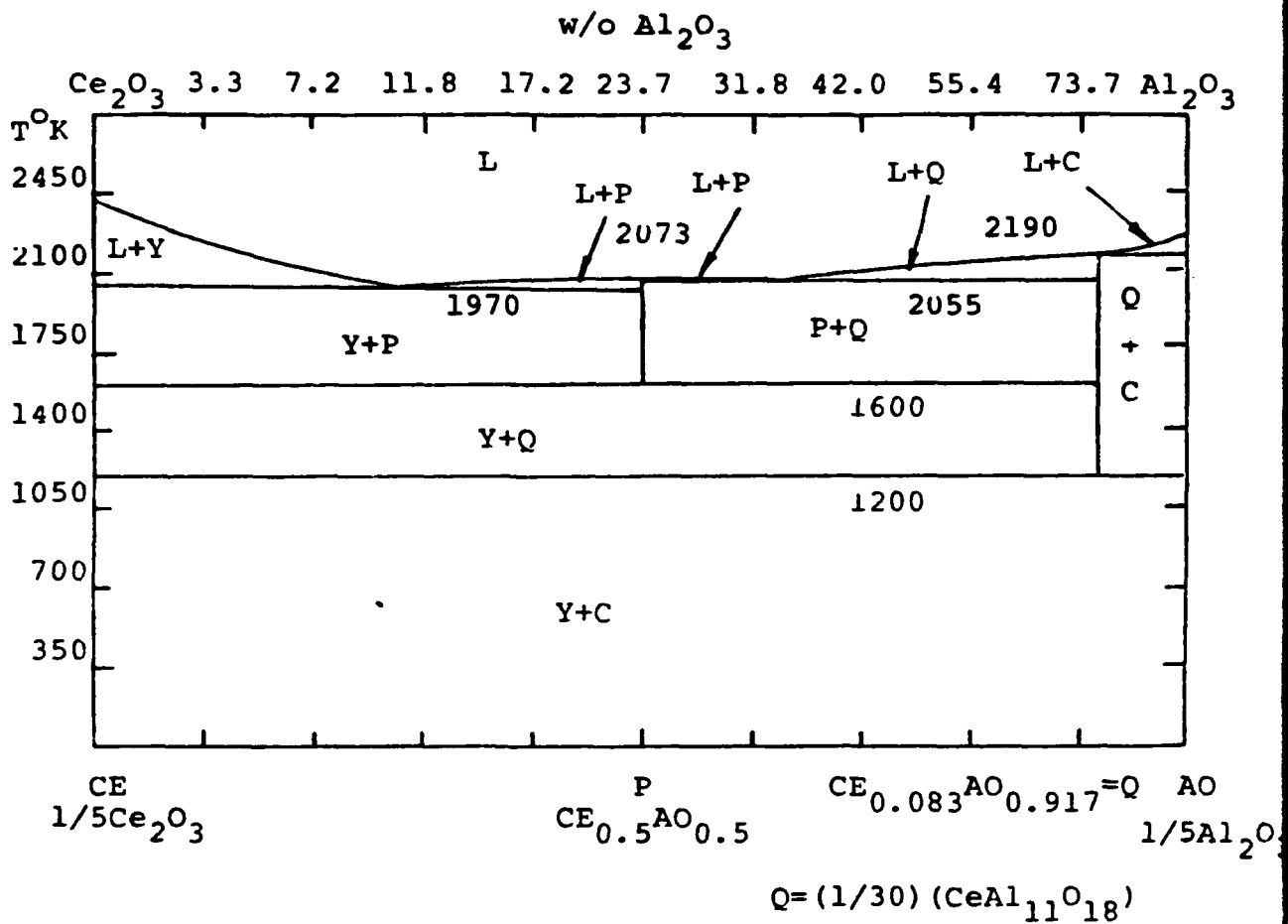


Figure 14. Calculated Ce_2O_3 - Al_2O_3 Phase Diagram.

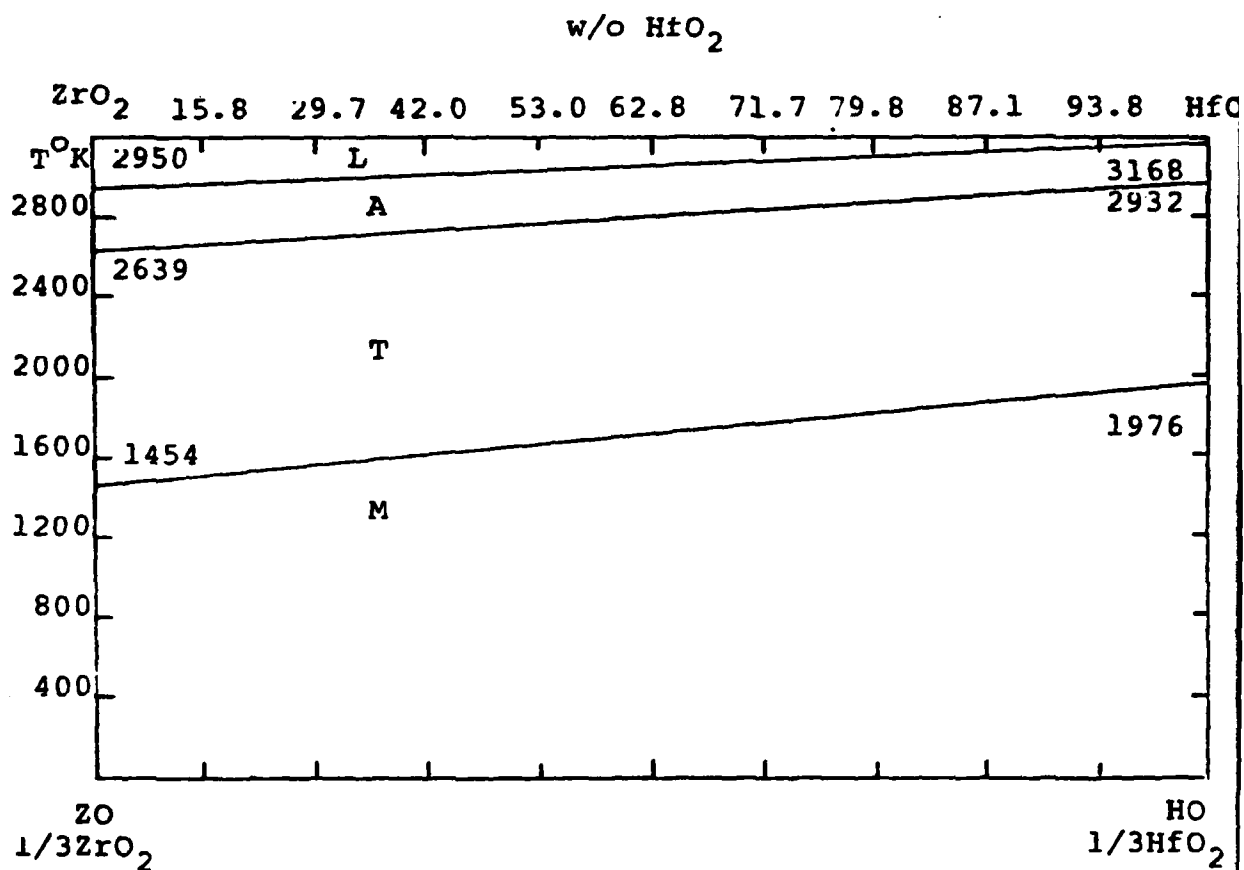


Figure 15. Calculated ZrO_2 - HfO_2 Phase Diagram.

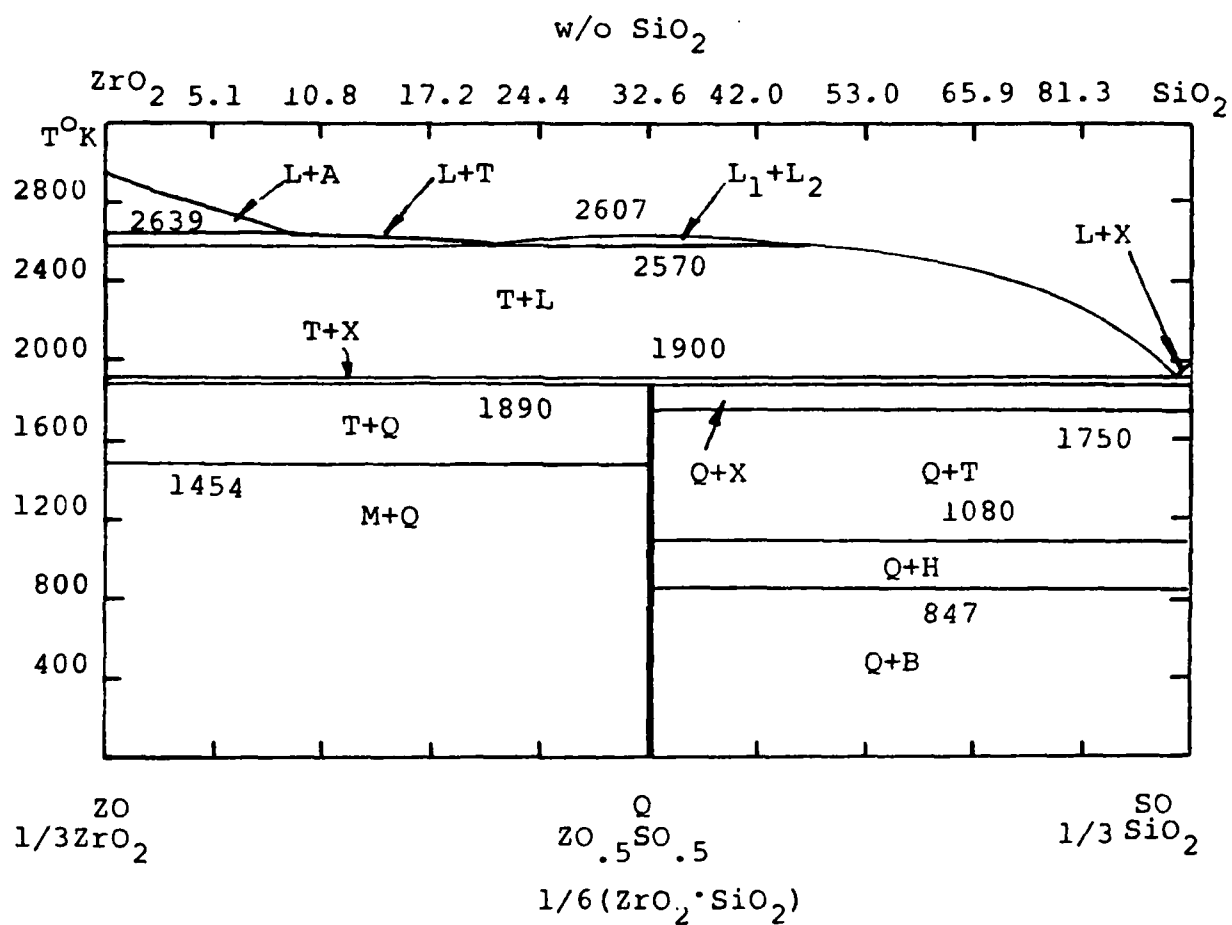


Figure 16. Calculated ZrO₂-SiO₂ Phase Diagram.

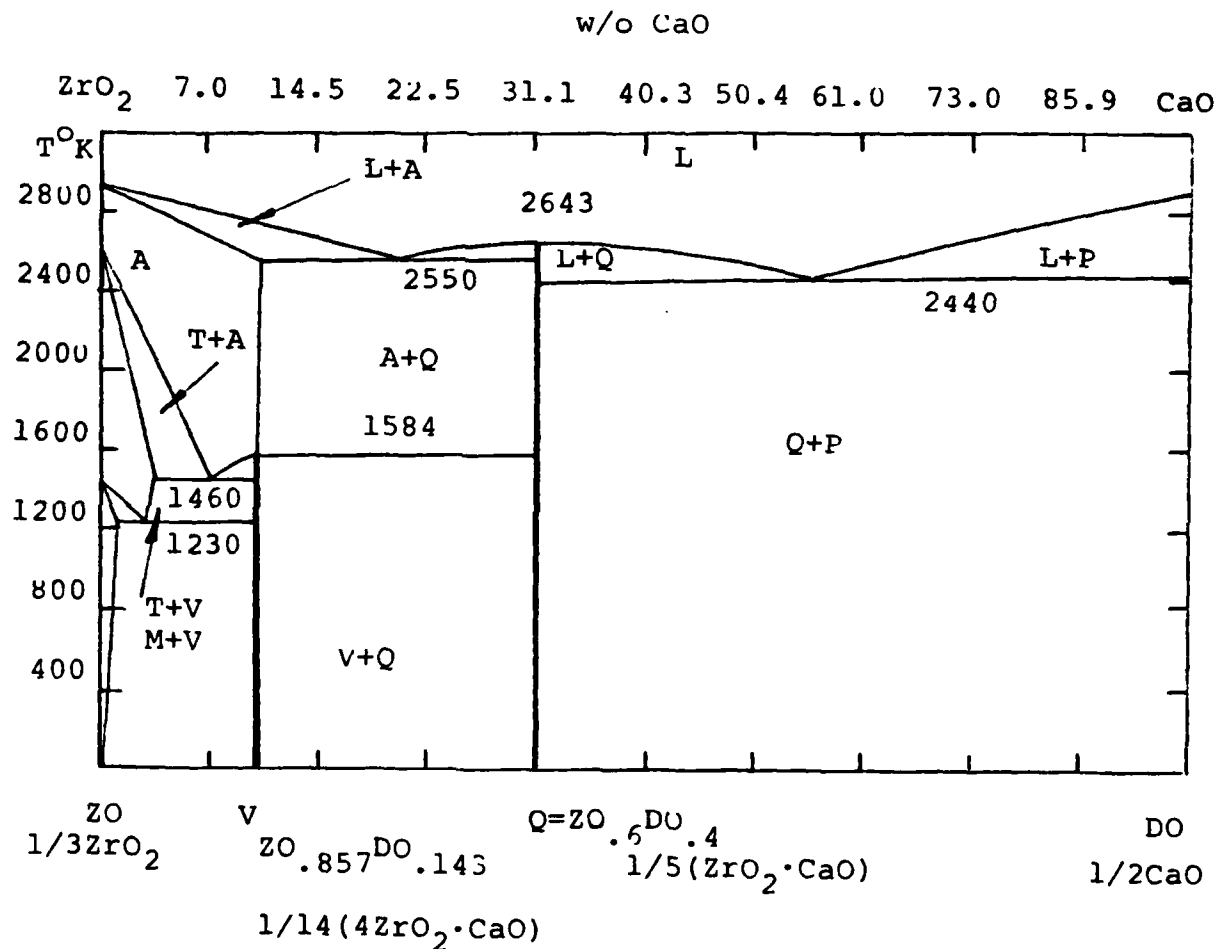


Figure 17. Calculated ZrO₂-CaO Phase Diagram.

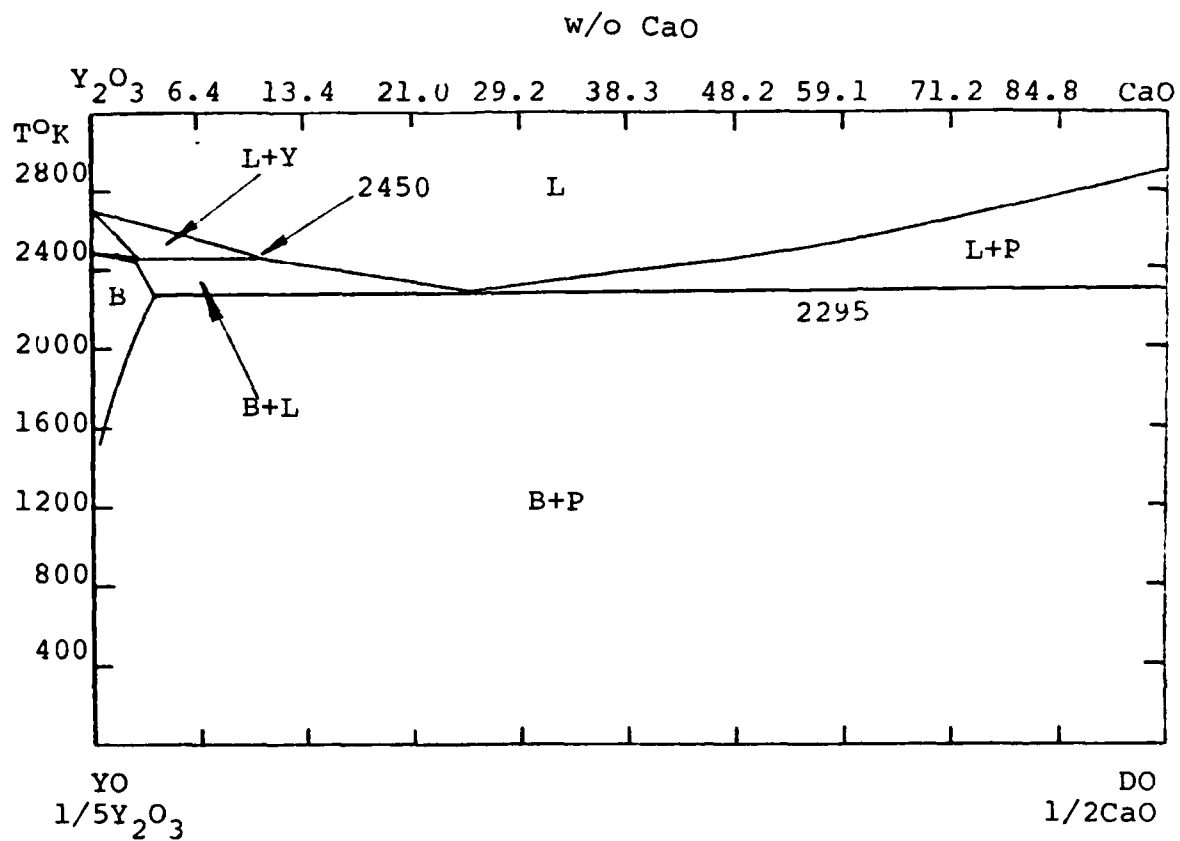


Figure 18. Calculated Y_2O_3 -CaO Phase Diagram.

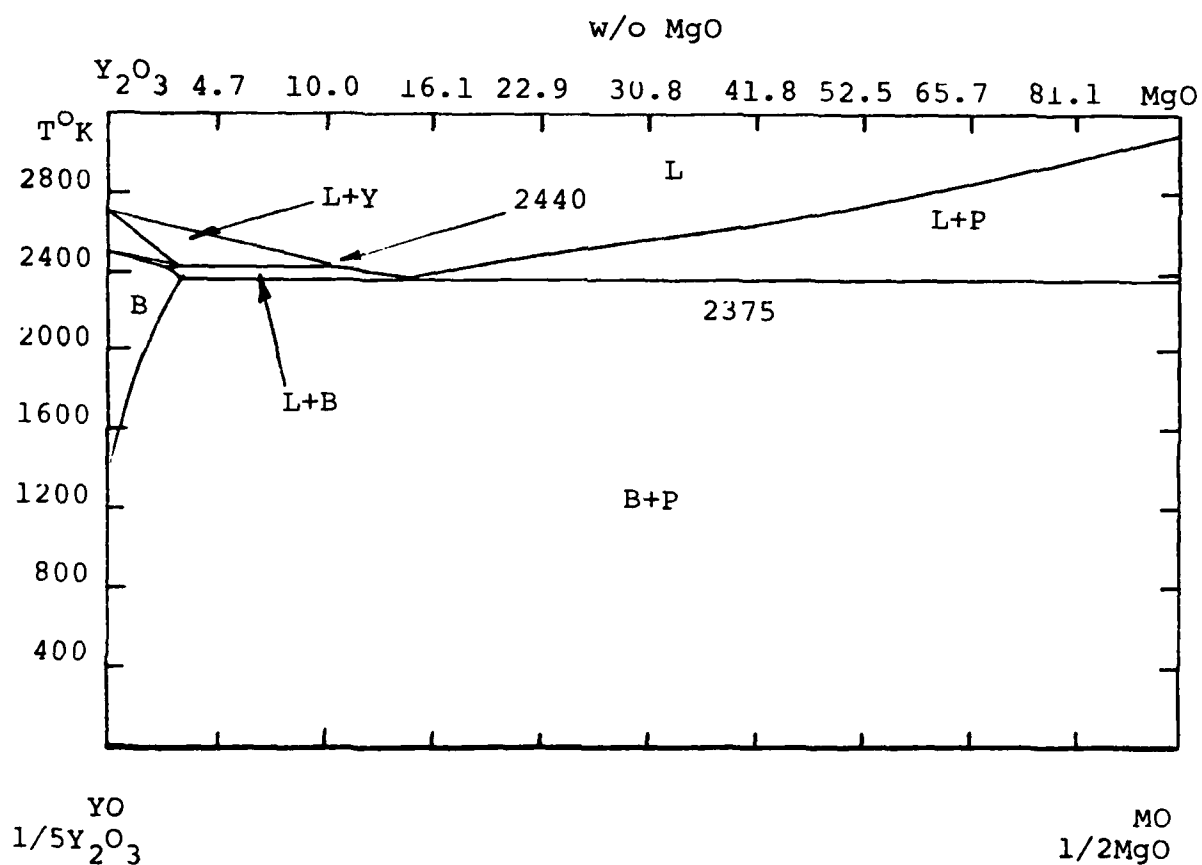


Figure 19. Calculated Y_2O_3 - MgO System.

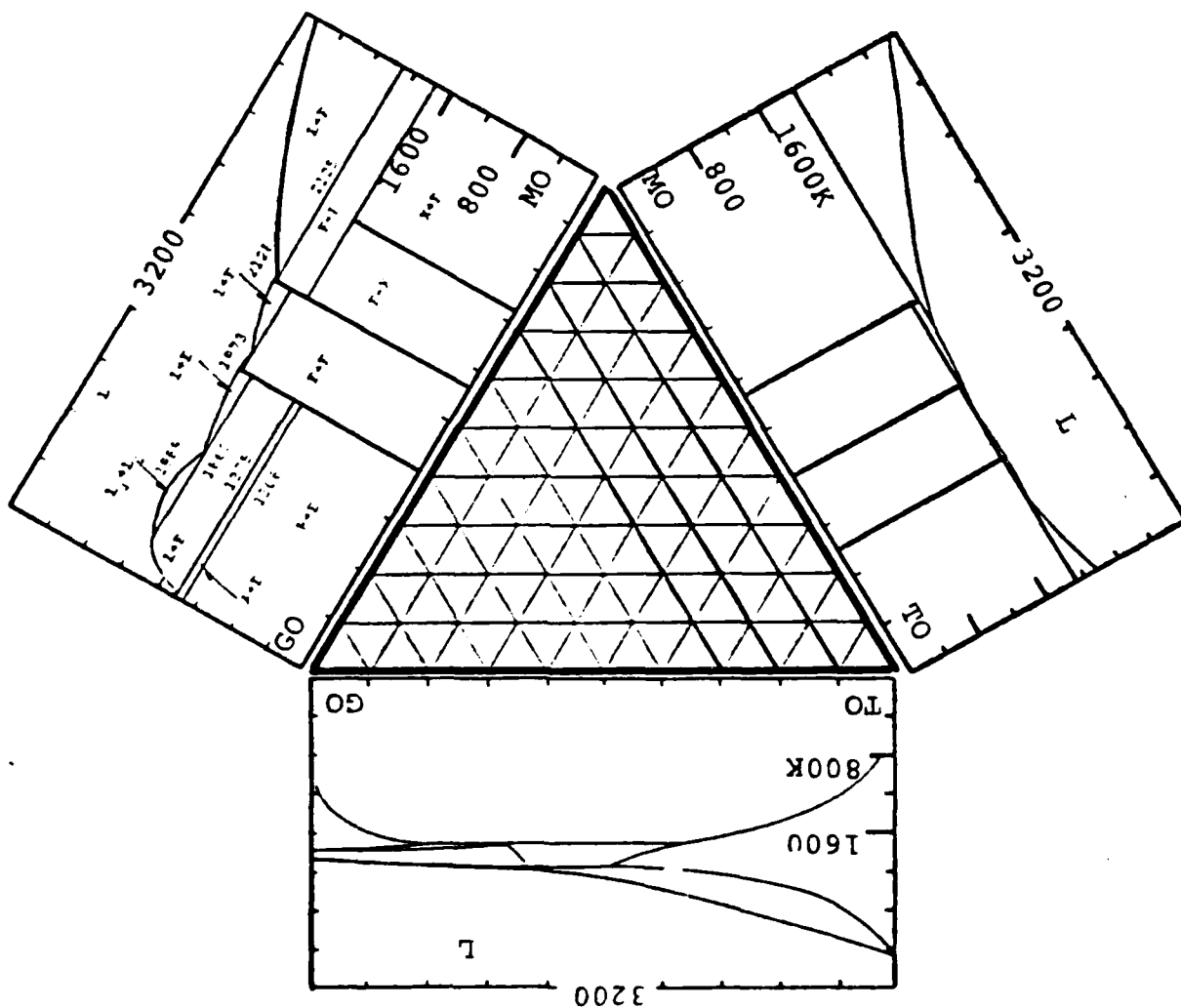


Figure 20 Calculated Isothermal Sections in the $\text{MO}(1/2\text{MgO})\text{-TO}(1/3\text{TiO}_2)\text{-GO}(1/3\text{GeO}_2)$ System.

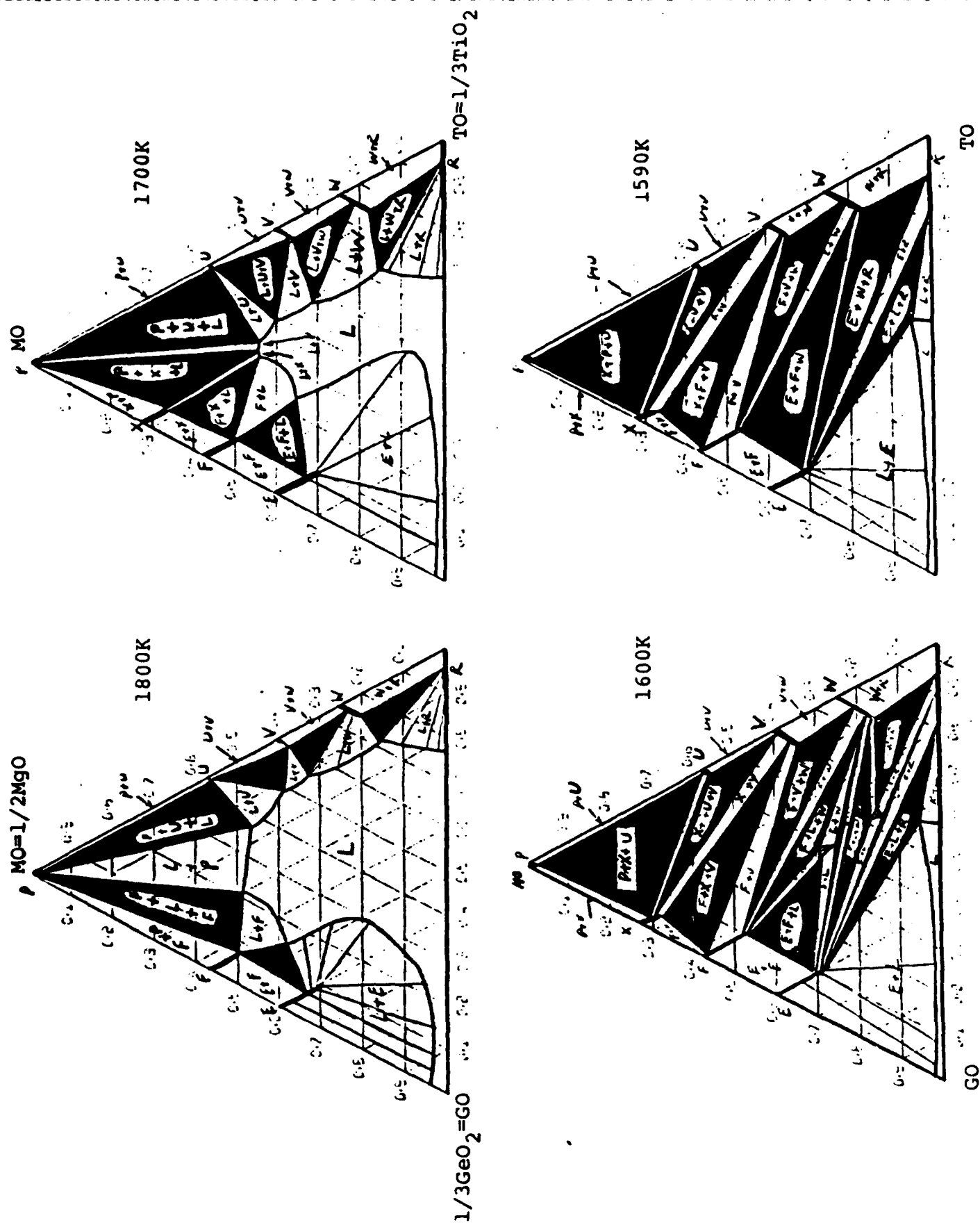


Figure 22. Calculated Isothermal Sections in MO-TO-GO.

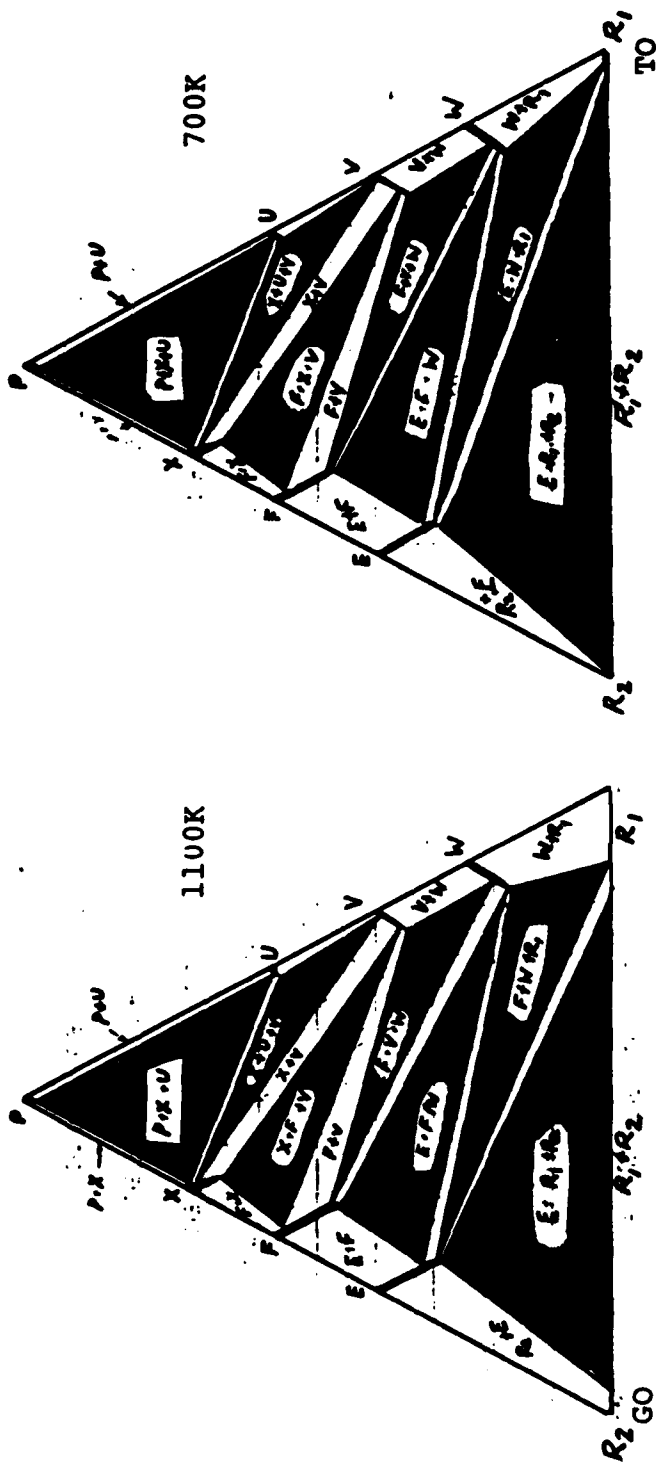
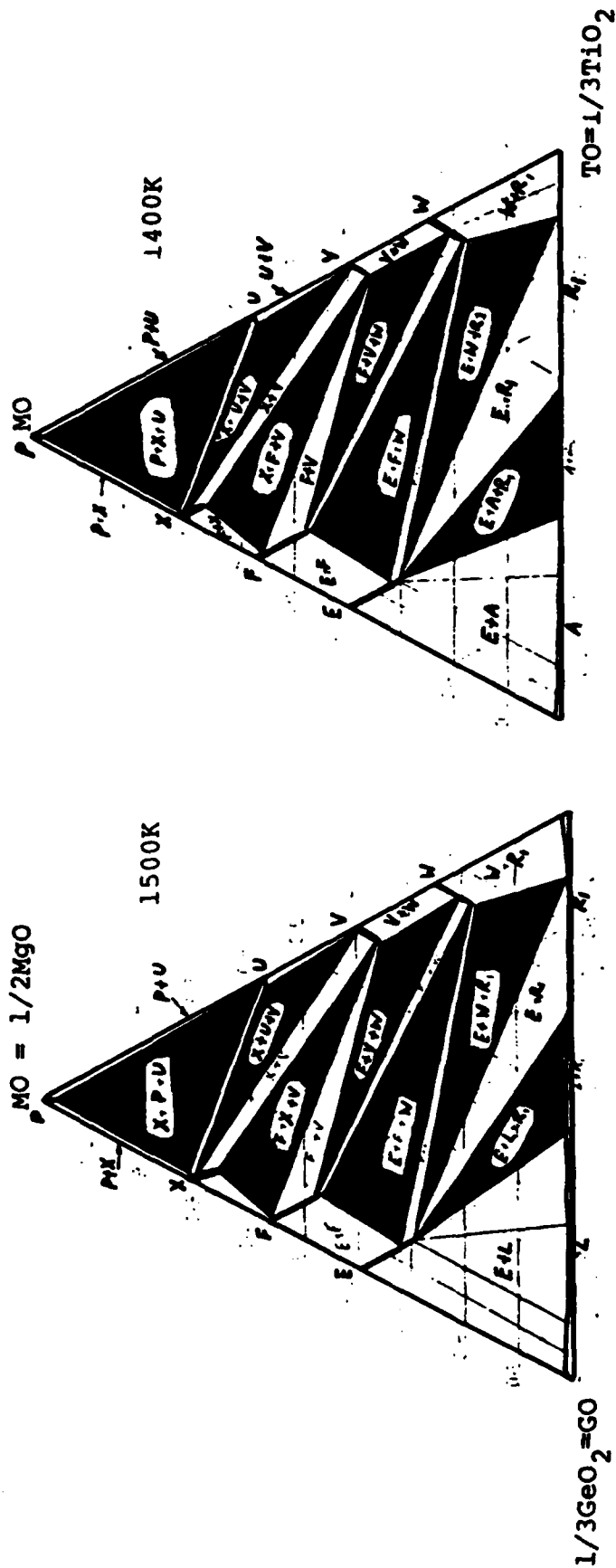


Figure 23. Calculated Isothermal Sections in MO-TO-GeO₂.

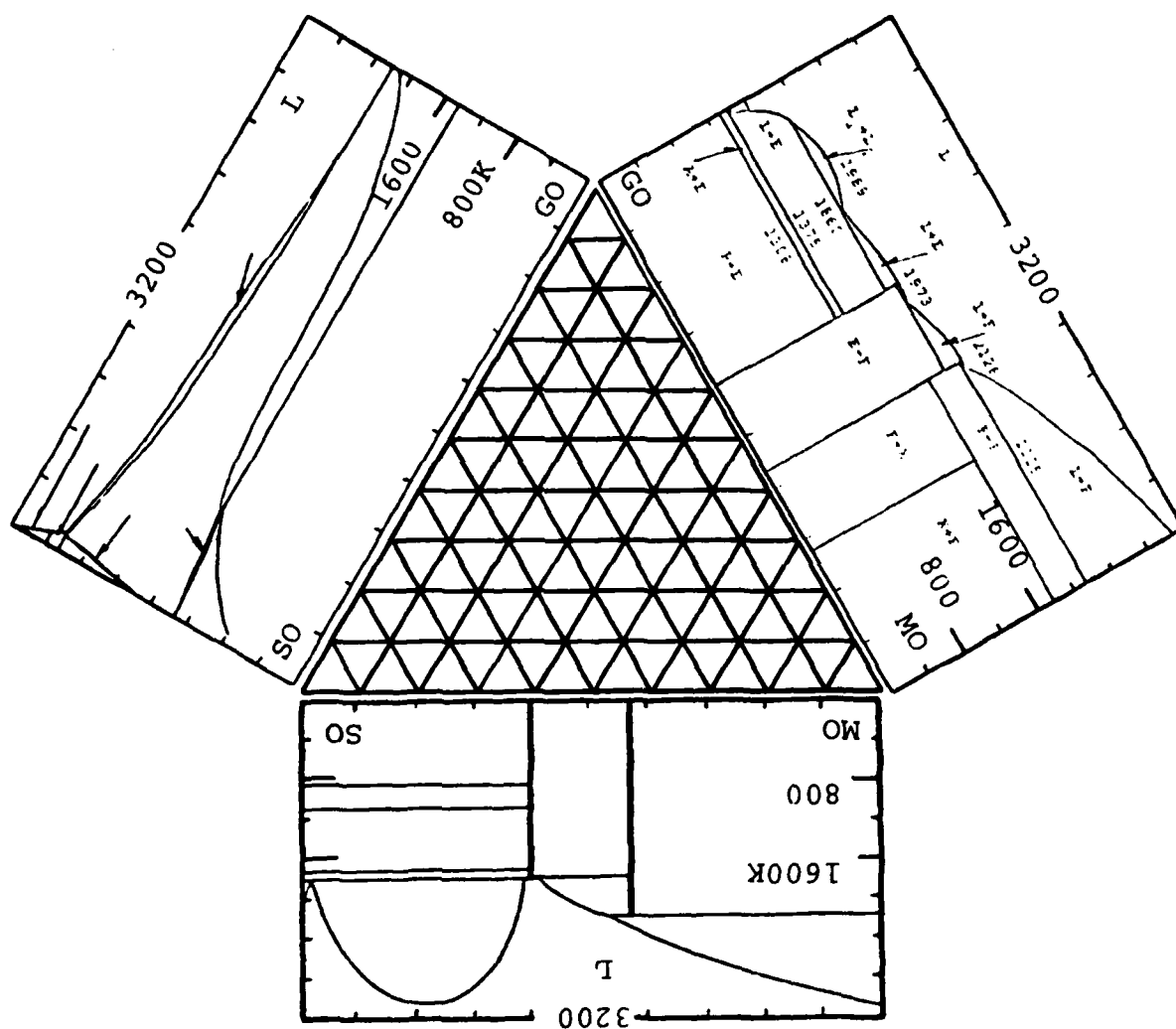


Figure 24. Calculated Isothermal Sections in the $\text{GO}(\frac{1}{3}\text{GeO}_2)$ - $\text{MO}(\frac{1}{2}\text{MgO})$ - $\text{SO}(\frac{1}{3}\text{SiO}_2)$ system.

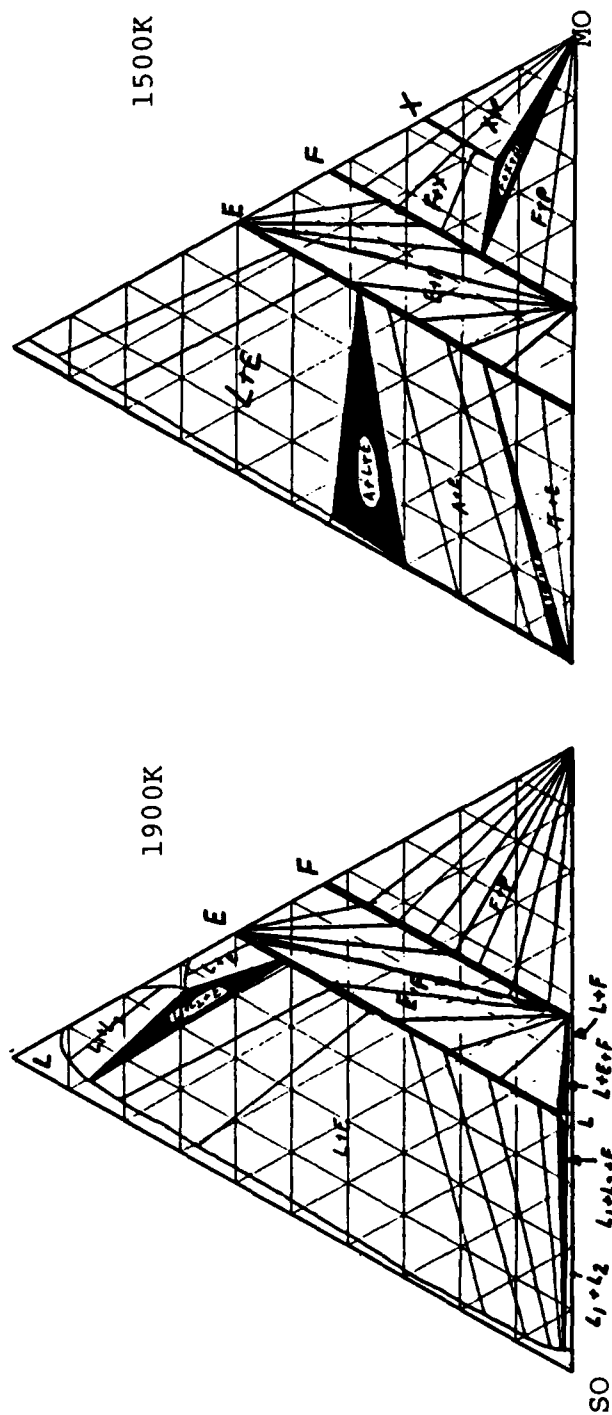
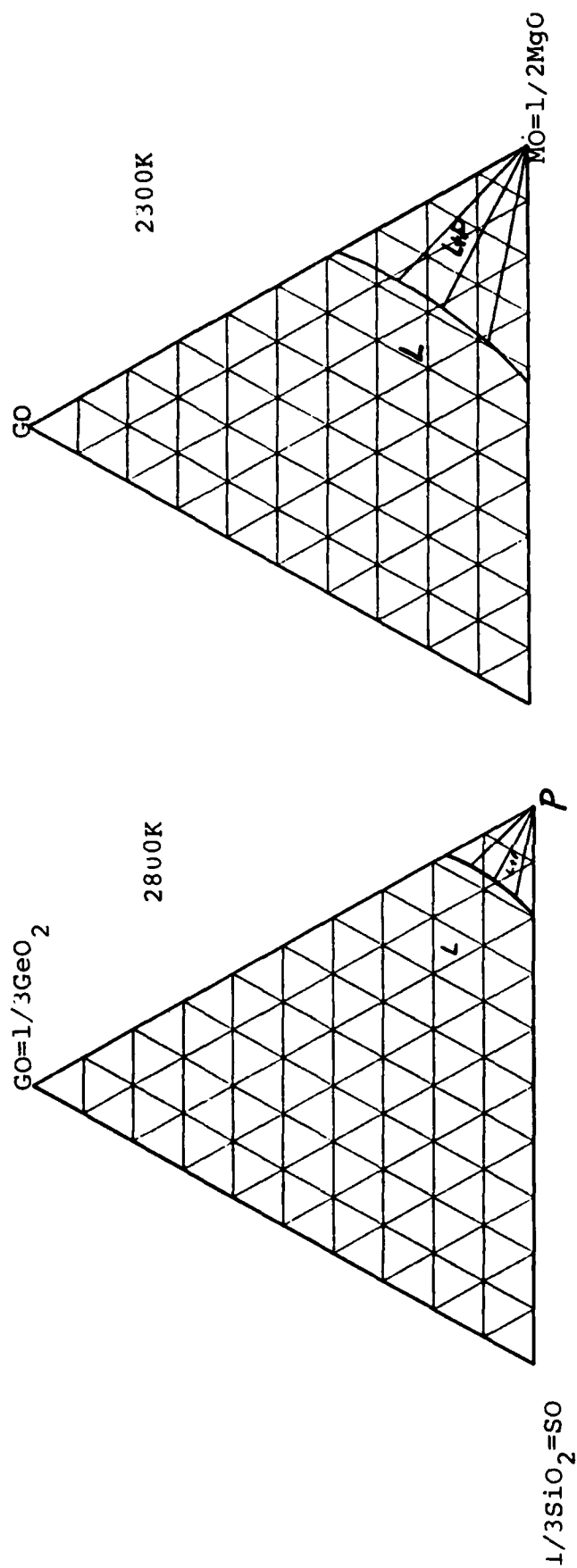


Figure 25. Calculated Isothermal Sections in GO-MO-SO.

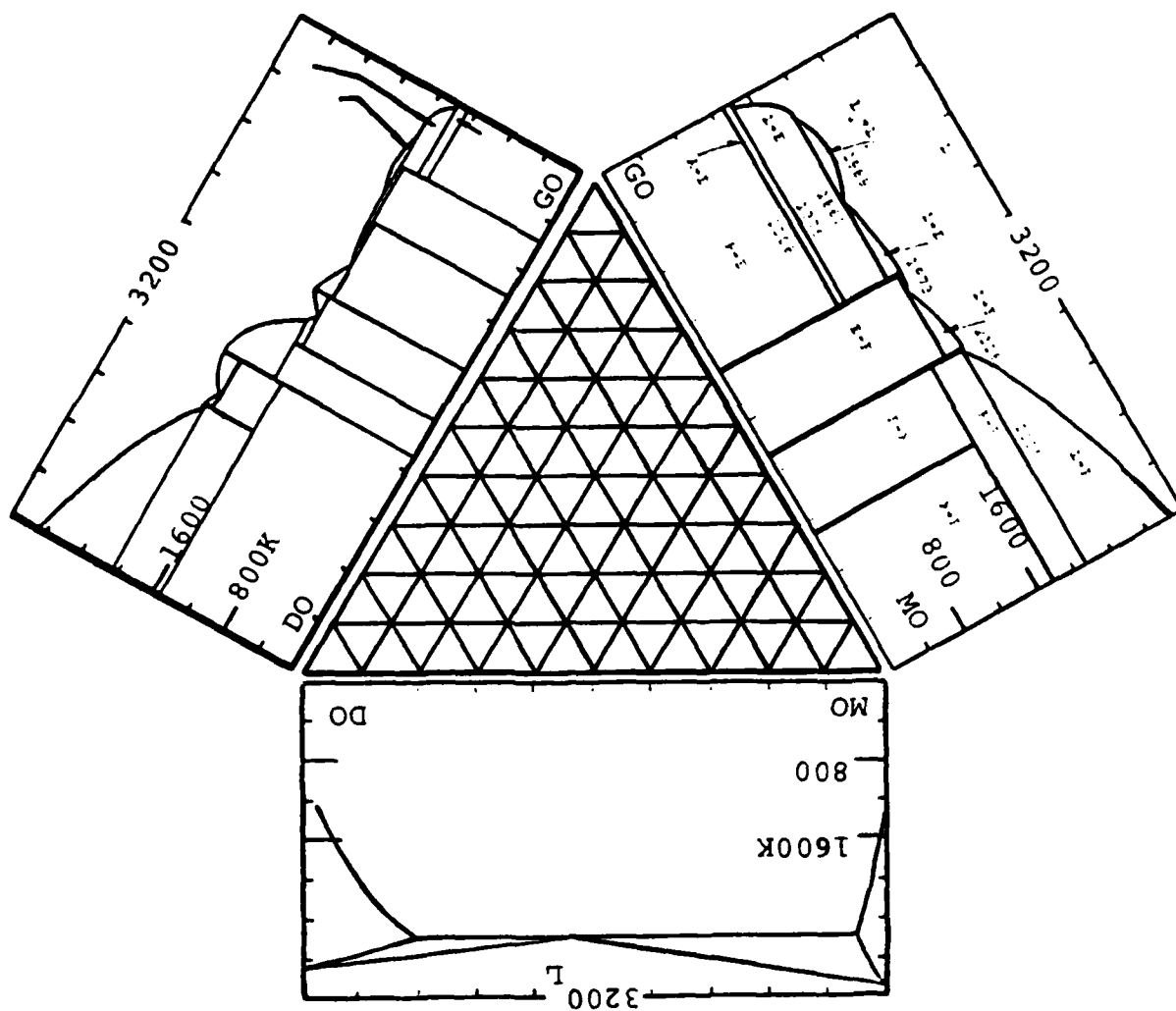


Figure 27 Calculated Isothermal Sections in the
GO ($1/3 \text{ GeO}_2$) - MO ($1/2 \text{ MgO}$) - DO ($1/2 \text{ CaO}$) System.

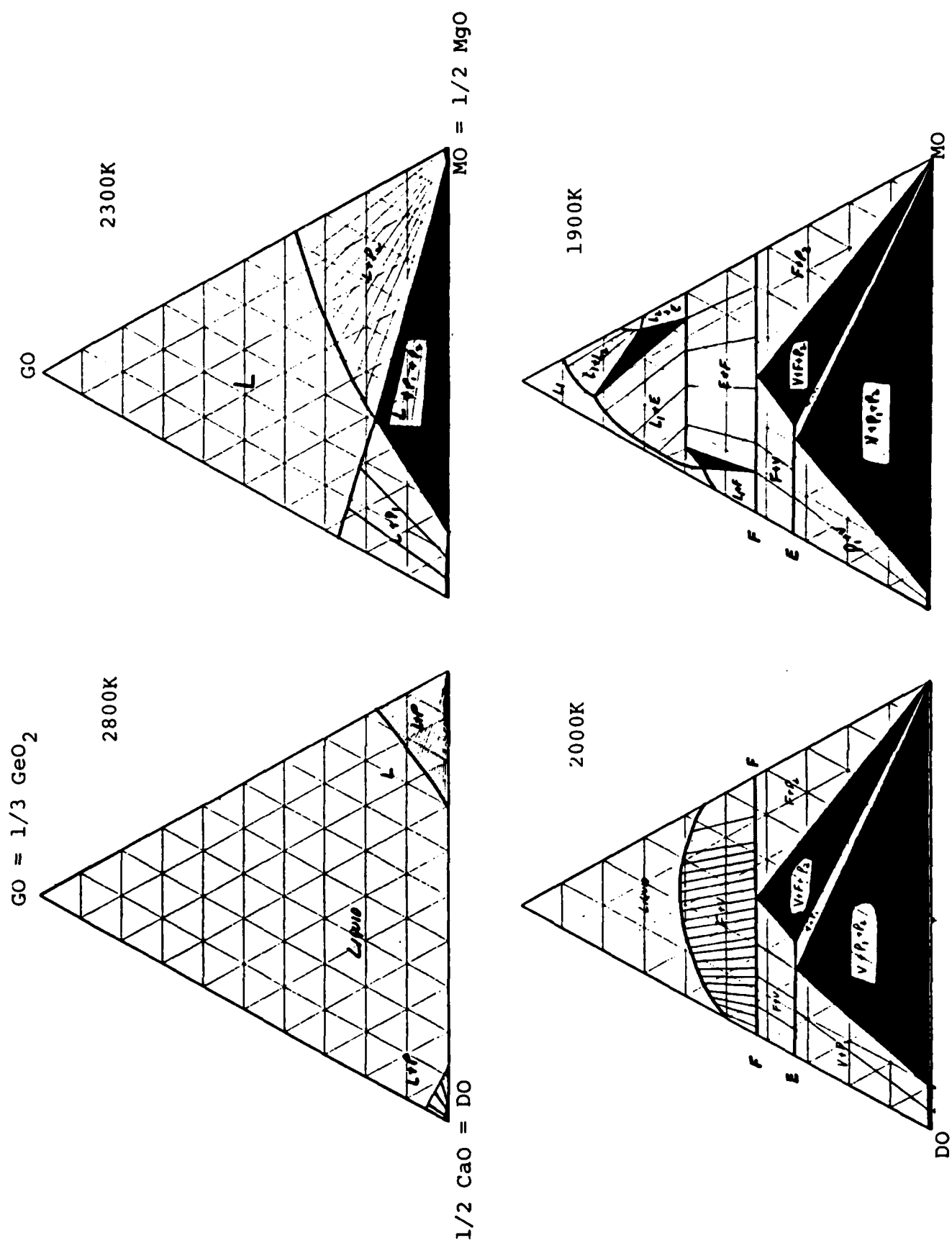
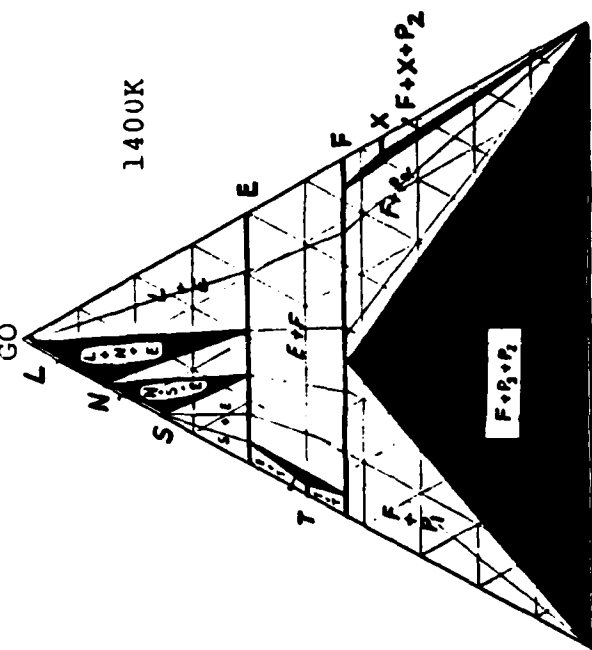
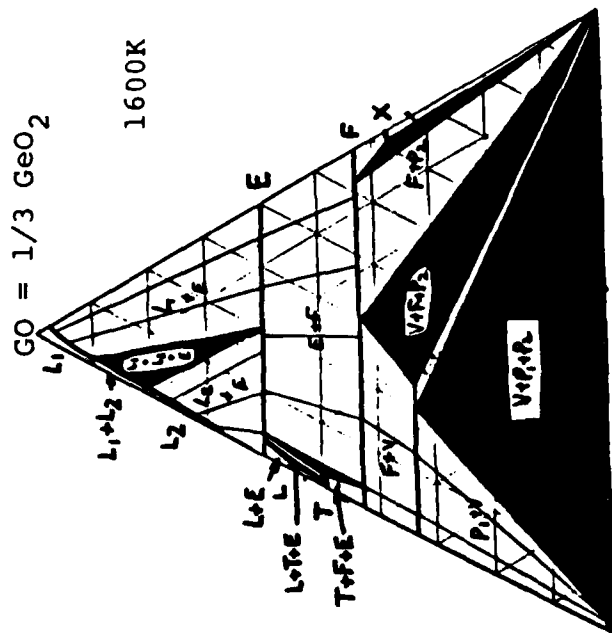
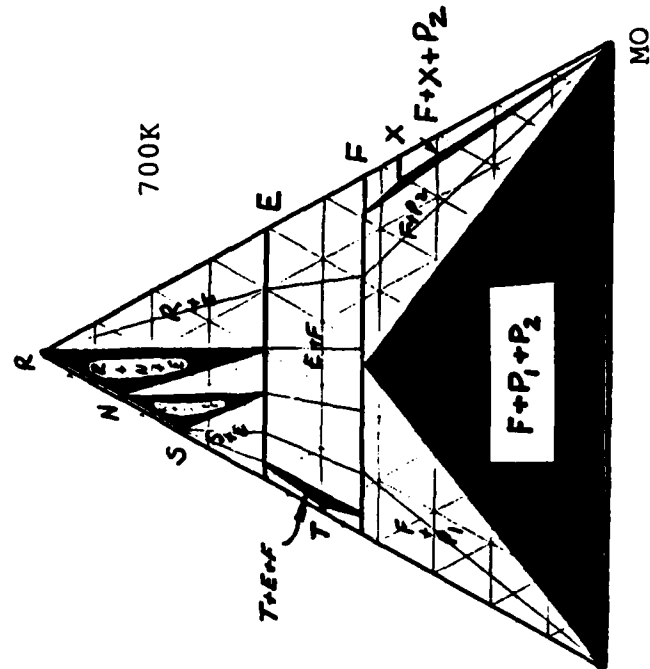


Figure 28. Calculated Isothermal Sections in GO-MO-DO



MO = 1/2 MgO



1/2 CaO = DO

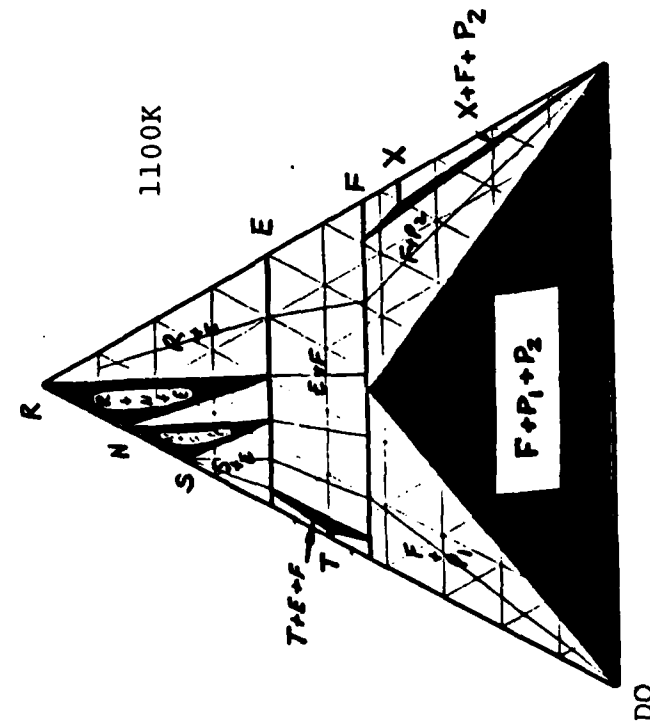


Figure 29. Calculated Isothermal Sections in GO-MO-DO

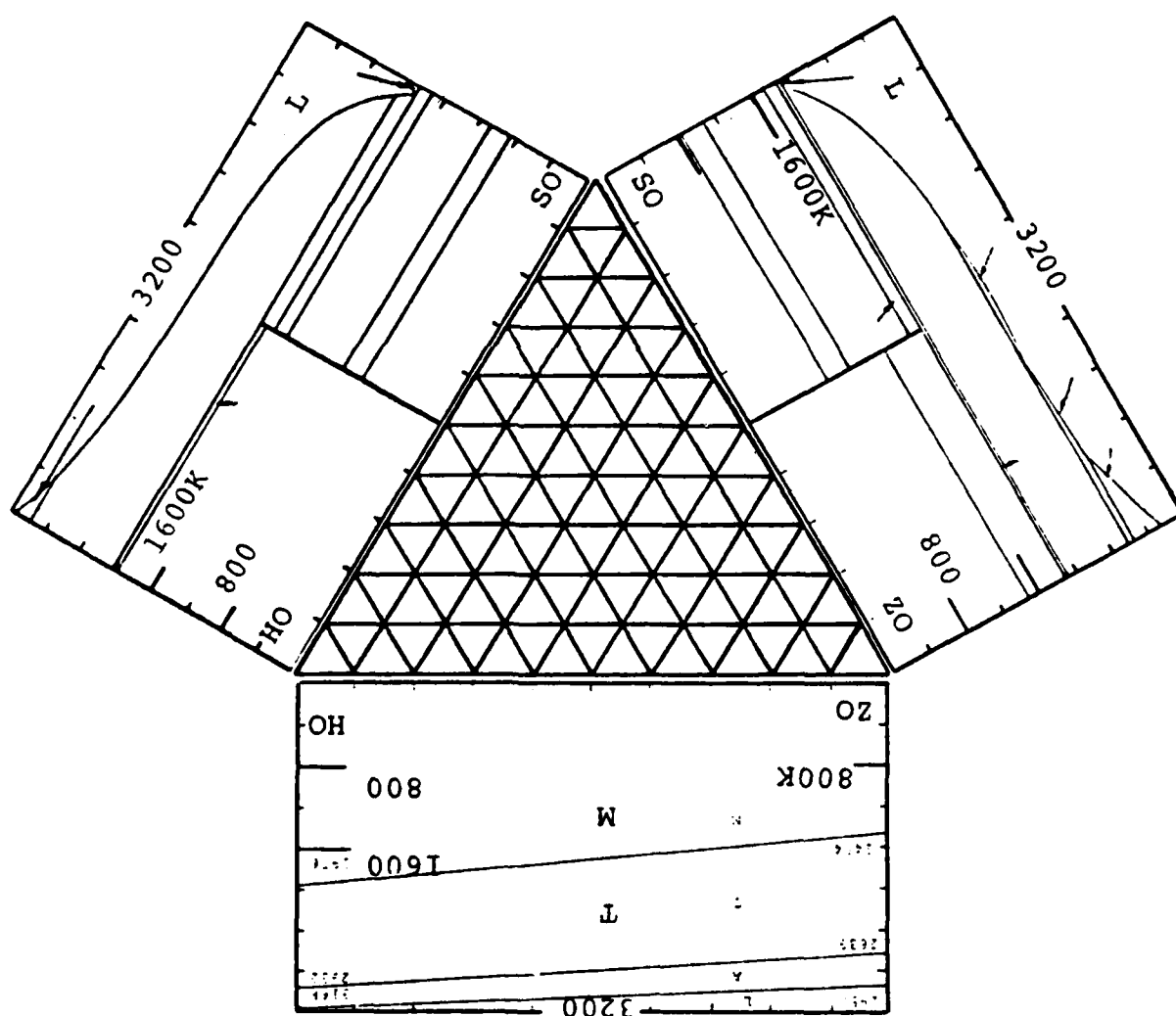


Figure 30 Calculated Isothermal Sections in the $\text{SO}(\frac{1}{3}\text{SiO}_2)$ - $\text{ZO}(\frac{1}{3}\text{ZrO}_2)$ - $\text{HO}(\frac{1}{3}\text{HfO}_2)$ System.

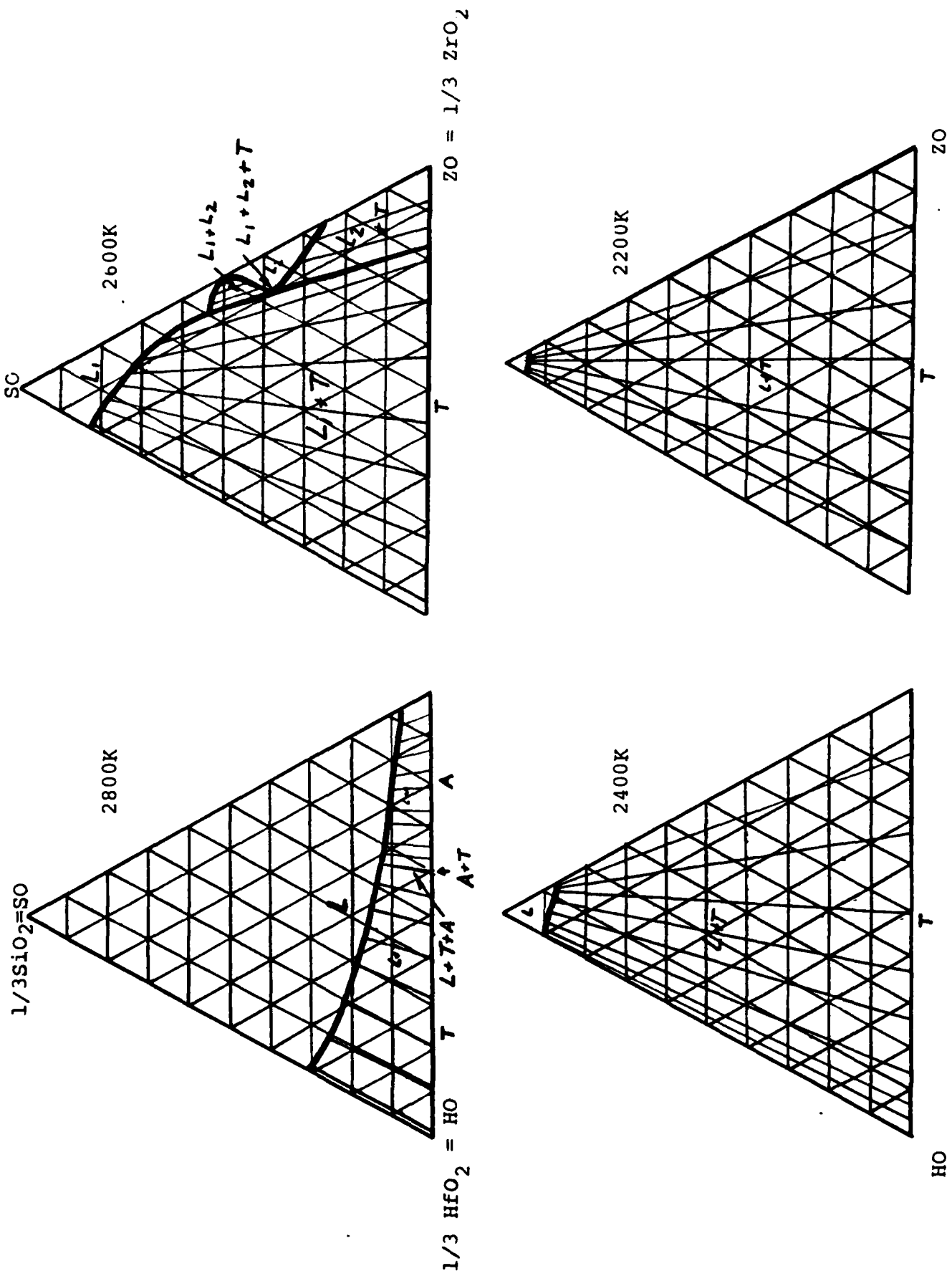


Figure 31. Calculated Isothermal Sections in SO-ZO-HO

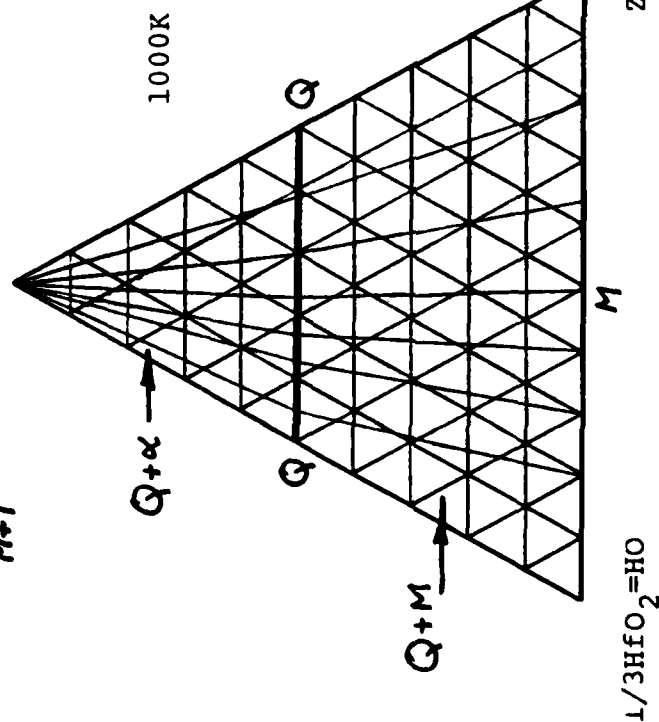
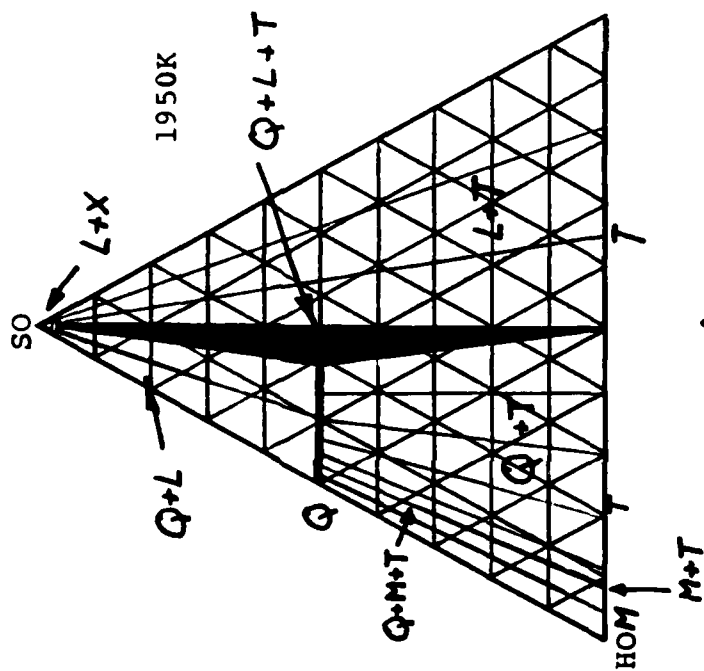
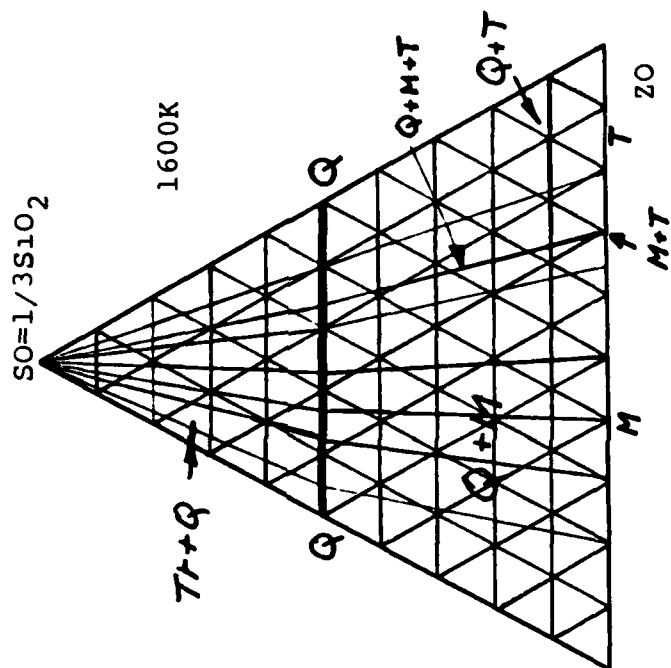


Figure 32 Calculated Isothermal Sections in SO-ZO-HO

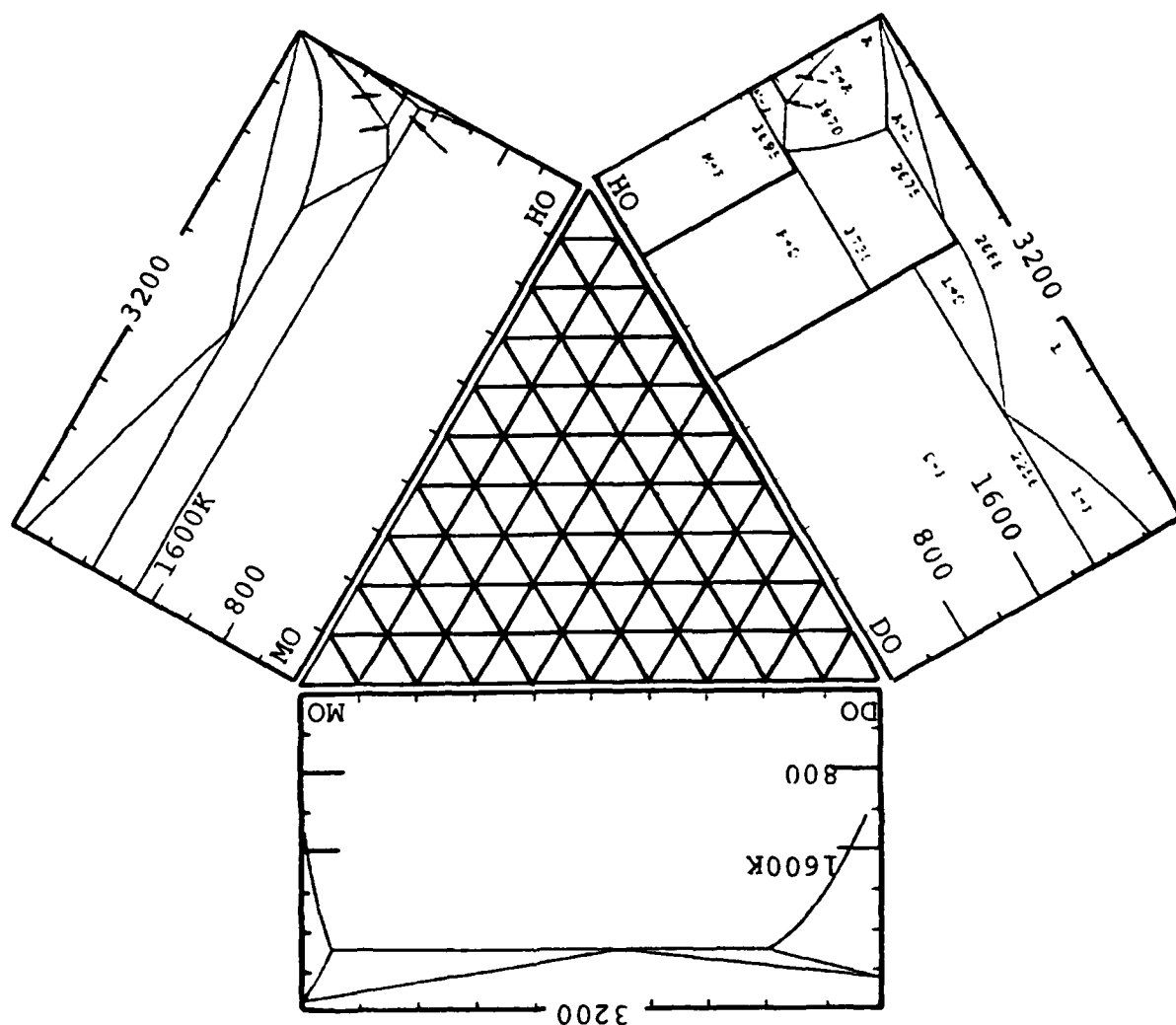


Figure 33. Calculated Isothermal Sections in the
 $\text{HO}(\frac{1}{3} \text{HfO}_2) - \text{DO}(\frac{1}{2} \text{CaO}) - \text{MO}(\frac{1}{2} \text{MgO})$

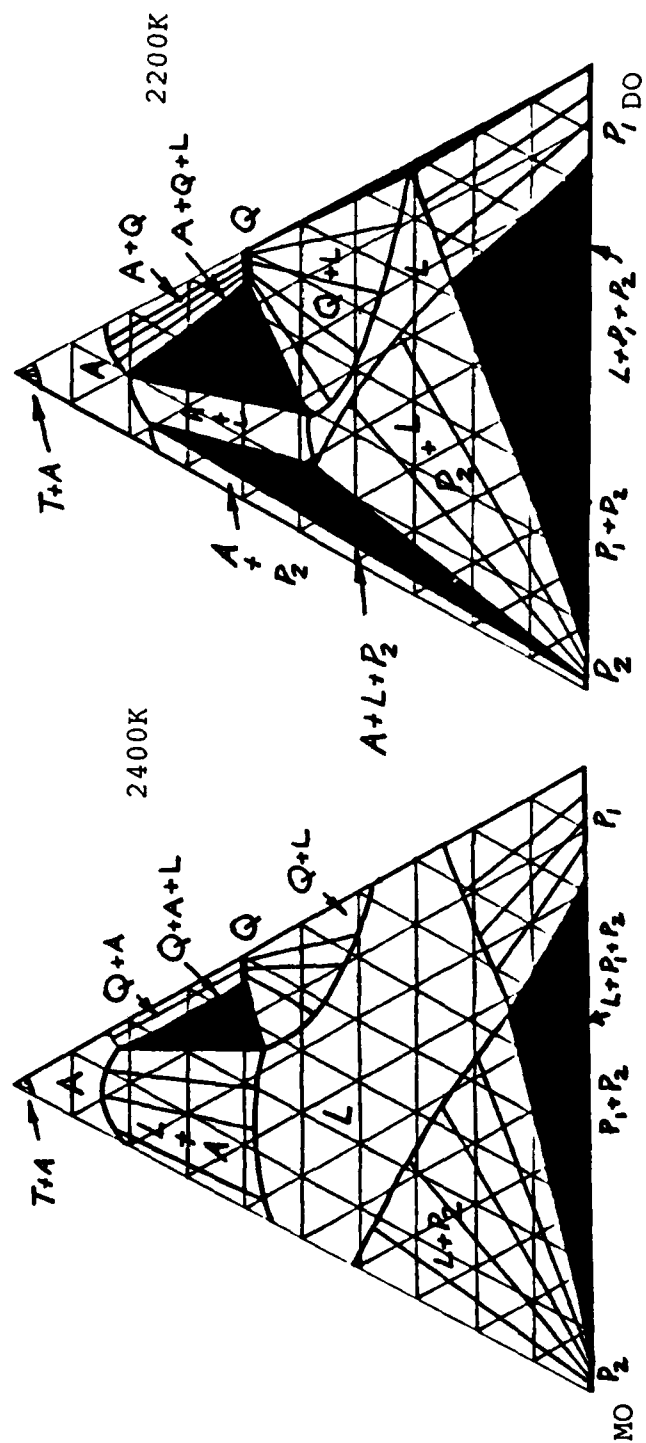
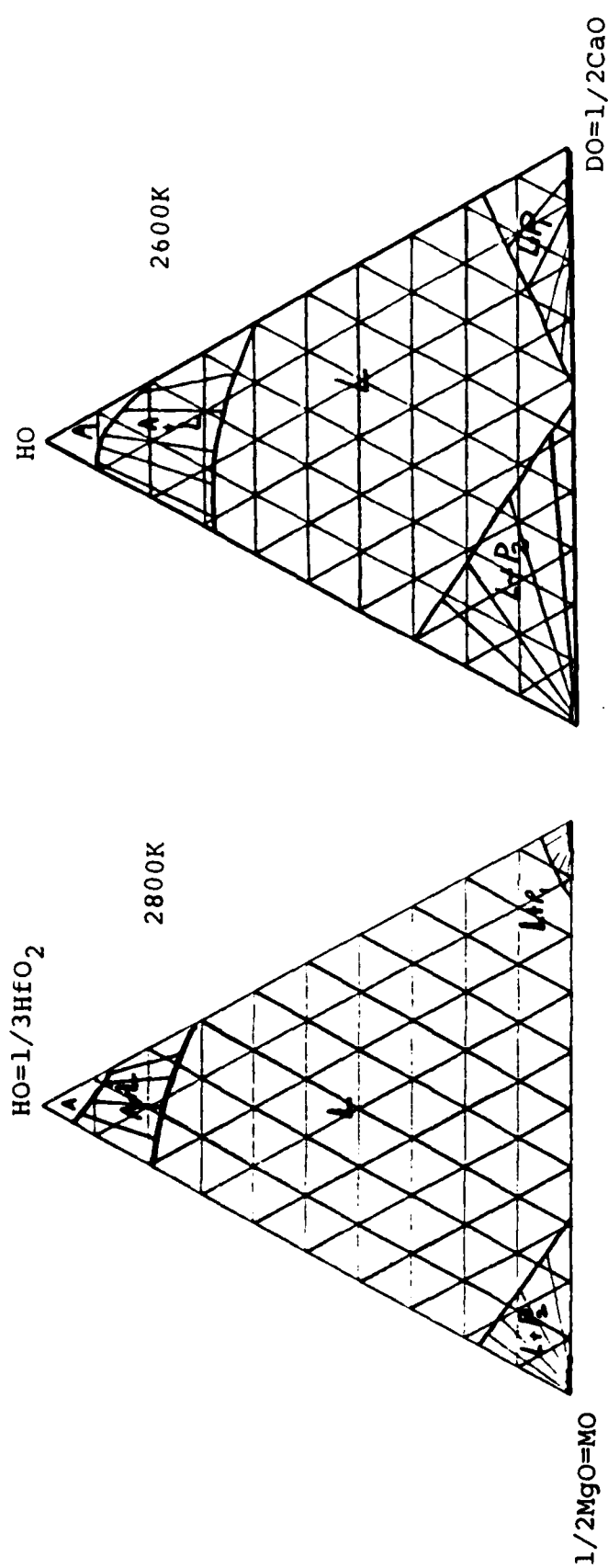


Figure 34. Calculated Isothermal Sections in HO-DO-MO.

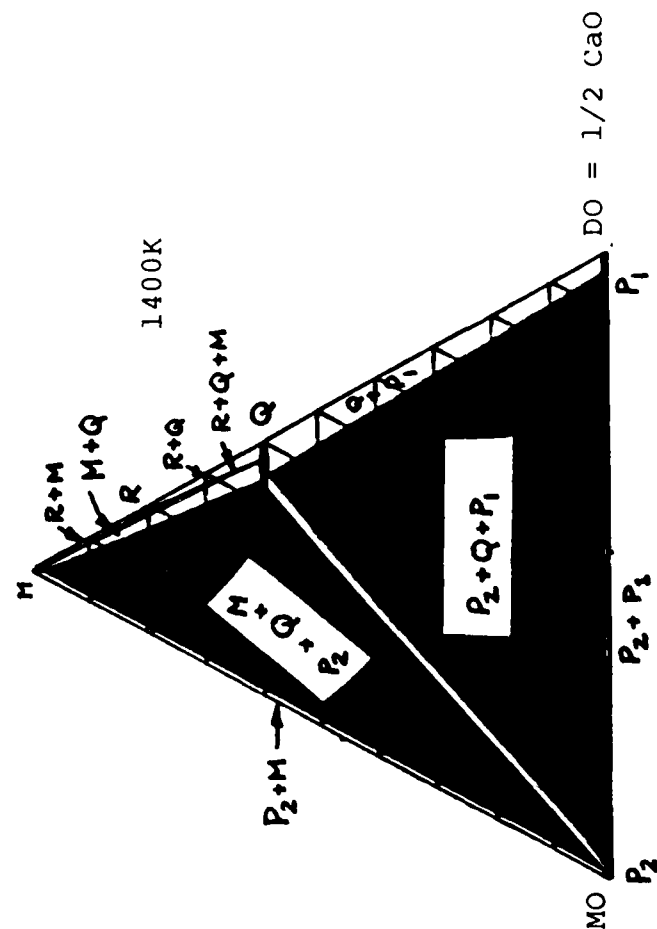
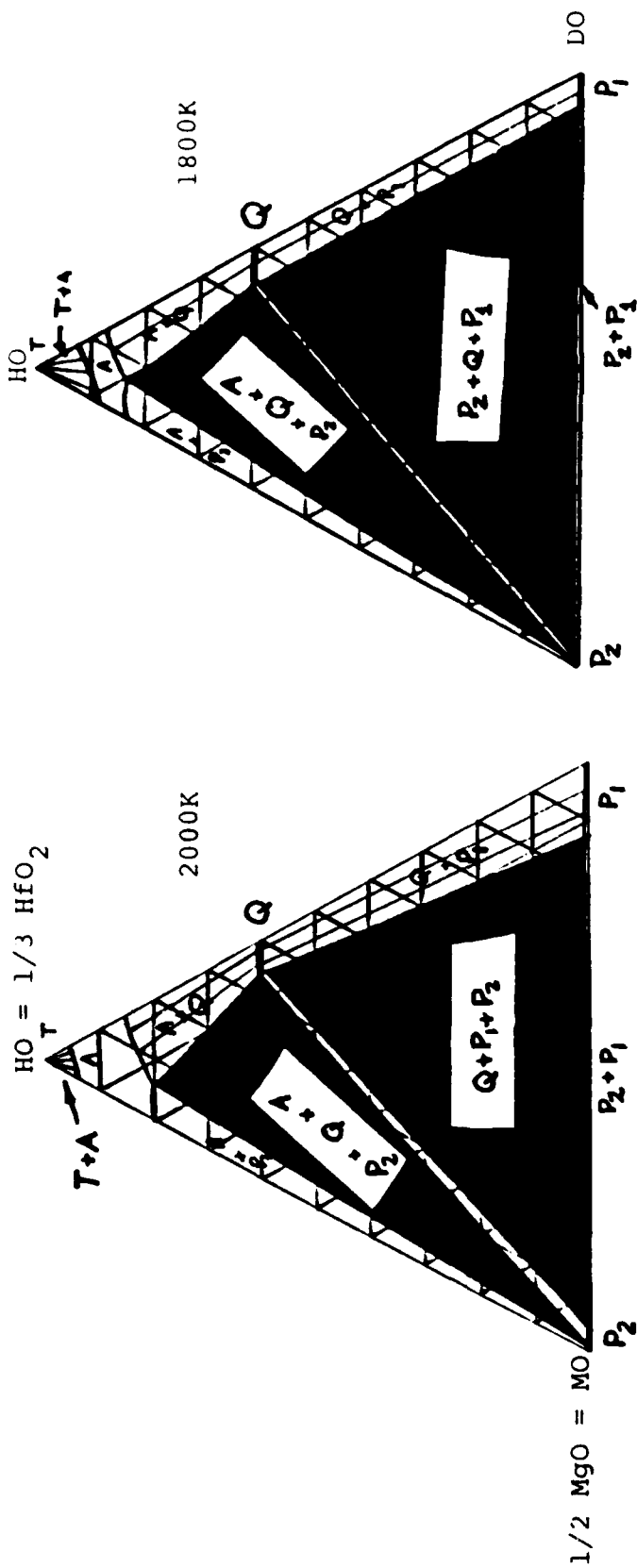


Figure 35. Calculated Isothermal Sections in HO-DO-MO.

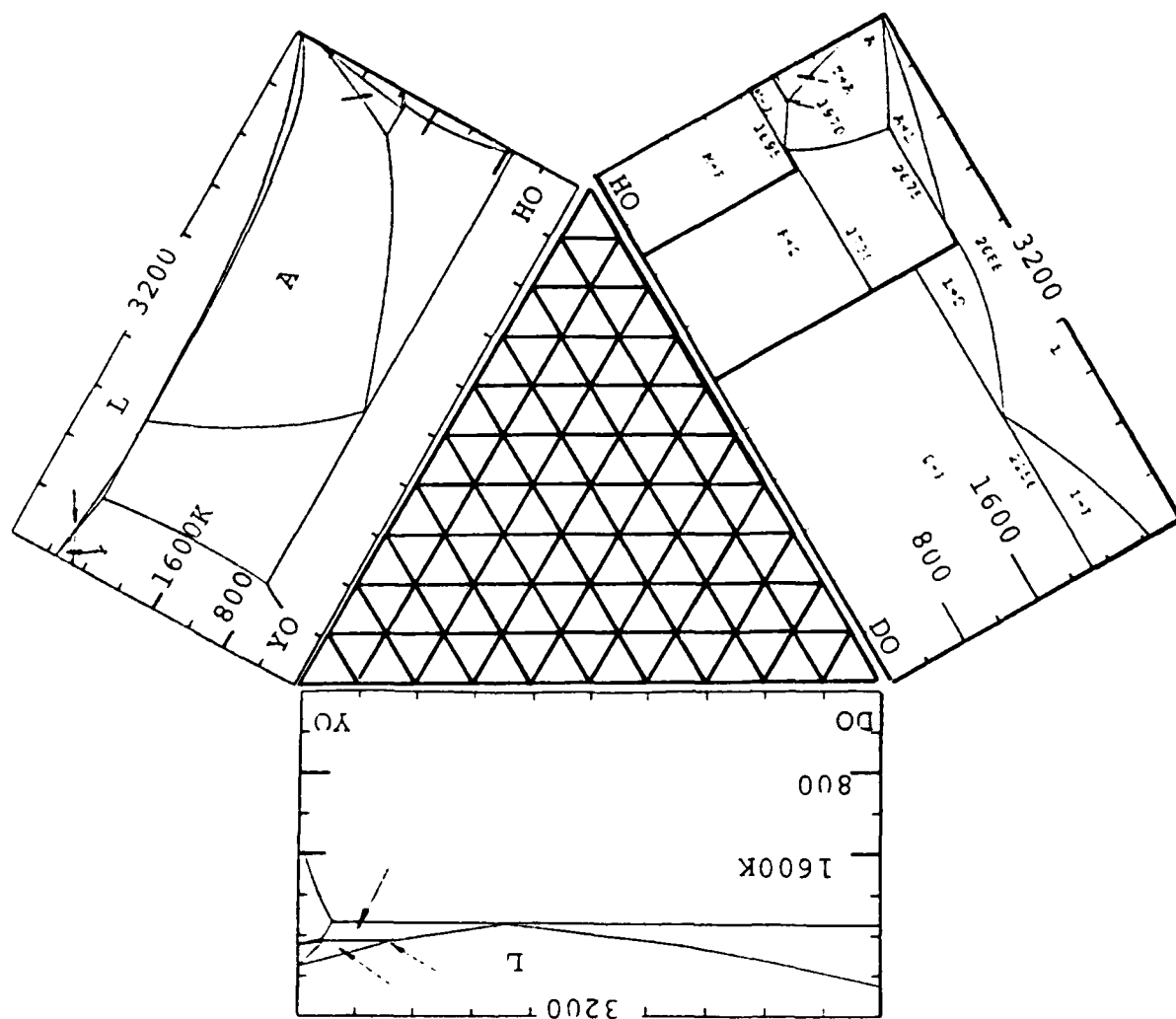


Figure 36. Calculated Isothermal Sections in the $\text{HO}(\frac{1}{3}\text{HfO}_2)\text{-DO}(\frac{1}{2}\text{CaO})\text{-YO}(\frac{1}{5}\text{Y}_2\text{O}_3)$ System.

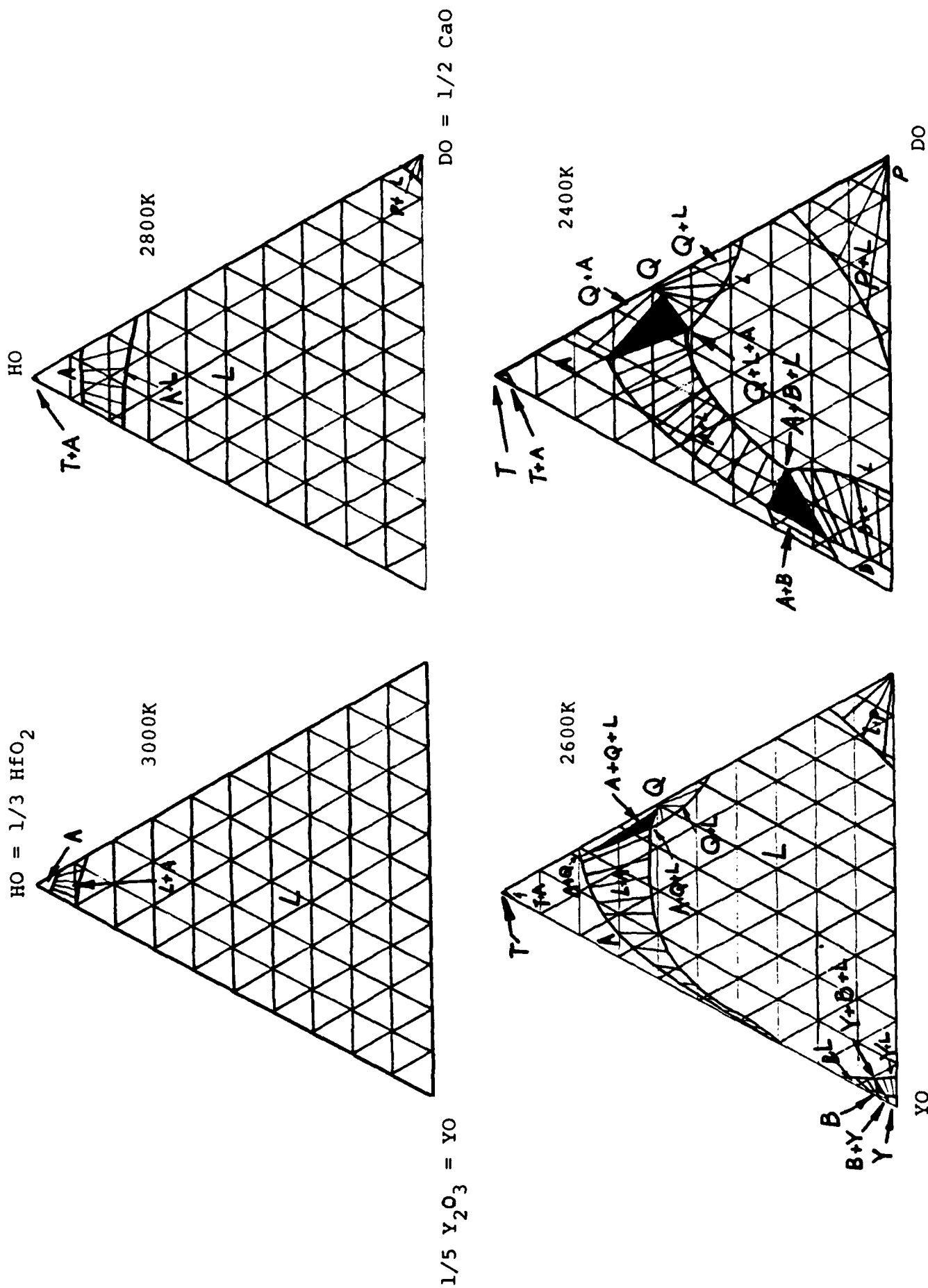


Figure 37. Calculated Isothermal Sections in HO-DO-YO.

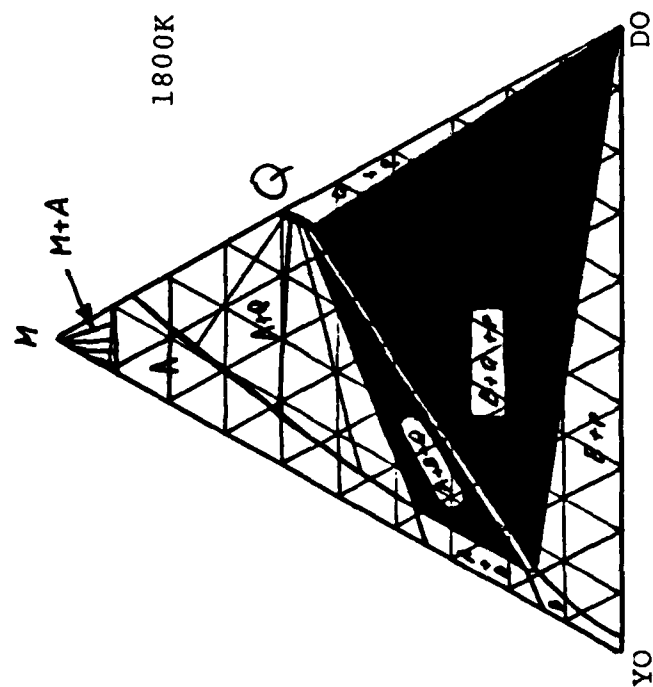
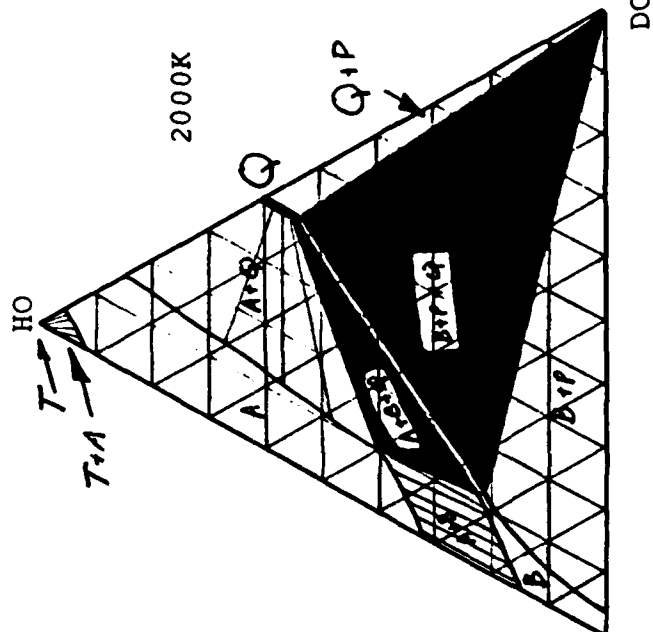
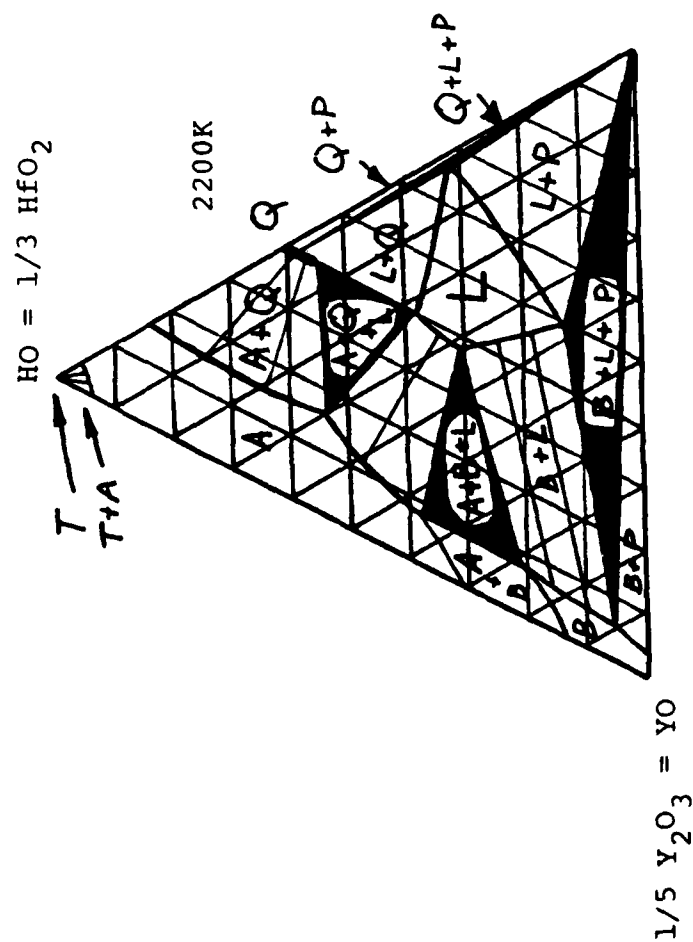


Figure 38. Calculated Isothermal Sections in HO-DO-YO.

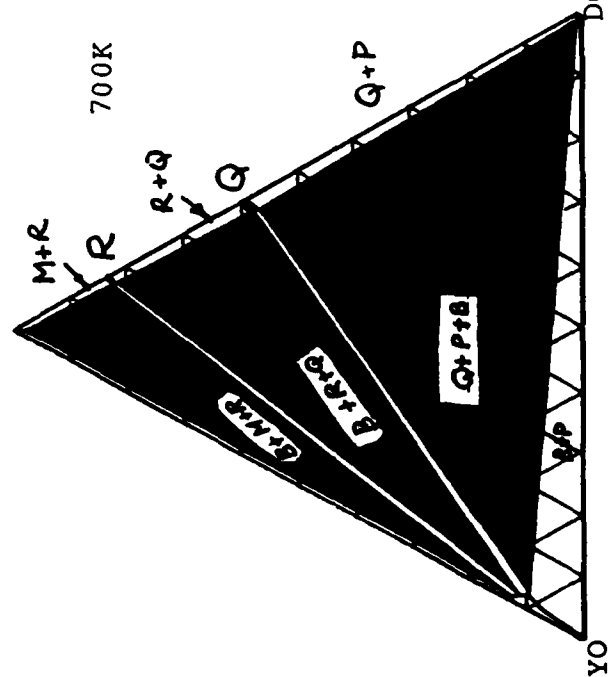
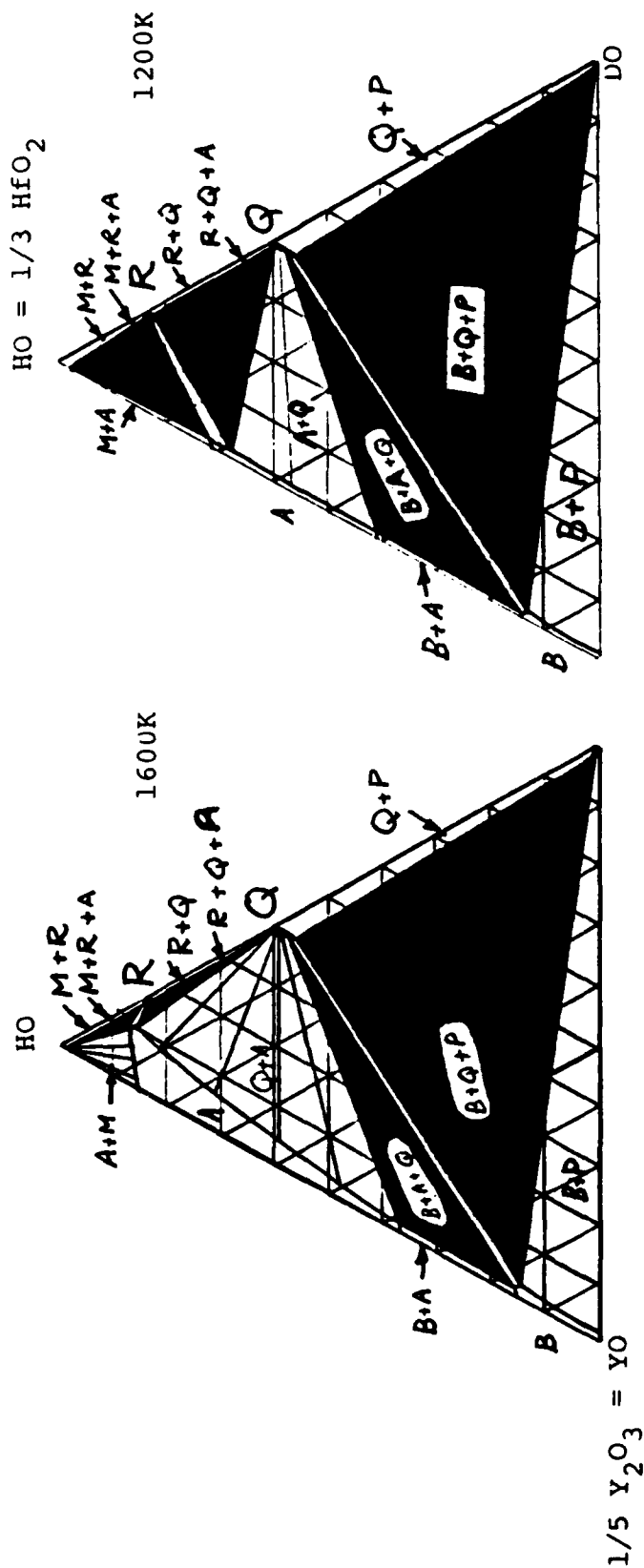


Figure 39. Calculated Isothermal Sections in HO-DO-YO.

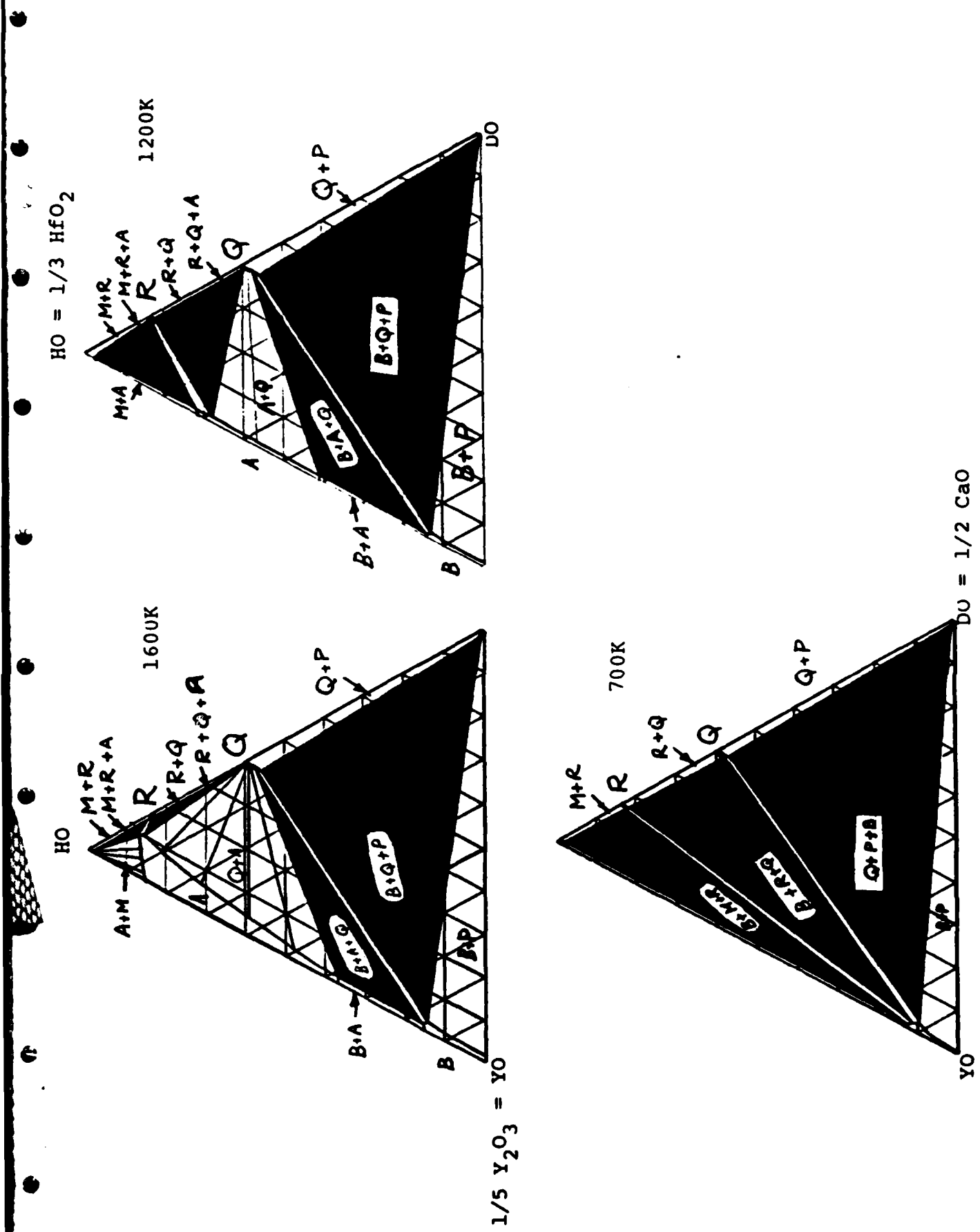


Figure 39. Calculated Isothermal Sections in HO-DO-YO .

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