AD-A179 167 APPLICATION OF COMPUTER METHODS FOR CALCULATION OF 1/1
MULTICOMPONENT PHASE D.. (U) MANLABS INC CAMBRIDGE MASS
L KAUFMAN 27 FEB 87 AFOSR-TR-87-0328 F49620-84-C-0070

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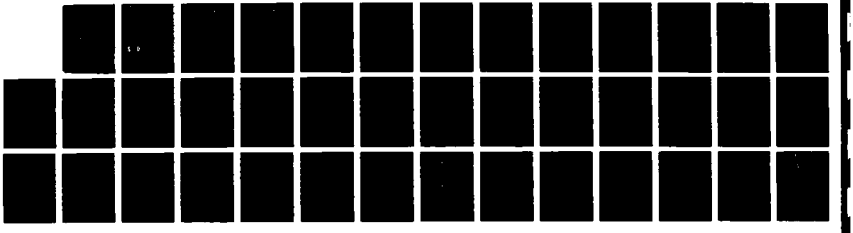

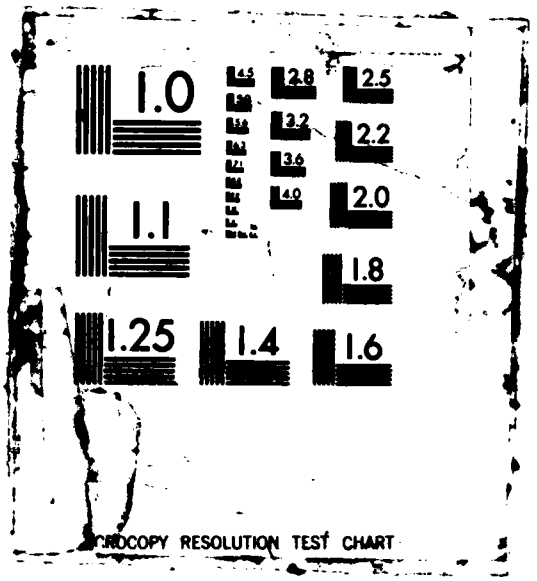
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AFOSR-TR- 87-0328

Annual Report

on

CONTRACT F49620-84-C0078

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

1 March 1986 to 27 February 1987

Air Force Scientific Research (AFSC)
Bolling Air Force Base, D.C. 20332

27 February 1987

by

Larry Kaufman
ManLabs, Inc.
21 Erie Street
Cambridge, Massachusetts 02139

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Quasi ternary Sytems
Titanium dioxide-Aluminum oxide, Silicon dioxide, Calcium oxide, Yttrium oxide, Hafnium oxide-Magnesium oxide, Zirconium oxide

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Computer Coupled Phase Diagrams and Thermochemical Data have been used to calculate the TiO_2-Al_2O_3, TiO_2-SiO_2, TiO_2-CaO, TiO_2-Y_2O_3 quasi binary systems as well as ternary sections over a wide range of temperature for the following systems, HfO_2-MgO-Y_2O_3, HfO_2-CaO-ZrO_2, SiO_2-HfO_2-Y_2O_3, MgO-SiO_2-HfO_2, TiO_2-Al_2O_3-MgO, Al_2O_3-TiO_2-SiO_2, TiO_2-Al_2O_3-HfO_2 and MgO-SiO_2-TiO_2

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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 were employed to carry out the following tasks during the past year of the current program (1)*.

1. A combined thermochemical and phase diagram analysis was performed to calculate isothermal sections in the HfO_2-MgO-Y_2O_3 and the HfO_2-CaO-ZrO_2 system based on the binary systems described earlier (1 - 8). The results are shown in Figures 40 - 45. The sequence of figure numbers is continued from the previous annual report (3) for convenience. The data provided in Figures 1 to 39 (3) and 40 - 45 will be published as reference (9).

2. A combined thermochemical and phase diagram analysis was performed to describe the TiO_2-Al_2O_3, TiO_2-SiO_2, TiO_2-CaO and TiO_2-Y_2O_3 quasi binary systems. The results are shown in Figures 46 - 49.

3. The results of item 2 above were combined with the earlier findings (1 - 9) to calculate isothermal sections in the following systems HfO_2-MgO-Y_2O_3, HfO_2-CaO-ZrO_2, SiO_2-HfO_2-Y_2O_3, MgO-SiO_2-HfO_2, TiO_2-Al_2O_3-MgO, Al_2O_3-TiO_2-SiO_2, TiO_2-Al_2O_3-HfO_2 and MgO-SiO_2-TiO_2 over a

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* Underscored numbers in parentheses denote references listed at the end of this report.

wide range of temperatures as shown in Figures 50 - 71. The material covered by items 2 and 3 will be presented and published in reference (10). Items 1 - 3 above as well as the results reported earlier (2, 3) complete the work described in the work statement year 1 and options I and II defined in April 1984. It should be noted that Figures 15 - 19 (3) represent analysis of five quasi binary systems which were not included in the original work statements (nor in options I and II) but were performed in order to complete the ternary calculations listed in options I and II.

4. Technical efforts toward installation of the KTH-Thermocalc Data Bank at NBS on a VAX Computer and demonstration of multicomponent metal-oxide and ceramic systems as outlined in 0001AB Option 1 dated April 1986 have been largely completed. The system is available at NBS and at MIT in Cambridge, Massachusetts. Modeling of the Fe-Ni-O, Fe-Cr-O, Ti-C-N, ZrO_2-Y_2O_3, ZrO_2-Al_2O_3, Y_2O_3-Al_2O_3 and ZrO_2-Y_2O_3-Al_2O_3 sytems on a gram atom and a mole of metal basis has been completed. The imput has been stored on standard 5 inch floppy disks which can be loaded via IBM P.C. on the VAX Linkage via telephone has been demonstrated in Cambridge and awaits trial at NBS when their communicaions network clears. Hard copy of the results will be included in the final report on the contract.

During the year the following personnel have been active in the program: L. Kaufman, E. P. Warekois, P. Neshe, J. Smith, D. Hay, V. Farber, W. S. Owen, M. Grujicic and J. Agren. The following technical lectures and discussions were presented in connection with work performed on this contract.

1. "Calculation of Multicomponent Oxide Phase Diagrams" CALPHAD XVI London, July 1986

2. "Calculation of Multicomponent Oxide Phase Diagrams" ASM Annual Meeting, Orlando, Florida, October 1986

3. Program Review with Major J. Hager - ManLabs, Inc. Cambridge, Massachusetts, December 1986

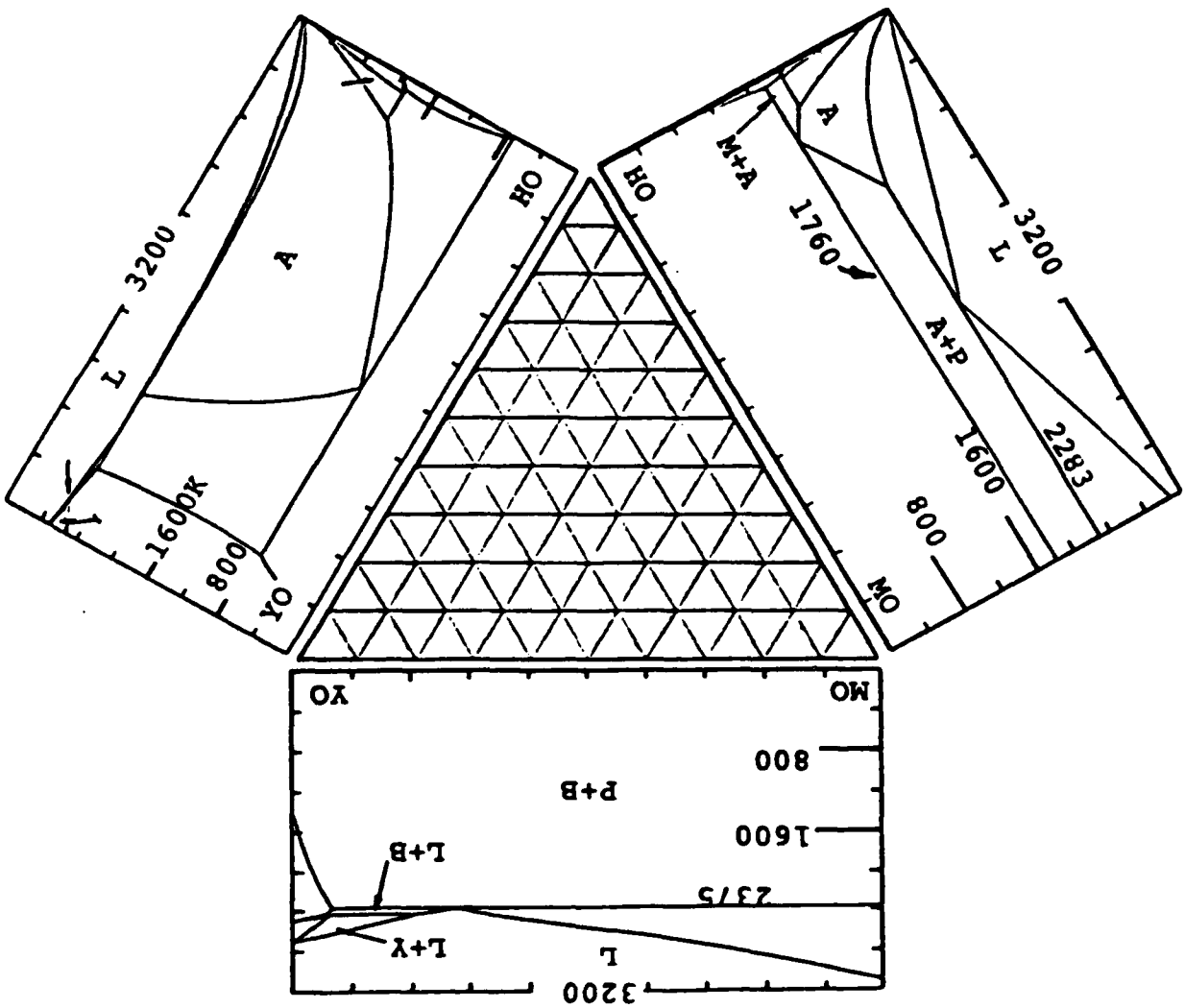


Figure 40. Calculated Isothermal Sections in the $HO(1/3HfO_2)$-$MO(1/2MgO)$-$YO(1/5Y_2O_3)$ system.

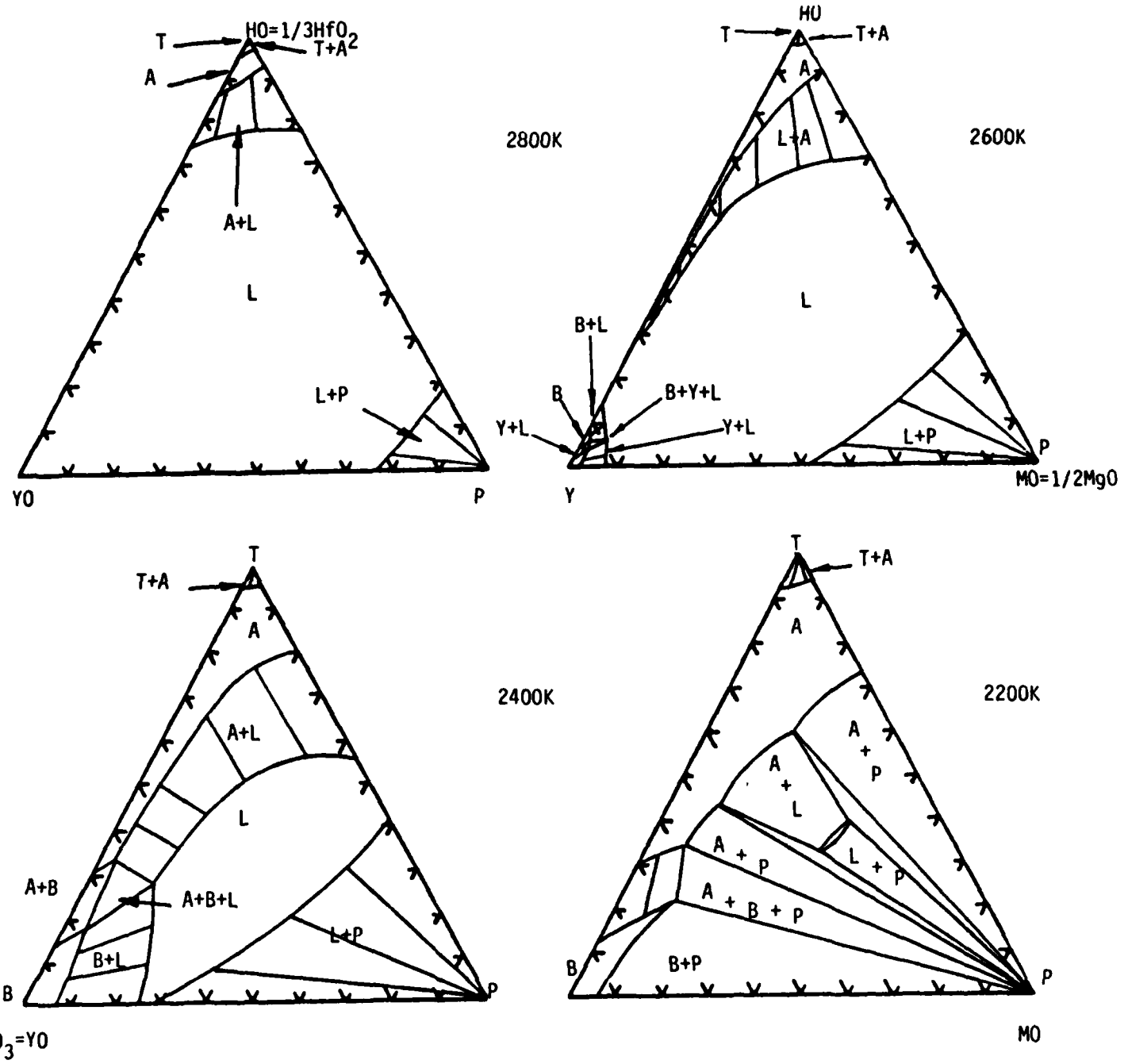


Figure 41. Calculated Isothermal Sections in HO-MO-YO

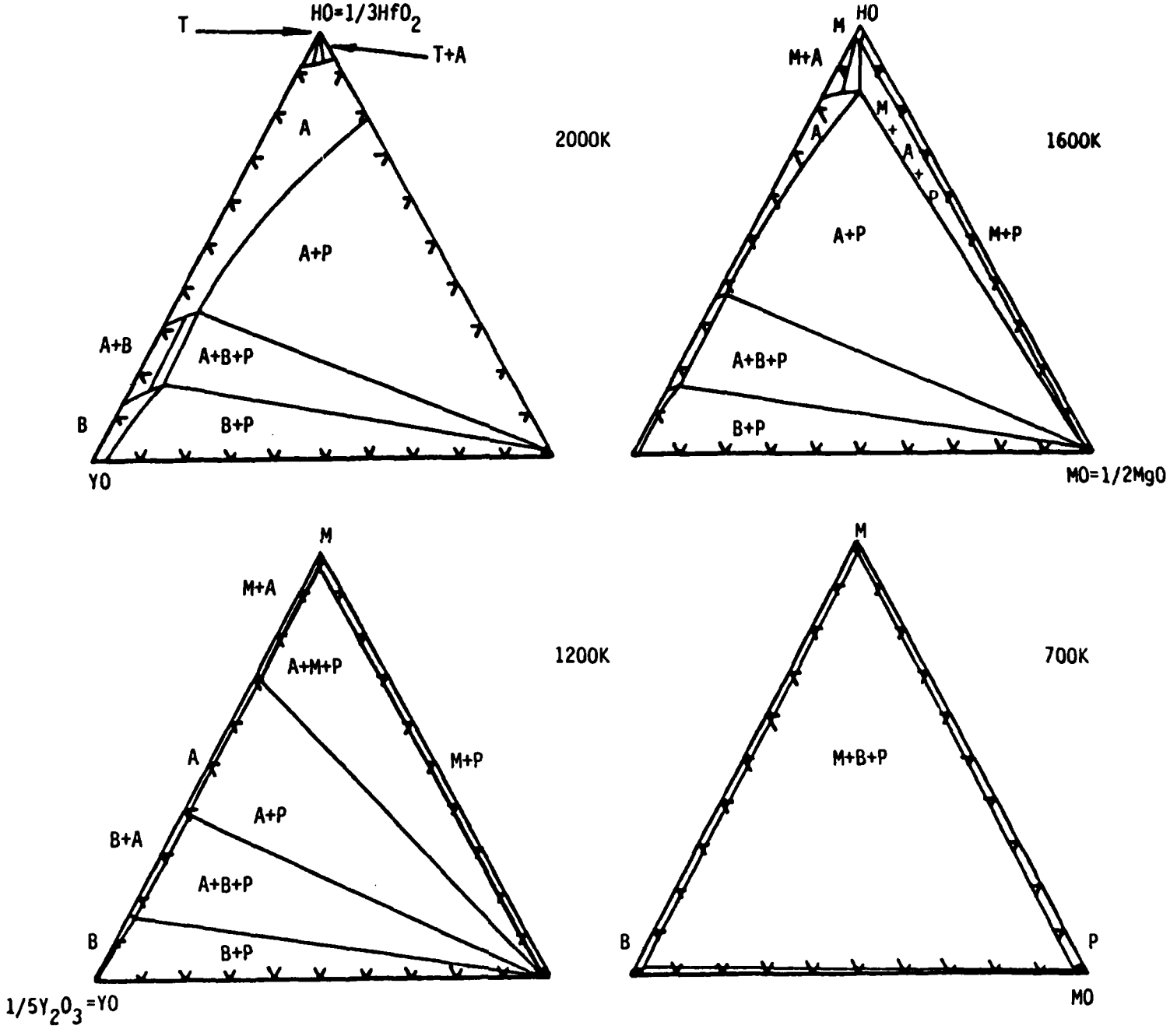


Figure 42. Calculated Isothermal Sections in HO-MO-YO

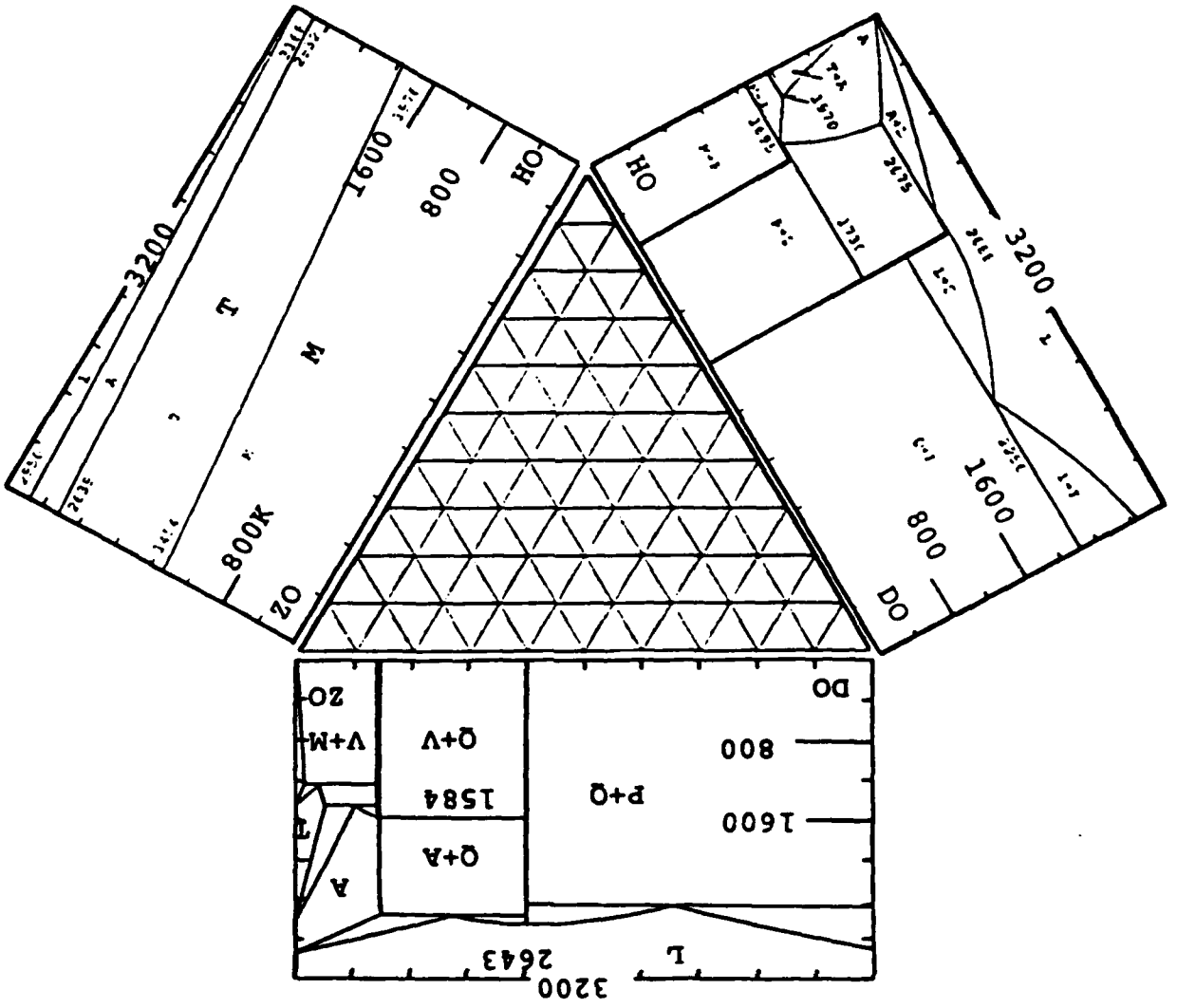


Figure 43. Calculated Isothermal Sections in the $HO(1/3HfO_2)$ - $DO(1/2CaO)$ - $ZO(1/3ZrO_2)$ System

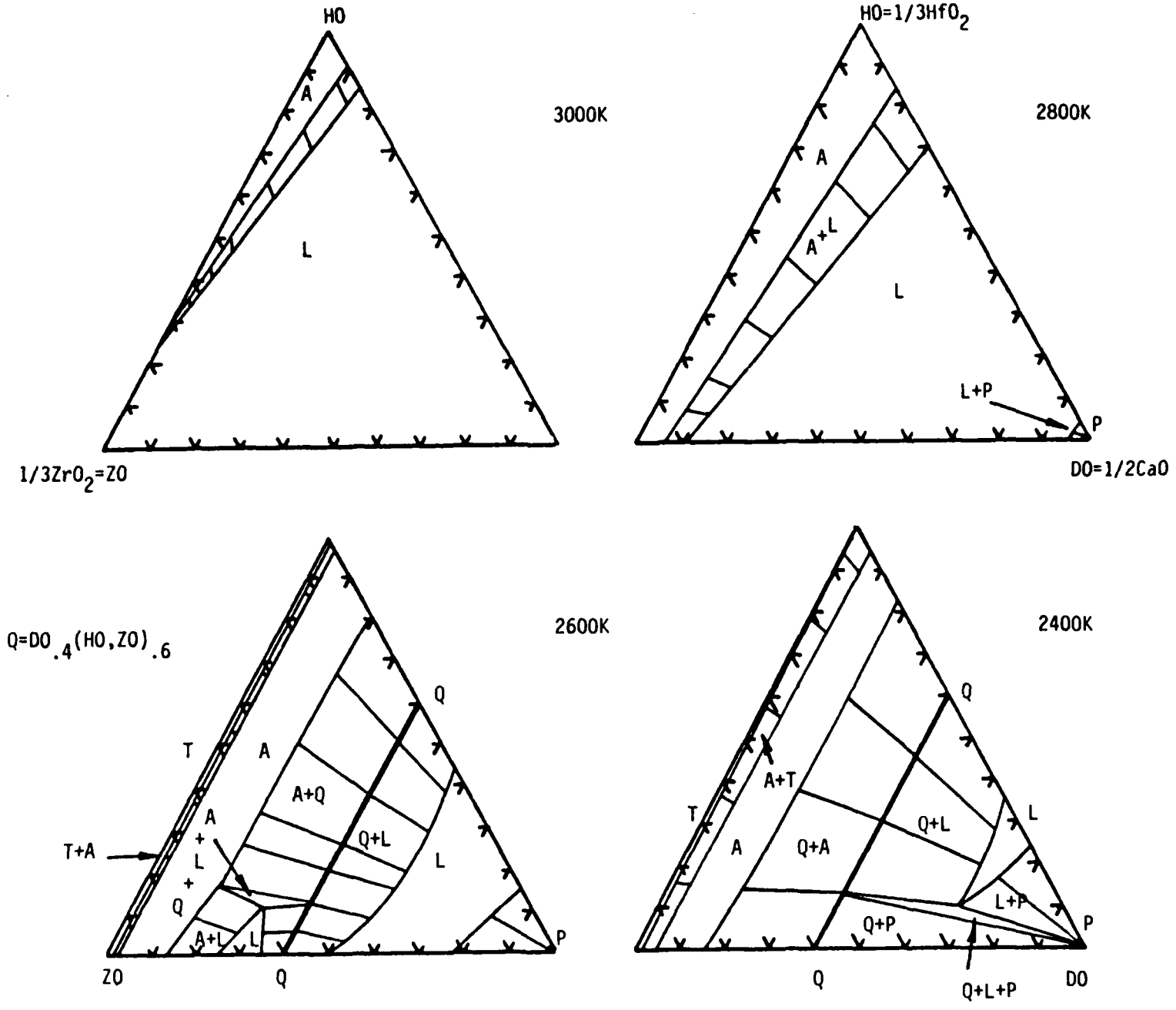


Figure 44. Calculated Isothermal Sections in HO-DO-ZO

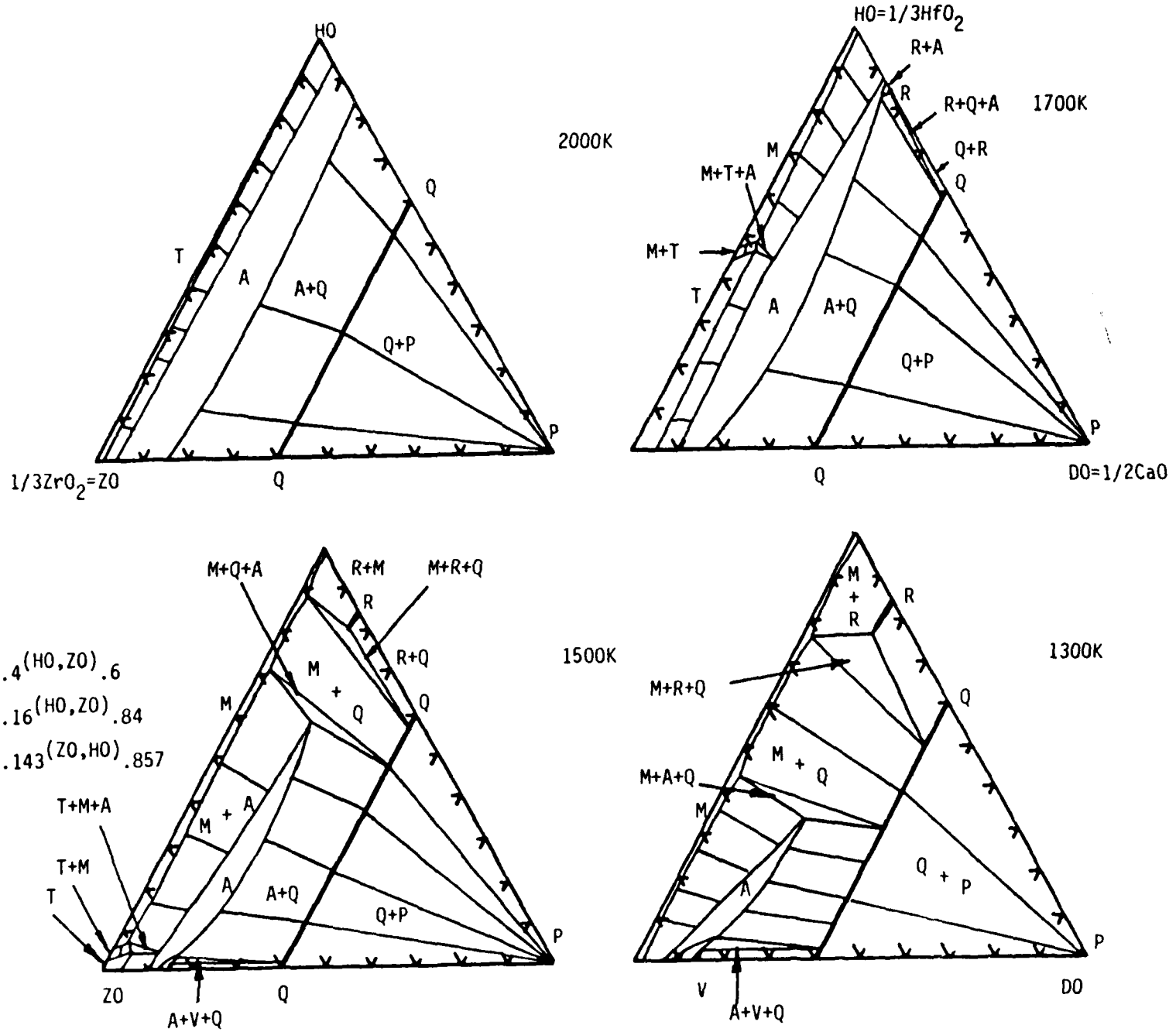


Figure 45. Calculated Isothermal Sections in HO-DO-ZO

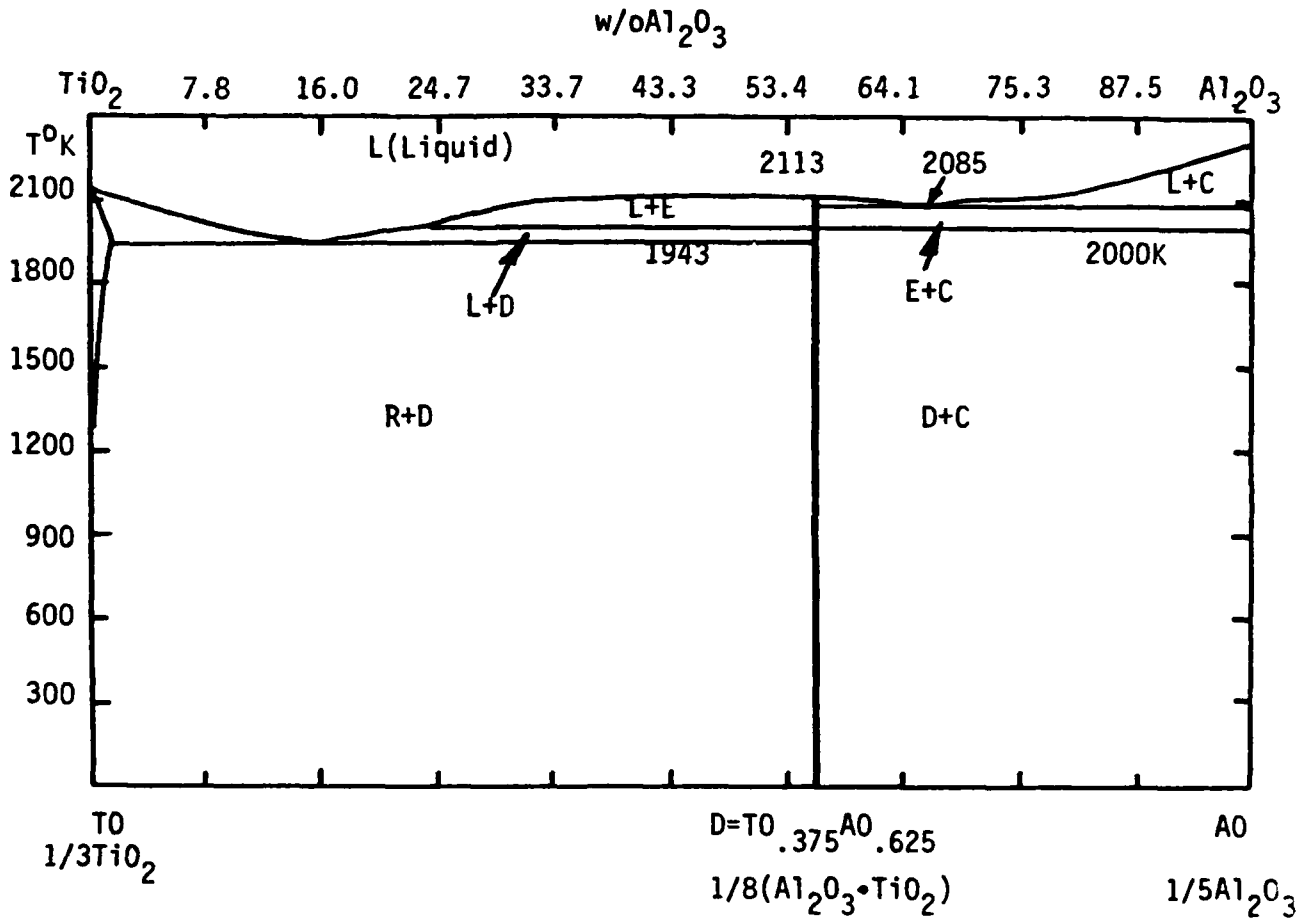


Figure 46. Calculated TiO_2-Al_2O_3 Phase Diagram.

E=High Temperature form of D

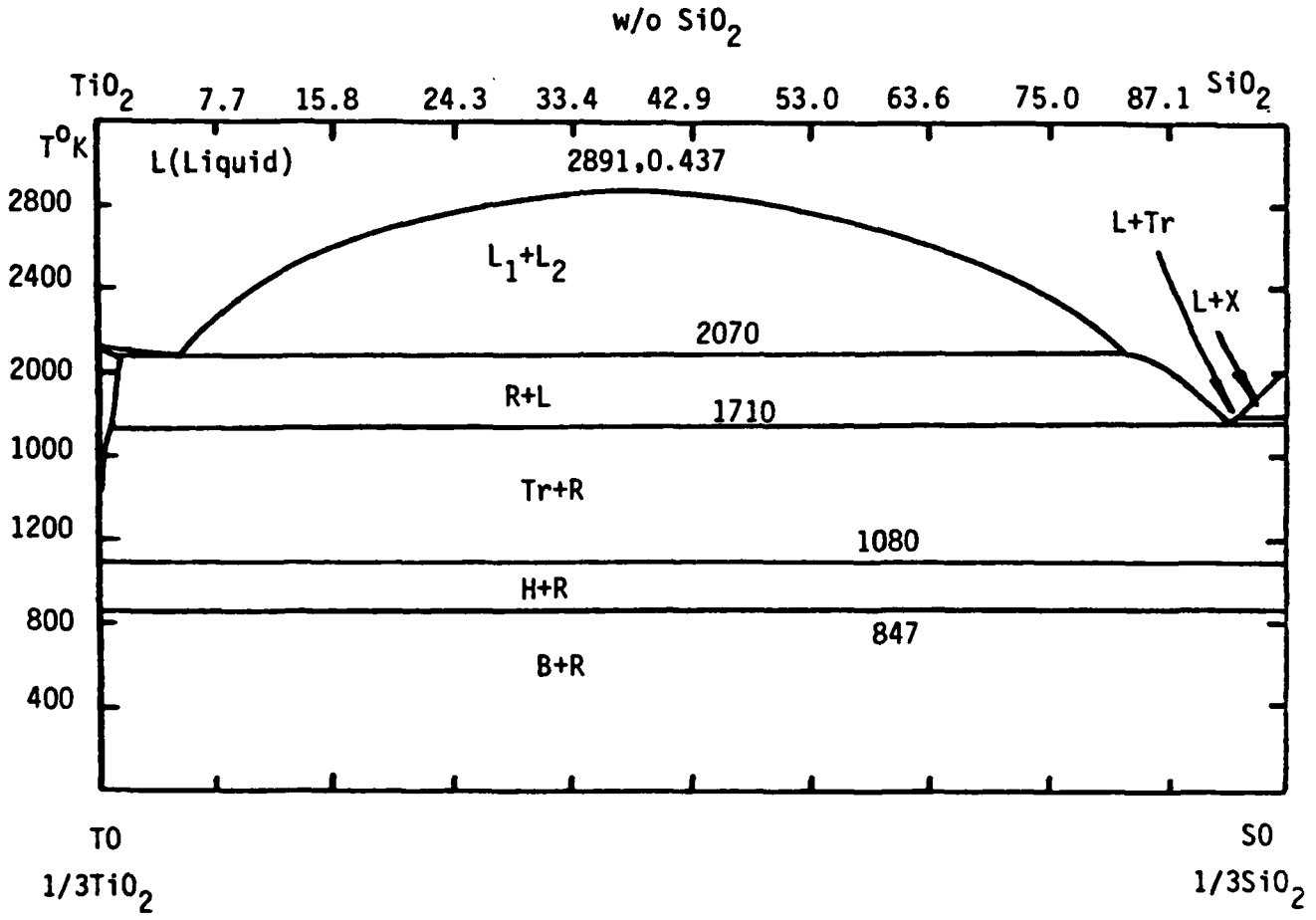


Figure 47. Calculated TiO_2-SiO_2 Phase Diagram

X=Crystoballite
Tr=Trydimite
H=α Quartz
B=β Quartz

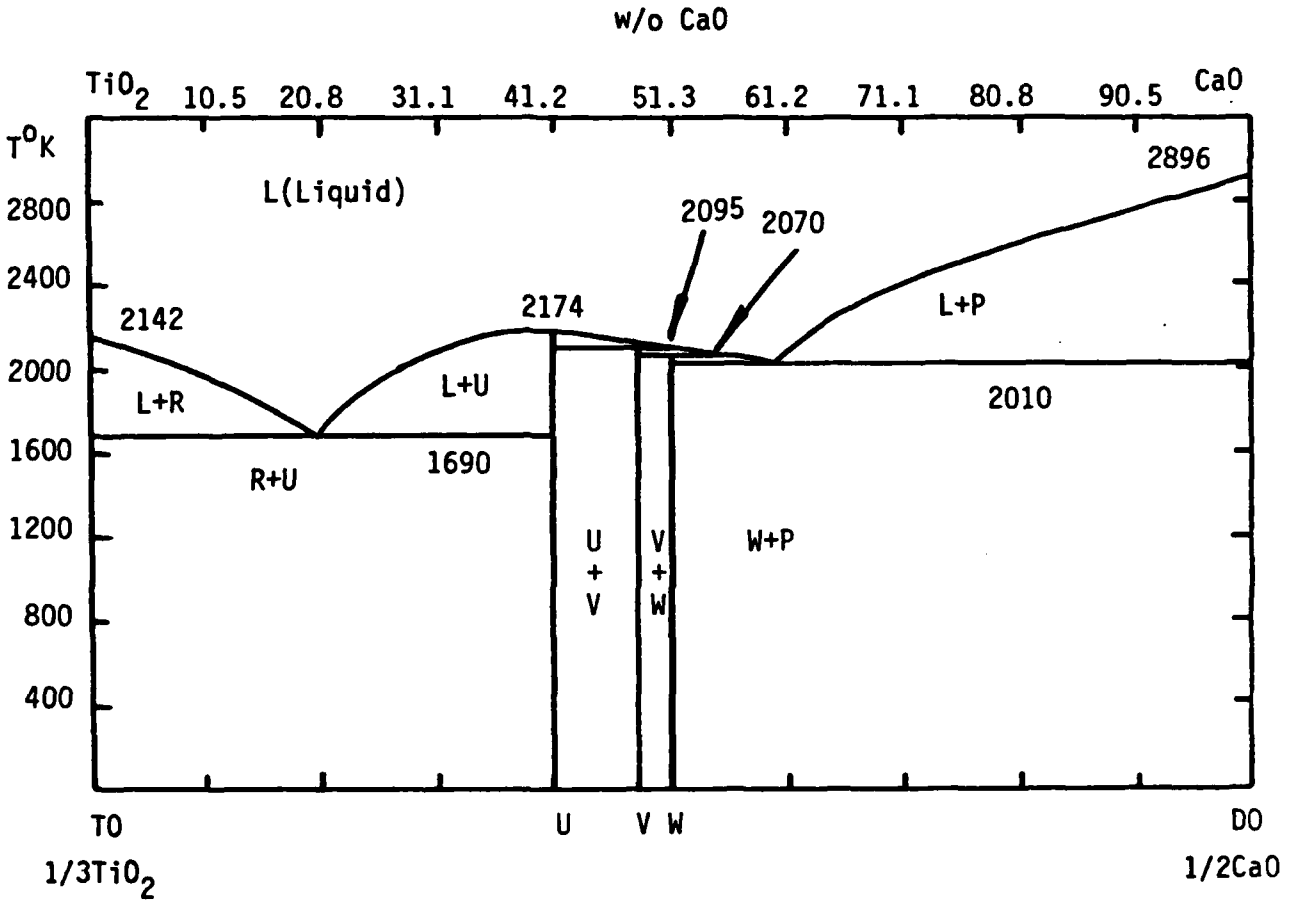


Figure 48. Calculated TiO_2-CaO Phase Diagram

$U=TO_{.6}DO_{.4}=1/5(TiO_2 \cdot CaO)$

$V=TO_{.529}DO_{.471}=1/17(3TiO_2 \cdot 4CaO)$

$W=TO_{.5}DO_{.5}=1/12(2TiO_2 \cdot 3CaO)$

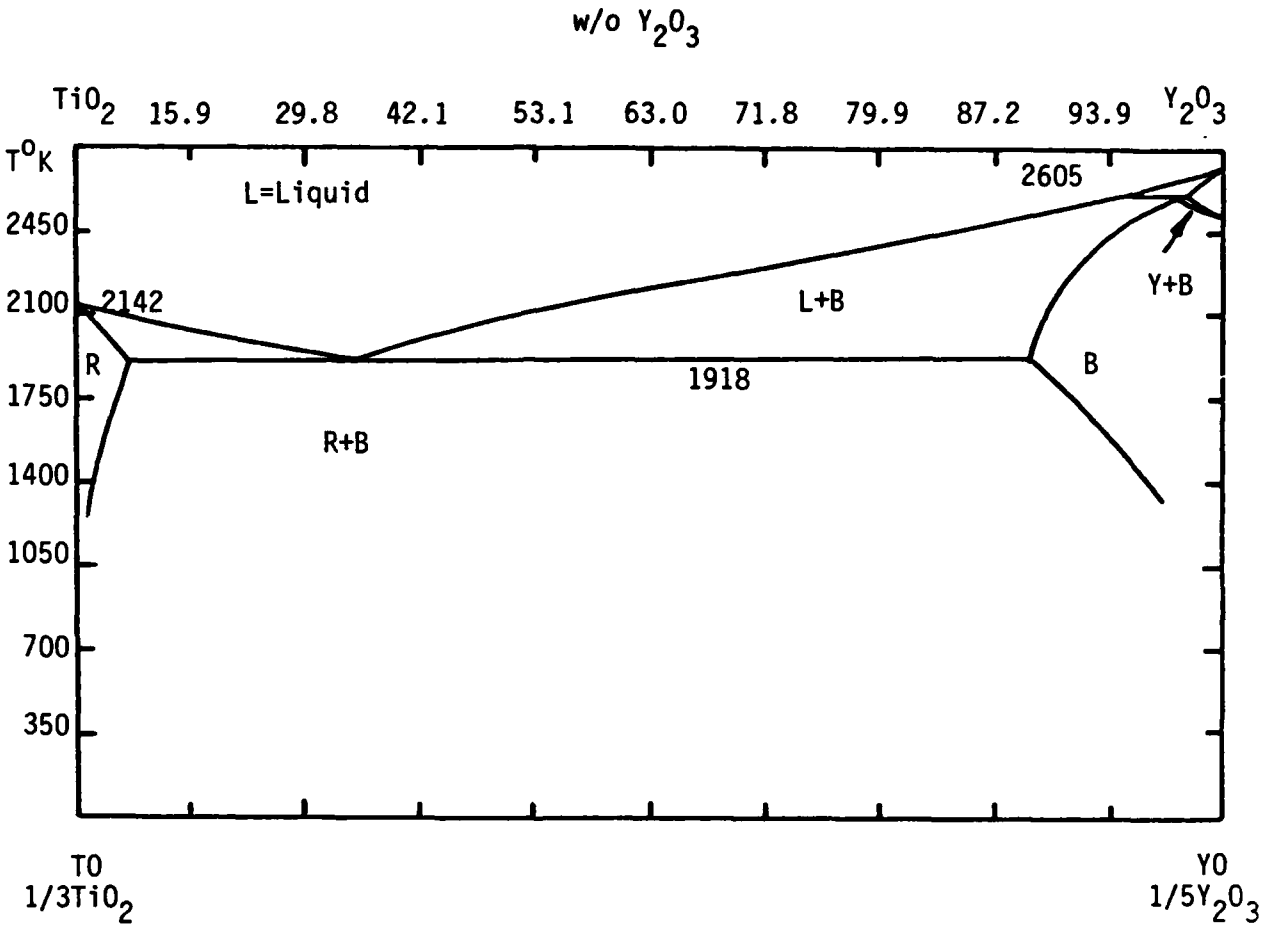


Figure 49. Calculated TiO_2-Y_2O_3 Phase Diagram

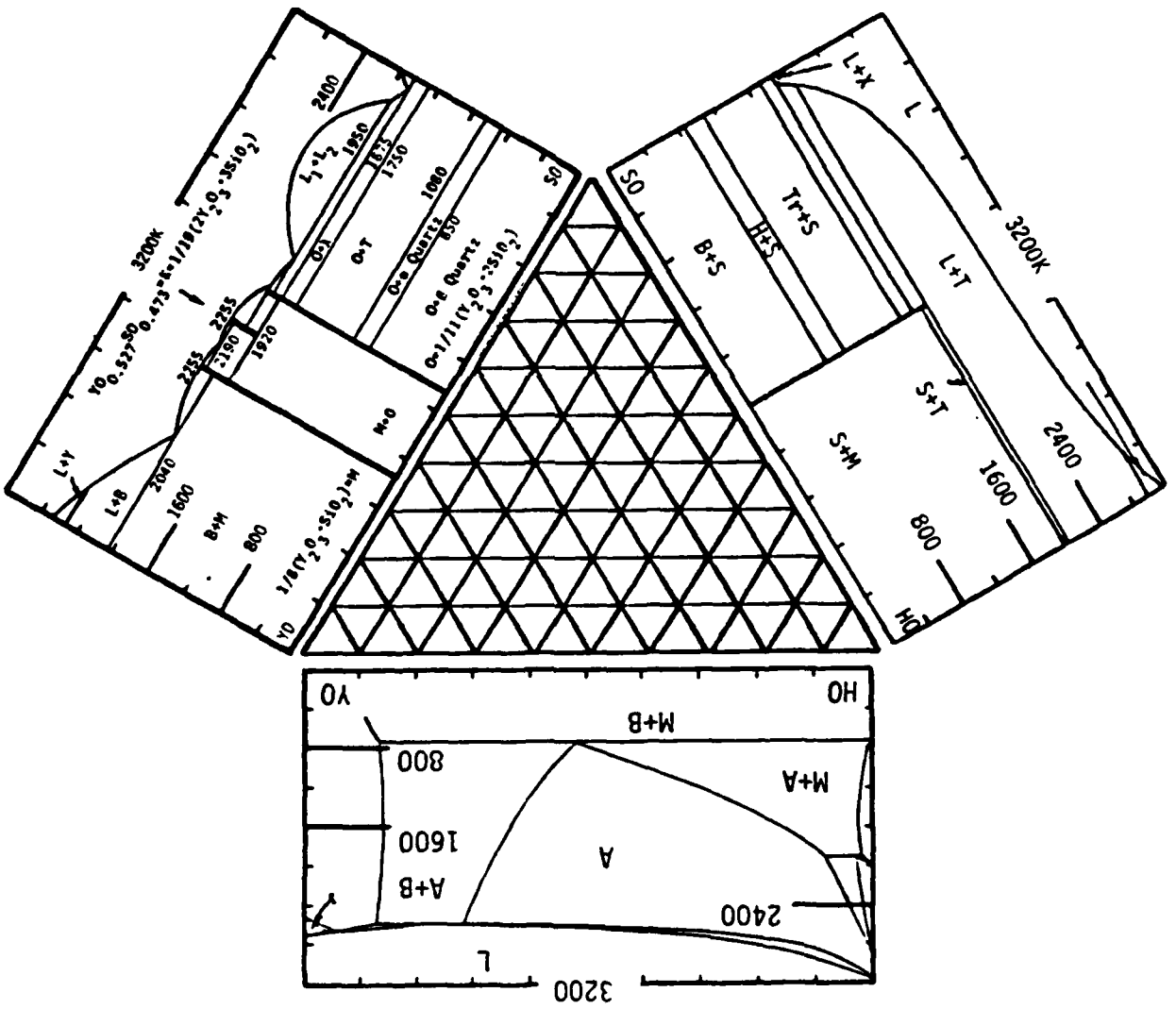


Figure 50. Calculated Isothermal Sections in the $SO(1/3SiO_2)$-$HO(1/3HfO_2)$-$YO(1/5Y_2O_3)$ System.

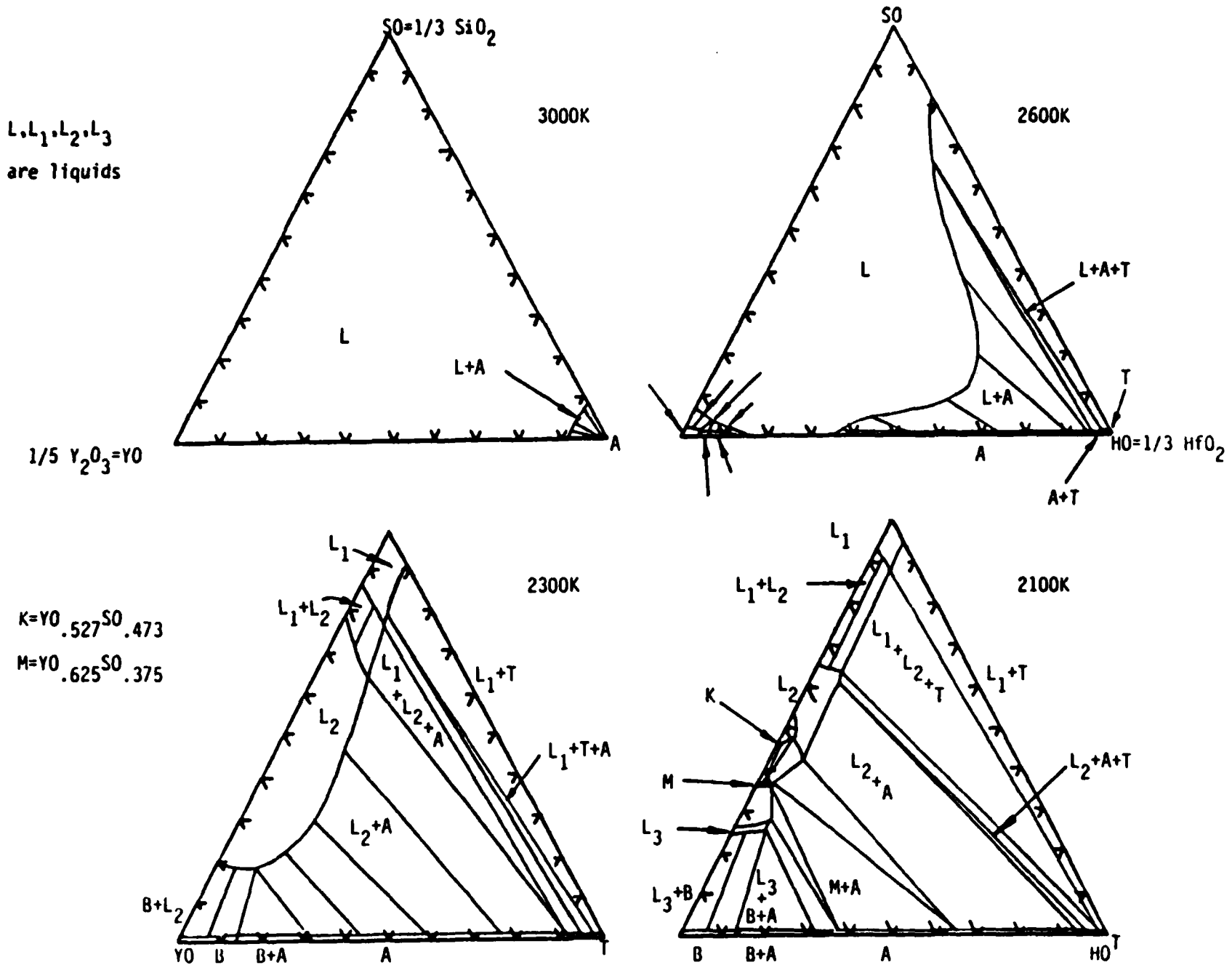


Figure 51. Calculated Isothermal Sections in SO-HO-YO

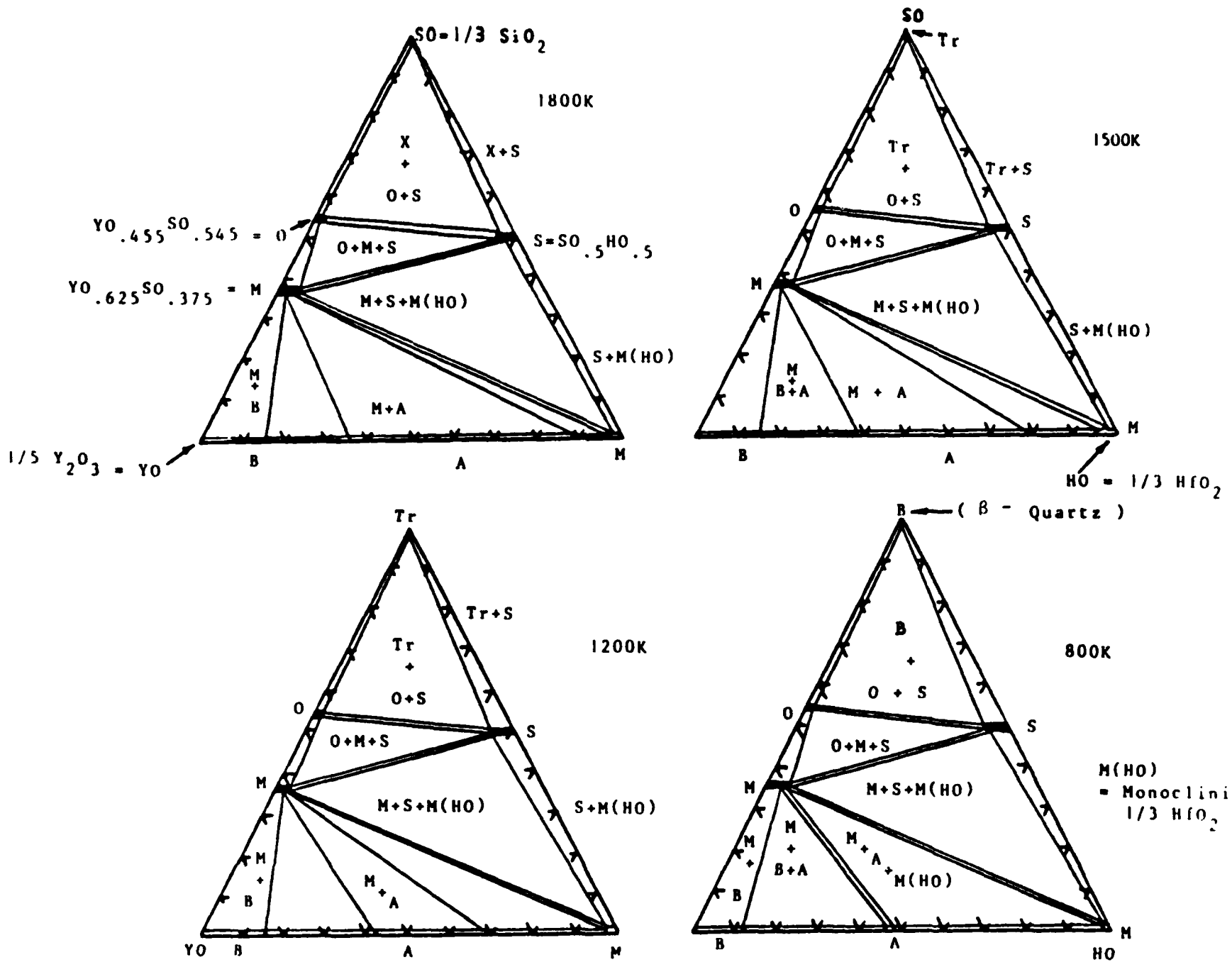


Figure 52. Calculated Isothermal Sections in SO-HO-YO

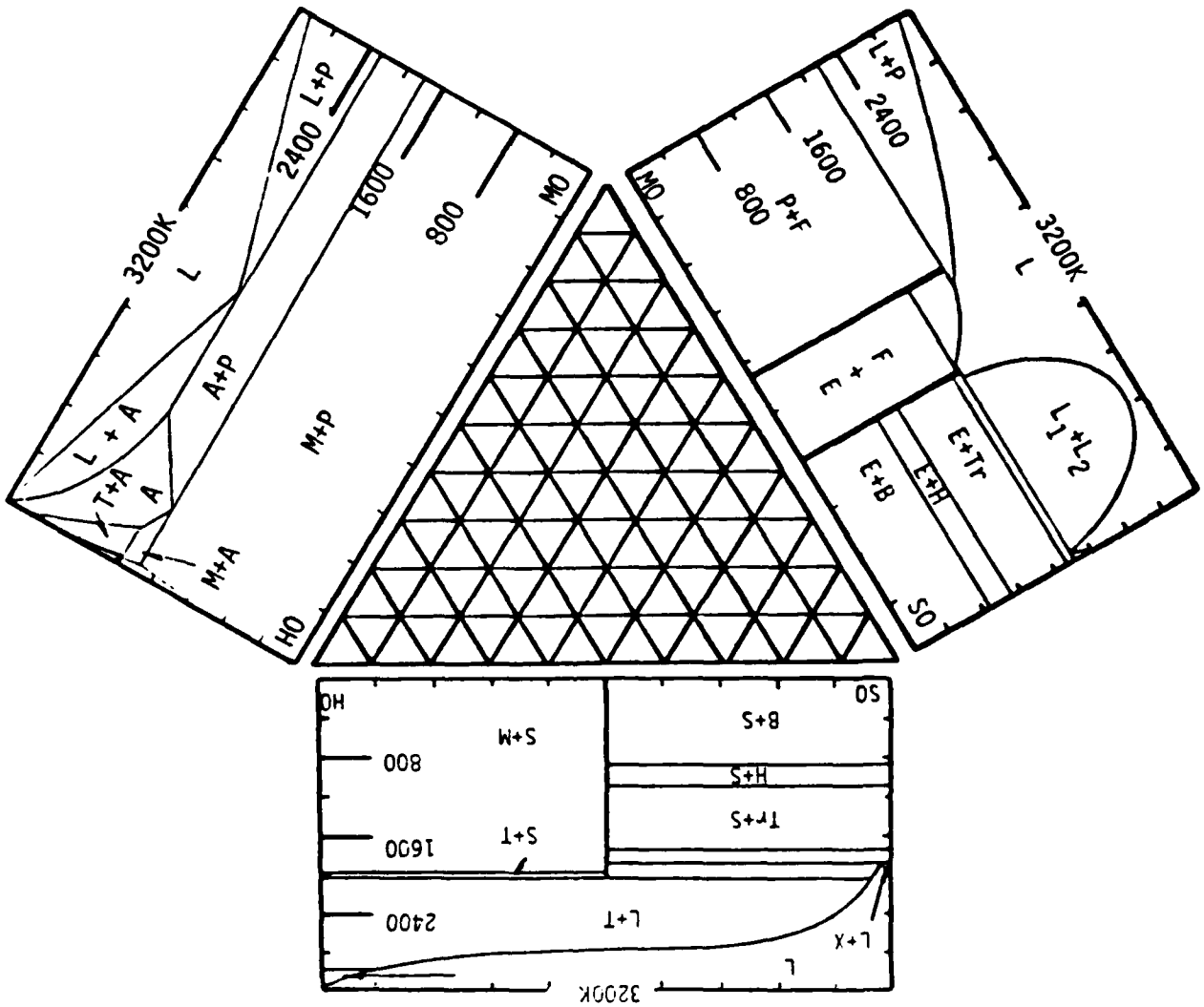


Figure 53. Calculated Isothermal Sections in the $MO(1/2MgO)$-$SO(1/3SiO_2)$-$HO(1/3HfO_2)$ System.

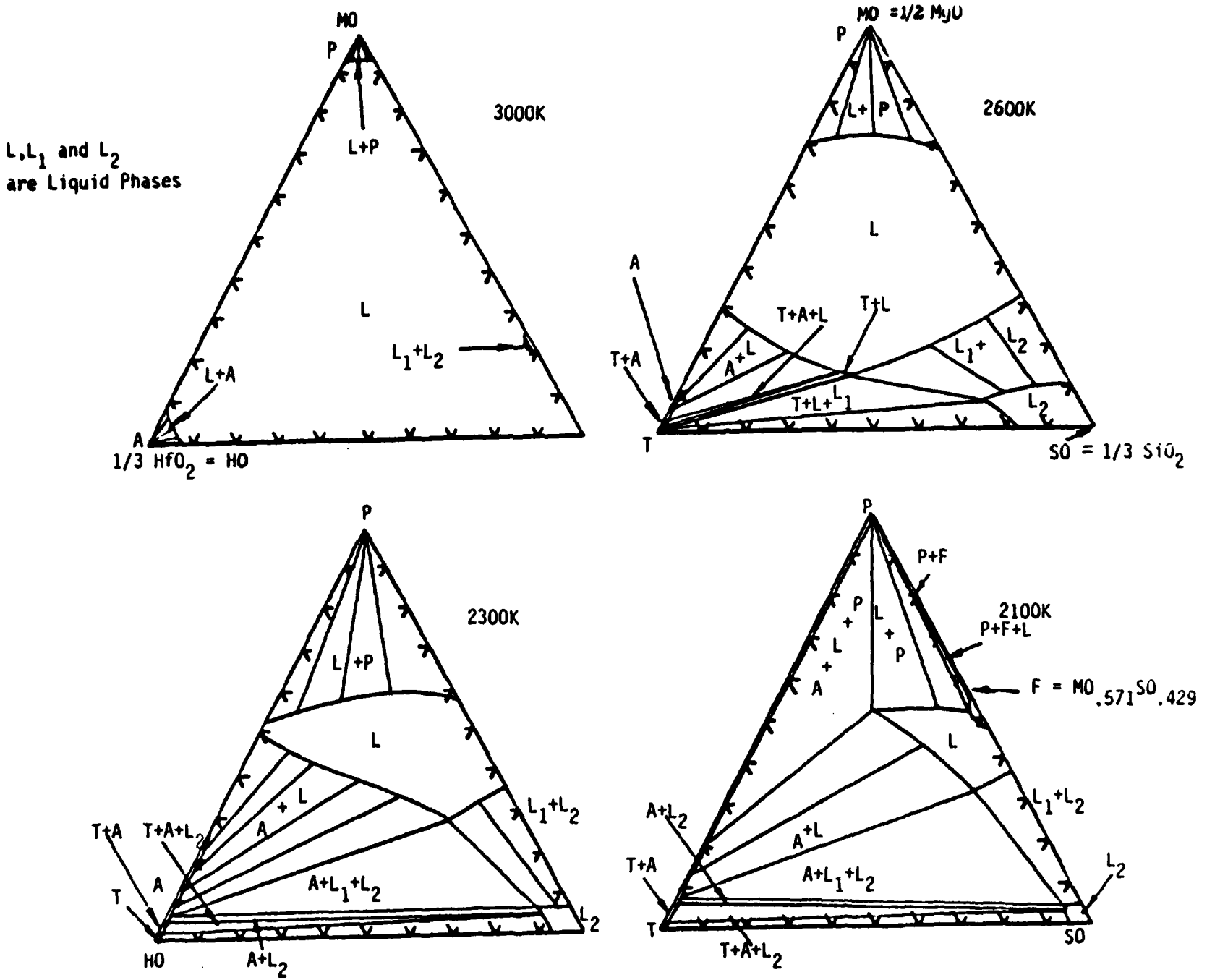


Figure 54. Calculated Isothermal Seactions in MO-SO-HO

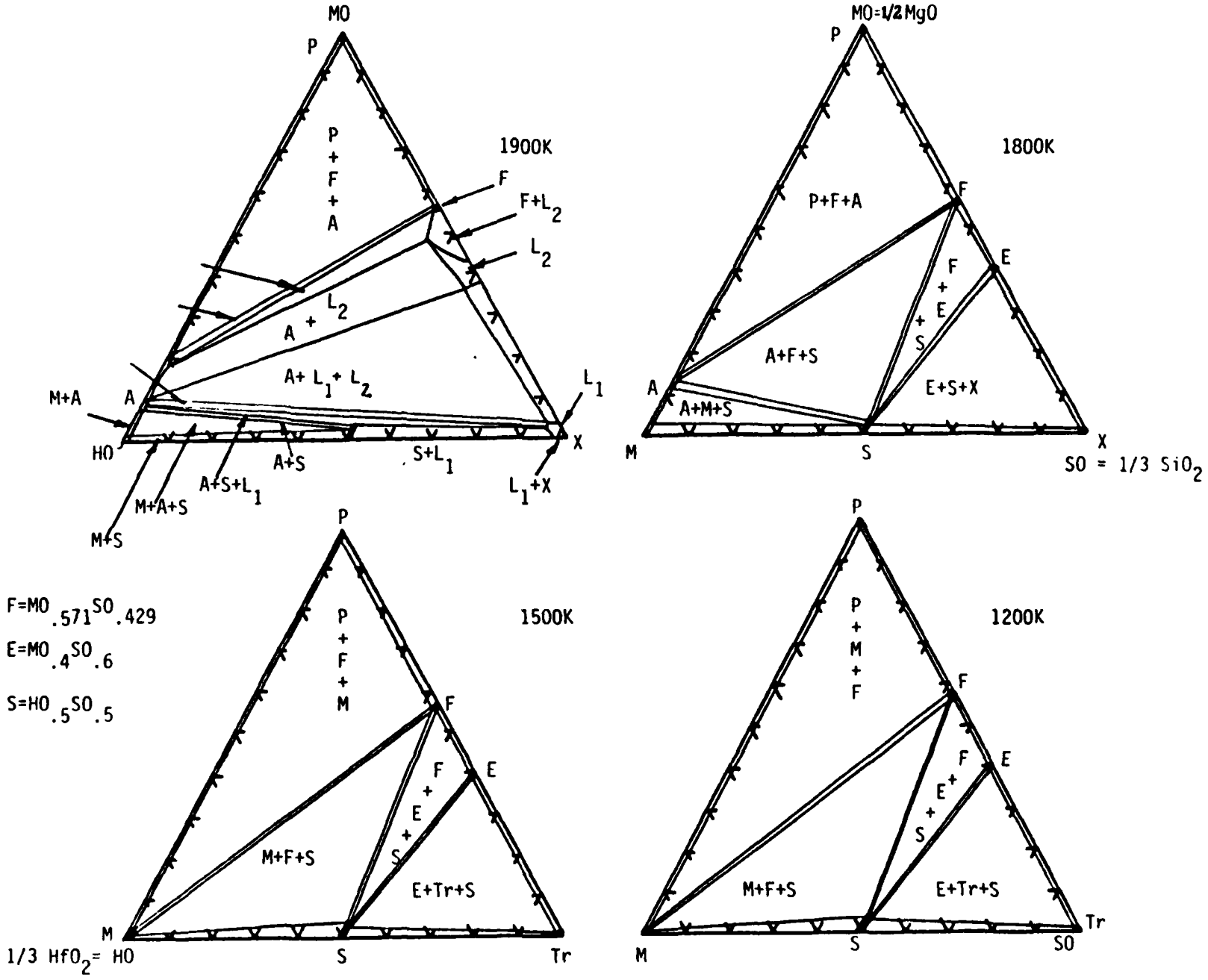


Figure 55. Calculated Isothermal Sections in MO-SO-HO

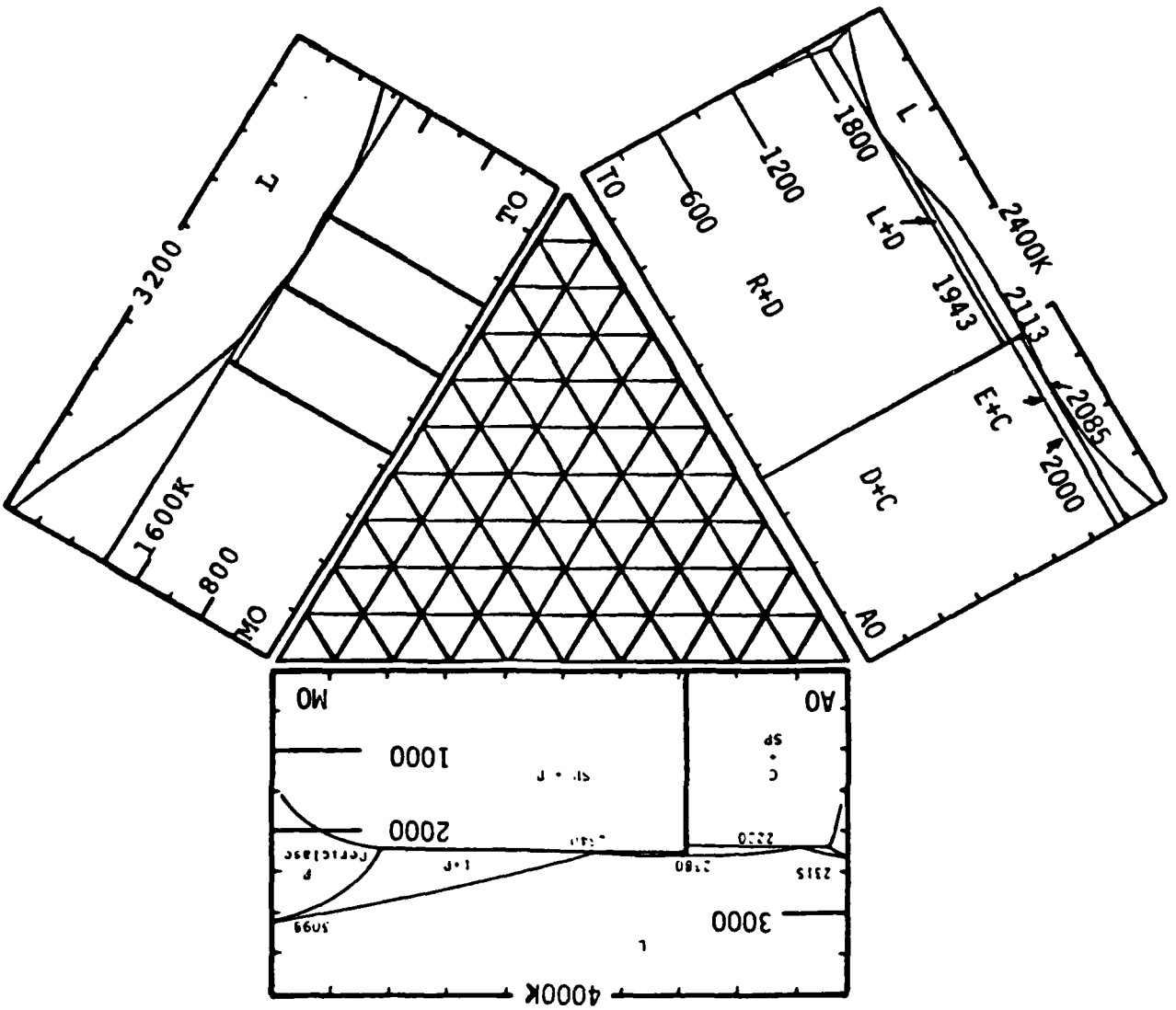


Figure 56. Calculated Isothermal Sections in the $TO(1/3\ TiO_2)$ - $AO(1/5\ Al_2O_3)$ - $MO(1/2\ Mg\ O)$ system.

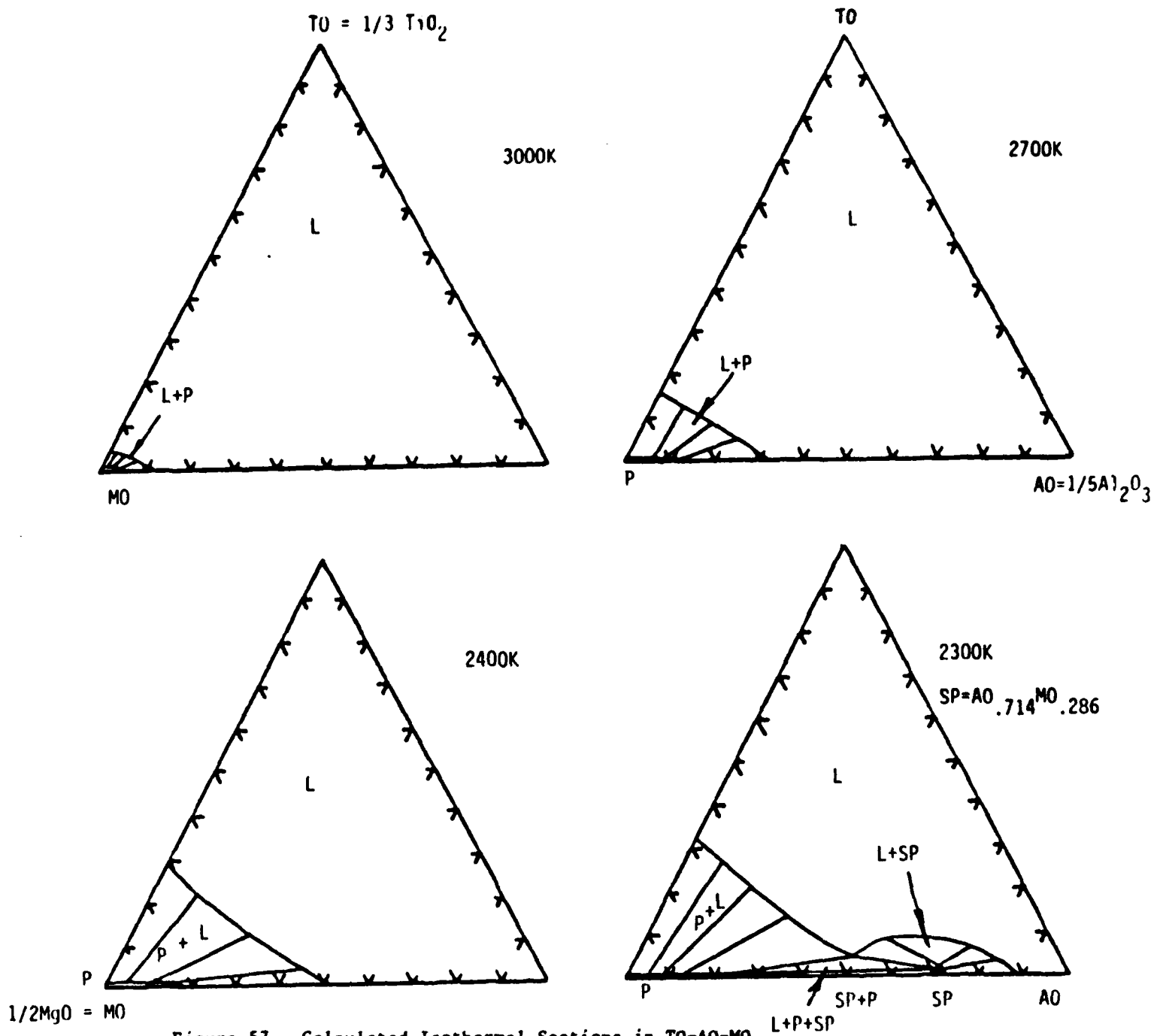


Figure 57. Calculated Isothermal Sections in TO-AO-MO.

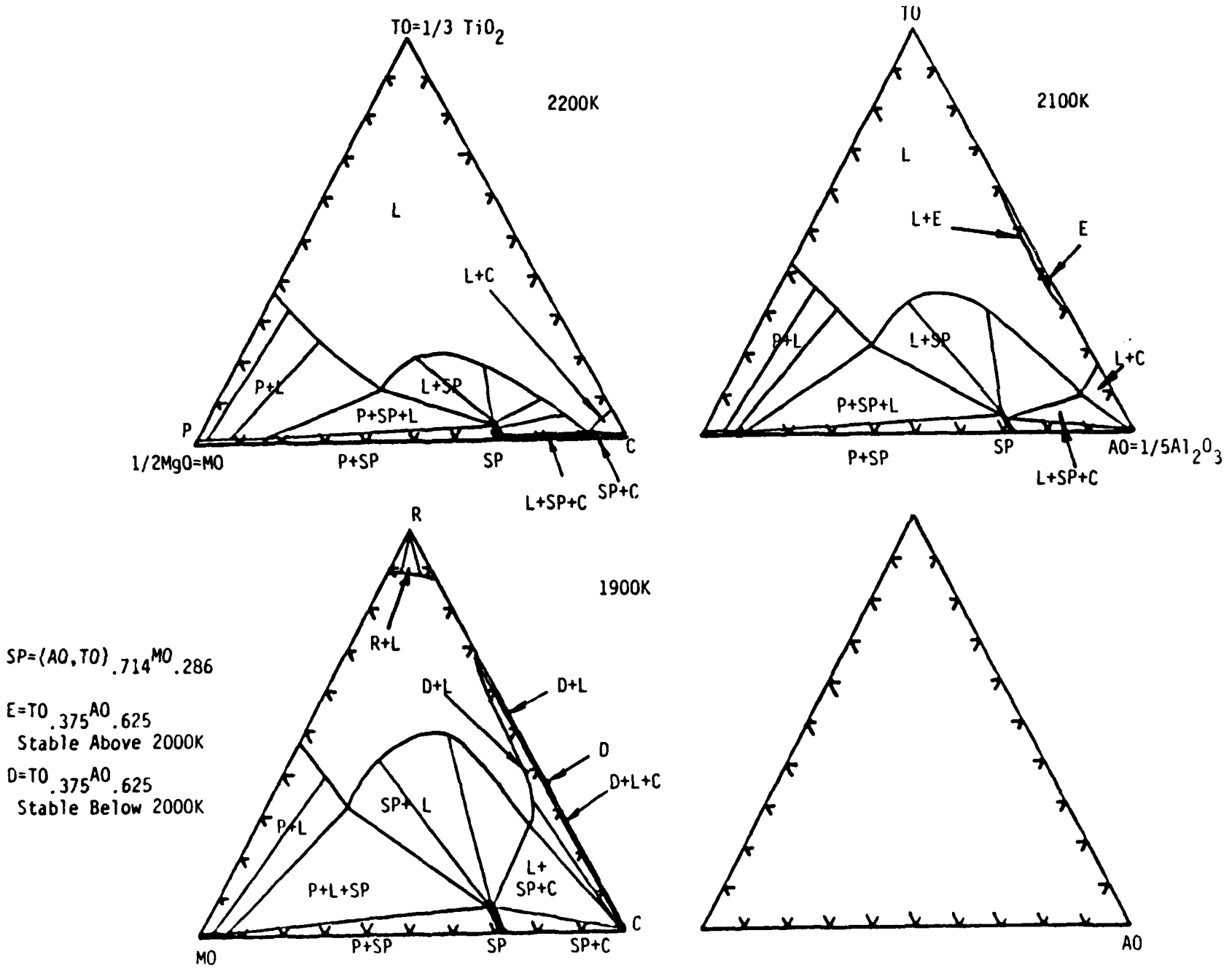


Figure 58. Calculated Isothermal Sections in TO-AO-MO

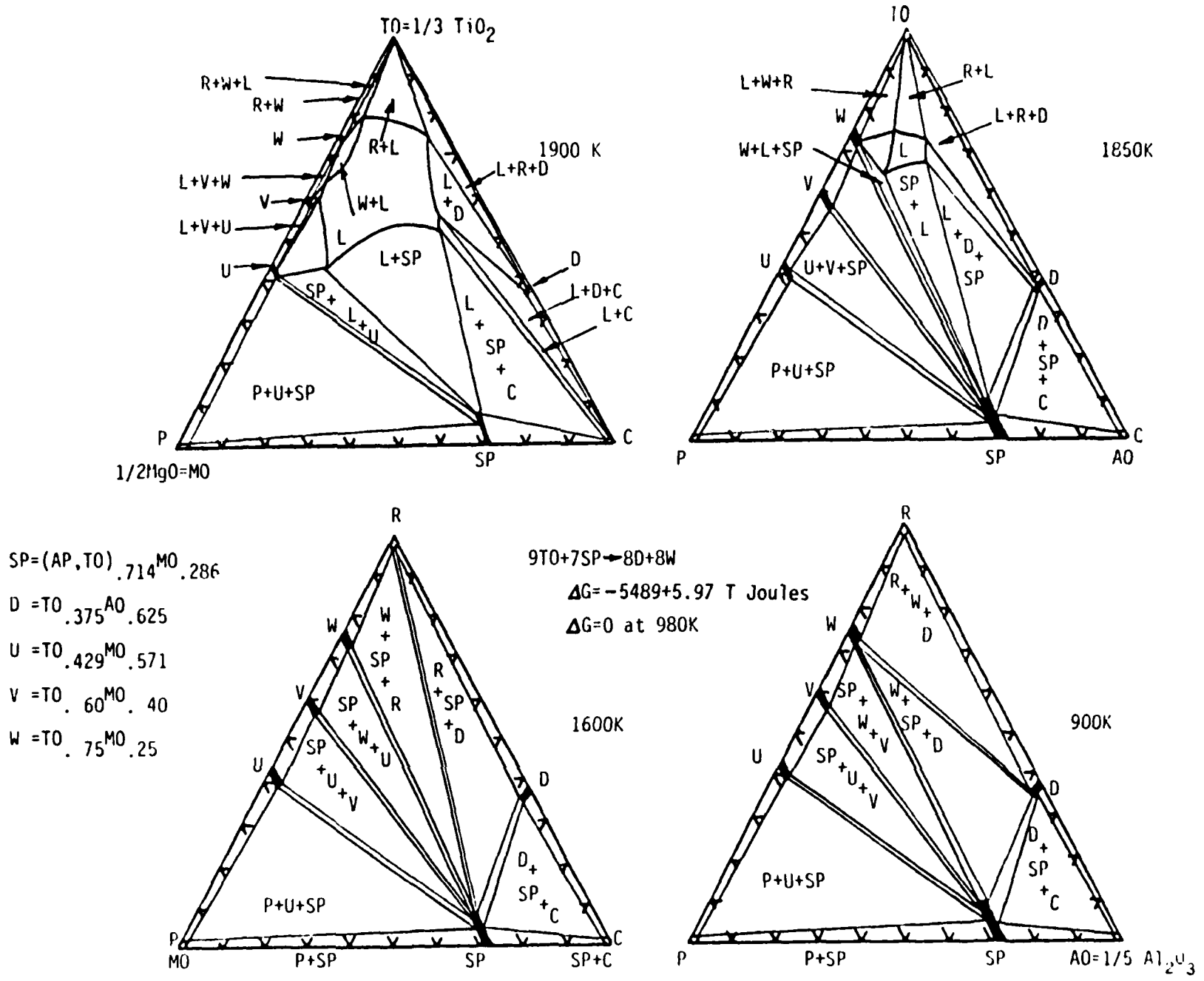


Figure 59. Calculated Isothermal Sections in TO-AO-MO

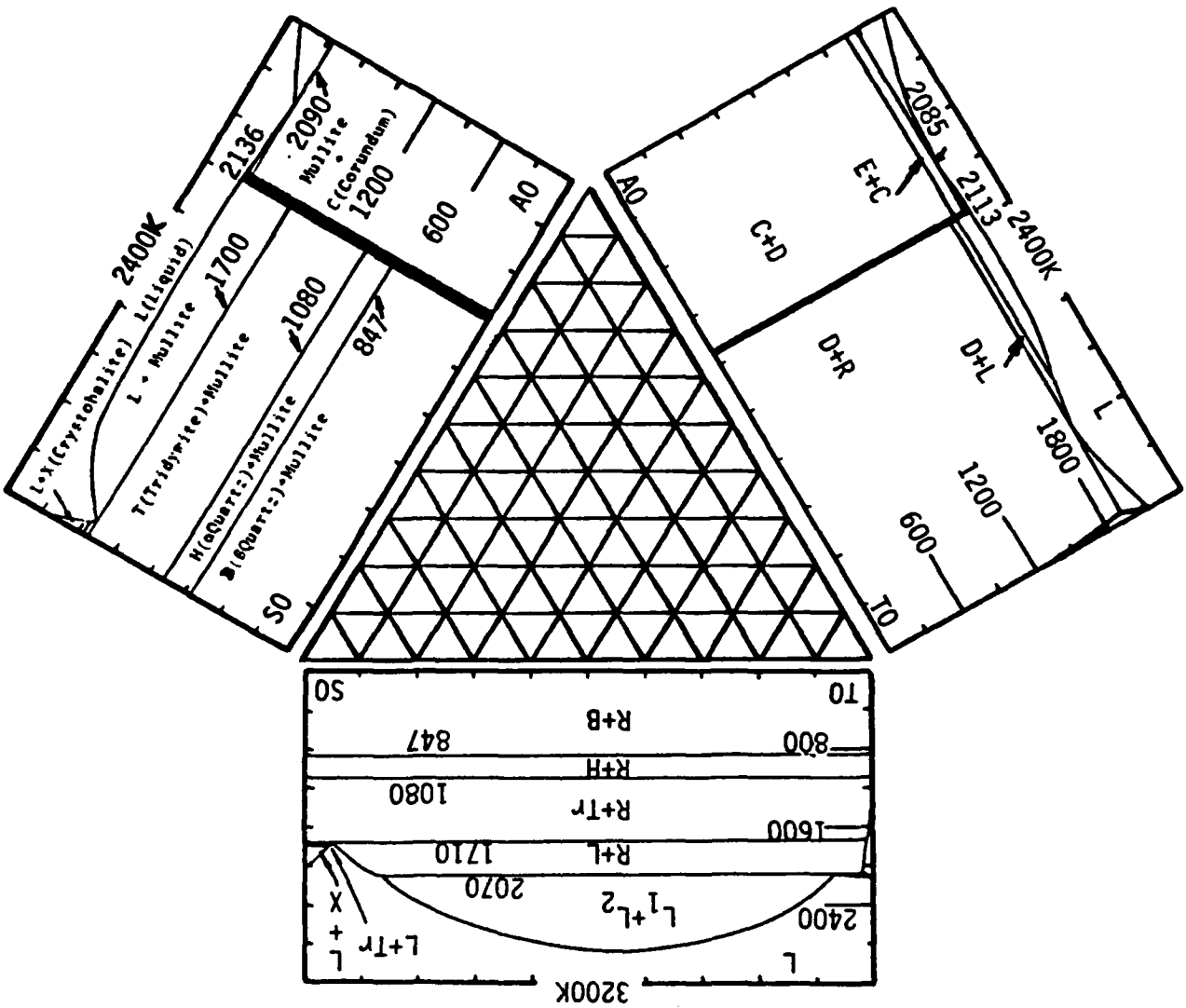


Figure 60. Calculated Isothermal Sections in the AO(1/5 Al_2O_3) - TO(1/3 TiO_2) - SO(1/3 SiO_2) system.

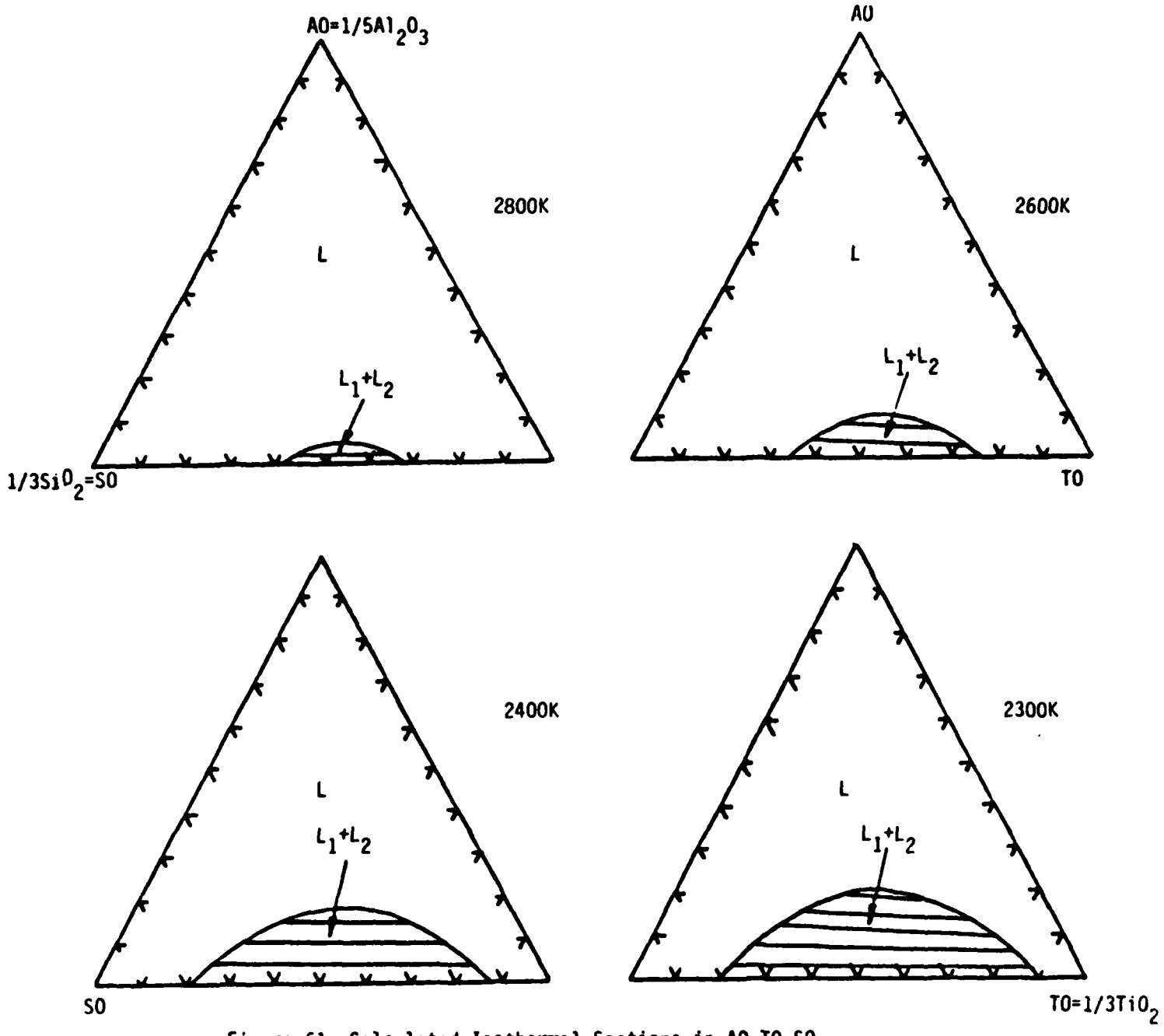


Figure 61. Calculated Isothermal Sections in AO-TO-SO

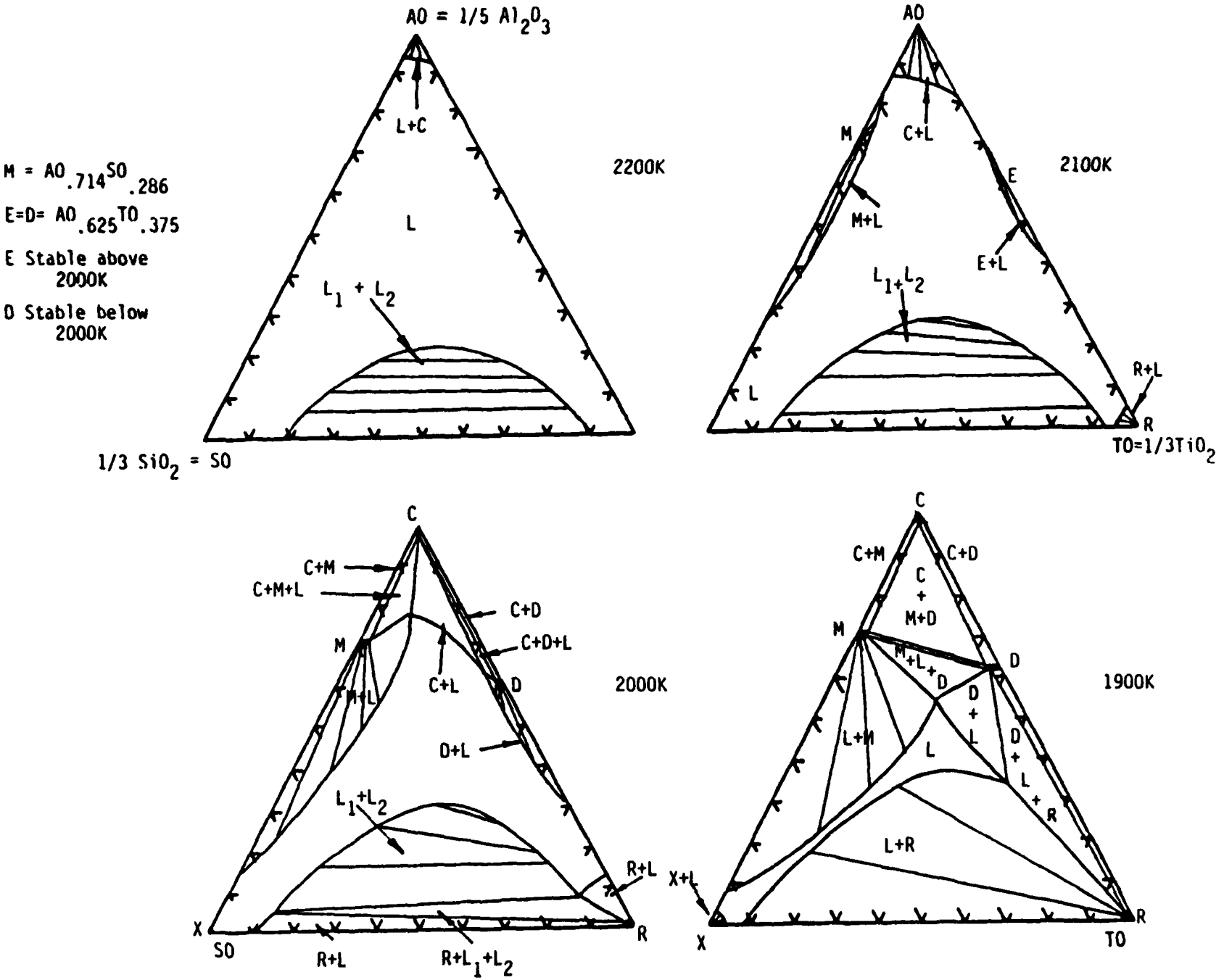


Figure 62. Calculated Isothermal Sections in AO-TO-SO

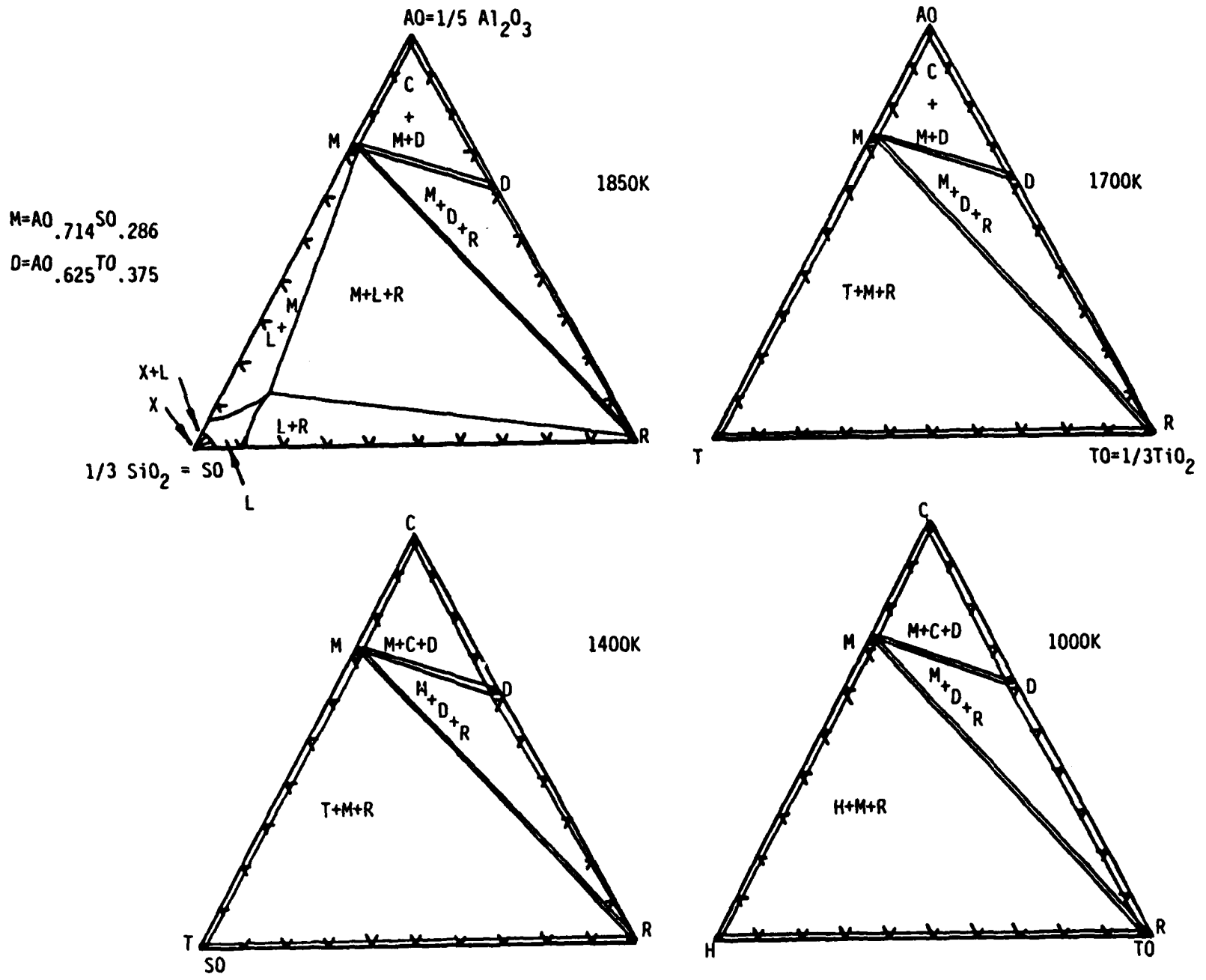


Figure 63. Calculated Isothermal Sections in AO-TO-SO

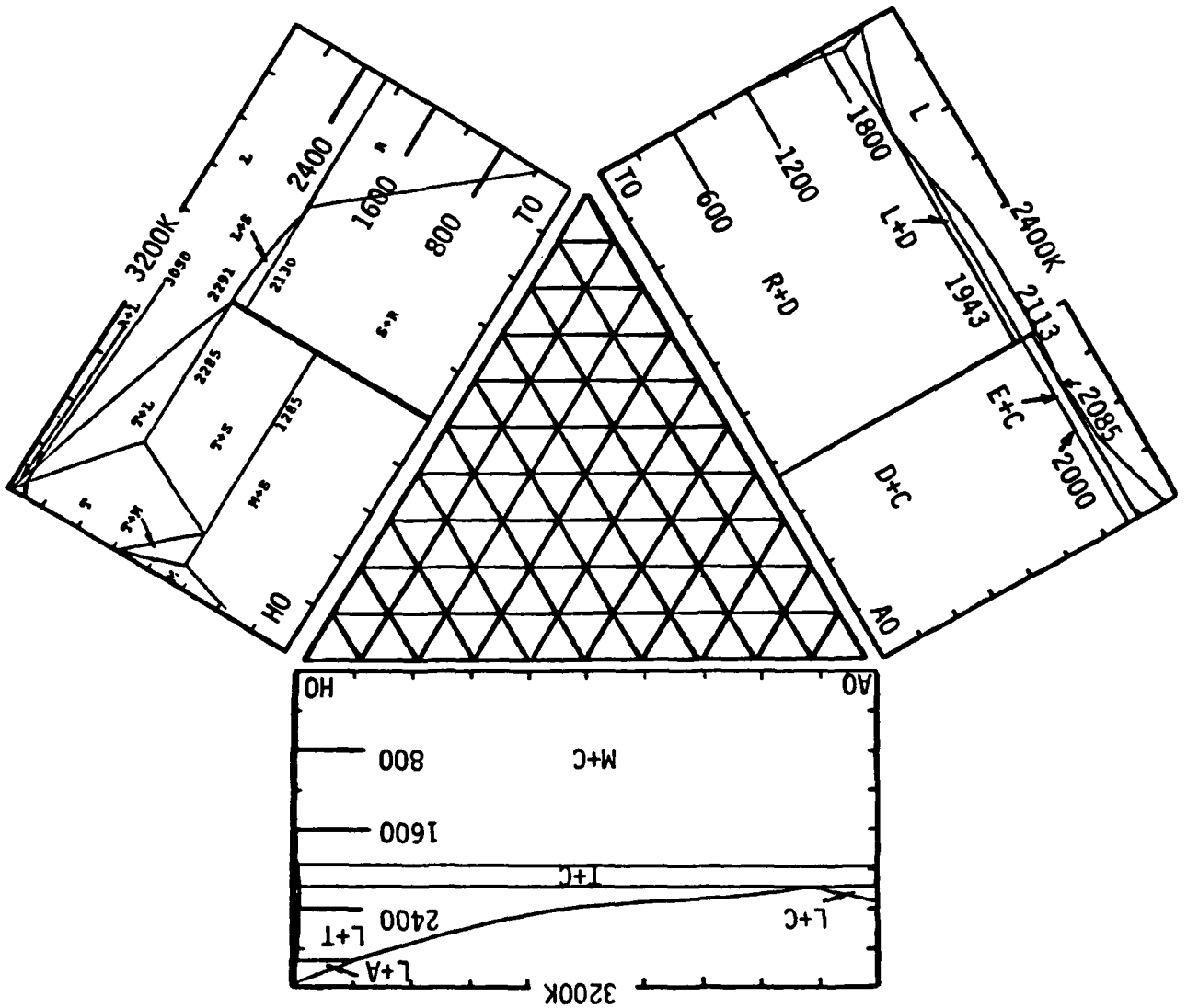


Figure 64. Calculated Isothermal Sections in the TO(1/3 TiO_2) - AO(1/5 Al_2O_3) - HO(1/3 HfO_2) system.

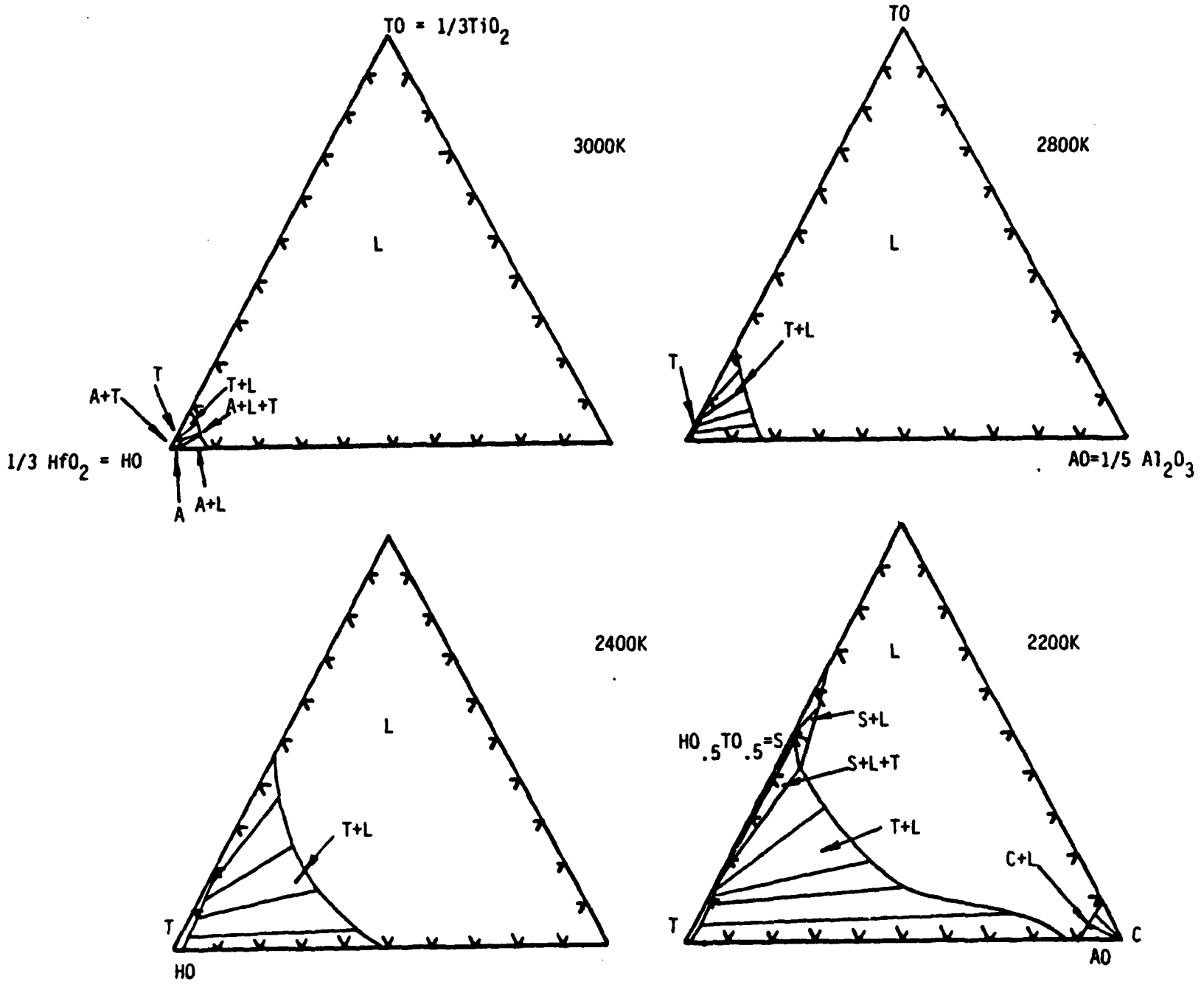


Figure 65. Calculated Isothermal Sections in TO-AO-HO

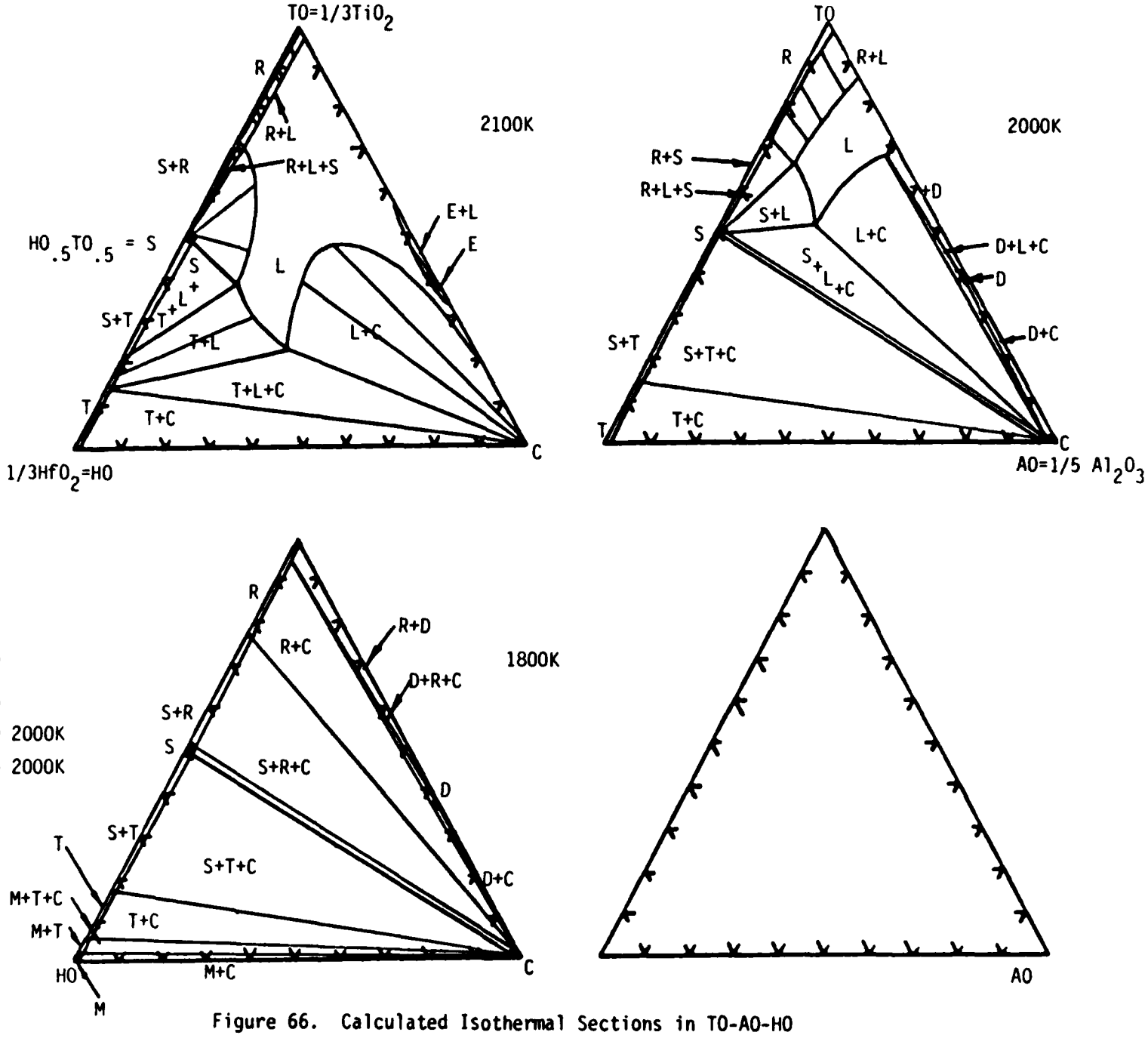


Figure 66. Calculated Isothermal Sections in TO-AO-HO

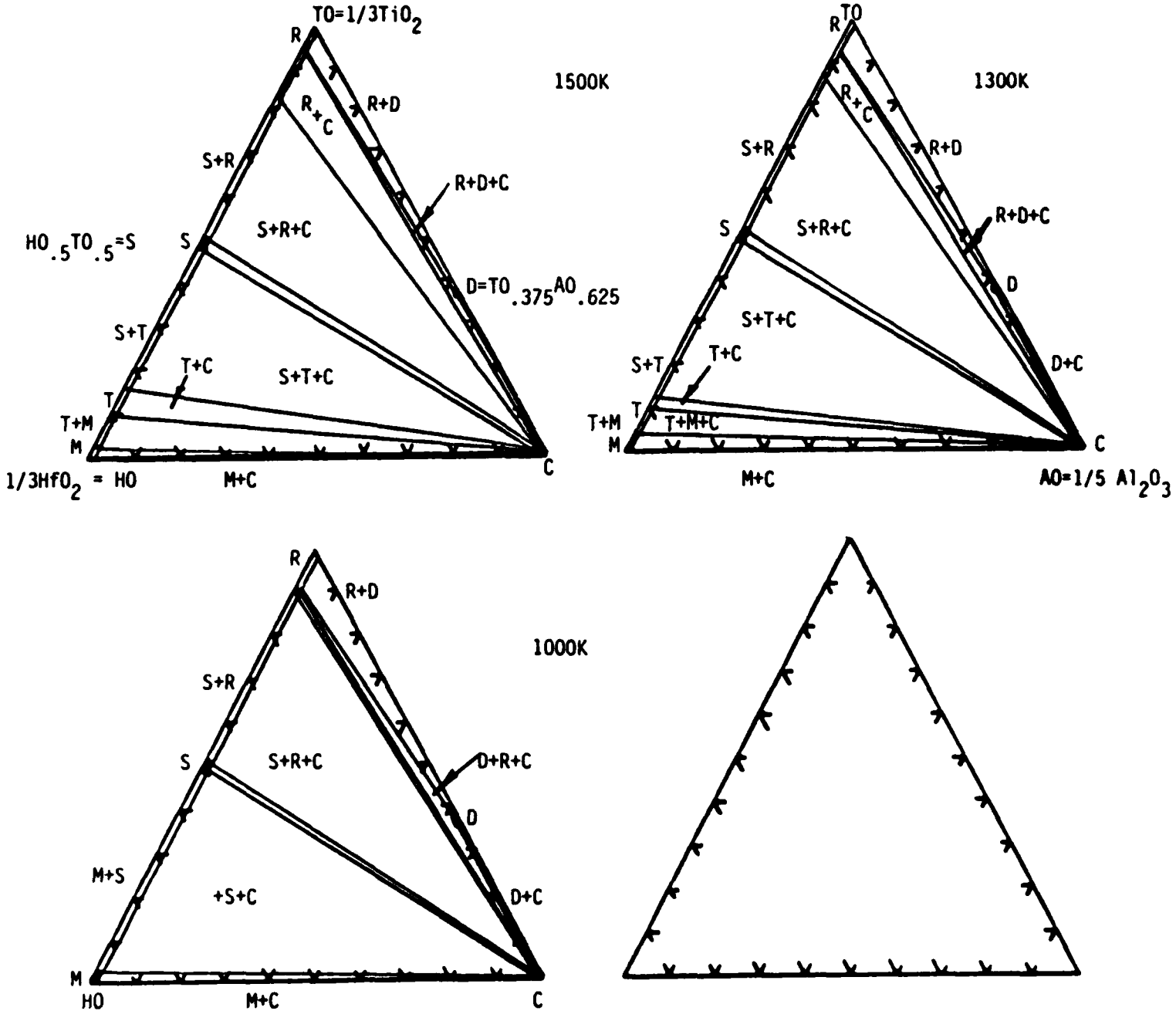


Figure 67. Calculated Isothermal Sections in TO-AO-HO

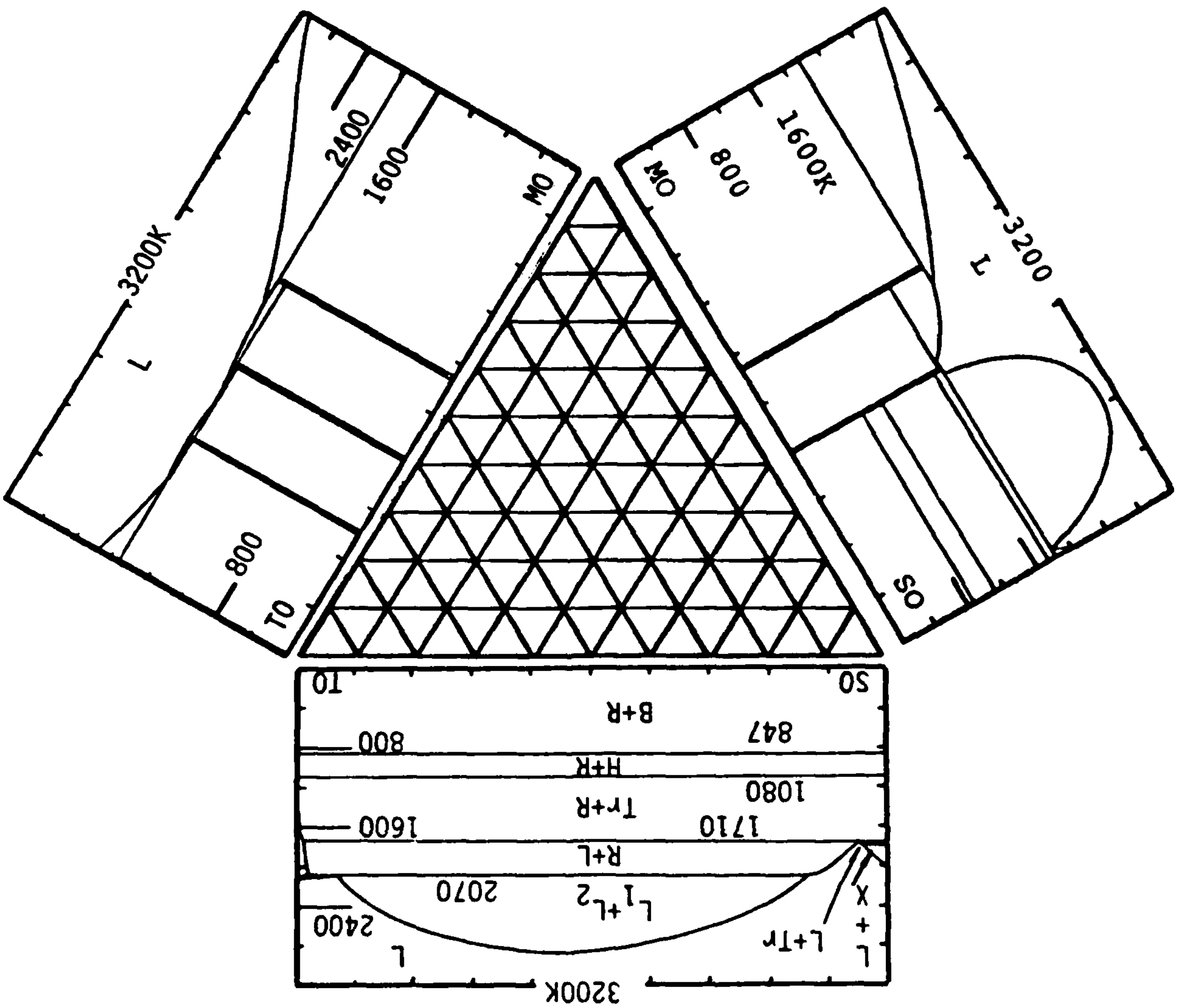
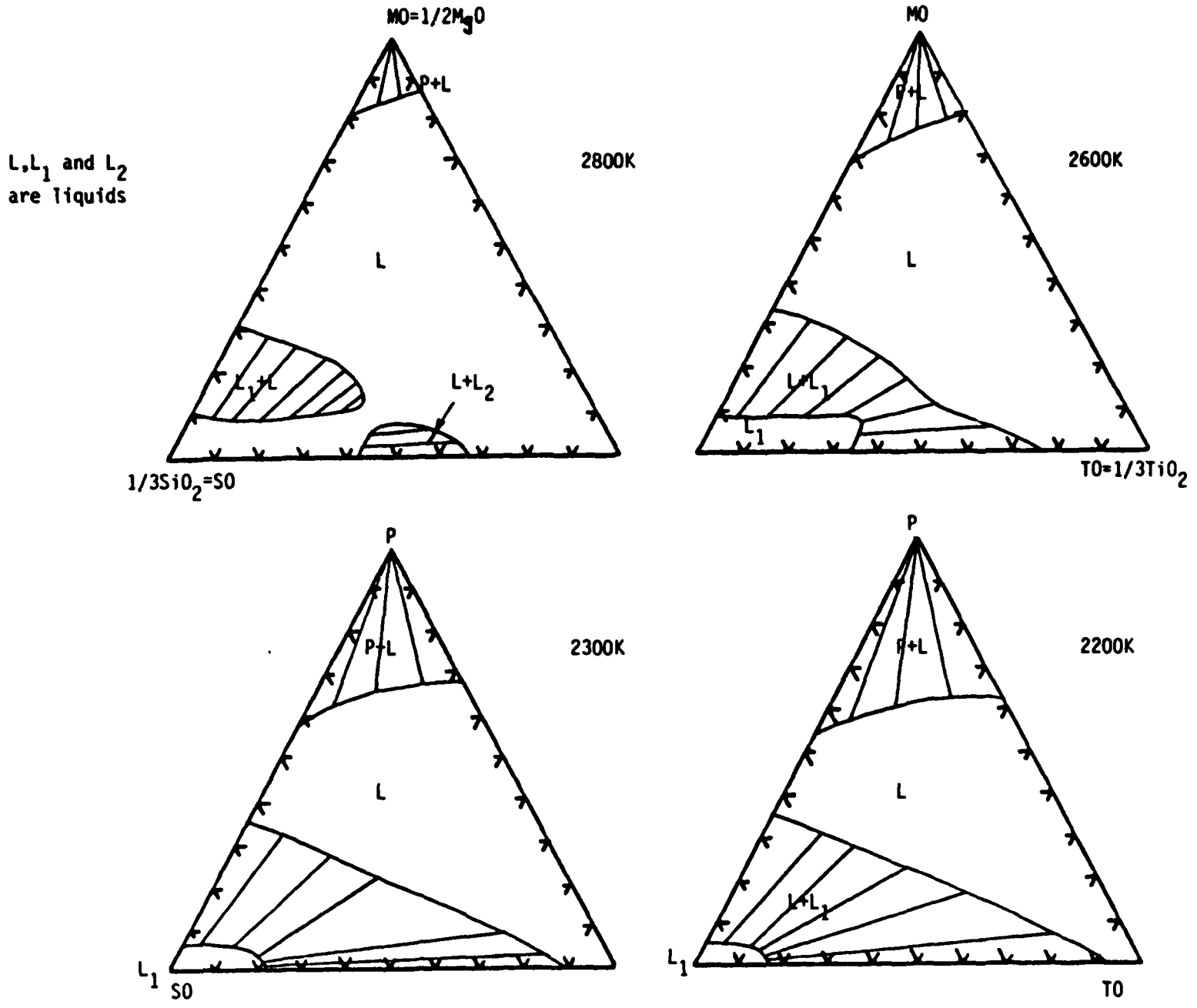
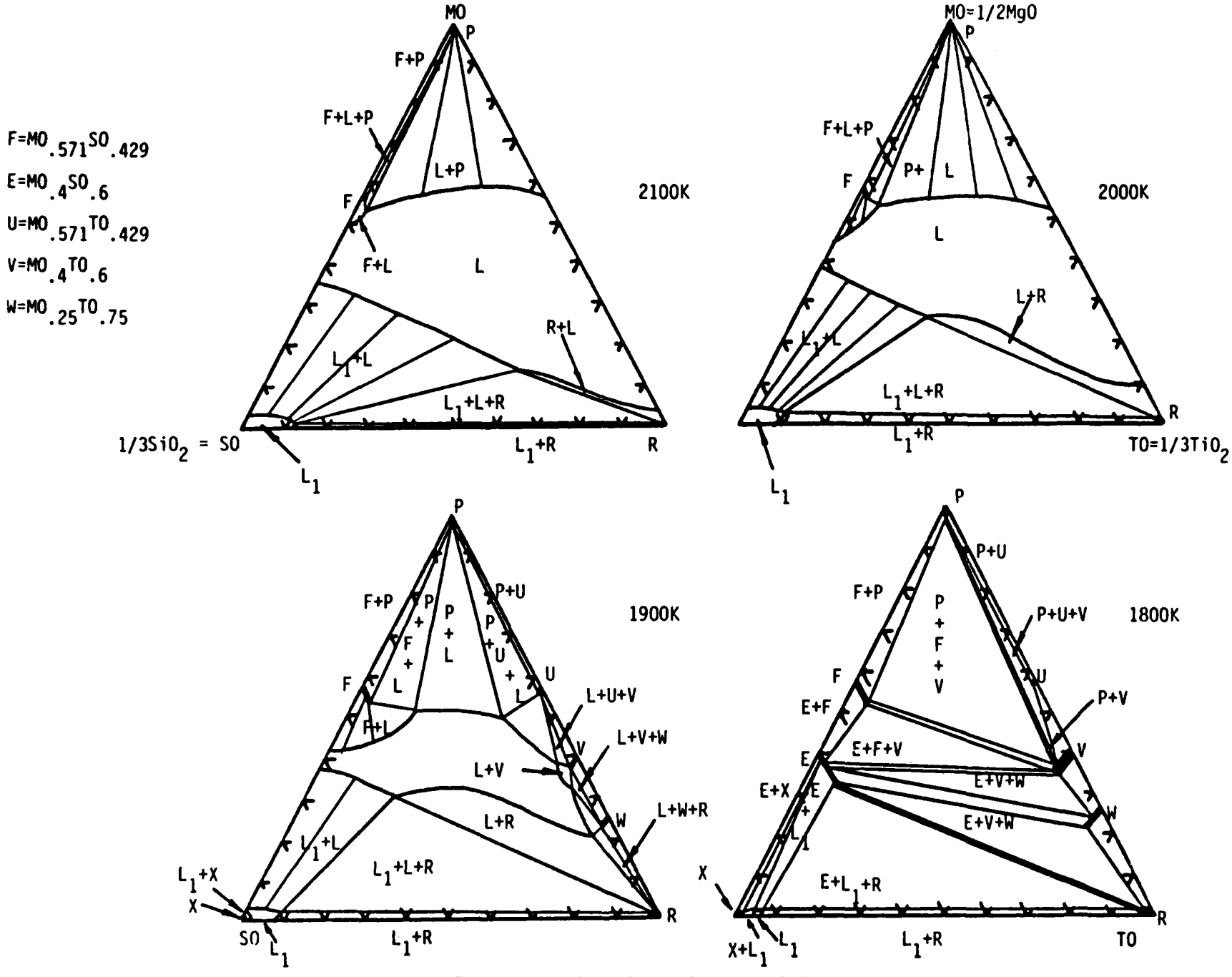


Figure 68. Calculated Isothermal Sections in the MO(1/2MgO)-SO(1/3SiO_2)-TO(1/3TiO_2) System.



L, L_1 and L_2 are liquids

Figure 69. Calculated Isothermal Sections in MO-TO-SO



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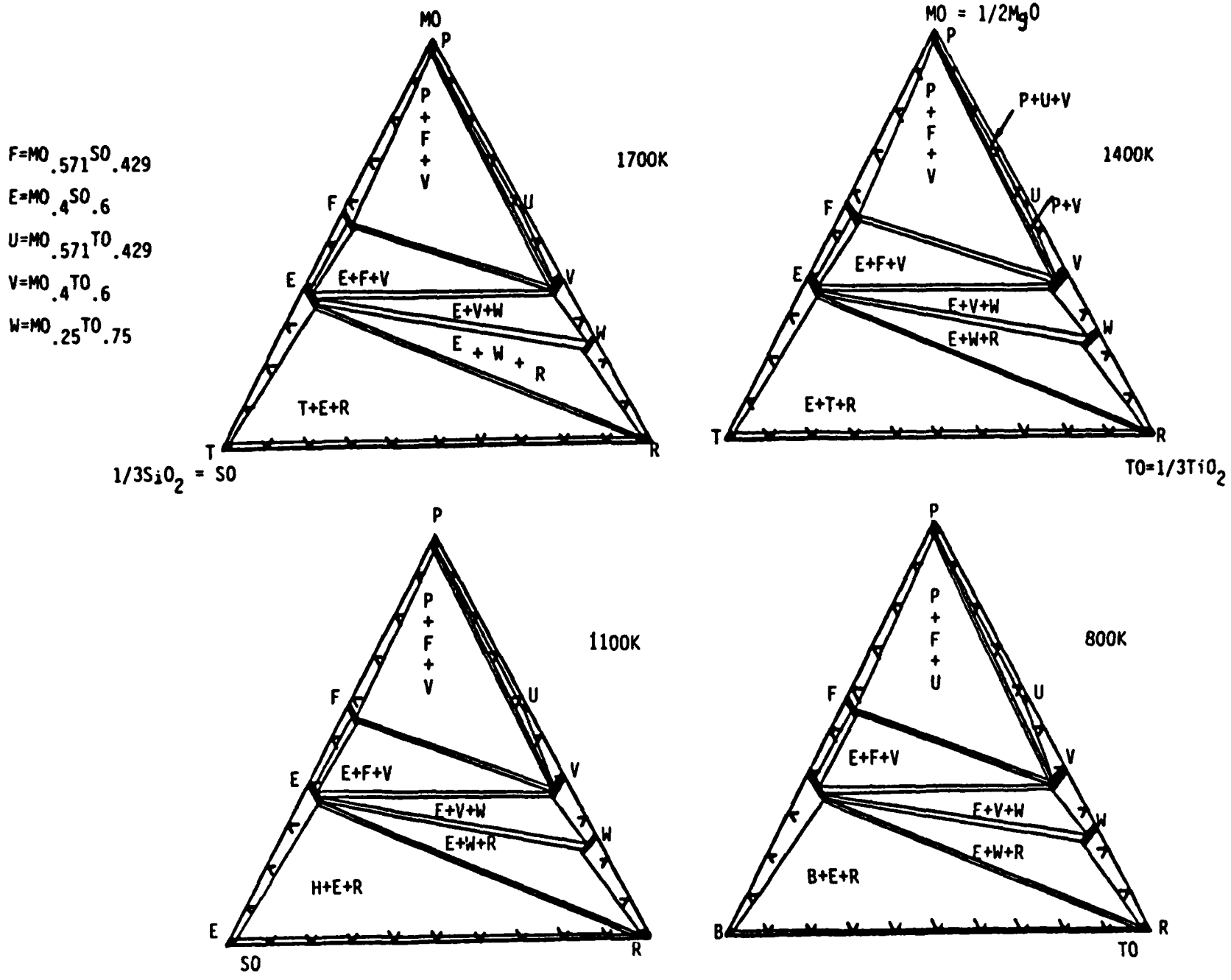

Figure 71. Calculated Isothermal Sections in MO-TO-SO

References

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