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6. "Theoretical dipole transition moments for transitions between bound electronic states and non-adiabatic coupling matrix elements between $^2\Sigma^+$ of HeH",
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J. Phys. Chem. 91, 2233 (1987).
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A. Metropoulos,
Z. Naturforsch. A 42, 731 (1987).
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- A. Metropoulos, C.A. Nicolaides and R.J. Buenker,
Chem. Phys. 114, 1(1987).
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A. Metropoulos and C.A. Nicolaides,
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C.A. Nicolaides and Y. Komninos,
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C.A. Nicolaides and T. Mercouris,
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Y. Komninos, M. Chrysos and C.A. Nicolaides,
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Z. Physik D 5, 1 (1987).
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A.N. Andriotis and C.A. Nicolaides,
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Synth. Met. 19, 481 (1987).
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Yiannopoulos,
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G.C. Papavassiliou, S.Y. Yiannopoulos, J.S. Zambounis, K. Kobayashi and K. Umemoto,
Chem. Lett. 7, 1279 (1987).
29. "Some new π -donors - Bis(propylene-dithio) tetrathiafulvalene, 4,5-Bis (alkylthio)-1,2-
dithiolium tTetrafluoroborates and similar compounds",
G.C. Papavassiliou, J.S. Zambounis and S.Y. Yiannopoulos,
Chem. Scripta 27, 261 (1987).

30. "Bis(Pyrazino)tetrathiafulvalene and similar π -donors",
G.C. Papavassiliou, S.Y. Yiannopoulos and J.S. Zambounis,
Chem. Scripta 27, 265 (1987).
31. "Electrical properties of α -(PEDTTTF) $_2$ BF $_4$ and α -(PEDTTTF) $_2$ IBr $_2$ ",
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Mater. Sci. 13, 185 (1987).
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G.D. Chryssikos and E.I. Kamitsos,
Solid State Commun. 63, 611 (1987).
33. "Electrical-conduction in cadmium germanate glasses",
G.D. Chryssikos, E.I. Kamitsos and J. Swiatek,
Solid State Commun. 63, 615 (1987).
34. "A Raman investigation of cadmium borate and borogermanate glasses",
G.D. Chryssikos, E.I. Kamitsos and W.M. Risen,
J. Non-Cryst. Solids 93, 155 (1987).
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S.J. Hamodrakas, E.I. Kamitsos and P.G. Papadopoulou,
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36. "Vibrational-spectra of magnesium-sodium-borate glasses . 1. Far-infrared investigation
of the cation-site interactions",
E.I. Kamitsos, G.D. Chryssikos and M.A. Karakassides,
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37. "Vibrational-spectra of magnesium-sodium-borate glasses. 2. Raman and midinfrared
investigation of the network structure",
E.I. Kamitsos, M.A. Karakassides and G.D. Chryssikos,
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38. "Cation network interactions in binary alkali-metal borate glasses - a far-infrared study",
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J. Phys. Chem. 91, 5807 (1987).
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| 2. Papers in Proceedings of International and National Conferences |
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1. "Pyrazinotetraheterofulvalenes and a few of their salts",
G.C. Papavassiliou, S.Y. Yiannopoulos and J.S. Zambounis
in "Organic and Inorganic Low Dimensional Crystalline Materials", Ed. P. Delhaes, Plenum
(NATO SERIES) 168, 305 (1987).
2. "Conducting solids based on some new molecules with isothiazolo-rings",
G.C. Papavassiliou, G.C. Mousdis, J.S. Zambounis and S.Y. Yiannopoulos
in "Organic and Inorganic Low Dimensional Crystalline Materials", Ed. P. Delhaes, Plenum
(NATO SERIES) 168, 301 (1987).
3. "New highly conducting systems",
H.J. Keller, G.C. Papavassiliou et al,
in "Organic and Inorganic Low-Dimensional Crystalline Materials", Edited by P. Delhaes and
M. Drillon, Plenum (NATO SERIES) 168, 457 (1987).

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| 3. Dissertations |
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a. PhD theses

1. "Nitrogen containing tetrathiafulvalens, selenium analogues and their conducting salts",
S.Y. Yiannopoulos, supervisor G.C. Papavassiliou, University of Athens (1987).
2. "Conducting compounds resulting from multisulfur π -Donors and π -Acceptors",
J.S. Zambounis, supervisor G.C. Papavassiliou, University of Athens (1987).

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