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AlOX(X=F,Cl,Br,I) AlOX (X=F, Cl, Br, I)	**Aluminum oxyhalides** Z. Varga, M. Hargittai Quantum chemical calculations, thermodynamic study Struct. Chem. **19** (2008)
C_2Th ThC_2	**Thorium dicarbid** A. Kovacs, R. J. M. Konings Quantum chemical calculations, thermodynamic study J. Nuclear Materials, accepted
C_4Th ThC_4	**Thorium tetracarbid** A. Kovacs, R. J. M. Konings Quantum chemical calculations, thermodynamic study J. Nuclear Materials, accepted
C_7H_5N	**Cyanobenzene** A. R. Campanelli, A. Domenicano, F. Ramondo, I. Hargittai Structure from ED, quantum chemical calculations J. Phys. Chem. A **112** (2008), 10998-11008
$C_8H_4N_2$	**1,4-Dicyanobenzene** A. R. Campanelli, A. Domenicano, F. Ramondo, I. Hargittai Structure from ED, quantum chemical calculations J. Phys. Chem. A **112** (2008), 10998-11008
$C_{10}H_2N_4$	**1,2,4,5-Tetracyanobenzene**

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Cl_2Cr $CrCl_2$	**Chromium dichloride** B. Vest, Z. Varga, M. Hargittai, A. Hermann, P. Schwerdtfeger Structure from ED, quantum chemical calculations, reinvestigation Chem. Eur. J. **14** (2008), 5130-5143
Cl_3Dy $DyCl_3$	**Dysprosium trichloride** G. Lanza, Z. Varga, M. Kolonits, M. Hargittai Structure from ED, quantum chemical calculations J. Chem. Phys. **128** (2008), 74301
CrF_2 CrF_2	**Chromium difluoride** B. Vest, P. Schwerdtfeger, M. Kolonits, M. Hargittai Structure from ED, quantum chemical calculations, reinvestigation Chem. Phys. Lett. (2008), in press
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	Mercury dihalides K. J. Donald, M. Hargittai, R. Hoffmann Quantum chemical calculations Chem. Eur. J. **15** (2008), 158-177
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