Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information.

Thermal stability and structures of the gaseous GeB_2O_4 and $GeMo_2O_7$

Sergey I. Lopatin,* Andrej I. Panin, Sergey M. Shugurov and Ksenia A. Emelyanova

Table S1. Cartesian coordinates (Å) and harmonic frequencies (cm^{-1}) corresponding to the equilibrium geometry of energetically favorable isomer of GeB_2O_4 calculated at MP2 and DFT M06 levels of theory.

$GeB_2O_4(C_s)$							
MP2				DFT M06			
O	0.063565410	0.915876040	0.000000000	O	0.653140000	-0.659239000	0.000000000
B	0.506896260	-0.408275920	0.000000000	B	0.000000000	0.554789000	0.000000000
O	1.827327700	-0.802957450	0.000000000	O	0.619485000	1.775523000	0.000000000
B	2.917379560	-0.038021160	0.000000000	B	1.889499000	2.111226000	0.000000000
O	3.960567340	0.603545320	0.000000000	O	3.038568000	2.484895000	0.000000000
Ge	-1.656177340	0.194268150	0.000000000	Ge	-1.031667000	-1.416261000	0.000000000
O	-0.554677110	-1.307731730	0.000000000	O	-1.365462000	0.397604000	0.000000000
Harmonic frequencies				Harmonic frequencies			
60 (A")				63 (A")			
76 (A')				68 (A')			
141 (A")				143 (A")			
337 (A')				337 (A')			
402 (A')				401 (A')			
515 (A')				524 (A')			
525 (A")				532 (A")			
580 (A')				584 (A')			
680 (A")				689 (A")			
710 (A')				716 (A')			
842 (A')				873 (A')			
1073 (A')				1126 (A')			
1205 (A')				1242 (A')			
1432 (A')				1452 (A')			
2052 (A')				2123 (A')			

Table S2. Cartesian coordinates (Å) and harmonic frequencies (cm^{-1}) corresponding to the equilibrium geometry of energetically favorable isomer of $GeMoO_4$ calculated at MP2 and DFT M06 levels of theory.

$GeMoO_4$ (C_{2v})							
MP2				DFT M06			
O	0.000000000	1.392710130	1.934309499	O	0.000000000	1.372807000	1.853963000
O	-1.325903465	0.000000000	-0.503480711	O	-1.286470000	0.000000000	-0.507444000
O	0.000000000	-1.392710130	1.934309499	O	0.000000000	-1.372807000	1.853963000
Mo	0.000000000	0.000000000	0.906481324	Mo	0.000000000	0.000000000	0.883741000
O	1.325903465	0.000000000	-0.503480711	O	1.286470000	0.000000000	-0.507444000
Ge	0.000000000	0.000000000	-1.819778206	Ge	0.000000000	0.000000000	-1.833170000
Harmonic frequencies				Harmonic frequencies			
111 (B_2) 199 (B_1) 231 (A_2) 260 (A_1) 289 (B_2) 353 (A_1) 384 (B_1) 629 (A_1) 655 (B_1) 687 (A_1) 903 (B_2) 939 (A_1)				120 (B_2) 231 (B_1) 255 (A_2) 274 (A_1) 320 (B_2) 377 (A_1) 406 (B_1) 636 (A_1) 691 (B_1) 754 (A_1) 1017 (B_2) 1041 (A_1)			

Table S3. Cartesian coordinates (Å) and harmonic frequencies (cm^{-1}) corresponding to the equilibrium geometry of energetically favorable isomer of $GeMo_2O_7$ calculated at MP2 and DFT M06 levels of theory.

$GeMo_2O_7$ (C_{2v})							
MP2				DFT M06			
Mo	0.000000000	1.717842923	-0.637576189	Mo	0.000000000	1.730010000	-0.617543000
Mo	0.000000000	-1.717842923	-0.637576189	Mo	0.000000000	-1.730010000	-0.617543000
O	1.372655715	2.659505545	-1.100799438	O	1.355807000	2.607701000	-1.061329000
O	1.372655715	-2.659505545	-1.100799438	O	1.355807000	-2.607701000	-1.061329000
O	0.000000000	1.390132174	1.244839620	O	0.000000000	1.359585000	1.216671000
O	0.000000000	-1.390132174	1.244839620	O	0.000000000	-1.359585000	1.216671000
O	0.000000000	0.000000000	-1.487753785	O	0.000000000	0.000000000	-1.378570000
O	-1.372655715	2.659505545	-1.100799438	O	-1.355807000	2.607701000	-1.061329000
O	-1.372655715	-2.659505545	-1.100799438	O	-1.355807000	-2.607701000	-1.061329000
Ge	0.000000000	0.000000000	2.424822351	Ge	0.000000000	0.000000000	2.418685000
Harmonic frequencies				Harmonic frequencies			
12 (B_1) 27 (A_2) 68 (B_1) 119 (B_2) 141 (A_1) 167 (A_2)				38 (B_1) 41 (A_2) 75 (B_1) 142 (B_2) 156 (A_1) 184 (A_2)			

183 (A_1)	202 (A_1)
218 (B_2)	238 (B_2)
233 (A_1)	253 (A_1)
237 (A_2)	266 (A_2)
243 (B_1)	274 (B_1)
267 (B_1)	306 (B_1)
322 (A_1)	350 (A_1)
326 (B_2)	355 (B_2)
432 (B_2)	437 (B_2)
435 (A_1)	451 (A_1)
519 (A_1)	534 (A_1)
603 (B_2)	635 (B_2)
825 (B_2)	861 (B_2)
852 (A_1)	869 (A_1)
902 (A_2)	1023 (A_2)
903 (B_1)	1028 (B_1)
944 (B_2)	1050 (B_2)
945 (A_1)	1061 (A_1)