Oxidizing Metal Oxides with Polynuclear Superhalogen: An *ab Initio* Study

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SUPPLEMENTARY MATERIALS

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Table S1. The MP2/6-311+G(d) geometrical parameters for the CoO/Mg_3F_7 compounds. E_R in kcal/mol, bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

Species	Geometrical parameters			
1 $CoOMg_3F_7$ (C_1) E_R=0.00	$r(Mg_1\text{-}F_1)$=1.802	$r(Mg_3\text{-}F_4)$=1.896	$\alpha(Mg_2F_7Co)$=128.99	$\alpha(F_5CoO)$=140.57
	$r(Mg_1\text{-}F_{2,4})$=1.991	$r(Mg_3\text{-}F_5)$=1.920	$\alpha(F_1Mg_1F_4)$=122.25	$\alpha(F_6CoO)$=163.03
	$r(Mg_1\text{-}F_3)$=2.074	$r(Mg_3\text{-}F_6)$=1.894	$\alpha(Mg_1F_2Mg_2)$=102.03	$\alpha(F_7CoO)$=96.68
	$r(Mg_2\text{-}F_2)$=1.896	$r(Co\text{-}F_6)$=1.956	$\alpha(Mg_1F_3Mg_2)$=95.70	$\omega(F_1Mg_1F_2Mg_2)$=142.65
	$r(Mg_2\text{-}F_3)$=2.001	$r(Co\text{-}F_7)$=1.877	$\alpha(Mg_1F_4Mg_3)$=102.05	$\omega(F_1Mg_1F_3Mg_3)$=134.42
	$r(Mg_2\text{-}F_5)$=1.919	r(Co-O)=1.551	$\alpha(Mg_2F_5Mg_3)$=95.26	$\omega(F_2Mg_2F_7Co)$=121.58
	$r(Mg_2\text{-}F_7)$=1.898	$\alpha(F_1Mg_1F_2)$=122.52	$\alpha(Mg_2F_5Co)$=70.87	$\omega(Mg_2F_7CoO)$=177.69
	$r(Mg_3\text{-}F_3)$=2.003	$\alpha(F_1Mg_1F_3)$=129.31		
2 $CoOMg_3F_7$ (C_1) E_R=0.01	$r(Mg_1\text{-}F_1)$=1.802	$r(Mg_3\text{-}F_3)$=2.000	$\alpha(F_1Mg_1F_2)$=122.20	$\alpha(Mg_2F_7Co)$=127.38
	$r(Mg_1\text{-}F_{2,4})$=1.991	$r(Mg_3\text{-}F_4)$=1.896	$\alpha(F_1Mg_1F_3)$=129.23	$\alpha(Mg_3F_6Co)$=129.06
	$r(Mg_1\text{-}F_3)$=2.074	$r(Mg_3\text{-}F_5)$=1.919	$\alpha(F_1Mg_1F_4)$=122.63	$\alpha(F_6CoO)$=96.65
	$r(Mg_2\text{-}F_2)$=1.896	$r(Mg_3\text{-}F_6)$=1.898	$\alpha(Mg_1F_2Mg_2)$=102.03	$\omega(F_1Mg_1F_2Mg_2)$=142.45
	$r(Mg_2\text{-}F_3)$=2.004	$r(Co\text{-}F_6)$=1.877	$\alpha(Mg_1F_3Mg_2)$=95.63	$\omega(F_1Mg_1F_3Mg_3)$=134.88
	$r(Mg_2\text{-}F_5)$=1.920	$r(Co\text{-}F_7)$=1.956	$\alpha(Mg_1F_4Mg_3)$=102.05	$\omega(F_2Mg_2F_7Co)$=120.87
	$r(Mg_2\text{-}F_7)$=1.893	r(Co-O)=1.551	$\alpha(Mg_2F_5Mg_3)$=95.26	$\omega(Mg_3F_7CoO)$=176.91
3 $CoOMg_3F_7$ (C_s) E_R=0.97	$r(Mg_1\text{-}F_1)$=1.789	$r(Mg_3\text{-}F_6)$=1.927	$\alpha(F_1Mg_1F_3)$=139.19	$\alpha(F_6CoO)$=105.52
	$r(Mg_1\text{-}F_2)$=1.922	$r(Mg_3\text{-}F_7)$=1.914	$\alpha(Mg_1F_2Mg_2)$=98.65	$\alpha(F_7CoO)$=171.92
	$r(Mg_1\text{-}F_3)$=1.923	$r(Co\text{-}F_6)$=1.859	$\alpha(F_2Mg_2F_{4,5})$=124.88	$\omega(F_1Mg_1F_2Mg_2)$=180.00
	$r(Mg_2\text{-}F_{2,3})$=1.932	$r(Co\text{-}F_7)$=1.930	$\alpha(Mg_2F_{4,5}Mg_3)$=98.09	$\omega(F_2Mg_2F_5Mg_3)$=127.40
	$r(Mg_2\text{-}F_{4,5})$=1.922	r(Co-O)=1.556	$\alpha(F_{4,5}Mg_3F_6)$=124.50	$\omega(F_5Mg_3F_6Co)$=127.49
	$r(Mg_3\text{-}F_{4,5})$=1.931	$\alpha(F_1Mg_1F_2)$=139.25	$\alpha(Mg_3F_6Co)$=99.10	$\omega(Mg_3F_6CoO)$=180.00
4 $CoOMg_3F_7$ (C_1) E_R=1.18	$r(Mg_1\text{-}F_1)$=1.799	$r(Mg_3\text{-}F_3)$=1.998	$\alpha(F_1Mg_1F_2)$=123.67	$\alpha(Mg_2F_7Co)$=104.31
	$r(Mg_1\text{-}F_2)$=1.981	$r(Mg_3\text{-}F_4)$=1.891	$\alpha(F_1Mg_1F_3)$=128.00	$\alpha(F_5CoO)$=142.35
	$r(Mg_1\text{-}F_3)$=2.105	$r(Mg_3\text{-}F_5)$=1.974	$\alpha(F_1Mg_1F_4)$=123.95	$\alpha(F_6CoO)$=141.73
	$r(Mg_1\text{-}F_4)$=1.979	$r(Mg_3\text{-}F_6)$=1.866	$\alpha(Mg_1F_2Mg_2)$=103.08	$\alpha(F_7CoO)$=95.04
	$r(Mg_2\text{-}F_2)$=1.889	$r(Co\text{-}F_5)$=2.220	$\alpha(Mg_1F_3Mg_2)$=95.44	$\omega(F_1Mg_1F_2Mg_2)$=137.70
	$r(Mg_2\text{-}F_3)$=1.990	$r(Co\text{-}F_6)$=2.067	$\alpha(Mg_1F_4Mg_3)$=103.39	$\omega(F_1Mg_1F_3Mg_3)$=132.59
	$r(Mg_2\text{-}F_5)$=1.967	$r(Co\text{-}F_7)$=1.940	$\alpha(Mg_2F_5Mg_3)$=95.77	$\omega(F_4Mg_3F_5Co)$=175.38
	$r(Mg_2\text{-}F_7)$=1.881	r(Co-O)=1.536	$\alpha(Mg_2F_5Co)$=92.04	$\omega(Mg_3F_5CoO)$=174.92
5 $CoOMg_3F_7$ (C_1) E_R=4.26	$r(Mg_1\text{-}F_1)$=1.800	$r(Mg_3\text{-}F_4)$=1.891	$\alpha(F_1Mg_1F_{2,4})$=123.99	$\alpha(F_5CoO)$=178.34
	$r(Mg_1\text{-}F_{2,4})$=1.975	$r(Mg_3\text{-}F_6)$=1.870	$\alpha(Mg_1F_2Mg_2)$=103.41	$\alpha(F_{6,7}CoO)$=101.73
	$r(Mg_1\text{-}F_3)$=2.104	$r(Co\text{-}F_5)$=2.188	$\alpha(Mg_1F_3Mg_2)$=103.41	$\omega(F_1Mg_1F_2Mg_2)$=136.09
	$r(Mg_2\text{-}F_2)$=1.891	$r(Co\text{-}F_{6,7})$=1.870	$\alpha(Mg_1F_3Mg_{2,3})$=95.11	$\omega(F_1Mg_1F_3Mg_3)$=132.08
	$r(Mg_{2,3}\text{-}F_3)$=2.007	r(Co-O)=1.666	$\alpha(Mg_2F_5Mg_3)$=98.01	$\omega(F_4Mg_3F_5Co)$=168.35
	$r(Mg_{2,3}\text{-}F_5)$=1.966	$\alpha(F_1Mg_1F_3)$=127.24	$\alpha(Mg_{2,3}F_5Co)$=88.93	$\omega(Mg_3F_5CoO)$=130.83
	$r(Mg_2\text{-}F_7)$=1.870	$\alpha(Mg_2F_7Co)$=95.62		
6 $CoOMg_3F_7$ (C_1) E_R=10.03	$r(Mg_1\text{-}F_1)$=1.791	$r(Mg_3\text{-}F_3)$=1.973	$\alpha(F_1Mg_1F_2)$=128.68	$\alpha(Mg_2F_5Co)$=94.85
	$r(Mg_1\text{-}F_2)$=1.920	$r(Mg_3\text{-}F_4)$=1.931	$\alpha(F_1Mg_1F_4)$=135.25	$\alpha(Mg_2F_7Co)$=103.02
	$r(Mg_1\text{-}F_4)$=1.887	$r(Mg_3\text{-}F_5)$=2.076	$\alpha(Mg_1F_2Mg_2)$=125.32	$\alpha(F_5CoO)$=172.20
	$r(Mg_2\text{-}F_2)$=1.883	$r(Mg_3\text{-}F_6)$=1.800	$\alpha(Mg_1F_4Mg_3)$=141.38	$\omega(F_1Mg_1F_2Mg_2)$=174.55
	$r(Mg_2\text{-}F_3)$=1.888	$r(Co\text{-}F_5)$=1.969	$\alpha(Mg_2F_3Mg_3)$=99.73	$\omega(Mg_1F_2Mg_2F_7)$=136.07
	$r(Mg_2\text{-}F_5)$=2.035	$r(Co\text{-}F_7)$=1.862	$\alpha(Mg_2F_5Mg_3)$=91.79	$\omega(F_4Mg_3F_5Co)$=175.18
	$r(Mg_2\text{-}F_7)$=1.906	r(Co-O)=1.539	$\alpha(F_4Mg_3F_6)$=132.50	$\omega(Mg_3F_5CoO)$=77.99

7 $CoOMg_3F_7$ (C_1) E_R=13.72	$r(Mg_1\text{-}F_1)$=1.797 $r(Mg_1\text{-}F_2)$=1.953 $r(Mg_{1,3}\text{-}F_3)$=2.232 $r(Mg_{1,3}\text{-}F_4)$=1.914 $r(Mg_2\text{-}F_{2,5})$=1.876 $r(Mg_2\text{-}F_3)$=2.124 $r(Mg_2\text{-}F_7)$=1.902	$r(Mg_3\text{-}F_6)$=1.797 $r(Co\text{-}F_3)$=1.999 $r(Co\text{-}F_7)$=1.860 r(Co-O)=1.531 $\alpha(F_1Mg_1F_2)$=123.86 $\alpha(F_1Mg_1F_3)$=113.97	$\alpha(F_1Mg_1F_4)$=135.46 $\alpha(Mg_1F_2Mg_2)$=106.66 $\alpha(Mg_1F_3Mg_3)$=91.48 $\alpha(Mg_1F_4Mg_3)$=113.28 $\alpha(Mg_2F_5Mg_3)$=106.66 $\alpha(Mg_2F_3Co)$=93.34 $\alpha(Mg_2F_7Co)$=105.78	$\alpha(F_3CoO)$=171.92 $\alpha(F_7CoO)$=105.51 $\omega(F_1Mg_1F_2Mg_2)$=123.25 $\omega(Mg_1F_4Mg_3F_6)$=116.24 $\omega(Mg_1F_3Mg_2F_7)$=134.24 $\omega(F_3Mg_2F_7Co)$=0.00 $\omega(Mg_1F_3CoO)$=87.27
8 $CoOMg_3F_7$ (C_s) E_R=24.58	$r(Mg_1\text{-}F_1)$=1.783 $r(Mg_1\text{-}F_{2,4})$=1.997 $r(Mg_1\text{-}F_3)$=2.058 $r(Mg_2\text{-}F_2)$=1.999 $r(Mg_{2,3}\text{-}F_3)$=2.033 $r(Mg_{2,3}\text{-}F_5)$=2.028	$r(Mg_2\text{-}F_7)$=1.782 $r(Mg_3\text{-}F_6)$=1.782 $r(Co\text{-}F_{2,4})$=2.109 $r(Co\text{-}F_5)$=1.971 r(Co-O)=1.513 $\alpha(F_1Mg_1F_{2,4})$=133.06	$\alpha(F_1Mg_1F_3)$=130.79 $\alpha(Mg_1F_2Mg_2)$=101.92 $\alpha(Mg_1F_3Mg_3)$=101.92 $\alpha(Mg_1F_3Mg_{2,3})$=98.68 $\alpha(F_3Mg_{2,3}F_5)$=79.25 $\alpha(Mg_{2,3}F_5Co)$=99.80	$\alpha(F_{2,4}CoO)$=141.88 $\omega(F_1Mg_1F_2Mg_2)$=127.08 $\omega(Mg_1F_3Mg_2F_7)$=131.32 $\omega(Mg_1F_4Mg_3F_6)$=130.63 $\omega(F_1Mg_1F_4Co)$=134.18 $\omega(Mg_1F_2CoO)$=172.95
9 $CoOMg_3F_7$ (C_s) E_R=26.83	$r(Mg_1\text{-}F_1)$=1.879 $r(Mg_1\text{-}F_2)$=1.934 $r(Mg_1\text{-}F_4)$=1.935 $r(Mg_{1,3}\text{-}F_3)$=1.982 $r(Mg_2\text{-}F_{2,6})$=2.001 $r(Mg_2\text{-}F_{4,5})$=2.003 $r(Mg_2\text{-}F_3)$=2.144	$r(Mg_3\text{-}F_5)$=1.935 $r(Mg_3\text{-}F_6)$=1.934 $r(Mg_3\text{-}F_7)$=1.898 $r(Co\text{-}F_3)$=2.146 $r(Co\text{-}F_{1,7})$=2.146 r(Co-O)=1.536	$\alpha(F_1Mg_1F_2)$=136.43 $\alpha(F_1Mg_1F_4)$=138.43 $\alpha(Mg_1F_2Mg_2)$=84.89 $\alpha(Mg_1F_4Mg_2)$=84.81 $\alpha(Mg_1F_3Mg_3)$=160.04 $\alpha(F_2Mg_2F_6)$=97.32 $\alpha(F_4Mg_2F_5)$=98.03	$\alpha(Mg_1F_1Co)$=103.41 $\alpha(Mg_2F_3Co)$=176.97 $\alpha(F_3CoO)$=177.17 $\omega(F_1Mg_1F_4Mg_2)$=116.65 $\omega(Mg_1F_2Mg_2F_6)$=117.07 $\omega(F_2Mg_2F_3Co)$=49.97 $\omega(Mg_1F_1CoO)$=178.72

Table S2. The MP2/6-311+G(d) geometrical parameters for the MeO/Mg_3F_7 (Me=Ni, Cu) compounds. E_R in kcal/mol, bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

Species	Geometrical parameters			
1 $NiOMg_3F_7$ (C_1) E_R=0.00	$r(Mg_1\text{-}F_1)$=1.797 $r(Mg_1\text{-}F_2)$=1.976 $r(Mg_1\text{-}F_3)$=2.123 $r(Mg_1\text{-}F_4)$=1.979 $r(Mg_2\text{-}F_2)$=1.887 $r(Mg_2\text{-}F_3)$=1.995 $r(Mg_2\text{-}F_5)$=1.996 $r(Mg_2\text{-}F_7)$=1.876	$r(Mg_3\text{-}F_3)$=1.984 $r(Mg_3\text{-}F_4)$=1.885 $r(Mg_3\text{-}F_5)$=1.989 $r(Mg_3\text{-}F_6)$=1.884 $r(Ni\text{-}F_5)$=2.143 $r(Ni\text{-}F_{6,7})$=2.009 r(Ni-O)=1.823	$\alpha(F_1Mg_1F_2)$=124.75 $\alpha(F_1Mg_1F_3)$=126.99 $\alpha(F_1Mg_1F_4)$=124.10 $\alpha(Mg_1F_2Mg_2)$=104.07 $\alpha(Mg_1F_3Mg_2)$=95.31 $\alpha(Mg_1F_4Mg_3)$=103.60 $\alpha(Mg_2F_5Mg_3)$=95.64 $\alpha(Mg_2F_5Ni)$=95.18	$\alpha(Mg_2F_7Ni)$=103.76 $\alpha(F_7NiO)$=107.31 $\alpha(F_5NiO)$=137.01 $\alpha(F_6NiO)$=137.53 $\omega(F_1Mg_1F_2Mg_2)$=135.13 $\omega(F_1Mg_1F_3Mg_3)$=131.52 $\omega(F_4Mg_3F_5Ni)$=177.85 $\omega(Mg_3F_5NiO)$=156.07
2 $NiOMg_3F_7$ (C_1) E_R=$1.3\cdot10^{-4}$	$r(Mg_1\text{-}F_1)$=1.797 $r(Mg_1\text{-}F_2)$=1.979 $r(Mg_1\text{-}F_3)$=2.124 $r(Mg_1\text{-}F_4)$=1.976 $r(Mg_2\text{-}F_2)$=1.885 $r(Mg_2\text{-}F_3)$=1.984 $r(Mg_2\text{-}F_5)$=1.989 $r(Mg_2\text{-}F_7)$=1.885	$r(Mg_3\text{-}F_3)$=1.995 $r(Mg_3\text{-}F_4)$=1.887 $r(Mg_3\text{-}F_5)$=1.996 $r(Mg_3\text{-}F_6)$=1.876 $r(Ni\text{-}F_5)$=2.143 $r(Ni\text{-}F_6)$=2.010 $r(Ni\text{-}F_7)$=2.009 r(Ni-O)=1.823	$\alpha(F_1Mg_1F_2)$=124.14 $\alpha(F_1Mg_1F_3)$=127.01 $\alpha(F_1Mg_1F_4)$=124.67 $\alpha(Mg_1F_2Mg_2)$=103.60 $\alpha(Mg_1F_3Mg_2)$=95.28 $\alpha(Mg_1F_4Mg_3)$=104.09 $\alpha(Mg_2F_5Mg_3)$=95.64 $\alpha(Mg_2F_5Ni)$=96.20	$\alpha(Mg_2F_7Ni)$=104.36 $\alpha(F_7NiO)$=137.51 $\alpha(F_5NiO)$=137.03 $\alpha(F_6NiO)$=137.32 $\omega(F_1Mg_1F_2Mg_2)$=135.29 $\omega(F_1Mg_1F_3Mg_3)$=131.99 $\omega(F_4Mg_3F_5Ni)$=178.31 $\omega(Mg_3F_5NiO)$=107.71
3 $NiOMg_3F_7$ (C_1) E_R=5.18	$r(Mg_1\text{-}F_1)$=1.797 $r(Mg_1\text{-}F_2)$=1.979 $r(Mg_1\text{-}F_3)$=2.122 $r(Mg_1\text{-}F_4)$=1.976 $r(Mg_2\text{-}F_2)$=1.885 $r(Mg_2\text{-}F_3)$=1.987 $r(Mg_2\text{-}F_5)$=1.983 $r(Mg_2\text{-}F_7)$=1.884	$r(Mg_3\text{-}F_3)$=1.997 $r(Mg_3\text{-}F_4)$=1.887 $r(Mg_3\text{-}F_5)$=1.990 $r(Mg_3\text{-}F_6)$=1.874 $r(Ni\text{-}F_5)$=2.174 $r(Ni\text{-}F_6)$=2.008 $r(Ni\text{-}F_7)$=2.003 r(Ni-O)=1.779	$\alpha(F_1Mg_1F_2)$=124.07 $\alpha(F_1Mg_1F_3)$=127.17 $\alpha(F_1Mg_1F_4)$=124.64 $\alpha(Mg_1F_2Mg_2)$=103.59 $\alpha(Mg_1F_3Mg_2)$=95.23 $\alpha(Mg_1F_4Mg_3)$=104.02 $\alpha(Mg_2F_5Mg_3)$=96.12 $\alpha(Mg_2F_5Ni)$=95.53	$\alpha(Mg_2F_7Ni)$=104.78 $\alpha(F_7NiO)$=132.69 $\alpha(F_6NiO)$=104.56 $\omega(F_1Mg_1F_2Mg_2)$=135.53 $\omega(F_1Mg_1F_3Mg_3)$=132.04 $\omega(F_4Mg_3F_5Ni)$=177.07 $\omega(Mg_3F_5NiO)$=103.88
4 $NiOMg_3F_7$ (C_{2V})E_R=8.07	$r(Mg_1\text{-}F_1)$=1.788 $r(Mg_1\text{-}F_{2,3})$=1.924 $r(Mg_2\text{-}F_{2,3})$=1.930 $r(Mg_2\text{-}F_{4,5})$=1.927	$r(Mg_3\text{-}F_{4,5})$=1.924 $r(Mg_3\text{-}F_{6,7})$=1.934 $r(Ni\text{-}F_{6,7})$=1.837 r(Ni-O)=1.642	$\alpha(F_1Mg_1F_{2,3})$=139.26 $\alpha(Mg_1F_{2,3}Mg_2)$=98.67 $\alpha(F_{2,3}Mg_2F_{4,5})$=125.04 $\alpha(Mg_2F_{4,5}Mg_3)$=98.19 $\alpha(F_{4,5}Mg_3F_{6,7})$=125.61 $\alpha(Mg_3F_{6,7}Ni)$=98.31	$\alpha(F_{6,7}NiO)$=137.89 $\omega(F_1Mg_1F_2Mg_2)$=180.00 $\omega(F_2Mg_2F_5Mg_3)$=127.37 $\omega(F_4Mg_3F_6Ni)$=126.30 $\omega(Mg_3F_6NiO)$=180.00
5 $NiOMg_3F_7$ (C_1) E_R=13.94	$r(Mg_1\text{-}F_1)$=1.795 $r(Mg_1\text{-}F_2)$=1.970 $r(Mg_1\text{-}F_3)$=2.198 $r(Mg_1\text{-}F_4)$=1.930 $r(Mg_2\text{-}F_2)$=1.866 $r(Mg_2\text{-}F_3)$=1.941 $r(Mg_2\text{-}F_5)$=2.023 $r(Mg_2\text{-}F_7)$=1.909	$r(Mg_3\text{-}F_3)$=2.065 $r(Mg_3\text{-}F_4)$=1.910 $r(Mg_3\text{-}F_5)$=2.056 $r(Mg_3\text{-}F_6)$=1.793 $r(Ni\text{-}F_5)$=1.999 $r(Ni\text{-}F_7)$=1.920 r(Ni-O)=1.781	$\alpha(F_1Mg_1F_2)$=124.35 $\alpha(F_1Mg_1F_3)$=124.12 $\alpha(F_1Mg_1F_4)$=131.87 $\alpha(Mg_1F_2Mg_2)$=102.77 $\alpha(Mg_1F_3Mg_2)$=92.62 $\alpha(Mg_1F_4Mg_3)$=109.11 $\alpha(Mg_2F_5Mg_3)$=97.41 $\alpha(Mg_2F_5Ni)$=96.82	$\alpha(Mg_2F_7Ni)$=103.55 $\alpha(F_7NiO)$=151.67 $\alpha(F_5NiO)$=120.56 $\omega(F_1Mg_1F_2Mg_2)$=131.38 $\omega(F_1Mg_1F_3Mg_3)$=128.90 $\omega(F_4Mg_3F_5Ni)$=179.23 $\omega(Mg_3F_5NiO)$=44.88
6 $NiOMg_3F_7$ (C_s) E_R=16.29	$r(Mg_1\text{-}F_1)$=1.801 $r(Mg_1\text{-}F_{2,4})$=1.975 $r(Mg_1\text{-}F_3)$=2.107 $r(Mg_2\text{-}F_2)$=1.891 $r(Mg_{2,3}\text{-}F_3)$=2.010 $r(Mg_{2,3}\text{-}F_5)$=1.955	$r(Mg_2\text{-}F_7)$=1.878 $r(Mg_3\text{-}F_4)$=1.891 $r(Mg_3\text{-}F_6)$=1.878 $r(Ni\text{-}F_5)$=2.301 $r(Ni\text{-}F_{6,7})$=2.028 r(Ni-O)=1.684	$\alpha(F_1Mg_1F_{2,4})$=123.57 $\alpha(F_1Mg_1F_3)$=127.87 $\alpha(Mg_1F_2Mg_2)$=103.39 $\alpha(Mg_1F_3Mg_{2,3})$=94.91 $\alpha(Mg_1F_4Mg_3)$=103.39 $\alpha(Mg_2F_5Mg_3)$=98.73 $\alpha(Mg_{2,3}F_5Ni)$=86.70	$\alpha(Mg_2F_7Ni)$=97.22 $\alpha(F_{6,7}NiO)$=103.71 $\omega(F_1Mg_1F_2Mg_2)$=137.35 $\omega(F_1Mg_1F_3Mg_3)$=132.23 $\omega(F_4Mg_3F_5Ni)$=166.35 $\omega(Mg_3F_5NiO)$=130.52

7 $NiOMg_3F_7$ (C_S) E_R=19.14	r(Mg_1-F_1)=1.796 r(Mg_1-F_2)=1.954 r($Mg_{1,3}$-F_3)=2.232 r($Mg_{1,3}$-F_4)=1.913 r(Mg_2-$F_{2,5}$)=1.874 r(Mg_2-F_3)=2.136 r(Mg_2-F_7)=1.900	r(Mg_3-F_5)=1.954 r(Mg_3-F_6)=1.796 r(Ni-F_3)=2.004 r(Ni-F_7)=1.916 r(Ni-O)=1.751 α($F_1Mg_1F_2$)=121.95 α($F_1Mg_1F_3$)=112.34	α($F_1Mg_1F_4$)=137.34 α($Mg_1F_2Mg_2$)=106.86 α($Mg_1F_3Mg_3$)=89.46 α($Mg_1F_4Mg_3$)=113.15 α($Mg_2F_5Mg_3$)=106.86 α(Mg_2F_3Ni)=95.45 α(Mg_2F_7Ni)=106.83	α(F_3NiO)=131.15 α(F_7NiO)=148.52 ω($F_1Mg_1F_2Mg_2$)=121.24 ω($Mg_1F_4Mg_3F_6$)=114.91 ω($Mg_1F_2Mg_2F_5$)=67.41 ω($F_2Mg_2F_7Ni$)=73.60 ω(Mg_2F_7NiO)=180.00
8 $NiOMg_3F_7$ (C_S) E_R=22.29	r(Mg_1-F_1)=1.907 r(Mg_1-F_2)=1.935 r(Mg_1-F_4)=1.918 r($Mg_{1,3}$-F_3)=2.024 r(Mg_2-$F_{2,6}$)=2.010 r(Mg_2-$F_{4,5}$)=1.998 r(Mg_2-F_3)=2.158	r(Mg_3-F_5)=1.918 r(Mg_3-F_6)=1.935 r(Mg_3-F_7)=1.907 r(Ni-F_3)=1.919 r(Ni-$F_{1,7}$)=1.927 r(Ni-O)=1.706	α($F_1Mg_1F_2$)=142.61 α($F_1Mg_1F_4$)=127.16 α($Mg_1F_2Mg_2$)=85.83 α($Mg_1F_4Mg_2$)=86.63 α($Mg_1F_3Mg_3$)=157.67 α($F_2Mg_2F_6$)=101.37 α($F_4Mg_2F_5$)=93.36	α(Mg_1F_1Ni)=102.05 α(Mg_2F_3Ni)=161.83 α(F_3NiO)=179.86 ω($F_1Mg_1F_4Mg_2$)=113.02 ω($Mg_1F_2Mg_2F_6$)=116.20 ω($F_5Mg_2F_3Ni$)=47.75 ω(Mg_1F_1NiO)=173.01
9 $NiOMg_3F_7$ (C_1) E_R=24.57	r(Mg_1-F_1)=1.779 r(Mg_1-$F_{2,3,4}$)=2.024 r(Mg_2-F_2)=2.031 r(Mg_2-F_4)=2.043 r(Mg_2-F_5)=2.015 r(Mg_2-F_7)=1.779	r(Mg_3-F_3)=2.042 r(Mg_3-F_4)=2.030 r(Mg_3-F_5)=2.016 r(Mg_3-F_6)=1.779 r(Ni-F_2)=2.048 r(Ni-F_4)=2.049 r(Ni-O)=1.804	α($F_1Mg_1F_2$)=131.78 α($F_1Mg_1F_3$)=134.64 α($F_1Mg_1F_4$)=131.92 α($Mg_1F_2Mg_2$)=100.48 α($Mg_1F_3Mg_3$)=100.07 α($Mg_1F_4Mg_3$)=100.45 α($Mg_2F_5Mg_3$)=101.29 α(Mg_2F_2Ni)=99.45	α(Mg_2F_5Ni)=99.44 α(F_2NiO)=140.13 α(F_5NiO)=115.04 ω($F_1Mg_1F_2Mg_2$)=131.18 ω($Mg_1F_3Mg_2F_7$)=126.38 ω($Mg_1F_4Mg_3F_6$)=125.38 ω($F_1Mg_1F_4Ni$)=126.80 ω(Mg_1F_2NiO)=153.58
1 $CuOMg_3F_7$ (C_S) E_R=0.00	r(Mg_1-F_1)=1.800 r(Mg_1-$F_{2,4}$)=1.992 r(Mg_1-F_3)=2.084 r(Mg_2-F_2)=1.891 r($Mg_{2,3}$-F_3)=1.998 r($Mg_{2,3}$-F_5)=1.918 r(Mg_2-F_7)=1.918	r(Mg_3-F_4)=1.891 r(Mg_3-F_6)=1.917 r(Cu-F_5)=3.483 r(Cu-$F_{6,7}$)=1.855 r(Cu-O)=1.652 α($F_1Mg_1F_{2,4}$)=122.83 α($F_1Mg_1F_3$)=129.00	α($Mg_1F_2Mg_2$)=102.39 α($Mg_1F_3Mg_2$)=95.68 α($Mg_1F_4Mg_3$)=102.38 α($Mg_2F_5Mg_3$)=95.29 α(Mg_2F_5Cu)=73.03 α(Mg_2F_7Cu)=132.32	α($F_{6,7}CuO$)=131.63 α(F_5CuO)=128.24 ω($F_1Mg_1F_2Mg_2$)=141.81 ω($F_1Mg_1F_3Mg_3$)=134.53 ω($F_4Mg_3F_5Cu$)=158.34 ω(Mg_3F_5CuO)=129.41
2 $CuOMg_3F_7$ (C_{2v}) E_R=2.64	r(Mg_1-F_1)=1.787 r(Mg_1-$F_{2,3}$)=1.925 r(Mg_2-$F_{2,3}$)=1.928 r(Mg_2-$F_{4,5}$)=1.929	r(Mg_3-$F_{4,5}$)=1.920 r(Mg_3-$F_{6,7}$)=1.940 r(Cu-$F_{6,7}$)=1.848 r(Cu-O)=1.650 α($F_1Mg_1F_{2,3}$)=139.29	α($Mg_1F_{2,3}Mg_2$)=98.67 α($F_{2,3}Mg_2F_{4,5}$)=125.09 α($Mg_2F_{4,5}Mg_3$)=98.24 α($F_{4,5}Mg_3F_{6,7}$)=126.02 α($Mg_3F_{6,7}Cu$)=100.02	α($F_{6,7}CuO$)=138.83 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($F_2Mg_2F_4Mg_3$)=127.27 ω($F_5Mg_3F_6Cu$)=125.79 ω(Mg_3F_6CuO)=180.00
3 $CuOMg_3F_7$ (C_1) E_R=12.00	r(Mg_1-F_1)=1.789 r(Mg_1-F_2)=1.924 r(Mg_1-F_4)=1.890 r(Mg_2-F_2)=1.876 r(Mg_2-F_3)=1.879 r(Mg_2-F_5)=2.078 r(Mg_2-F_7)=1.916	r(Mg_3-F_3)=1.969 r(Mg_3-F_4)=1.927 r(Mg_3-F_5)=2.133 r(Mg_3-F_6)=1.794 r(Cu-F_5)=1.868 r(Cu-F_7)=1.848 r(Cu-O)=1.634 α($F_1Mg_1F_2$)=129.26	α($F_1Mg_1F_3$)=158.08 α($F_1Mg_1F_4$)=136.32 α($Mg_1F_2Mg_2$)=125.59 α($Mg_1F_3Mg_2$)=65.16 α($Mg_1F_4Mg_3$)=144.74 α($F_4Mg_3F_6$)=133.48 α($Mg_2F_5Mg_3$)=90.35	α(Mg_2F_5Cu)=97.50 α(Mg_2F_7Cu)=104.19 α(F_5CuO)=140.05 ω($F_1Mg_1F_2Mg_2$)=174.32 ω($F_1Mg_1F_3Mg_3$)=121.22 ω($F_4Mg_3F_5Cu$)=178.24 ω(Mg_3F_5CuO)=78.58
4 $CuOMg_3F_7$ (C_1) E_R=12.93	r(Mg_1-F_1)=1.792 r(Mg_1-F_2)=2.089 r(Mg_1-F_3)=2.049 r(Mg_1-F_4)=1.905 r(Mg_2-F_2)=2.056 r(Mg_2-F_3)=1.936 r(Mg_2-F_5)=1.863 r(Mg_2-F_7)=1.909	r(Mg_3-F_3)=2.221 r(Mg_3-F_4)=1.931 r(Mg_3-F_5)=1.969 r(Mg_3-F_6)=1.794 r(Cu-F_2)=1.878 r(Cu-F_7)=1.850 r(Cu-O)=1.628 α($F_1Mg_1F_2$)=106.80	α($F_1Mg_1F_3$)=126.37 α($F_1Mg_1F_4$)=145.42 α($Mg_1F_2Mg_2$)=102.68 α($Mg_1F_3Mg_2$)=96.51 α($Mg_1F_4Mg_3$)=109.44 α($Mg_2F_5Mg_3$)=103.56 α(Mg_2F_2Cu)=97.98	α(Mg_2F_7Cu)=104.44 α(F_2CuO)=141.93 α(F_7CuO)=136.30 ω($F_1Mg_1F_2Mg_2$)=134.91 ω($F_1Mg_1F_3Mg_3$)=153.24 ω($F_1Mg_1F_2Cu$)=22.68 ω(Mg_2F_2CuO)=176.77

5 $CuOMg_3F_7$ (C_s) E_R=21.64	r(Mg_1-F_1)=1.799 r(Mg_1-$F_{2,4}$)=1.942 r(Mg_1-F_3)=2.176 r(Mg_3-F_3)=2.101 r(Mg_2-$F_{2,4}$)=1.939 r(Mg_2-$F_{5,6}$)=1.992	r(Mg_2-F_3)=2.847 r(Mg_3-$F_{5,6}$)=1.894 r(Mg_3-F_7)=1.904 r(Cu-F_3)=1.873 r(Cu-F_7)=1.852 r(Cu-O)=1.633	α($F_1Mg_1F_{2,4}$)=139.36 α($Mg_1F_{2,4}Mg_2$)=92.52 α($Mg_1F_3Mg_3$)=131.32 α($F_2Mg_2F_6$)=89.75 α($F_4Mg_2F_6$)=143.04 α(Mg_2F_3Cu)=161.75	α(Mg_3F_7Cu)=104.73 α(F_3CuO)=150.12 ω($F_1Mg_1F_4Mg_2$)=164.21 ω($Mg_1F_2Mg_2F_6$)=115.29 ω($F_6Mg_3F_3Cu$)=138.72 ω(Mg_3F_3CuO)=180.00
6 $CuOMg_3F_7$ (C_1) E_R=31.76	r(Mg_1-F_1)=1.775 r(Mg_1-$F_{2,3}$)=2.088 r(Mg_1-F_4)=1.960 r(Mg_2-F_2)=2.093 r($Mg_{2,3}$-F_4)=2.077 r($Mg_{2,3}$-F_5)=1.930	r(Mg_2-F_7)=1.781 r(Mg_3-F_6)=1.781 r(Cu-$F_{2,3}$)=1.878 r(Cu-O)=1.620 α($F_1Mg_1F_{2,3}$)=128.53 α($F_1Mg_1F_4$)=142.91	α($Mg_1F_2Mg_2$)=98.11 α($Mg_1F_3Mg_3$)=98.11 α($Mg_1F_4Mg_{2,3}$)=102.89 α($Mg_2F_5Mg_3$)=105.61 α(Mg_2F_2Cu)=112.48 α(Mg_2F_5Cu)=89.28	α($F_{2,3}CuO$)=139.46 ω($F_1Mg_1F_2Mg_2$)=140.09 ω($Mg_1F_4Mg_2F_7$)=107.45 ω($Mg_1F_3Mg_3F_6$)=112.94 ω($F_1Mg_1F_3Cu$)=105.21 ω(Mg_1F_2CuO)=155.37

Table S3. The MP2/6-311+G(d) geometrical parameters for the MeO/Mg_3F_7 (Me=Mg, Zn) species. E_R in kcal/mol, bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

Species	Geometrical parameters			
1 $MgOMg_3F_7$ (C_S) E_R=0.00	r(Mg_1-F_1)=1.797 r(Mg_1-$F_{2,4}$)=1.977 r(Mg_1-F_3)=2.128 r(Mg_2-$F_{2,7}$)=1.884 r($Mg_{2,3}$-F_3)=1.993	r($Mg_{2,3}$-F_5)=1.989 r(Mg_3-$F_{4,6}$)=1.884 r(Mg_4-F_5)=2.141 r(Mg_4-$F_{6,7}$)=1.980 r(Mg_4-O)=1.899	α($F_1Mg_1F_{2,4}$)=124.57 α($F_1Mg_1F_3$)=126.61 α($Mg_1F_2Mg_2$)=104.02 α($Mg_1F_3Mg_2$)=95.17 α($Mg_1F_4Mg_3$)=104.02 α($Mg_2F_5Mg_3$)=96.30	α($Mg_2F_7Mg_4$)=104.17 α($F_{6,7}Mg_4O$)=123.60 ω($F_1Mg_1F_2Mg_2$)=134.52 ω($F_1Mg_1F_3Mg_3$)=131.71 ω($F_4Mg_3F_6Mg_4$)=150.15 ω($Mg_2F_7Mg_4O$)=138.14
3 $MgOMg_3F_7$ (C_{2V})E_R=11.16	r(Mg_1-F_1)=1.788 r(Mg_1-$F_{2,3}$)=1.924 r(Mg_2-$F_{2,3}$)=1.930 r(Mg_2-$F_{4,5}$)=1.927 r(Mg_3-$F_{4,5}$)=1.926	r(Mg_3-$F_{6,7}$)=1.930 r(Mg_4-$F_{6,7}$)=1.926 r(Mg_4-O)=1.891 α($F_{6,7}Mg_4O$)=139.23	α($F_1Mg_1F_{2,3}$)=139.25 α($Mg_1F_{2,3}Mg_2$)=98.67 α($F_{2,3}Mg_2F_{4,5}$)=125.01 α($Mg_2F_{4,5}Mg_3$)=98.10 α($F_{4,5}Mg_3F_{6,7}$)=124.95	α($Mg_3F_{6,7}Mg_4$)=98.56 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($F_2Mg_2F_5Mg_3$)=127.42 ω($F_4Mg_3F_6Mg_4$)=126.91 ω($Mg_3F_{6,7}Mg_4O$)=180.00
4 $MgOMg_3F_7$ (C_S) E_R=16.19	r(Mg_1-F_1)=1.893 r(Mg_1-F_2)=1.942 r(Mg_1-F_4)=1.907 r($Mg_{1,3}$-F_3)=2.026 r(Mg_2-$F_{2,6}$)=1.999 r(Mg_2-$F_{4,5}$)=1.993	r(Mg_3-F_5)=1.907 r(Mg_3-F_6)=1.942 r(Mg_3-F_7)=1.893 r(Mg_4-$F_{1,7}$)=2.015 r(Mg_4-F_3)=2.045 r(Mg_4-O)=1.903	α($F_1Mg_1F_2$)=147.93 α($F_1Mg_1F_4$)=123.06 α($Mg_1F_2Mg_2$)=85.56 α($Mg_1F_4Mg_2$)=86.66 α($F_2Mg_2F_6$)=104.34 α($Mg_1F_3Mg_3$)=149.03	α($Mg_{1,3}F_3Mg_4$)=99.81 α($F_{1,7}Mg_4O$)=110.31 ω($F_1Mg_1F_4Mg_2$)=117.38 ω($F_2Mg_1F_3Mg_3$)=79.44 ω($F_6Mg_3F_3Mg_4$)=151.92 ω($Mg_3F_7Mg_4O$)=135.95
5 $MgOMg_3F_7$ (C_S)E_R=29.88	r(Mg_1-F_1)=1.778 r(Mg_1-$F_{2,4}$)=2.030 r(Mg_1-F_3)=2.029 r(Mg_2-$F_{2,5}$)=2.030 r($Mg_{2,3}$-F_3)=2.033	r(Mg_2-F_7)=1.778 r(Mg_3-$F_{4,5}$)=2.030 r(Mg_4-$F_{2,4}$)=2.038 r(Mg_4-O)=1.880 α($F_1Mg_1F_3$)=133.59	α($F_1Mg_1F_{2,4}$)=132.35 α($Mg_1F_2Mg_2$)=100.09 α($Mg_1F_3Mg_{2,3}$)=100.03 α($Mg_2F_5Mg_3$)=100.24 α($Mg_1F_{2,4}Mg_4$)=100.36	α($F_{2,3}Mg_4O$)=134.22 ω($F_1Mg_1F_2Mg_2$)=129.87 ω($F_1Mg_1F_3Mg_3$)=128.92 ω($F_1Mg_1F_4Mg_4$)=127.87 ω($Mg_1F_2Mg_4O$)=131.97
1 $ZnOMg_3F_7$ (C_1) E_R=0.00	r(Mg_1-F_1)=1.798 r(Mg_1-$F_{2,4}$)=1.980 r(Mg_1-F_3)=2.114 r(Mg_2-F_2)=1.886 r($Mg_{2,3}$-F_3)=1.994 r($Mg_{2,3}$-F_5)=1.966 r(Mg_2-F_7)=1.890	r(Mg_3-F_4)=1.886 r(Mg_3-F_6)=1.890 r(Zn-F_5)=2.330 r(Zn-$F_{6,7}$)=1.984 r(Zn-O)=1.827 α($F_1Mg_1F_{2,4}$)=124.20 α($F_1Mg_1F_3$)=127.33	α($Mg_1F_2Mg_2$)=103.55 α($Mg_1F_3Mg_2$)=95.31 α($Mg_1F_4Mg_3$)=103.55 α($Mg_2F_5Mg_3$)=96.33 α(Mg_2F_5Zn)=92.44 α(Mg_2F_7Zn)=106.86	α($F_{6,7}ZnO$)=125.43 α(F_5ZnO)=128.24 ω($F_1Mg_1F_2Mg_2$)=136.44 ω($F_1Mg_1F_3Mg_3$)=132.48 ω($F_4Mg_3F_5Zn$)=174.20 ω(Mg_3F_5ZnO)=131.78
2 $ZnOMg_3F_7$ (C_1) E_R=0.52	r(Mg_1-F_1)=1.800 r(Mg_1-$F_{2,4}$)=1.987 r(Mg_1-F_3)=2.090 r(Mg_2-F_2)=1.891 r(Mg_2-F_3)=2.002 r($Mg_{2,3}$-F_5)=1.923 r(Mg_2-F_7)=1.903	r(Mg_3-F_3)=2.003 r(Mg_3-F_4)=1.891 r(Mg_3-F_6)=1.903 r(Zn-F_5)=3.326 r(Zn-$F_{6,7}$)=1.941 r(Zn-O)=1.819 α($F_1Mg_1F_2$)=123.24 α($F_1Mg_1F_3$)=128.33	α($F_1Mg_1F_4$)=123.22 α($Mg_1F_2Mg_2$)=102.68 α($Mg_1F_3Mg_2$)=95.45 α($Mg_1F_4Mg_3$)=102.67 α($Mg_2F_5Mg_3$)=96.44 α(Mg_2F_5Zn)=75.39 α(Mg_2F_7Zn)=124.16	α(F_6ZnO)=127.72 α(F_7ZnO)=127.70 α(F_5ZnO)=151.68 ω($F_1Mg_1F_2Mg_2$)=140.10 ω($F_1Mg_1F_3Mg_3$)=133.99 ω($F_4Mg_3F_5Zn$)=158.22 ω(Mg_3F_5ZnO)=129.56
3 $ZnOMg_3F_7$ (C_{2V}) E_R=5.94	r(Mg_1-F_1)=1.788 r(Mg_1-$F_{2,3}$)=1.924 r(Mg_2-$F_{2,3}$)=1.930 r(Mg_2-$F_{4,5}$)=1.926	r(Mg_3-$F_{4,5}$)=1.927 r(Mg_3-$F_{6,7}$)=1.930 r(Zn-$F_{6,7}$)=1.939 r(Zn-O)=1.809 α($F_1Mg_1F_{2,3}$)=139.25	α($Mg_1F_{2,3}Mg_2$)=98.67 α($F_{2,3}Mg_2F_{4,5}$)=125.01 α($Mg_2F_{4,5}Mg_3$)=98.15 α($F_{4,5}Mg_3F_{6,7}$)=124.89 α($Mg_3F_{6,7}Zn$)=98.63	α($F_{6,7}ZnO$)=139.43 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($F_2Mg_2F_5Mg_3$)=127.42 ω($F_5Mg_3F_6Zn$)=127.01 ω(Mg_3F_6ZnO)=180.00

4 ZnOMg$_3$F$_7$ (C_S) E_R=16.63	r(Mg$_1$-F$_1$)=1.795 r(Mg$_1$-F$_2$)=1.952 r(Mg$_{1,3}$-F$_3$)=2.251 r(Mg$_{1,3}$-F$_4$)=1.912 r(Mg$_2$-F$_{2,5}$)=1.873 r(Mg$_2$-F$_3$)=2.148	r(Mg$_2$-F$_7$)=1.902 r(Mg$_3$-F$_5$)=1.952 r(Mg$_3$-F$_6$)=1.795 r(Zn-F$_3$)=2.015 r(Zn-F$_7$)=1.928 r(Zn-O)=1.802	α(F$_1$Mg$_1$F$_2$)=122.97 α(F$_1$Mg$_1$F$_3$)=112.16 α(F$_1$Mg$_1$F$_4$)=136.64 α(Mg$_1$F$_2$Mg$_2$)=107.42 α(Mg$_1$F$_3$Mg$_3$)=90.82 α(Mg$_1$F$_4$Mg$_3$)=113.90 α(Mg$_2$F$_5$Mg$_3$)=107.42	α(F$_{2,5}$Mg$_2$F$_7$)=121.15 α(Mg$_2$F$_7$Zn)=105.77 α(F$_7$ZnO)=142.16 ω(F$_1$Mg$_1$F$_2$Mg$_2$)=121.57 ω(Mg$_1$F$_4$Mg$_3$F$_6$)=114.27 ω(F$_2$Mg$_2$F$_7$Zn)=74.24 ω(Mg$_2$F$_{3,7}$ZnO)=180.00
5 ZnOMg$_3$F$_7$ (C_S) E_R=32.19	r(Mg$_1$-F$_1$)=1.797 r(Mg$_1$-F$_{2,4}$)=1.979 r(Mg$_1$-F$_3$)=2.122 r(Mg$_2$-F$_2$)=1.885 r(Mg$_{2,3}$-F$_3$)=1.993 r(Mg$_{2,3}$-F$_5$)=1.976	r(Mg$_2$-F$_7$)=1.893 r(Mg$_3$-F$_4$)=1.885 r(Mg$_3$-F$_6$)=1.893 r(Zn-F$_5$)=2.242 r(Zn-F$_{6,7}$)=1.973 r(Zn-O)=1.802 α(F$_1$Mg$_1$F$_{2,4}$)=124.35	α(F$_1$Mg$_1$F$_3$)=127.03 α(Mg$_1$F$_2$Mg$_2$)=103.80 α(Mg$_1$F$_3$Mg$_{2,3}$)=95.24 α(Mg$_1$F$_4$Mg$_3$)=103.80 α(Mg$_2$F$_5$Mg$_3$)=96.45 α(Mg$_{2,3}$F$_5$Zn)=93.30	α(Mg$_2$F$_7$Zn)=105.25 α(F$_{6,7}$ZnO)=124.77 ω(F$_1$Mg$_1$F$_2$Mg$_2$)=135.56 ω(F$_1$Mg$_1$F$_3$Mg$_3$)=132.07 ω(F$_4$Mg$_3$F$_5$Zn)=174.61 ω(Mg$_3$F$_5$ZnO)=131.67

Table S4. The binding energies (BE in eV, see text for definition), the charge flow values (Δq^{ESP} and ε_{SOMO} in a.u.), the spin density of the unpaired electron (localized over MeO_n molecules), HOMO-LUMO gap (GAP in eV) calculated for the MeO_n/Mg_3F_7 systems. The BE values were calculated at the CCSD(T)/6-311+G(d) for the MP2/6-311+G(d) structures (M=Co, Cu, Mn, Ti). The spin densities are the sums of the spin density population on the atoms of MeO_n molecule.

Species *(Symmetry)*	E_R	q_{Me}	Δq^{ESP}	**Spin density (MeO_n)**	**GAP**	**BE**	**VIP**
1 CoO/Mg_3F_7 *(C_1)*	0.00	1.26	0.57	-	12.593	6.18*	
2 CoO/Mg_3F_7 *(C_1)*	0.01	1.26	0.57	-	12.593	6.18*	
3 CoO/Mg_3F_7 *(C_s)*	0.97	1.23	0.53	-	12.880	5.81	10.240
4 CoO/Mg_3F_7 *(C_1)*	1.18	1.26	0.54	-	12.079	6.13*	9.732
5 CoO/Mg_3F_7 *(C_1)*	4.26	1.23	0.47	-	10.787	5.48	
6 CoO/Mg_3F_7 *(C_1)*	10.03	1.21	0.57	-	13.248	5.74*	8.978
7 CoO/Mg_3F_7 *(C_1)*	13.72	1.21	0.59	-	13.197	5.58*	8.889
8 CoO/Mg_3F_7 *(C_s)*	24.58	1.23	0.56	-	13.340	5.11*	11.605
9 CoO/Mg_3F_7 *(C_s)*	12.02	1.14	0.50	-	12.624	4.37	9.248
1 CuO/Mg_3F_7 *(C_s)*	0.00	1.00	0.63	-	12.095	4.50	
2 CuO/Mg_3F_7 *(C_s)*	2.64	0.99	0.60	-	11.985	4.41	13.821
3 CuO/Mg_3F_7 *(C_1)*	12.00	0.97	0.64	-	12.320	4.00	
4 CuO/Mg_3F_7 *(C_1)*	12.93	0.94	0.63	-	12.437	3.96	
5 CuO/Mg_3F_7 *(C_s)*	21.64	0.97	0.62	-	12.287	3.59	6.481
6 CuO/Mg_3F_7 *(C_1)*	31.76	0.96	0.66	-	12.596	3.10	
1 MnO_2/Mg_3F_7 *(C_s)*	0.00	1.34	0.43	-	12.469	5.83	13.458
2 MnO_2/Mg_3F_7 *(C_1)*	10.66	1.32	0.45	-	12.443	5.40	12.753
3 MnO_2/Mg_3F_7 *(C_{2v})*	11.18	1.31	0.68	-	12.405	5.38	13.307
4 MnO_2/Mg_3F_7 *(C_1)*	11.86	1.29	0.39	-	12.288	5.36	12.497
5 MnO_2/Mg_3F_7 *(C_{2v})*	17.09	1.24	0.35	-	11.449	4.86	12.764
6 MnO_2/Mg_3F_7 *(C_s)*	33.13	1.27	0.46	-	12.426	4.40	13.232
1 TiO_2/Mg_3F_7 *(C_s)*	0.00	1.74	0.53	0.992	13.828	6.41	12.448
2 TiO_2/Mg_3F_7 *(C_s)*	0.17	1.81	0.57	0.989	13.997	6.25	12.585
3 TiO_2/Mg_3F_7 *(C_s)*	8.98	1.82	0.53	1.008	14.327	5.92	12.668
4 TiO_2/Mg_3F_7 *(C_s)*	18.76	1.80	0.56	0.997	14.051	5.49	12.726
5 TiO_2/Mg_3F_7 *(C_1)*	20.50	1.81	0.62	0.993	14.170	5.43	12.575
6 TiO_2/Mg_3F_7 *(C_s)*	38.18		0.59	0.990	15.101	4.59	13.516

* BE values calculated without counterpoise approach

Table S5. The MP2/6-311+G(d) geometrical parameters for the TiO_2/Mg_3F_7 and MnO_2/Mg_3F_7 compounds. E_R in kcal/mol, bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

Species	Geometrical parameters			
1 TiO_2/Mg_3F_7 (C_S) E_R=0.00	r(Mg_1-F_1)=1.798	r(Mg_2-F_6)=1.906	α($F_1Mg_1F_{2,4}$)=124.16	α($F_{6,7}TiO_1$)=109.75
	r(Mg_1-$F_{2,4}$)=1.981	r(Mg_3-F_4)=1.885	α($F_1Mg_1F_3$)=127.32	α($F_{6,7}TiO_2$)=113.65
	r(Mg_1-F_3)=2.112	r(Mg_3-F_7)=1.906	α($Mg_1F_2Mg_2$)=103.47	ω($F_1Mg_1F_2Mg_2$)=136.90
	r(Mg_2-F_2)=1.885	r(Ti-$F_{6,7}$)=2.018	α($Mg_1F_3Mg_{2,3}$)=95.11	ω($F_1Mg_1F_3Mg_3$)=132.85
	r($Mg_{2,3}$-F_3)=2.002	r(Ti-O_1)=1.601	α($Mg_1F_4Mg_3$)=103.47	ω($F_2Mg_2F_6Ti$)=158.32
	r($Mg_{2,3}$-F_5)=1.938	r(Ti-O_2)=1.872	α($Mg_2F_5Mg_3$)=97.96	ω($Mg_3F_7TiO_1$)=157.29
			α(Mg_2F_6Ti)=115.32	ω($F_7TiO_1O_2$)=121.70
2 TiO_2/Mg_3F_7 (C_S) E_R=0.17	r(Mg_1-F_1)=1.799	r(Mg_3-F_4)=1.887	α($F_1Mg_1F_{2,4}$)=123.66	α($F_{6,7}TiO_1$)=110.74
	r(Mg_1-$F_{2,4}$)=1.985	r(Mg_3-F_7)=1.910	α($F_1Mg_1F_3$)=127.88	α($F_{6,7}TiO_2$)=113.87
	r(Mg_1-F_3)=2.100	r(Ti-F_5)=3.343	α($Mg_1F_2Mg_2$)=103.10	ω($F_1Mg_1F_2Mg_2$)=138.78
	r(Mg_2-F_2)=1.887	r(Ti-$F_{6,7}$)=2.005	α($Mg_1F_3Mg_2$)=95.17	ω($F_1Mg_1F_3Mg_3$)=133.56
	r($Mg_{2,3}$-F_3)=2.008	r(Ti-O_1)=1.601	α($Mg_1F_4Mg_3$)=103.10	ω($F_2Mg_2F_6Ti$)=125.26
	r($Mg_{2,3}$-F_5)=1.921	r(Ti-O_2)=1.871	α($Mg_2F_5Mg_3$)=97.92	ω($Mg_2F_6TiO_1$)=109.80
	r(Mg_2-F_6)=1.910		α(Mg_2F_6Ti)=123.65	ω($F_6TiO_1O_2$)=122.56
3 $TiO_2Mg_3F_7$ (C_S) E_R=8.98	r(Mg_1-F_1)=1.788	r(Mg_3-F_5)=1.919	α($Mg_1F_{2,3}Mg_2$)=98.66	α($F_{6,7}TiO_1$)=112.97
	r(Mg_1-$F_{2,3}$)=1.925	r(Mg_3-$F_{6,7}$)=1.942	α($F_{2,3}Mg_2F_4$)=124.95	α($F_{6,7}TiO_2$)=122.70
	r(Mg_2-$F_{2,3}$)=1.929	r(Ti-$F_{6,7}$)=1.997	α($Mg_2F_5Mg_3$)=98.12	ω($F_1Mg_1F_2Mg_2$)=179.91
	r(Mg_2-F_4)=1.928	r(Ti-O_1)=1.607	α($F_4Mg_3F_{6,7}$)=123.90	ω($F_2Mg_2F_5Mg_3$)=127.26
	r(Mg_2-F_5)=1.929	r(Ti-O_2)=1.874	α($Mg_3F_{6,7}Ti$)=100.23	ω($F_4Mg_3F_6Ti$)=127.71
	r(Mg_3-F_4)=1.922		α($F_1Mg_1F_{2,3}$)=139.28	ω($F_6TiO_1O_2$)=136.66
4 $TiO_2Mg_3F_7$ (C_S) E_R=18.76	r(Mg_1-F_1)=1.789	r(Mg_3-F_4)=1.899	α($F_1Mg_1F_3$)=132.41	α($F_{5,6}TiO_2$)=112.97
	r(Mg_1-$F_{2,3}$)=1.900	r(Mg_3-F_7)=1.789	α($Mg_1F_2Mg_2$)=142.18	ω($F_1Mg_1F_2Mg_2$)=180.00
	r(Mg_2-F_2)=1.895	r(Ti-$F_{5,6}$)=1.999	α($Mg_1F_3Mg_3$)=145.62	ω($Mg_1F_2Mg_2F_5$)=131.84
	r(Mg_2-F_4)=1.894	r(Ti-O_1)=1.874	α($Mg_2F_4Mg_3$)=142.38	ω($F_2Mg_2F_5Ti$)=121.26
	r(Mg_2-$F_{5,6}$)=1.943	r(Ti-O_2)=1.606	α($Mg_2F_{5,6}Ti$)=99.97	ω($Mg_2F_6TiO_1$)=124.37
	r(Mg_3-F_3)=1.901	α($F_1Mg_1F_2$)=131.89	α($F_{5,6}TiO_1$)=122.63	ω($F_6TiO_1O_2$)=131.22
5 $TiO_2Mg_3F_7$ (C_1) E_R=20.50	r(Mg_1-F_1)=1.794	r(Mg_3-F_3)=2.053	α($F_1Mg_1F_2$)=124.67	α(Mg_2F_6Ti)=104.64
	r(Mg_1-F_2)=1.966	r(Mg_3-F_4)=1.907	α($F_1Mg_1F_3$)=123.38	α(F_7TiO_1)=111.73
	r(Mg_1-F_3)=2.218	r(Mg_3-F_5)=2.072	α($F_1Mg_1F_4$)=131.89	α(F_7TiO_2)=122.36
	r(Mg_1-F_4)=1.929	r(Mg_3-F_7)=1.793	α($Mg_1F_2Mg_2$)=103.55	ω($F_1Mg_1F_2Mg_2$)=128.88
	r(Mg_2-F_2)=1.865	r(Ti-F_5)=2.059	α($Mg_1F_3Mg_2$)=92.50	ω($F_1Mg_1F_3Mg_3$)=128.61
	r(Mg_2-F_3)=1.940	r(Ti-F_6)=2.016	α($Mg_1F_4Mg_3$)=109.40	ω($F_4Mg_3F_5Ti$)=178.72
	r(Mg_2-F_5)=2.059	r(Ti-O_1)=1.594	α($Mg_2F_5Mg_3$)=96.83	ω($Mg_3F_5TiO_2$)=124.17
	r(Mg_2-F_6)=1.902	r(Ti-O_2)=1.867	α(Mg_2F_5Ti)=97.74	ω($F_6TiO_2O_1$)=128.82
6 $TiO_2Mg_3F_7$ (C_S) E_R=38.18	r(Mg_1-F_1)=1.777	r(Mg_2-F_6)=1.780	α($F_1Mg_1F_{2,4}$)=131.85	α($F_{2,4}TiO_1$)=105.97
	r(Mg_1-$F_{2,4}$)=2.065	r(Mg_3-F_4)=2.053	α($F_1Mg_1F_3$)=135.08	α($F_{2,4}TiO_2$)=130.46
	r(Mg_1-F_3)=1.997	r(Mg_3-F_7)=1.780	α($Mg_1F_2Mg_2$)=99.19	ω($F_1Mg_1F_2Mg_2$)=132.54
	r(Mg_2-F_2)=2.053	r(Ti-$F_{2,3}$)=2.084	α($Mg_1F_4Mg_3$)=99.19	ω($Mg_1F_3Mg_2F_6$)=118.91
	r($Mg_{2,3}$-F_3)=2.052	r(Ti-O_1)=1.592	α($Mg_1F_3Mg_{2,3}$)=101.51	ω($F_1Mg_1F_4Ti$)=116.06
	r($Mg_{2,3}$-F_5)=1.968	r(Ti-O_2)=1.858	α($Mg_2F_5Mg_3$)=102.94	ω($Mg_1F_2TiO_1$)=83.32
			α($Mg_1F_{2,4}Ti$)=99.53	ω($F_2TiO_1O_2$)=139.85
1 MnO_2/Mg_3F_7 (C_S) E_R=0.00	r(Mg_1-F_1)=1.801	r(Mg_3-F_4)=1.893	α($F_1Mg_1F_{2,4}$)=122.40	α($F_{6,7}MnO_2$)=109.47
	r(Mg_1-$F_{2,4}$)=1.994	r(Mg_3-F_7)=1.912	α($Mg_1F_2Mg_2$)=101.99	ω($F_1Mg_1F_2Mg_2$)=143.27
	r(Mg_1-F_3)=2.077	r(Mn-$F_{6,7}$)=1.914	α($Mg_1F_3Mg_{2,3}$)=95.77	ω($Mg_1F_4Mg_3F_7$)=84.38
	r(Mg_2-F_2)=1.893	r(Mn-O_1)=1.578	α($Mg_1F_4Mg_3$)=101.99	ω($F_2Mg_2F_6Mn$)=115.82
	r($Mg_{2,3}$-F_3)=1.996	r(Mn-O_2)=1.579	α(Mg_2F_6Mn)=135.01	ω($Mg_3F_7MnO_1$)=115.08
	r($Mg_{2,3}$-F_5)=1.916	α($F_1Mg_1F_3$)=129.69	α($F_{6,7}MnO_1$)=109.76	ω($F_7MnO_1O_2$)=130.24
	r(Mg_2-F_6)=1.912	α($Mg_2F_5Mg_3$)=94.56		

2 $MnO_2Mg_3F_7$ (C_1) E_R=10.66	r(Mg_1-F_1)=1.795 r(Mg_1-F_2)=2.126 r(Mg_1-F_3)=1.968 r(Mg_1-F_4)=1.929 r(Mg_2-F_2)=2.047 r(Mg_2-F_3)=1.884 r(Mg_2-F_5)=1.878 r(Mg_2-F_6)=1.909	r(Mg_3-F_4)=1.889 r(Mg_3-F_5)=1.922 r(Mg_3-F_7)=1.790 r(Mn-F_2)=1.922 r(Mn-F_6)=1.907 r(Mn-O_1)=1.578 r(Mn-O_2)=1.583 α($F_1Mg_1F_2$)=117.33	α($F_1Mg_1F_3$)=130.63 α($F_1Mg_1F_4$)=131.95 α($Mg_1F_3Mg_2$)=101.26 α($Mg_1F_4Mg_3$)=144.44 α($Mg_1F_2Mg_2$)=91.06 α($Mg_2F_5Mg_3$)=125.03 α(Mg_2F_2Mn)=98.89	α(F_2MnO_1)=111.70 α(F_6MnO_2)=112.87 ω($F_1Mg_1F_4Mg_3$)=179.35 ω($F_1Mg_1F_2Mg_2$)=148.83 ω($F_3Mg_2F_2Mn$)=127.83 ω($Mg_2F_6MnO_1$)=108.23 ω($F_6MnO_1O_2$)=138.53
3 $MnO_2Mg_3F_7$ (C_{2v}) E_R=11.18	r(Mg_1-F_1)=1.789 r(Mg_1-F_2)=1.898 r($Mg_{1,3}$-F_3)=1.901 r(Mg_2-$F_{2,4}$)=1.896 r(Mg_2-$F_{5,6}$)=1.930	r(Mg_3-F_4)=1.898 r(Mg_3-F_7)=1.789 r(Mn-$F_{5,6}$)=1.899 r(Mn-$O_{1,2}$)=1.591 α($F_1Mg_1F_2$)=132.26	α($F_1Mg_1F_3$)=131.96 α($Mg_1F_2Mg_2$)=142.71 α($Mg_1F_3Mg_3$)=145.12 α($Mg_2F_4Mg_3$)=142.71 α($F_{2,4}Mg_2F_{5,6}$)=120.60 α($Mg_2F_{5,6}Mn$)=100.90	α($F_{5,6}MnO_{1,2}$)=112.27 ω($F_1Mg_1F_3Mg_3$)=180.00 ω($Mg_1F_3Mg_3F_4$)=0.00 ω($F_2Mg_2F_5Mn$)=118.81 ω($Mg_2F_6MnO_1$)=110.04 ω($F_6MnO_1O_2$)=136.09
4 $MnO_2Mg_3F_7$ (C_1) E_R=11.86	r(Mg_1-F_1)=1.792 r(Mg_1-F_2)=2.081 r(Mg_1-F_3)=2.054 r(Mg_1-F_4)=1.908 r(Mg_2-F_2)=2.028 r(Mg_2-F_3)=1.944 r(Mg_2-F_5)=1.865 r(Mg_2-F_6)=1.912	r(Mg_3-F_3)=2.207 r(Mg_3-F_4)=1.931 r(Mg_3-F_5)=1.967 r(Mg_3-F_7)=1.795 r(Mn-F_2)=1.933 r(Mn-F_6)=1.912 r(Mn-O_1)=1.572 r(Mn-O_2)=1.581 α($F_1Mg_1F_2$)=109.64	α($F_1Mg_1F_3$)=128.85 α($F_1Mg_1F_4$)=142.26 α($Mg_1F_2Mg_2$)=97.40 α($Mg_1F_3Mg_3$)=94.51 α($Mg_1F_4Mg_3$)=109.25 α($Mg_2F_5Mg_3$)=103.15 α(Mg_2F_2Mn)=99.15 α(Mg_2F_6Mn)=104.59	α(F_2MnO_1)=111.70 α(F_2MnO_2)=110.37 ω($F_1Mg_1F_2Mg_2$)=138.05 ω($Mg_1F_4Mg_3F_7$)=119.02 ω($Mg_1F_3Mg_2F_6$)=76.91 ω($F_1Mg_1F_2Mn$)=23.19 ω($Mg_1F_2MnO_1$)=4.44 ω($F_6MnO_1O_2$)=139.74
5 $MnO_2Mg_3F_7$ (C_{2v}) E_R=17.09	r(Mg_1-F_1)=1.788 r(Mg_1-$F_{2,3}$)=1.924 r(Mg_2-$F_{2,3}$)=1.929 r(Mg_2-$F_{4,5}$)=1.928 r(Mg_3-$F_{4,5}$)=1.922	r(Mg_3-$F_{6,7}$)=1.931 r(Mn-$F_{6,7}$)=1.902 r(Mn-$O_{1,2}$)=1.713 α($F_1Mg_1F_{2,3}$)=139.26	α($Mg_1F_{2,3}Mg_2$)=98.65 α($F_{2,3}Mg_2F_{4,5}$)=125.05 α($Mg_2F_{4,5}Mg_3$)=98.16 α($F_{4,5}Mg_3F_{6,7}$)=125.79 α($Mg_3F_{6,7}Mn$)=100.83	α($F_{6,7}MnO_{1,2}$)=114.31 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($F_2Mg_2F_5Mg_3$)=127.34 ω($F_4Mg_3F_6Mn$)=126.04 ω($F_6MnO_1O_2$)=135.20
6 $MnO_2Mg_3F_7$ (C_S) E_R=33.13	r(Mg_1-F_1)=1.778 r(Mg_1-$F_{2,4}$)=2.082 r(Mg_1-F_3)=1.950 r(Mg_2-F_2)=2.098 r($Mg_{2,3}$-F_3)=2.083 r($Mg_{2,3}$-F_5)=1.911	r(Mg_2-F_7)=1.785 r(Mg_3-F_4)=2.098 r(Mg_3-F_6)=1.785 r(Mn-$F_{2,4}$)=1.932 r(Mn-O_1)=1.572 r(Mn-O_2)=1.577	α($F_1Mg_1F_{2,4}$)=128.65 α($F_1Mg_1F_3$)=142.43 α($Mg_1F_2Mg_2$)=98.03 α($Mg_1F_3Mg_{2,3}$)=102.91 α($Mg_2F_5Mg_3$)=105.75 α($Mg_1F_{2,4}Mn$)=98.16	α($F_{2,4}MnO_1$)=110.91 α($F_{2,4}MnO_2$)=113.88 ω($F_1Mg_1F_2Mg_2$)=140.36 ω($F_1Mg_1F_3Mg_3$)=131.38 ω($F_1Mg_1F_4Mn$)=95.69 ω($F_2MnO_1O_2$)=138.08

Table S6. The MP2/6-311+G(d) geometrical parameters for the SiO_2/Mg_3F_7 compounds. The E_R values (in kcal/mol) stand for the relative energies estimated for the SiO_2/Mg_3F_7 isomers with respect to corresponding global minimum (labeled **1**). Bond lengths (r) in Å, valence angles (α) and dihedral angles (ω) in degrees.

1 SiO_2/Mg_3F_7 (C_1) E_R=0.00	r(Mg_1-F_1)=1.788 r(Mg_1-$F_{2,3}$)=1.925 r(Mg_2-F_2)=1.928 r(Mg_2-$F_{3,4,5}$)=1.929 r(Mg_3-F_4)=1.919 r(Mg_3-F_5)=1.920	r(Mg_3-F_6)=2.192 r(Mg_3-O_1)=1.936 r(Si-F_6)=1.691 r(Si-F_7)=1.590 r(Si-O_1)=1.579 r(Si-O_2)=1.663	α($F_1Mg_1F_2$)=139.24 α($F_1Mg_1F_3$)=139.32 α($Mg_1F_2Mg_2$)=98.67 α($Mg_1F_3Mg_2$)=98.64 α($F_2Mg_2F_4$)=125.41 α($F_2Mg_2F_5$)=125.46 α($Mg_2F_4Mg_3$)=98.23	α(O_1SiO_2)=116.47 α(F_6SiO_7)=103.58 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($Mg_1F_2Mg_2F_5$)=126.86 ω($F_4Mg_3F_6Si$)=133.59 ω($F_6SiO_1O_2$)=116.32 ω($F_7SiO_2O_1$)=139.13
2 SiO_2/Mg_3F_7 (C_1) E_R=1.26	r(Mg_1-F_1)=1.790 r(Mg_1-F_2)=2.077 r(Mg_1-F_3)=1.971 r(Mg_2-F_2)=1.996 r(Mg_2-F_4)=1.978 r(Mg_2-F_5)=2.086 r(Mg_2-F_6)=1.790	r(Mg_3-F_3)=1.881 r(Mg_3-F_4)=1.873 r(Si-F_5)=1.669 r(Si-F_7)=1.589 r(Si-O_1)=1.590 r(Si-O_2)=1.659	α($F_1Mg_1F_2$)=126.83 α($F_1Mg_1F_3$)=142.65 α($Mg_1F_3Mg_2$)=145.51 α($Mg_1F_3Mg_3$)=87.27 α($F_2Mg_2F_6$)=131.27 α($F_2Mg_2F_5$)=89.23 α($F_3Mg_3F_4$)=157.61	α(Mg_2F_5Si)=130.07 α(O_1SiO_2)=114.27 ω($F_1Mg_1F_2Mg_2$)=90.68 ω($Mg_1F_2Mg_2F_6$)=87.11 ω($F_6Mg_2F_5Si$)=174.29 ω($Mg_2F_5SiF_7$)=110.23 ω($F_7SiO_1O_2$)=128.39
3 SiO_2/Mg_3F_7 (C_1) E_R=11.51	r(Mg_1-F_1)=1.871 r(Mg_1-$F_{2,3}$)=1.995 r(Mg_1-F_4=1.970 r(Mg_2-$F_{2,3}$)=2.132 r(Mg_3-$F_{2,3}$)=1.997 r(Mg_3-F_4)=1.971 r(Mg_3-F_5)=1.870	r(Mg_2-F_1)=2.126 r(Mg_3-O_1)=1.860 r(Si-F_6)=1.611 r(Si-F_7)=1.608 r(Si-O_1)=1.574 r(Si-O_2)=1.680 α($F_1Mg_1F_{2,3}$)=83.24	α($F_1Mg_1F_4$)=158.62 α($Mg_1F_2Mg_2$)=85.50 α($Mg_1F_3Mg_3$)=83.53 α($Mg_1F_4Mg_3$)=84.87 α($Mg_2F_5Mg_3$)=88.83 α($F_2Mg_2O_1$)=143.02 α(Mg_2O_1Si)=163.15	α(F_6SiF_7)=103.23 α(O_1SiO_2)=109.52 ω($F_1Mg_1F_3Mg_2$)=40.20 ω($F_1Mg_1F_3Mg_3$)=126.19 ω($F_2Mg_2O_1Si$)=97.96 ω($F_6SiO_1O_2$)=120.79 ω($F_7SiO_2O_1$)=125.01
4 SiO_2/Mg_3F_7 (C_1) E_R=15.96	r(Mg_1-F_1)=1.878 r(Mg_1-F_2)=1.992 r(Mg_1-F_3)=1.976 r(Mg_1-F_4=1.978 r(Mg_2-F_2)=2.120 r(Mg_3-F_2)=1.993 r(Mg_3-F_3)=1.975 r(Mg_3-F_4)=1.978 r(Mg_3-F_5)=1.878	r(Mg_2-$F_{1,5}$)=2.113 r(Mg_3-O_1)=1.953 r(Si-F_6)=1.599 r(Si-F_7)=1.600 r(Si-O_1)=1.574 r(Si-O_2)=1.740 α($F_1Mg_1F_2$)=83.49 α($F_1Mg_1F_3$)=83.87	α($F_1Mg_1F_4$)=158.67 α($Mg_1F_2Mg_2$)=86.11 α($Mg_1F_3Mg_3$)=84.08 α($Mg_1F_4Mg_3$)=83.96 α($Mg_2F_5Mg_3$)=89.28 α($F_2Mg_2O_1$)=122.47 α(Mg_2O_1Si)=102.91	α(F_6SiF_7)=105.95 α(O_1SiO_2)=102.62 ω($F_1Mg_1F_3Mg_2$)=40.50 ω($F_1Mg_1F_3Mg_3$)=125.08 ω($F_1Mg_2O_2Si$)=105.79 ω($F_6SiO_2O_1$)=124.36 ω($F_7SiO_1O_2$)=114.48
2 SiO_2/Mg_3F_7 (C_S) E_R=27.04	r(Mg_1-F_1)=1.797 r(Mg_1-$F_{2,4}$)=1.994 r(Mg_1-F_3)=2.096 r(Mg_2-F_2)=1.884 r($Mg_{2,3}$-F_3)=1.997 r($Mg_{2,3}$-F_5)=1.909	r(Mg_2-F_6)=1.968 r(Mg_3-F_4)=1.884 r(Mg_3-F_7)=1.968 r(Si-$F_{6,7}$)=1.732 r(Si-O_1)=1.526 r(Si-O_2)=1.666 α($F_1Mg_1F_3$)=128.84	α($F_1Mg_1F_{2,4}$)=123.13 α($Mg_1F_2Mg_2$)=102.88 α($Mg_1F_3Mg_{2,3}$)=95.63 α($Mg_1F_4Mg_3$)=102.88 α($Mg_2F_5Mg_3$)=96.43 α($F_2Mg_2F_6$)=163.05 α(Mg_2F_6Si)=134.31	α($F_{6,7}SiO_1$)=116.24 α($F_{6,7}SiO_2$)=100.12 ω($F_1Mg_1F_2Mg_2$)=141.16 ω($F_1Mg_1F_3Mg_3$)=134.26 ω($F_2Mg_2F_6Si$)=116.59 ω($Mg_2F_6SiO_1$)=94.43 ω($F_6SiO_1O_2$)=125.30
3 SiO_2/Mg_3F_7 (C_S) E_R=27.35	r(Mg_1-F_1)=1.797 r(Mg_1-$F_{2,4}$)=1.995 r(Mg_1-F_3)=2.105 r(Mg_2-F_2)=1.884 r($Mg_{2,3}$-F_3)=1.989 r($Mg_{2,3}$-F_5)=1.916	r(Mg_2-F_6)=1.966 r(Mg_3-F_4)=1.884 r(Mg_3-F_7)=1.966 r(Si-$F_{6,7}$)=1.732 r(Si-O_1)=1.525 r(Si-O_2)=1.667 α($F_1Mg_1F_3$)=130.07	α($F_1Mg_1F_{2,4}$)=123.06 α($Mg_1F_2Mg_2$)=102.84 α($Mg_1F_3Mg_{2,3}$)=95.66 α($Mg_1F_4Mg_3$)=102.84 α($Mg_2F_5Mg_3$)=95.78 α($F_2Mg_2F_6$)=164.23 α(Mg_2F_6Si)=136.74	α($F_{6,7}SiO_1$)=116.45 α($F_{6,7}SiO_2$)=99.90 ω($F_1Mg_1F_2Mg_2$)=142.22 ω($F_1Mg_1F_3Mg_3$)=134.08 ω($F_2Mg_2F_6Si$)=90.90 ω($Mg_3F_7SiO_1$)=110.36 ω($F_5SiO_1O_2$)=125.07

4 SiO_2/Mg_3F_7 (C_S) E_R=29.59	r(Mg_1-F_1)=1.796 r(Mg_1-$F_{2,4}$)=1.994 r(Mg_1-F_3)=2.102 r(Mg_2-F_2)=1.883 r($Mg_{2,3}$-F_3)=1.993 r($Mg_{2,3}$-F_5)=1.913 r(Mg_2-F_6)=1.971	r(Mg_3-F_4)=1.883 r(Mg_3-F_7)=1.971 r(Si-$F_{6,7}$)=1.721 r(Si-O_1)=1.565 r(Si-O_2)=1.568 α($F_1Mg_1F_3$)=128.96	α($F_1Mg_1F_{2,4}$)=123.32 α($Mg_1F_2Mg_2$)=102.98 α($Mg_1F_3Mg_{2,3}$)=95.60 α($Mg_1F_4Mg_3$)=102.98 α($Mg_2F_5Mg_3$)=96.19 α($F_2Mg_2F_6$)=163.82 α(Mg_2F_6Si)=135.79	α($F_{6,7}SiO_1$)=112.84 α($F_{6,7}SiO_2$)=112.17 ω($F_1Mg_1F_2Mg_2$)=140.94 ω($F_1Mg_1F_3Mg_3$)=134.15 ω($F_2Mg_2F_6Si$)=110.76 ω($Mg_3F_7SiO_1$)=136.51 ω($F_5SiO_1O_2$)=127.12
5 SiO_2/Mg_3F_7 (C_{2v}) E_R=31.69	r(Mg_1-F_1)=1.786 r(Mg_1-$F_{2,3}$)=1.929 r(Mg_2-$F_{2,3}$)=1.922 r(Mg_2-$F_{4,5}$)=1.939 r(Mg_3-$F_{4,5}$)=1.903	r(Mg_3-$F_{6,7}$)=1.983 r(Si-$F_{6,7}$)=1.730 r(Si-$O_{1,2}$)=1.564 α($F_1Mg_1F_{2,3}$)=139.42	α($Mg_1F_{2,3}Mg_2$)=98.68 α($F_{2,3}Mg_2F_{4,5}$)=125.25 α($Mg_2F_{4,5}Mg_3$)=98.29 α($F_{4,5}Mg_3F_{6,7}$)=127.52 α($Mg_3F_{6,7}Si$)=102.09	α($F_{6,7}SiO_{1,2}$)=114.49 ω($F_1Mg_1F_2Mg_2$)=180.00 ω($F_2Mg_2F_5Mg_3$)=126.95 ω($F_4Mg_3F_6Si$)=123.63 ω($F_7SiO_1O_2$)=132.54