Table 1. Atomic coordinates, isotropic displacement parameters, and selected interatomic distances and bonding angles for $Mg_2Fe_2(C_4O_{13})$, monoclinic, *C*2/*c*, *a* = 9.822(3) *b* = 3.9023(13) *c* = 13.154(5) Å, β = 108.02(3)°, and *V* = 479.4(3) Å^3 at 135 GPa

Atom	*x*	*y*	*z*	*U* (Å^2)	Bond distances (Å) and angles (°)	
$(Mg,Fe)_1$	0.8848(5)	−0.0245(9)	0.4113(3)	0.0237(13)	C_1-O_4	1.24(5)
$(Mg,Fe)_2$	0.6619(5)	−0.4841(9)	0.3355(3)	0.0186(13)	C_1-O_5	1.35(4)
O_1	0.808(2)	0.317(3)	0.2843(13)	0.020(4)	C_1-O_6	1.31(3)
O_2	0.5	−0.197(5)	0.25	0.024(6)	C_1-O_7	1.31(2)
O_3	0.9380(18)	0.798(3)	0.3018(12)	0.006(3)	C_2-O_1	1.18(3)
O_4	0.997(2)	−0.376(3)	0.5881(13)	0.013(3)	C_2-O_2	1.36(3)
O_5	0.8149(18)	−0.524(3)	0.6211(13)	0.013(3)	C_2-O_3	1.291(19)
O_6	0.813(2)	−0.424(3)	0.4581(15)	0.012(3)	C_2-O_4	1.51(3)
O_7	0.909(2)	−0.880(3)	0.5420(15)	0.021(4)		
C_1	0.889(3)	−0.552(5)	0.550(2)	0.015(5)	C_2-O_2-C_2	122.1(17)
C_2	1.084(2)	−0.472(4)	0.7012(18)	0.005(3)	C_1-O_4-C_2	114.3(19)

Table 2. Atomic coordinates, isotropic displacement parameters, and Fe-O interatomic distances in octahedral sites for $Fe_{13}O_{19}$, monoclinic, *C*2/*m*, *a* = 19.233(2) *b* = 2.5820(13) *c* = 9.550(11) Å, β = 118.39(3)°, and *V* = 417.2(5) Å^3 at 135 GPa

Atom	*x*	*y*	*z*	*U* (Å^2)	Bond distances (Å)	
Fe_1	0.4267(5)	−0.5	0.4606(5)	0.0128(11)	Fe_6-O_9 (×2)	1.68(3)
Fe_2	0.2641(4)	0	0.3647(4)	0.0110(10)	Fe_6-O_{10} (×4)	1.706(11)
Fe_3	0.4645(4)	−1	0.2289(5)	0.0134(11)	Fe_1-O_1 (×2)	1.814(6)
Fe_4	0.6273(4)	−1	0.3428(5)	0.0110(10)	Fe_1-O_2	1.76(2)
Fe_5	0.3501(4)	0	0.0691(4)	0.0120(10)	Fe_1-O_5	1.76(2)
Fe_6	0.5	−0.5	0	0.0181(16)	Fe_1-O_6 (×2)	1.66(2)
Fe_7	0.3142(4)	0	0.1576(5)	0.0107(10)		
O_1	0.5	0	0.5	0.022(8)		
O_2	0.4017(16)	−0.5	0.258(2)	0.017(5)		
O_3	0.3012(16)	0.5	0.5243(19)	0.006(4)		
O_4	0.1609(15)	0	0.2278(18)	0.007(4)		
O_5	0.4525(19)	−0.5	0.664(2)	0.026(5)		
O_6	0.367(2)	0	0.426(2)	0.018(5)		
O_7	0.3024(18)	−0.5	−0.003(2)	0.015(4)		
O_8	0.2469(13)	0	−0.2223(17)	0.000(4)		
O_9	0.5692(16)	−0.5	−0.059(2)	0.013(4)		
O_{10}	0.4566(17)	0	−0.130(2)	0.011(4)		

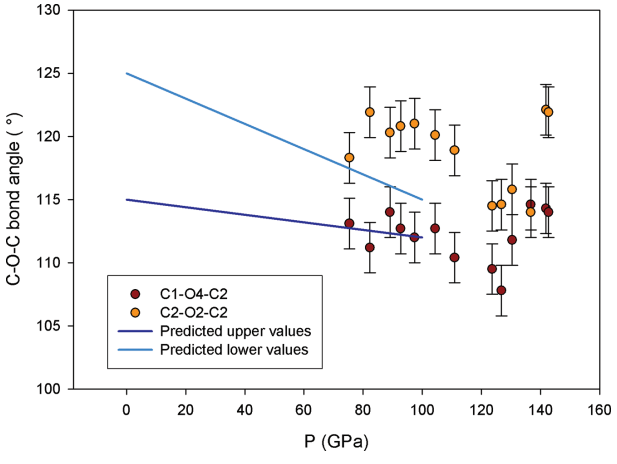

Figure 4. C-O-C bond angles determined at various pressures and a comparison with predicted values (Oganov et al. 2008; Oganov et al. 2013). The experimental values are in close agreement with prediction, taking into account the experimental accuracy and chemical difference between $H_6C_2O_6$ used in the computation and $Mg_2Fe_2(C_4O_{13})$.

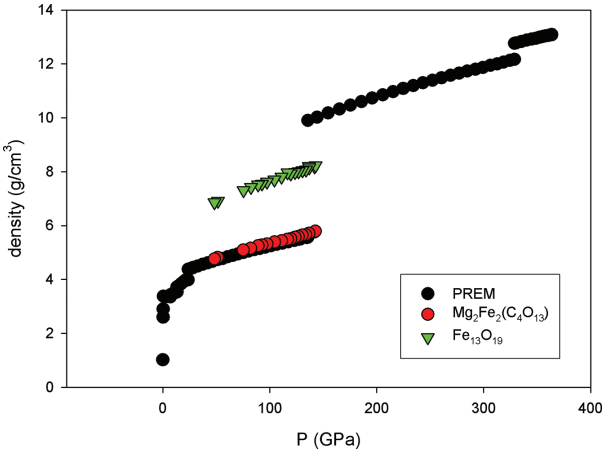

Figure 5. Density of $Mg_2Fe_2(C_3O_{13})$ and $Fe_{13}O_{19}$ as function of pressure, compared with PREM model.