

Electronic Supplementary Information

**Planar tetracoordinate fluorine in  $\text{FMg}_4\text{Se}_4^-$  cluster**

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**Contents**

Cartesian Coordinates for the structures shown in **Fig. 1** and **Fig. 2**.

Cartesian Coordinates for the structures shown in **Fig. 1** and **Fig. 2**.

B2PLYP-D3(BJ)/aug-cc-pVTZ-optimized structures (in Cartesian coordinates) shown in **Fig. 1**.

**1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | 0.00000000  | 0.00000000  | 0.78220000  |
| Mg | 0.00000000  | 1.99567000  | -0.00253000 |
| Mg | 1.99567000  | 0.00000000  | -0.00253000 |
| Mg | -1.99567000 | 0.00000000  | -0.00253000 |
| Mg | 0.00000000  | -1.99567000 | -0.00253000 |
| O  | 1.84761700  | 1.84761700  | -0.21619800 |
| O  | -1.84761700 | 1.84761700  | -0.21619800 |
| O  | -1.84761700 | -1.84761700 | -0.21619800 |
| O  | 1.84761700  | -1.84761700 | -0.21619800 |

**2**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | 2.15078600  | 0.00000000 |
| Mg | 2.15078600  | 0.00000000  | 0.00000000 |
| Mg | -2.15078600 | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | -2.15078600 | 0.00000000 |
| S  | -2.30309800 | 2.30309800  | 0.00000000 |
| S  | -2.30309800 | -2.30309800 | 0.00000000 |
| S  | 2.30309800  | 2.30309800  | 0.00000000 |
| S  | 2.30309800  | -2.30309800 | 0.00000000 |

**3**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | 2.17744400  | 0.00000000 |
| Mg | 2.17744400  | 0.00000000  | 0.00000000 |
| Mg | -2.17744400 | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | -2.17744400 | 0.00000000 |
| Se | 2.41554600  | 2.41554600  | 0.00000000 |
| Se | -2.41554600 | 2.41554600  | 0.00000000 |
| Se | -2.41554600 | -2.41554600 | 0.00000000 |
| Se | 2.41554600  | -2.41554600 | 0.00000000 |

**4**

|    |            |             |             |
|----|------------|-------------|-------------|
| F  | 0.00000000 | 0.00000000  | -0.23927600 |
| Mg | 0.00000000 | 0.00000000  | -2.40220400 |
| Mg | 0.00000000 | 2.00968300  | -0.01961800 |
| Mg | 0.00000000 | -2.00968300 | -0.01961800 |

|    |            |             |             |
|----|------------|-------------|-------------|
| Mg | 0.00000000 | 0.00000000  | 2.75339600  |
| Te | 0.00000000 | 2.62914500  | -2.59511500 |
| Te | 0.00000000 | -2.62914500 | -2.59511500 |
| Te | 0.00000000 | -2.59284200 | 2.57982700  |
| Te | 0.00000000 | 2.59284200  | 2.57982700  |

MP2/aug-cc-pVQZ-optimized structures (in Cartesian coordinates) of FMg<sub>4</sub>S<sub>4</sub><sup>-</sup> (**2**) and FMg<sub>4</sub>Se<sub>4</sub><sup>-</sup> (**3**) shown in Fig. 1.

**2**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | 2.16003200  | 0.00000000 |
| Mg | 2.16003200  | 0.00000000  | 0.00000000 |
| Mg | -2.16003200 | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | -2.16003200 | 0.00000000 |
| S  | -2.30964900 | 2.30964900  | 0.00000000 |
| S  | -2.30964900 | -2.30964900 | 0.00000000 |
| S  | 2.30964900  | 2.30964900  | 0.00000000 |
| S  | 2.30964900  | -2.30964900 | 0.00000000 |

**3**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | -1.54475000 | 1.54475200  | 0.00000000 |
| Mg | 1.54475000  | 1.54474900  | 0.00000000 |
| Mg | -1.54475000 | -1.54474900 | 0.00000000 |
| Mg | 1.54475000  | -1.54475200 | 0.00000000 |
| Se | 0.00000000  | 3.41322900  | 0.00000000 |
| Se | -3.41323200 | 0.00000400  | 0.00000000 |
| Se | 0.00000000  | -3.41322900 | 0.00000000 |
| Se | 3.41323200  | -0.00000400 | 0.00000000 |

B2PLYP-D3(BJ)/aug-cc-pVTZ -optimized structures (in Cartesian coordinates) shown in Fig. 2.

**2**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | 2.15078600  | 0.00000000 |
| Mg | 2.15078600  | 0.00000000  | 0.00000000 |
| Mg | -2.15078600 | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | -2.15078600 | 0.00000000 |
| S  | -2.30309800 | 2.30309800  | 0.00000000 |
| S  | -2.30309800 | -2.30309800 | 0.00000000 |
| S  | 2.30309800  | 2.30309800  | 0.00000000 |

|   |            |             |            |
|---|------------|-------------|------------|
| S | 2.30309800 | -2.30309800 | 0.00000000 |
|---|------------|-------------|------------|

**2a**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | 0.00000000  | 0.00000000  | -3.58487500 |
| Mg | 1.44166900  | 0.83234800  | 0.86691600  |
| Mg | 0.00000000  | -1.66469600 | 0.86691600  |
| Mg | 0.00000000  | 0.00000000  | -1.77854700 |
| Mg | -1.44166900 | 0.83234800  | 0.86691600  |
| S  | 0.00000000  | 2.22642500  | -0.42000100 |
| S  | 0.00000000  | 0.00000000  | 2.65984600  |
| S  | 1.92814000  | -1.11321200 | -0.42000100 |
| S  | -1.92814000 | -1.11321200 | -0.42000100 |

**2b**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | 0.76600400  | -2.72720300 | 0.00000000  |
| Mg | 0.77318400  | -1.45079800 | 1.45451700  |
| Mg | -0.45190800 | 1.20592100  | 1.51698400  |
| Mg | 0.77318400  | -1.45079800 | -1.45451700 |
| Mg | -0.45190800 | 1.20592100  | -1.51698400 |
| S  | -1.51697500 | 2.60915000  | 0.00000000  |
| S  | 1.50799800  | 0.32959500  | 0.00000000  |
| S  | -0.45190800 | -0.51868900 | 3.14400300  |
| S  | -0.45190800 | -0.51868900 | -3.14400300 |

**2c**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | -2.78354400 | 0.34799800  | 0.48139900  |
| Mg | 1.38581000  | 1.03722900  | 0.67207300  |
| Mg | 1.06744500  | -1.46192200 | -0.50899400 |
| Mg | -1.45227200 | 1.06320100  | -0.77480100 |
| Mg | -1.68858700 | -1.18017200 | 0.73623800  |
| S  | 0.33458800  | -1.11360300 | 1.84043600  |
| S  | -1.11567900 | -1.26337500 | -1.59536800 |
| S  | 2.96601200  | -0.15264600 | -0.62145500 |
| S  | -0.10347400 | 2.74012300  | 0.01221200  |

**3**

|    |             |             |            |
|----|-------------|-------------|------------|
| F  | 0.00000000  | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | 2.17744400  | 0.00000000 |
| Mg | 2.17744400  | 0.00000000  | 0.00000000 |
| Mg | -2.17744400 | 0.00000000  | 0.00000000 |
| Mg | 0.00000000  | -2.17744400 | 0.00000000 |

|    |             |             |            |
|----|-------------|-------------|------------|
| Se | 2.41554600  | 2.41554600  | 0.00000000 |
| Se | -2.41554600 | 2.41554600  | 0.00000000 |
| Se | -2.41554600 | -2.41554600 | 0.00000000 |
| Se | 2.41554600  | -2.41554600 | 0.00000000 |

**3a**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | -3.77786200 | 0.00006900  | 0.00000100  |
| Mg | 0.75409500  | 0.88078400  | -1.46595300 |
| Mg | 0.75406900  | -1.70995400 | -0.02980200 |
| Mg | -1.97560300 | 0.00000800  | 0.00000000  |
| Mg | 0.75409500  | 0.82916500  | 1.49575600  |
| Se | -0.59341200 | 2.36625900  | 0.04124100  |
| Se | 2.67918400  | -0.00002100 | 0.00000000  |
| Se | -0.59346100 | -1.14741300 | -2.06985500 |
| Se | -0.59346100 | -1.21884500 | 2.02861400  |

**3b**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | 0.93061500  | -2.90447700 | 0.00000000  |
| Mg | 0.93059500  | -1.65694300 | 1.47158400  |
| Mg | -0.39716700 | 1.03469200  | 1.55815400  |
| Mg | 0.93059500  | -1.65694300 | -1.47158400 |
| Mg | -0.39716700 | 1.03469200  | -1.55815400 |
| Se | -1.57950400 | 2.50828500  | 0.00000000  |
| Se | 1.75096000  | 0.25348400  | 0.00000000  |
| Se | -0.39716700 | -0.77685100 | 3.27632600  |
| Se | -0.39716700 | -0.77685100 | -3.27632600 |

**3c**

|    |             |             |             |
|----|-------------|-------------|-------------|
| F  | -2.95374000 | 0.53405500  | 0.66753200  |
| Mg | 1.31456300  | 0.97130000  | 0.63963100  |
| Mg | -1.67027800 | 1.17349800  | -0.66083600 |
| Mg | -1.99635800 | -1.08921200 | 0.89007700  |
| Mg | 0.76105600  | -1.59720200 | -0.48965400 |
| Se | 2.85775700  | -0.38985200 | -0.75980200 |
| Se | -1.54529600 | -1.27994000 | -1.58917600 |
| Se | 0.15531600  | -1.17865000 | 2.01426400  |
| Se | -0.12436900 | 2.89823300  | 0.02417300  |