

**Supplementary Information Table 3** Crystallographic data for sulfoxides **17** to **19**, **23** to **25**, **29** and **30**.

Compound	<b>17</b>	<b>18</b>	<b>19</b>	<b>R*R*-23</b>	<b>R*R*-24</b>	<b>R*S*-25</b>	<b>R*S*-28</b>	<b>R*S*-29</b>	<b>R*R*-30</b>
Formula	C <sub>15</sub> H <sub>16</sub> O <sub>3</sub> S	C <sub>13</sub> H <sub>10</sub> F <sub>2</sub> OS	C <sub>13</sub> H <sub>11</sub> BrOS	C <sub>14</sub> H <sub>14</sub> OS	C <sub>14</sub> H <sub>12</sub> F <sub>2</sub> OS	C <sub>16</sub> H <sub>18</sub> O <sub>3</sub> S	C <sub>14</sub> H <sub>12</sub> F <sub>2</sub> OS	C <sub>16</sub> H <sub>18</sub> O <sub>3</sub> S	C <sub>16</sub> H <sub>18</sub> O <sub>3</sub> S
Formula Weight	276.34	252.27	295.19	230.31	266.30	290.36	266.30	290.36	290.36
T/K	180(2)	100(2)	180(2)	120(2)	120(2)	123(2)	180(2)	100(2)	293(2)
Crystal System	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Orthorhombic
Space Group	<i>Pc</i>	<i>Pca</i> 2 <sub>1</sub>	<i>Pca</i> 2 <sub>1</sub>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>Pn</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> $\bar{1}$	<i>Pca</i> 2 <sub>1</sub>
<i>a</i> /Å	15.4234(11)	8.1909(9)	8.2638(2)	28.2961(6)	15.5607(3)	8.5839(6)	13.5661(5)	7.1117(12)	12.4822(15)
<i>b</i> /Å	5.4410(4)	5.4433(5)	5.42770(10)	5.75060(10)	5.81098(11)	5.5077(3)	5.7383(2)	8.5497(7)	8.0394(9)
<i>c</i> /Å	8.1642(5)	24.948(2)	27.4202(9)	15.7264(3)	14.3987(3)	15.7646(11)	15.7552(7)	23.495(2)	14.9907(9)
$\alpha$ /°	90	90	90	90	90	90	90	89.756(7)	90
$\beta$ /°	105.124(2)	90	90	112.1590(10)	107.8650(10)	104.481(7)	93.6250(10)	89.579(10)	90
$\gamma$ /°	90	90	90	90	90	90	90	89.428(10)	90
<i>V</i> /Å <sup>3</sup>	661.40(8)	1112.3(2)	1229.89(6)	2369.99(8)	1239.19(4)	721.63(8)	1224.03(8)	1428.5(3)	1504.3(3)
<i>Z</i>	2	4	4	8	4	2	4	4	4
$\rho_{\text{calc}}$ /gcm <sup>-3</sup>	1.388	1.506	1.594	1.291	1.427	1.336	1.445	1.350	1.282
$\mu$ /mm <sup>-1</sup>	0.246	0.296	3.487	0.248	2.433	2.032	0.273	0.231	0.219
2 $\theta$ max/°	54.18	56.80	49.98	54.92	136.26	135.36	54.94	60.28	50.94
Total reflections	5584	7201	6583	2936	8951	6211	8959	21334	3012
Unique reflections	2873	2747	1873	2712	2200	2330	2796	8198	2800
Refls <i>I</i> >2 $\sigma$ ( <i>I</i> )	2753	2661	1563	2407	2005	2257	2240	7513	1783
<i>R</i> <sub>int</sub>	0.0198	0.0210	0.0694	0.0270	0.0702	0.0384	0.0451	0.0116	0.0531
Parameters	174	154	145	146	165	185	164	367	184
<i>R</i> <sub>1</sub> [ <i>F</i> , <i>I</i> >2 $\sigma$ ( <i>I</i> )]	0.0349	0.0312	0.0539	0.0311	0.0394	0.0314	0.0418	0.0364	0.0522
<i>wR</i> <sub>2</sub> ( <i>F</i> <sup>2</sup> , all data)	0.0922	0.0827	0.1312	0.0846	0.1088	0.0838	0.1113	0.0876	0.1320
Flack	0.06(7)	0.03(6)	-0.019(18)	-	-	0.392(16)	-	-	0.07(13)
Hoofit <sup>a</sup>	0.11(3)	0.03(2)	-0.024(8)	-	-	0.385(7) <sup>b</sup>	-	-	0.11(7)

<sup>a</sup> as implemented in PLATON

<sup>b</sup> racemic twin