

## Supplementary Materials

### Synthesis and structural features of chiral cyclic squaramides and their application in asymmetric catalytic reactions

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	<b>4a</b>	<b>4b</b>	<b>4c</b>	<b>4d</b>
CCDC deposition number	783604	783602	783603	783605
formula	C <sub>20</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>48</sub> H <sub>50</sub> N <sub>4</sub> O <sub>5</sub>	C <sub>28</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>32</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Formula weight	318.36	762.92	426.54	470.55
T [K]	273(2)	273(2)	273(2)	273(2)
Wavelength	0.71073 Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
space group	<i>P</i> 2(1)	<i>P</i> 2(1)	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>C</i> 222(1)
<i>Unit cell dimensions</i>				
<i>a</i> [Å]	8.9343(19)	9.6536(12)	8.7372(8)	11.9819(8)
<i>b</i> [Å]	6.5722(14)	16.123(2)	16.3550(16)	16.2372(11)
<i>c</i> [Å]	14.533(3)	13.6848(17)	17.5772(17)	25.7415(18)
$\alpha$ [deg]	90	90	90	90
$\beta$ [deg]	97.941(3)	97.426(2)	90	90
$\gamma$ [deg]	90	90	90	90
V [Å <sup>3</sup> ]	845.2(3)	2112.2(5)	2511.7(4)	5008.1(6)
Z	2	2	4	8
Calculated density [Mg/m <sup>3</sup> ]	1.251	1.200	1.128	1.248
Absorption coefficient [mm <sup>-1</sup> ]	0.082	0.078	0.071	0.078
F(000)	336	812	912	1984

Crystal size [mm]	0.28 × 0.27 × 0.24	0.32 × 0.28 × 0.28	0.32 × 0.28 × 0.27	0.37 × 0.35 × 0.32
Theta range for data collection [deg]	2.30-26.49	1.96-26.49	2.32-26.00	2.11-26.00
Limiting indices	$-11 \leq h \leq 9$	$-12 \leq h \leq 5$	$-8 \leq h \leq 10$	$-14 \leq h \leq 14$
	$-7 \leq k \leq 8$	$-20 \leq k \leq 20$	$-18 \leq k \leq 20$	$-14 \leq k \leq 19$
	$-17 \leq l \leq 18$	$-17 \leq l \leq 17$	$-21 \leq l \leq 21$	$-30 \leq l \leq 31$
Reflections collected	5076	12835	14684	14645
Unique reflections	3019 [R(int) = 0.0176]	8458 [R(int) = 0.0205]	4927 [R(int) = 0.0359]	4927 [R(int) = 0.0196]
Completeness to theta = 26.49	99.6 %	99.7 %	99.8 %	99.7 %
Transmission Max/min	0.9806/0.9775	0.9785/0.9755	0.9811/0.9777	0.9755/0.9717
Refinement method	Full-matrix	Full-matrix	Full-matrix	Full-matrix
	least-squares on $F^2$	least-squares on $F^2$	least-squares on $F^2$	least-squares on $F^2$
Data/restraints/parameters	3019/1/220	8458/22/517	4927/1/292	4927/0/326
Goodness-of-fit on $F^2$	0.996	1.032	0.977	1.014
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0347,$ $wR_2 = 0.0740$	$R_1 = 0.0775,$ $wR_2 = 0.2161$	$R_1 = 0.0690,$ $wR_2 = 0.1580$	$R_1 = 0.0323,$ $wR_2 = 0.0644$
	$R_1 = 0.0455,$ $wR_2 = 0.0808$	$R_1 = 0.1062,$ $wR_2 = 0.2499$	$R_1 = 0.1276,$ $wR_2 = 0.1897$	$R_1 = 0.0394,$ $wR_2 = 0.0677$
Absolute structure parameter	0.3(15)	0(2)	0(3)	0.5(12)
Extinction coefficient	0.040(3)	0.012(3)	0.0021(10)	0.00559(18)