

# Synthesis, structural, thermal, and Hirshfeld surface analysis of In(III) tris (N-methyl-N-phenyl dithiocarbamate)

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**Table S1.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>).

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub> */ <i>U</i> <sub>eq</sub>
<b>In1</b>	-0.02270 (2)	0.68802 (3)	0.15580 (2)	0.02275 (12)
<b>S1</b>	0.07453 (9)	0.78311 (10)	-0.01197 (9)	0.0266 (3)
<b>S2</b>	-0.13027 (9)	0.86419 (10)	0.04961 (9)	0.0252 (3)
<b>S3</b>	-0.13589 (9)	0.67652 (10)	0.31926 (9)	0.0256 (3)
<b>S4</b>	0.06313 (9)	0.71388 (10)	0.26633 (9)	0.0261 (3)
<b>S5</b>	0.07573 (9)	0.49475 (10)	0.20586 (10)	0.0266 (3)
<b>S6</b>	-0.10882 (9)	0.58524 (10)	0.11754 (10)	0.0280 (3)
<b>N1</b>	-0.0407 (3)	0.6885 (3)	0.4397 (3)	0.0242 (9)
<b>N2</b>	-0.0396 (3)	0.9562 (3)	-0.1277 (3)	0.0241 (9)
<b>N3</b>	-0.0214 (3)	0.3874 (3)	0.1777 (3)	0.0232 (9)
<b>C1</b>	-0.0324 (3)	0.8753 (4)	-0.0390 (4)	0.0227 (10)
<b>C2</b>	-0.0387 (4)	0.6926 (4)	0.3503 (4)	0.0243 (11)
<b>C3</b>	-0.0187 (3)	0.4806 (4)	0.1673 (3)	0.0212 (10)
<b>C4</b>	-0.1302 (4)	1.0349 (4)	-0.1496 (4)	0.0326 (13)
<b>C5</b>	-0.1233 (4)	0.6672 (5)	0.5152 (4)	0.0382 (14)
<b>C6</b>	-0.1022 (4)	0.3739 (5)	0.1457 (5)	0.0424 (15)
<b>C13</b>	0.0386 (3)	0.9686 (4)	-0.2065 (4)	0.0228 (11)
<b>C14</b>	0.0459 (4)	0.9248 (4)	-0.2705 (4)	0.0294 (12)
<b>C15</b>	0.1172 (4)	0.9413 (4)	-0.3502 (4)	0.0283 (11)
<b>C16</b>	0.1793 (4)	1.0032 (4)	-0.3670 (4)	0.0274 (11)
<b>C17</b>	0.1703 (4)	1.0474 (4)	-0.3026 (4)	0.0258 (11)
<b>C18</b>	0.0998 (3)	1.0300 (4)	-0.2218 (4)	0.0251 (11)
<b>C19</b>	0.0535 (3)	0.2960 (4)	0.2212 (4)	0.0231 (10)
<b>C20</b>	0.1272 (4)	0.2618 (4)	0.1602 (4)	0.0282 (11)
<b>C21</b>	0.1962 (4)	0.1720 (4)	0.2028 (4)	0.0319 (12)
<b>C22</b>	0.1907 (4)	0.1159 (4)	0.3032 (4)	0.0326 (12)
<b>C23</b>	0.1161 (4)	0.1496 (4)	0.3639 (4)	0.0310 (12)

<b>C24</b>	0.0475 (4)	0.2397 (4)	0.3225 (4)	0.0291 (12)
<b>C25</b>	0.0423 (3)	0.6984 (4)	0.4672 (3)	0.0212 (10)
<b>C26</b>	0.0625 (4)	0.7957 (4)	0.4325 (4)	0.0274 (11)
<b>C27</b>	0.1411 (4)	0.8030 (4)	0.4606 (4)	0.0333 (13)
<b>C28</b>	0.1986 (4)	0.7160 (5)	0.5248 (4)	0.0372 (13)
<b>C29</b>	0.1781 (4)	0.6203 (5)	0.5604 (4)	0.0366 (13)
<b>C30</b>	0.0989 (4)	0.6114 (4)	0.5324 (4)	0.0293 (12)
<b>In2</b>	0.47645 (2)	0.16387 (3)	0.65457 (2)	0.02313 (12)
<b>S7</b>	0.35653 (9)	0.09363 (10)	0.81209 (9)	0.0250 (3)
<b>S8</b>	0.55345 (9)	-0.02228 (10)	0.76913 (10)	0.0271 (3)
<b>S9</b>	0.57842 (9)	0.17766 (10)	0.48689 (9)	0.0253 (3)
<b>S10</b>	0.37774 (9)	0.14587 (11)	0.54664 (9)	0.0275 (3)
<b>S11</b>	0.39644 (9)	0.35767 (10)	0.61295 (10)	0.0266 (3)
<b>S12</b>	0.57941 (9)	0.24118 (10)	0.70531 (10)	0.0262 (3)
<b>N4</b>	0.4632 (3)	0.2005 (3)	0.3634 (3)	0.0243 (9)
<b>N5</b>	0.5022 (3)	0.4403 (3)	0.6612 (3)	0.0245 (9)
<b>N6</b>	0.4424 (3)	-0.0921 (3)	0.9383 (3)	0.0237 (9)
<b>C7</b>	0.4927 (3)	0.3557 (4)	0.6593 (3)	0.0228 (6)
<b>C8</b>	0.3710 (4)	0.2066 (5)	0.3350 (4)	0.0332 (13)
<b>C9</b>	0.4310 (4)	0.5396 (4)	0.6225 (4)	0.0320 (12)
<b>C10</b>	0.3549 (4)	-0.0910 (4)	1.0098 (4)	0.0382 (14)
<b>C11</b>	0.4491 (3)	-0.0145 (4)	0.8492 (4)	0.0228 (6)
<b>C12</b>	0.4723 (3)	0.1764 (4)	0.4562 (3)	0.0228 (6)
<b>C31</b>	0.5215 (3)	-0.1820 (4)	0.9687 (4)	0.0226 (10)
<b>C32</b>	0.5354 (4)	-0.2568 (4)	0.9348 (4)	0.0244 (11)
<b>C33</b>	0.6128 (4)	-0.3427 (4)	0.9628 (4)	0.0269 (11)
<b>C34</b>	0.6719 (4)	-0.3544 (4)	1.0270 (4)	0.0292 (12)
<b>C35</b>	0.6556 (4)	-0.2789 (4)	1.0620 (4)	0.0298 (12)
<b>C36</b>	0.5807 (4)	-0.1934 (4)	1.0331 (4)	0.0288 (12)
<b>C37</b>	0.5380 (4)	0.2362 (4)	0.2834 (4)	0.0240 (11)
<b>C38</b>	0.6172 (4)	0.1660 (4)	0.2642 (4)	0.0274 (11)
<b>C39</b>	0.6858 (4)	0.2037 (4)	0.1868 (4)	0.0300 (12)
<b>C40</b>	0.6776 (4)	0.3087 (4)	0.1291 (4)	0.0335 (13)
<b>C41</b>	0.5969 (4)	0.3785 (4)	0.1479 (4)	0.0321 (12)
<b>C42</b>	0.5264 (4)	0.3422 (4)	0.2260 (4)	0.0277 (11)
<b>C43</b>	0.5752 (4)	0.4372 (4)	0.7135 (4)	0.0235 (11)
<b>C44</b>	0.5621 (4)	0.3924 (4)	0.8164 (4)	0.0274 (11)

<b>C45</b>	0.6278 (4)	0.3929 (4)	0.8675 (4)	0.0295 (12)
<b>C46</b>	0.7056 (4)	0.4389 (4)	0.8161 (4)	0.0329 (13)
<b>C47</b>	0.7164 (4)	0.4837 (4)	0.7138 (4)	0.0341 (13)
<b>C48</b>	0.6512 (4)	0.4826 (4)	0.6624 (4)	0.0285 (12)

**Table S2.** Selected bond distances (Å) and angles (°) obtained by X-ray diffraction.

<b>Bond length (Å)</b>			
In1—S1	2.6033 (13)	In2—S7	2.6047 (13)
In1—S2	2.6018 (13)	In2—S8	2.5668 (13)
In1—S3	2.6258 (13)	In2—S9	2.6067 (13)
In1—S4	2.5561 (14)	In2—S10	2.5880 (14)
In1—S5	2.6352 (13)	In2—S11	2.5980 (13)
In1—S6	2.5817 (14)	In2—S12	2.5815 (13)
S1—C1	1.725 (5)	S7—C11	1.717 (5)
S2—C1	1.716 (5)	S8—C11	1.730 (5)
S3—C2	1.713 (5)	S9—C12	1.730 (5)
S4—C2	1.726 (5)	S10—C12	1.713 (5)
S5—C3	1.727 (5)	S11—C7	1.708 (5)
S6—C3	1.696 (5)	S12—C7	1.737 (5)
N1—C2	1.343 (7)	N4—C8	1.476 (6)
N1—C5	1.461 (6)	N4—C12	1.331 (6)
N1—C25	1.442 (6)	N4—C37	1.449 (6)
N2—C1	1.338 (6)	N5—C7	1.328 (6)
N2—C4	1.465 (6)	N5—C9	1.474 (6)
N2—C13	1.440 (6)	N5—C43	1.460 (6)
N3—C3	1.339 (6)	N6—C10	1.478 (6)
N3—C6	1.479 (7)	N6—C11	1.326 (6)
N3—C19	1.449 (6)	N6—C31	1.445 (6)
C13—C14	1.387 (7)	C31—C32	1.387 (7)
C13—C18	1.377 (7)	C31—C36	1.383 (7)
C14—C15	1.386 (7)	C32—C33	1.395 (7)
C15—C16	1.388 (7)	C33—C34	1.380 (8)
C16—C17	1.390 (7)	C34—C35	1.402 (8)
C17—C18	1.389 (7)	C35—C36	1.371 (7)
C19—C20	1.392 (7)	C37—C38	1.385 (7)
C19—C24	1.380 (7)	C37—C42	1.387 (7)
C20—C21	1.385 (7)	C38—C39	1.375 (7)

C21—C22	1.369 (8)	C39—C40	1.381 (8)
C22—C23	1.392 (8)	C40—C41	1.391 (8)
C23—C24	1.381 (7)	C41—C42	1.394 (7)
C25—C26	1.396 (7)	C43—C44	1.393 (7)
C25—C30	1.381 (7)	C43—C48	1.363 (7)
C26—C27	1.369 (8)	C44—C45	1.382 (7)
C27—C28	1.381 (8)	C45—C46	1.390 (7)
C28—C29	1.375 (8)	C46—C47	1.385 (8)
C29—C30	1.386 (8)	C47—C48	1.382 (8)
<b>Bond Angles (°)</b>			
S1—In1—S3	154.08 (4)	S7—In2—S9	156.95 (4)
S1—In1—S5	101.07 (4)	S8—In2—S7	70.24 (4)
S2—In1—S1	69.67 (4)	S8—In2—S9	100.21 (4)
S2—In1—S3	92.39 (4)	S8—In2—S10	105.54 (5)
S2—In1—S5	156.78 (5)	S8—In2—S11	153.82 (4)
S3—In1—S5	102.20 (4)	S8—In2—S12	92.26 (4)
S4—In1—S1	97.67 (4)	S10—In2—S7	92.11 (4)
S4—In1—S2	109.61 (4)	S10—In2—S9	69.75 (4)
S4—In1—S3	70.12 (4)	S10—In2—S11	95.94 (4)
S4—In1—S5	92.45 (4)	S11—In2—S7	94.56 (4)
S4—In1—S6	153.67 (4)	S11—In2—S9	101.18 (4)
S6—In1—S1	104.01 (5)	S12—In2—S7	103.64 (4)
S6—In1—S2	92.02 (4)	S12—In2—S9	97.53 (4)
S6—In1—S3	94.88 (4)	S12—In2—S10	159.50 (4)
S6—In1—S5	69.04 (4)	S12—In2—S11	70.13 (4)
C1—S1—In1	85.15 (16)	C11—S7—In2	84.59 (16)
C1—S2—In1	85.38 (17)	C11—S8—In2	85.53 (17)
C2—S3—In1	83.93 (17)	C12—S9—In2	84.39 (16)
C2—S4—In1	85.87 (18)	C12—S10—In2	85.31 (17)
C3—S5—In1	84.50 (17)	C7—S11—In2	85.20 (18)
C3—S6—In1	86.82 (18)	C7—S12—In2	85.16 (17)
C2—N1—C5	122.0 (5)	C12—N4—C8	121.2 (4)
C2—N1—C25	120.8 (4)	C12—N4—C37	121.7 (4)
C25—N1—C5	117.1 (4)	C37—N4—C8	116.5 (4)
C1—N2—C4	120.6 (4)	C7—N5—C9	121.6 (4)
C1—N2—C13	122.4 (4)	C7—N5—C43	122.1 (4)
C13—N2—C4	117.0 (4)	C43—N5—C9	115.8 (4)

C3—N3—C6	120.9 (4)	C11—N6—C10	122.1 (4)
C3—N3—C19	121.8 (4)	C11—N6—C31	120.6 (4)
C19—N3—C6	117.3 (4)	C31—N6—C10	117.4 (4)
S2—C1—S1	119.5 (3)	S11—C7—S12	119.5 (3)
N2—C1—S1	121.0 (4)	N5—C7—S11	121.1 (4)
N2—C1—S2	119.5 (4)	N5—C7—S12	119.4 (4)
S3—C2—S4	119.9 (3)	S7—C11—S8	119.4 (3)
N1—C2—S3	120.7 (4)	N6—C11—S7	121.3 (4)
N1—C2—S4	119.4 (4)	N6—C11—S8	119.3 (4)
S6—C3—S5	119.5 (3)	S10—C12—S9	119.2 (3)
N3—C3—S5	120.2 (4)	N4—C12—S9	120.7 (4)
N3—C3—S6	120.3 (4)	N4—C12—S10	120.1 (4)
C14—C13—N2	118.8 (4)	C32—C31—N6	119.3 (4)
C18—C13—N2	119.9 (5)	C36—C31—N6	119.6 (5)
C18—C13—C14	121.1 (5)	C36—C31—C32	121.0 (5)
C15—C14—C13	119.6 (5)	C31—C32—C33	119.4 (5)
C14—C15—C16	120.1 (5)	C34—C33—C32	119.7 (5)
C15—C16—C17	119.5 (5)	C33—C34—C35	120.1 (5)
C16—C17—C18	120.6 (5)	C36—C35—C34	120.3 (5)
C20—C19—N3	119.7 (5)	C38—C37—N4	120.6 (4)
C24—C19—N3	119.7 (4)	C38—C37—C42	121.5 (5)
C24—C19—C20	120.5 (5)	C42—C37—N4	117.9 (4)
C21—C20—C19	119.1 (5)	C39—C38—C37	118.4 (5)
C22—C21—C20	120.7 (5)	C38—C39—C40	121.8 (5)
C21—C22—C23	120.1 (5)	C39—C40—C41	119.4 (5)
C24—C23—C22	119.8 (5)	C40—C41—C42	119.9 (5)
C19—C24—C23	119.8 (5)	C37—C42—C41	119.0 (5)
C26—C25—N1	120.5 (4)	C44—C43—N5	118.3 (4)
C30—C25—N1	119.3 (4)	C48—C43—N5	120.5 (5)
C30—C25—C26	120.2 (5)	C48—C43—C44	121.1 (5)
C27—C26—C25	119.3 (5)	C45—C44—C43	119.4 (5)
C26—C27—C28	120.8 (5)	C44—C45—C46	119.9 (5)
C29—C28—C27	120.1 (5)	C47—C46—C45	119.4 (5)
C28—C29—C30	119.9 (5)	C48—C47—C46	120.8 (5)
C25—C30—C29	119.7 (5)	C43—C48—C47	119.3 (5)