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### Private Communications Cambridge Crystallographic Data Centre

#### 1. Summary of Data CCDC 154821

Authors: K.Harms, M.Marsch

Journal: Private Communication (1078), 2000

Compound: C<sub>10</sub> H<sub>13</sub> N<sub>1</sub>

Unit cell parameters: a 6.3611(16) b 16.313(4) c 8.6460(15) beta 96.089(18)

Space group P21/n

#### 2. Summary of Data CCDC 154822

Authors: K.Harms, M.Marsch

Journal: Private Communication (1078), 2000

Compound: C<sub>23</sub> H<sub>23</sub> N<sub>1</sub> O<sub>2</sub>

Unit cell parameters: a 8.3847(2) b 6.8914(4) c 14.8257(4) beta 98.280(3)

Space group P21/m

#### 3. Summary of Data CCDC 154823

Authors: K.Harms, M.Marsch

Journal: Private Communication (1078), 2000

Compound: C<sub>24</sub> H<sub>60</sub> Cl<sub>4</sub> Li<sub>2</sub> Mo<sub>2</sub> O<sub>17</sub>

Unit cell parameters: a 20.449(2) b 12.7631(12) c 16.5388(15)

Space group Pca21

#### 4. Summary of Data CCDC 154824

Authors: K.Harms, M.Marsch

Journal: Private Communication (1078), 2000

Compound: C<sub>19</sub> H<sub>16</sub> O<sub>1</sub>

Unit cell parameters: a 30.5918(13) c 7.7464(10) gamma 120.00

Space group R-3

#### 5. Summary of Data CCDC 160017

Authors: K.Harms, M.Marsch, G.Boche

Journal: Private Communication (1078), 2001

Formula: C<sub>28</sub> H<sub>35</sub> Li<sub>1</sub> N<sub>2</sub> O<sub>4</sub> S<sub>1</sub>

Unit cell parameters: a 11.738(9) b 12.401(8) c 12.538(8)

alpha 115.51(3) beta 95.46(4) gamma 115.22(3)

Space group P-1

6.Summary of Data CCDC 166308

Authors: K.Harms, G.Boche, M.Marsch

Journal: Private Communication (1078), 2001

Compound: C<sub>18</sub> H<sub>16</sub> Cd<sub>1</sub> F<sub>10</sub> N<sub>2</sub>

Unit cell parameters: a 18.110(2) b 7.2290(10) c 17.624(2) beta 118.150(10)

Space group C2/c

7.Summary of Data CCDC 166309

Authors: K.Harms, G.Boche, M.Marsch

Journal: Private Communication (1078), 2001

Compound: C<sub>18</sub> H<sub>21</sub> N<sub>1</sub> O<sub>2</sub>

Unit cell parameters: a 8.4490(10) b 9.8950(7) c 17.837(2) beta 101.507(6)

Space group P21/c

8.Summary of Data CCDC 166310

Authors: K.Harms, G.Boche, M.Marsch

Journal: Private Communication (1078), 2001

Compound: C<sub>16</sub> H<sub>23</sub> N<sub>1</sub> O<sub>4</sub>

Unit cell parameters: a 29.6297(13) b 8.8309(6) c 12.8246(8) beta 91.360(5)

Space group C2/c

9.Summary of Data CCDC 171753

Authors: G.Boche, M.Adler, S.Adler, M.Marsch, K.Harms

Journal: Private Communication (1078), 2001

Formula: C<sub>22</sub> H<sub>26</sub> F<sub>3</sub> Li<sub>1</sub> O<sub>3</sub>

Unit cell parameters: a 10.1124(17) b 10.7593(18) c 10.8940(17) alpha 114.874(16) beta 99.970(9)  
gamma 98.896(12)

space group P-1

10.Summary of Data CCDC 171754

Authors: G.Boche, M.Adler, S.Adler, M.Marsch, K.Harms

Journal: Private Communication (1078), 2001

Formula: C<sub>28</sub> H<sub>22</sub> F<sub>6</sub> O<sub>2</sub>

Unit cell parameters: a 8.249(4) b 11.771(9) c 12.354(8) alpha 92.23(8) beta 98.82(7) gamma 90.19(8)

space group P-1

11.Summary of Data CCDC 171790

Authors: G.Boche, M.Marsch, K.Harms

Journal: Private Communication (1078), 2001

Formula: C<sub>24</sub> H<sub>45</sub> Li<sub>2</sub> N<sub>5</sub> O<sub>1</sub>

Unit cell parameters: a 16.2540(6) b 14.6690(6) c 11.6570(5)

space group Pnma

12.Summary of Data CCDC 780552

Authors: B.Eckhardt, A.Geyer, K.Harms, M.Marsch

Journal: Private Communication (1078), 2010

Formula: C<sub>12</sub> H<sub>16</sub> N<sub>4</sub> O<sub>5</sub> S<sub>1</sub>

Unit cell parameters: a 6.4513(9) b 8.0413(11) c 8.3415(11)

alpha 74.668(16) beta 69.467(16) gamma 71.102(16)

space group P1

13. Summary of Data CCDC 781526  
Authors: P.Schueler, M.Oberthuer, M.Marsch  
Journal: Private Communication (1078), 2010  
Formula: C16 H22 N2 O5  
Unit cell parameters: a 4.7806(3) b 9.9198(4) c 18.0281(11) beta 90.350(5)  
space group P21

14. Summary of Data CCDC 1477552  
Authors: H.Seger, M.Marsch, A.Geyer  
Journal: Private Communication 2016  
Formula: C13 H19 N O8 S  
Unit cell parameters: a 5.680(<1) b 13.089(1) c 19.706(2) 90 90 90  
Space group P212121

15. Summary of Data CCDC 1477581  
Authors: A.Wuttke, M.Marsch, A.Geyer  
Journal: Private Communication 2016  
Formula: C26 H32 N6 O8 S, C H4 O  
Unit cell parameters: a 7.715(<1) b 11.708(<1) c 15.984(<1) beta 97.64  
Space group P21

16. Summary of Data CCDC 1004643  
Authors: André Wuttke, Michael Marsch, Armin Geyer  
Formula: C9 H12 N4 O5 S, C H4 O  
Unit cell a 4.96110(10)Å b 15.8494(5)Å c 17.3184(6)Å  
alpha 90° beta 90° gamma 90°  
Space group P 21 21 21  
DOI: 10.5517/ccdc.csd.cc12qdv1

17. Summary of Data CCDC 1004218  
Authors: André Wuttke, Michael Marsch, Armin Geyer  
Formula: C12 H16 N4 O5 S  
Unit cell a 6.4331(4)Å b 23.0497(14)Å c 10.2566(7)Å  
alpha 90° beta 90° gamma 90°  
Space group P 21 (4)  
DOI: 10.5517/ccdc.csd.cc12pz4w

18. Summary of Data CCDC 1004379  
Authors: André Wuttke, Michael Marsch, Armin Geyer  
Formula: C9 H12 N4 O5 S  
Unit cell a 6.4115(6)Å b 11.7145(12)Å c 16.3996(12)Å  
alpha 90° beta 90° gamma 90°  
Space group P 21 21 21  
DOI: 10.5517/ccdc.csd.cc12q4b8

19. Summary of Data CCDC 996510  
Authors: André Wuttke, Michael Marsch, Armin Geyer  
Formula: C15 H21 N5 O7 S  
Unit cell a 9.6748(6) Å b 13.6980(7) Å c 14.3131(10) Å  
alpha 90.00° beta 90.00° gamma 90.00°  
Space group P 21 21 21  
DOI: 10.5517/ccdc.csd.cc12fyhy

20. Summary of Data CCDC 1901488  
Authors: Michael Marsch, Ferdinand Bosold, Armin Geyer  
Formula: C10 H10 Cl1 N1 O4 S1  
Unit Cell Parameters: a 5.9481(4) b 9.1869(8) c 21.3378(18)  
Spacegroup P 21 21 21  
DOI: 10.5517/ccdc.csd.cc21tnbw
21. Summary of Data CCDC 1901636  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C16 H19 N1 O7 S1 \* H2 O1  
Unit Cell Parameters: a 8.2695(8) b 5.6479(3) c 18.3087(16)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21tt3t
22. Summary of Data CCDC 1901639  
Authors: Michael Marsch, Dominik Kohr, Armin Geyer  
Formula: C22 H34 N6 O8 \* H2 O1  
Unit Cell Parameters: a 12.7600(10) b 10.2294(6) c 19.5823(15)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21tt6x
23. Summary of Data CCDC 1901652  
Authors: Michael Marsch, Rolf Hörger, Armin Geyer  
Formula: C10 H15 N1 O7 S1 \* H2 O1  
Unit Cell Parameters: a 5.0040(2) b 6.9495(4) c 36.737(3)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21ttmb
24. Summary of Data CCDC 1901665  
Authors: Michael Marsch, Rolf Hörger, Armin Geyer  
Formula: C18 H23 N1 O9 S2  
Unit Cell Parameters: a 7.1842(3) b 8.8671(4) c 31.8062(16)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21tv1s
25. Summary of Data CCDC 1901682  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C13 H19 N1 O7 S1  
Unit Cell Parameters: a 10.5589(13) b 5.7632(8) c 13.2192(16)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21tv1b
26. Summary of Data CCDC 1901686  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C7 H9 N1 O4 S2  
Unit Cell Parameters: a 10.7345(12) b 5.1188(7) c 16.8496(18)  
Spacegroup P21/c  
DOI: 10.5517/ccdc.csd.cc21tvqg
27. Summary of Data CCDC 1901923  
Authors: Michael Marsch, Timm Schlosser, Armin Geyer  
Formula: C8 H14 O1 C8 H10 O1  
Unit Cell Parameters: a 8.3400(8) b 16.2352(14) c 11.3420(10)  
Spacegroup P21/n  
DOI: 10.5517/ccdc.csd.cc21v3cd

28. Summary of Data CCDC 1901931  
Authors: Michael Marsch, Rolf Hörger, Armin Geyer  
Formula: C17 H25 N1 O7 S1,0.13(H2 O1)  
Unit Cell Parameters: a 7.8870(8) b 12.1889(10) c 20.227(2)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21v3mn
29. Summary of Data CCDC 1901932  
Authors: Michael Marsch, Miriam Lauz, Armin Geyer  
Formula: C20 H21 N1 O5  
Unit Cell Parameters: a 11.5656(9) b 6.4796(4) c 11.6160(7)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21v3np
30. Summary of Data CCDC 1901933  
Formula: C14 H15 N1 O4 S1  
Authors: Michael Marsch, Sonja Eckhardt, Armin Geyer  
Unit Cell Parameters: a 9.010(7) b 9.721(6) c 15.109(8)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21v3pq
31. Summary of Data CCDC 1901934  
Authors: Michael Marsch, Björn Eckhardt, Armin Geyer  
Formula: C17 H26 N2 O7 S1  
Unit Cell Parameters: a 8.7771(8) b 11.0771(7) c 20.6432(16)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21v3qr
32. Summary of Data CCDC 1902308  
Authors: Michael Marsch, Sebastain Enck, Armin Geyer  
Formula: C28 H57 N1 O7 S1 Si3  
Unit Cell Parameters: a 19.997(3) b 16.246(3) c 23.468(3) C2  
DOI: 10.5517/ccdc.csd.cc21vhs6
33. Summary of Data CCDC 1902313  
Authors: Michael Marsch, Björn Eckhardt, Armin Geyer  
Formula: C14 H21 N3 O6 S1  
Unit Cell Parameters: a 6.9509(3) b 10.1853(4) c 23.1326(7)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21vhyc
34. Summary of Data CCDC 1902320  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C16 H21 N1 O10 S1  
Unit Cell Parameters: a 9.3157(5) b 8.3219(4) c 12.5309(9)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21vj5m
35. Summary of Data CCDC 1902321  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C22 H30 N6 O12 S2,3(H2 O1)  
Unit Cell Parameters: a 9.0051(13) b 17.0620(16) c 9.4081(13)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21vj6n

36. Summary of Data CCDC 1902323  
Authors: Michael Marsch, Timm Schlosser, Armin Geyer  
Formula: C12 H14 O2  
Unit Cell Parameters: a 11.1851(14) b 11.5962(12) c 8.0539(8)  
Spacegroup P21/c  
DOI: 10.5517/ccdc.csd.cc21vj8q

37. Summary of Data CCDC 1902339  
Authors: Michael Marsch, Dominik Kohr, Armin Geyer  
Formula: C6 H11 N4 O2 1+ C2 F3 O2 1-  
Unit Cell Parameters: a 7.4788(5) b 8.8087(5) c 9.2674(7)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21vjs7

38. Summary of Data CCDC 1902342  
Authors: Michael Marsch, Harald Seger, Armin Geyer  
Formula: C14 H19 N1 O7 S1  
Unit Cell Parameters: a 8.2360(3) b 12.0518(4) c 15.8231(6)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21vjwb

39. Summary of Data CCDC 1902640  
Authors: Michael Marsch, Sonja Eckhardt, Armin Geyer  
Formula: C13 H11 F3 N2 O4 S2  
Unit Cell Parameters: a 12.9234(5) b 8.4914(3) c 13.7005(5)  
Spacegroup P21/c  
DOI: 10.5517/ccdc.csd.cc21vvh8

40. Summary of Data CCDC 1902643  
Authors: Michael Marsch, Sonja Eckhardt, Armin Geyer  
Formula: C10 H13 N1 O5 S1  
Unit Cell Parameters: a 5.4364(6) b 5.2336(3) c 19.791(2)  
Spacegroup P21  
DOI: 10.5517/ccdc.csd.cc21vvlc

41. Summary of Data CCDC 1902644  
Authors: Michael Marsch, Magdalena Wasielak, Armin Geyer  
Formula: C9 H11 N1 O4  
Unit Cell Parameters: a 8.9839(3) b 30.5977(14) c 6.9839(4)  
Spacegroup P21/c  
DOI: 10.5517/ccdc.csd.cc21vvmd

42. Summary of Data CCDC 1902646  
Authors: Michael Marsch, Christoph Klotz, Armin Geyer  
Formula: C9 H13 N1 O6 S1  
Unit Cell Parameters: a 7.3767(2) b 18.1465(5) c 24.5676(8)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21vvpq

43. Summary of Data CCDC 1902649  
Authors: Michael Marsch, Björn Eckhardt, Armin Geyer  
Formula: C23 H30 N6 O9 S2  
Unit Cell Parameters: a 6.2422(3) b 20.5181(13) c 21.1418(13)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21vvsq

44. Summary of Data CCDC 1902966  
Authors: Michael Marsch, Sonja Eckhardt, Armin Geyer  
Formula: C15 H13 F3 N2 O6 S2  
Unit Cell Parameters: a 5.9381(2) b 8.1449(3) c 36.8782(16)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21w605
45. Summary of Data CCDC 1902989  
Authors: Michael Marsch, Susanne Kümmel, Armin Geyer  
Formula: C10 H9 N1 O4 S1  
Unit Cell Parameters: a 6.3391(4) b 21.1230(12) c 7.5907(5)  
Spacegroup P21/a  
DOI: 10.5517/ccdc.csd.cc21w6rx
46. Summary of Data CCDC 1902991  
Authors: Michael Marsch, Susanne Kümmel, Armin Geyer  
Formula: C14 H18 N2 2+,2(C11 1-)  
Unit Cell Parameters: a 11.2477(15) b 5.7441(5) c 11.3629(18)  
Spacegroup P21/n  
DOI: 10.5517/ccdc.csd.cc21w6tz
47. Summary of Data CCDC 1902999  
Authors: Michael Marsch, Felix Weiher, Armin Geyer  
Formula: C15 H24 N2 O6,H2 O1  
Unit Cell Parameters: a 10.4194(6) b 10.5401(8) c 16.0334(9)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21w728
48. Summary of Data CCDC 1903002  
Authors: Michael Marsch, Sebastian Enck, Armin Geyer  
Formula: C6 H6 N2 O3 S1  
Unit Cell Parameters: a 7.2504(5) b 9.1044(4) c 11.7134(8)  
Spacegroup P21/n  
DOI: 10.5517/ccdc.csd.cc21w75c
49. Summary of Data CCDC 1903005  
Authors: Michael Marsch, Frauke Messik, Markus Oberthür  
Formula: C6 H11 N1 O4  
Unit Cell Parameters: a 6.8969(3) b 9.3139(5) c 11.0526(4)  
Spacegroup P212121  
DOI: 10.5517/ccdc.csd.cc21w78g
50. Summary of Data CCDC 1904104  
Authors: Michael Marsch, Felix Weiher, Armin Geyer  
Formula: C10 H14 O3  
Unit Cell Parameters: a 21.4580(14) b 7.0850(6) c 6.3150(7)  
Spacegroup Pna21  
DOI: 10.5517/ccdc.csd.cc21xcq2
51. Summary of Data CCDC 1904125  
Authors: Michael Marsch, Lennart Nicke, Armin Geyer  
Formula: C15 H19 N1 O5  
Unit Cell Parameters: a 9.5463(4) b 16.6629(8) c 10.0255(5)  
Spacegroup P21/c

DOI: 10.5517/ccdc.csd.cc21xdds

52. Summary of Data CCDC 1904126

Authors: Michael Marsch, Christoph Priem, Armin Geyer

Formula: C12 H21 N1 O7 S1

Unit Cell Parameters: a 8.1297(8) b 10.7261(11) c 17.974(2)

Spacegroup P212121 DOI: 10.5517/ccdc.csd.cc21xdft

53. Summary of Data CCDC 1904127

Authors: Michael Marsch, Christoph Priem, Armin Geyer

Formula: C13 H20 N2 O5

Unit Cell Parameters: a 9.0857(5) b 12.9140(5) c 12.9884(6)

Spacegroup P21

DOI: 10.5517/ccdc.csd.cc21xdgv

54. Summary of Data CCDC 1904134

Authors: Michael Marsch, Christoph Priem, Armin Geyer

Formula: C21 H23 N1 O7 S1

Unit Cell Parameters: a 9.7727(4) b 9.5061(4) c 22.7303(10)

Spacegroup P21

DOI: 10.5517/ccdc.csd.cc21xdp2

55. Summary of Data CCDC 1904136

Authors: Michael Marsch, Lennart Nicke, Armin Geyer

Formula: C18 H19 N1 O3

Unit Cell Parameters: a 9.1412(4) b 15.5254(6) c 22.3430(11)

Spacegroup Pbca

DOI: 10.5517/ccdc.csd.cc21xdr4

56. Summary of Data CCDC 1904138

Authors: Michael Marsch, Lennart Nicke, Armin Geyer

Formula: C18 H17 N1 O3, C2 H6 O1 S1

Unit Cell Parameters: a 9.5160(4) b 9.6784(4) c 12.2712(5)

Spacegroup P-1

DOI: 10.5517/ccdc.csd.cc21xdt6

57. Summary of Data CCDC 1904139

Authors: Michael Marsch, Lennart Nicke, Armin Geyer

Formula: C25 H22 N2 O5

Unit Cell Parameters: a 12.298(3) b 5.4805(16) c 15.083(4)

Spacegroup P21

DOI: 10.5517/ccdc.csd.cc21xdv7

58. Summary of Data CCDC 1904140

Authors: Michael Marsch, Lennart Nicke, Armin Geyer

Formula: C25 H22 N2 O5

Unit Cell Parameters: a 8.811(7) b 14.177(8) c 17.112(10)

Spacegroup P212121

DOI: 10.5517/ccdc.csd.cc21xdw8



59. Summary of Data CCDC 1904148

Authors: Michael Marsch, Christoph Priem, Armin Geyer

Formula: C<sub>17</sub> H<sub>23</sub> N<sub>1</sub> O<sub>4</sub> Se<sub>1</sub>

Unit Cell Parameters: a 11.7613(9) b 5.9773(5) c 12.7129(10)

Spacegroup P21

DOI: 10.5517/ccdc.csd.cc21xf4k

60. Summary of Data CCDC 1857550

Authors: Klaus Harms, Michael Marsch

Formula: C<sub>18</sub> H<sub>18</sub> Br<sub>1</sub> N<sub>2</sub> 1<sup>+</sup>,F<sub>6</sub> P<sub>1</sub> 1<sup>-</sup>

Unit Cell Parameters: a 12.7402(2) b 15.3208(2) c 19.8461(3)

Spacegroup P21/c

DOI: 10.13140/RG.2.2.17659.87841