# 6-Carboxamido-5,4-Hydroxypyrimidinones: A New Class of Heterocyclic Ligands and their Evaluation as Gadolinium Chelating Agents

## Supplementary Information

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Contribution from

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Submitted to *Inorganic Chemistry*
March 14, 2001
Revised September 4, 2001

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 O(6)   1.2219(2)    0.2451(2)    0.3678(2)    0          Uij ? ?
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 C(1)   0.4379(2)    -0.3835(2)   -0.1025(2)   0          Uij ? ?
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 C(3)   0.4625(2)    -0.1378(2)   0.1066(2)    0          Uij ? ?
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 C(6)   0.6511(3)    -0.2900(3)   -0.1385(3)   0          Uij ? ?
 C(7)   0.2599(2)    -0.2561(2)   0.1432(2)    0          Uij ? ?
 C(8)   0.1273(3)    -0.0903(3)   0.0672(3)    0          Uij ? ?
 C(9)   0.0592(3)    -0.1848(3)   0.2149(3)    0          Uij ? ?
 C(10)  0.9456(2)    0.4257(2)    0.6141(2)    0          Uij ? ?
 C(11)  0.7839(2)    0.2701(2)    0.3930(2)    0          Uij ? ?
 C(12)  0.9112(2)    0.2185(2)    0.3706(2)    0          Uij ? ?
 C(13)  1.0415(2)    0.2722(2)    0.4696(2)    0          Uij ? ?
 C(14)  0.9625(3)    0.5376(2)    0.7471(2)    0          Uij ? ?
 C(15)  0.6802(2)    0.4239(2)    0.5502(2)    0          Uij ? ?
 C(16)  1.1766(2)    0.2208(2)    0.4480(2)    0          Uij ? ?
 C(17)  1.1912(3)    0.1162(3)    0.6123(3)    0          Uij ? ?
 C(18)  1.3752(3)    0.1016(3)    0.5035(3)    0          Uij ? ?
 H(1)   0.333(3)     -0.580(3)    -0.239(2)    0          Uij ? ?
 H(2)   0.510(3)     -0.560(2)    -0.202(2)    0          Uij ? ?
 H(3)   0.414(3)     -0.495(2)    -0.296(3)    0          Uij ? ?
 H(4)   0.690(3)     -0.378(3)    -0.149(2)    0          Uij ? ?
 H(5)   0.615(3)     -0.284(2)    -0.221(3)    0          Uij ? ?
 H(6)   0.732(3)     -0.220(3)    -0.087(3)    0          Uij ? ?
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 H(8)   0.113(3)     -0.188(2)    0.299(3)     0          Uij ? ?
 H(9)   0.026(3)     -0.093(3)    0.243(2)     0          Uij ? ?
 H(10)  0.027(3)     -0.122(2)    0.002(2)     0          Uij ? ?
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 H(12)  0.201(3)     -0.091(2)    0.023(2)     0          Uij ? ?
 H(13)  0.548(3)     0.048(3)     0.228(2)     0          Uij ? ?
 H(14)  0.690(3)     0.517(3)     0.565(2)     0          Uij ? ?
 H(15)  0.677(3)     0.406(2)     0.627(3)     0          Uij ? ?
 H(16)  0.595(3)     0.370(3)     0.472(3)     0          Uij ? ?
 H(17)  0.923(3)     0.621(3)     0.738(2)     0          Uij ? ?
 H(18)  0.903(3)     0.506(2)     0.790(2)     0          Uij ? ?
 H(19)  1.063(3)     0.564(3)     0.800(3)     0          Uij ? ?
 H(20)  1.099(3)     0.146(3)     0.611(2)     0          Uij ? ?
 H(21)  1.176(3)     0.017(3)     0.589(2)     0          Uij ? ?
 H(22)  1.252(3)     0.166(3)     0.698(3)     0          Uij ? ?
 H(23)  1.447(3)     0.156(3)     0.576(3)     0          Uij ? ?
 H(24)  1.385(3)     0.107(3)     0.429(3)     0          Uij ? ?
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0.0396(9)
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0.0019(6)
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0.0214(7)
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0.0151(8)
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0.0088(7)
 N(5)   0.0187(9)   0.0191(9)   0.0205(9)   0.0039(7)   0.0069(7)
0.0088(7)
 N(6)   0.0188(9)   0.0246(9)   0.0231(9)   0.0084(7)   0.0095(8)
0.0126(8)
 C(1)   0.016(1)    0.022(1)    0.021(1)    0.0058(8)   0.0044(9)
0.0094(9)
 C(2)   0.017(1)    0.022(1)    0.0147(10)  0.0031(9)   0.0026(8)
0.0077(8)
 C(3)   0.021(1)    0.019(1)    0.015(1)    0.0063(9)   0.0067(9)
0.0077(8)
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0.0119(9)
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0.0040(10)
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0.005(1)
 C(7)   0.022(1)    0.021(1)    0.024(1)    0.0041(9)   0.0095(9)
0.0105(9)
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0.024(1)
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0.021(1)
 C(10)  0.020(1)    0.0170(10)  0.021(1)    0.0035(8)   0.0071(9)
0.0120(9)
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0.0095(8)
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0.0098(9)
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0.0071(9)
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0.0088(9)
 C(16)  0.017(1)    0.0158(10)  0.020(1)    0.0005(8)   0.0056(9)
0.0054(8)
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0.019(1)
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    O(3)      C(7)      1.233(3)   ? ? yes
    O(4)      C(11)     1.239(2)   ? ? yes
    O(5)      C(12)     1.349(2)   ? ? yes
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    O(6)      C(16)     1.230(3)   ? ? yes
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    N(1)      C(4)      1.377(3)   ? ? yes
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   N(5)      C(10)     1.307(3)   ? ? yes
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   C(2)      C(3)      1.435(3)   ? ? yes
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   C(5)      H(3)      0.96(3)    ? ? no
   C(6)      H(4)      0.99(2)    ? ? no
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   C(6)      H(6)      0.93(3)    ? ? no
   C(8)      H(10)     0.99(3)    ? ? no
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   C(8)      H(12)     1.00(2)    ? ? no
   C(9)      H(7)      0.94(3)    ? ? no
   C(9)      H(8)      0.96(3)    ? ? no
   C(9)      H(9)      1.00(2)    ? ? no
   C(10)     C(14)     1.491(3)   ? ? yes
   C(11)     C(12)     1.443(3)   ? ? yes
   C(12)     C(13)     1.354(3)   ? ? yes
   C(13)     C(16)     1.512(3)   ? ? yes
   C(14)     H(17)     1.00(2)    ? ? no
   C(14)     H(18)     0.99(3)    ? ? no
   C(14)     H(19)     0.95(3)    ? ? no
   C(15)     H(14)     0.92(3)    ? ? no
   C(15)     H(15)     0.97(3)    ? ? no
   C(15)     H(16)     0.98(3)    ? ? no
   C(17)     H(20)     0.97(3)    ? ? no
   C(17)     H(21)     0.96(3)    ? ? no
   C(17)     H(22)     0.91(3)    ? ? no
   C(18)     H(23)     0.88(3)    ? ? no
   C(18)     H(24)     0.90(3)    ? ? no
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|---|---|---|---|---|
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| N(1) | H(1) | N(2) | 45.7(4) | ? ? ? no |
| N(5) | H(1) | N(6) | 65.0(5) | ? ? ? no |
| N(5) | H(1) | N(2) | 124.3(8) | ? ? ? no |
| N(6) | H(1) | N(2) | 148.3(9) | ? ? ? no |
| O(3) | H(2) | N(2) | 118.1(9) | ? ? ? no |
| O(3) | H(2) | N(1) | 63.9(6) | ? ? ? no |
| O(3) | H(2) | N(1) | 147(1) | ? ? ? no |
| N(2) | H(2) | N(1) | 97.2(7) | ? ? ? no |
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| N(1) | H(2) | N(1) | 87.4(6) | ? ? ? no |
| N(2) | H(3) | O(4) | 67.0(5) | ? ? ? no |
| N(2) | H(3) | N(1) | 48.2(4) | ? ? ? no |
| N(2) | H(3) | N(5) | 123.4(8) | ? ? ? no |
| O(4) | H(3) | N(1) | 81.1(6) | ? ? ? no |
| O(4) | H(3) | N(5) | 88.4(6) | ? ? ? no |
| N(1) | H(3) | N(5) | 79.2(6) | ? ? ? no |
| N(2) | H(4) | O(3) | 127(1) | ? ? ? no |
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| N(2) | H(5) | O(4) | 79.5(7) | ? ? ? no |
| N(2) | H(5) | O(1) | 46.0(5) | ? ? ? no |
| N(2) | H(5) | O(2) | 93.2(8) | ? ? ? no |
| O(6) | H(5) | O(4) | 111.2(9) | ? ? ? no |
| O(6) | H(5) | O(1) | 119.3(8) | ? ? ? no |
| O(6) | H(5) | O(2) | 84.0(7) | ? ? ? no |
| O(4) | H(5) | O(1) | 87.1(6) | ? ? ? no |
| O(4) | H(5) | O(2) | 52.1(4) | ? ? ? no |
| O(1) | H(5) | O(2) | 62.5(4) | ? ? ? no |
| N(2) | H(6) | O(1) | 63.6(7) | ? ? ? no |
| N(2) | H(6) | O(6) | 126(1) | ? ? ? no |
| O(1) | H(6) | O(6) | 131.3(10) | ? ? ? no |
| N(3) | H(7) | O(3) | 50.5(6) | ? ? ? no |
| N(3) | H(8) | O(3) | 59.3(6) | ? ? ? no |
| N(3) | H(8) | N(4) | 136(1) | ? ? ? no |
| N(3) | H(8) | N(5) | 146(1) | ? ? ? no |
| N(3) | H(8) | N(6) | 99.0(9) | ? ? ? no |
| O(3) | H(8) | N(4) | 77.4(7) | ? ? ? no |
| O(3) | H(8) | N(5) | 105.8(8) | ? ? ? no |
| O(3) | H(8) | N(6) | 120.5(9) | ? ? ? no |
| N(4) | H(8) | N(5) | 41.5(3) | ? ? ? no |
| N(4) | H(8) | N(6) | 105.3(7) | ? ? ? no |
| N(5) | H(8) | N(6) | 114.0(7) | ? ? ? no |
| N(3) | H(9) | O(5) | 131(1) | ? ? ? no |
| N(3) | H(9) | N(6) | 104.2(9) | ? ? ? no |
| N(3) | H(9) | O(6) | 92.9(8) | ? ? ? no |
| O(5) | H(9) | N(6) | 79.1(6) | ? ? ? no |
| O(5) | H(9) | O(6) | 59.1(5) | ? ? ? no |
| N(6) | H(9) | O(6) | 39.0(3) | ? ? ? no |
| N(3) | H(10) | O(5) | 123(1) | ? ? ? no |
| N(3) | H(11) | O(6) | 117(1) | ? ? ? no |
| N(3) | H(11) | O(5) | 108.1(9) | ? ? ? no |
| N(3) | H(11) | O(2) | 70.6(7) | ? ? ? no |
| O(6) | H(11) | O(5) | 62.8(5) | ? ? ? no |
| O(6) | H(11) | O(2) | 83.8(6) | ? ? ? no |
| O(5) | H(11) | O(2) | 142.1(9) | ? ? ? no |
| N(3) | H(12) | O(1) | 160(1) | ? ? ? no |
| N(3) | H(12) | O(2) | 82.5(8) | ? ? ? no |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N(3) | H(12) | O(5) | 141(1) | ? | ? | ? | no |
| N(3) | H(12) | N(1) | 75.5(7) | ? | ? | ? | no |
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| O(1) | H(12) | O(5) | 56.9(5) | ? | ? | ? | no |
| O(1) | H(12) | N(1) | 100.0(8) | ? | ? | ? | no |
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| O(2) | H(12) | N(1) | 73.6(5) | ? | ? | ? | no |
| O(5) | H(12) | N(1) | 95.6(7) | ? | ? | ? | no |
| O(2) | H(13) | O(4) | 156(2) | ? | ? | ? | no |
| O(2) | H(13) | O(1) | 107(1) | ? | ? | ? | no |
| O(2) | H(13) | O(1) | 82(1) | ? | ? | ? | no |
| O(2) | H(13) | O(5) | 146(1) | ? | ? | ? | no |
| O(4) | H(13) | O(1) | 95(1) | ? | ? | ? | no |
| O(4) | H(13) | O(1) | 100.9(10) | ? | ? | ? | no |
| O(4) | H(13) | O(5) | 55.0(7) | ? | ? | ? | no |
| O(1) | H(13) | O(1) | 69.7(6) | ? | ? | ? | no |
| O(1) | H(13) | O(5) | 50.7(5) | ? | ? | ? | no |
| O(1) | H(13) | O(5) | 106.9(7) | ? | ? | ? | no |
| N(4) | H(14) | O(6) | 121(1) | ? | ? | ? | no |
| N(4) | H(14) | O(4) | 43.2(5) | ? | ? | ? | no |
| O(6) | H(14) | O(4) | 135.9(9) | ? | ? | ? | no |
| N(4) | H(15) | O(3) | 118(1) | ? | ? | ? | no |
| N(4) | H(15) | O(4) | 41.1(5) | ? | ? | ? | no |
| O(3) | H(15) | O(4) | 128.3(9) | ? | ? | ? | no |
| N(4) | H(16) | O(4) | 65.4(7) | ? | ? | ? | no |
| O(6) | H(17) | N(4) | 93.8(8) | ? | ? | ? | no |
| O(6) | H(17) | N(5) | 124.1(9) | ? | ? | ? | no |
| O(6) | H(17) | O(5) | 65.9(6) | ? | ? | ? | no |
| N(4) | H(17) | N(5) | 47.1(4) | ? | ? | ? | no |
| N(4) | H(17) | O(5) | 125.7(8) | ? | ? | ? | no |
| N(5) | H(17) | O(5) | 102.4(7) | ? | ? | ? | no |
| O(3) | H(18) | N(4) | 89.5(8) | ? | ? | ? | no |
| O(3) | H(18) | N(5) | 114.6(8) | ? | ? | ? | no |
| N(4) | H(18) | N(5) | 47.6(4) | ? | ? | ? | no |
| N(5) | H(19) | N(1) | 103.4(9) | ? | ? | ? | no |
| N(5) | H(19) | N(4) | 46.3(4) | ? | ? | ? | no |
| N(1) | H(19) | N(4) | 149.6(9) | ? | ? | ? | no |
| N(6) | H(20) | N(5) | 83.7(9) | ? | ? | ? | no |
| N(6) | H(21) | O(5) | 166(1) | ? | ? | ? | no |
| N(6) | H(21) | O(4) | 132.6(10) | ? | ? | ? | no |
| O(5) | H(21) | O(4) | 51.1(4) | ? | ? | ? | no |
| N(6) | H(22) | O(2) | 103.9(9) | ? | ? | ? | no |
| N(6) | H(22) | O(1) | 149(1) | ? | ? | ? | no |
| N(6) | H(22) | N(5) | 65.3(7) | ? | ? | ? | no |
| O(2) | H(22) | O(1) | 49.8(4) | ? | ? | ? | no |
| O(2) | H(22) | N(5) | 160.3(8) | ? | ? | ? | no |
| O(1) | H(22) | N(5) | 144.5(8) | ? | ? | ? | no |
| N(6) | H(23) | O(3) | 140(1) | ? | ? | ? | no |
| N(6) | H(23) | O(6) | 44.5(5) | ? | ? | ? | no |
| N(6) | H(23) | O(2) | 107.8(10) | ? | ? | ? | no |
| O(3) | H(23) | O(6) | 127.5(8) | ? | ? | ? | no |
| O(3) | H(23) | O(2) | 73.1(6) | ? | ? | ? | no |
| O(6) | H(23) | O(2) | 152.3(9) | ? | ? | ? | no |
| N(6) | H(24) | O(6) | 62.6(7) | ? | ? | ? | no |
| N(6) | H(24) | O(2) | 154(1) | ? | ? | ? | no |
| O(6) | H(24) | O(2) | 105.0(10) | ? | ? | ? | no |
| N(6) | H(25) | O(2) | 100.6(8) | ? | ? | ? | no |

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   N(6)      H(25)     N(3)      95.5(8)    ? ? ? no
   N(6)      H(25)     O(6)      38.1(5)    ? ? ? no
   O(2)      H(25)     N(3)      154.5(9)   ? ? ? no
   O(2)      H(25)     O(6)      131.2(8)   ? ? ? no
   N(3)      H(25)     O(6)      72.4(5)    ? ? ? no
   O(5)      H(26)     O(1)      157(2)     ? ? ? no
   O(5)      H(26)     O(4)      104(1)     ? ? ? no
   O(5)      H(26)     O(2)      142(1)     ? ? ? no
   O(1)      H(26)     O(4)      98(1)      ? ? ? no
   O(1)      H(26)     O(2)      55.4(7)    ? ? ? no
   O(4)      H(26)     O(2)      52.8(5)    ? ? ? no
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