

Supporting Information

Photoluminescent chromium molybdate cluster coordinated with rare-earth cations: Synthesis, structure, optical and magnetic properties

Dinesh Kumar^a, Shahab Ahmad^b, G.Vijaya Prakash^{b*}, Kandalam V.

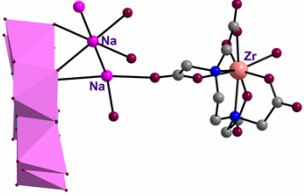
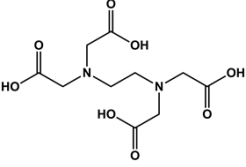
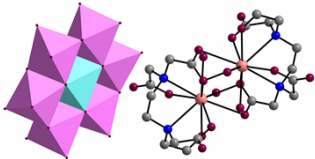
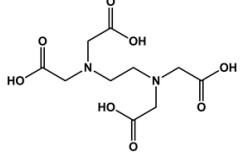
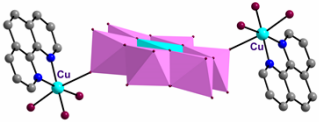
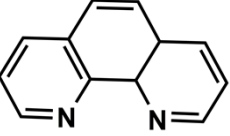
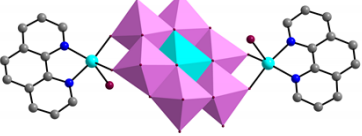
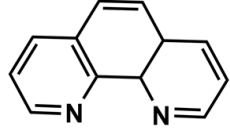
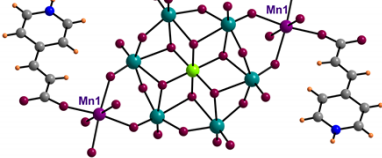
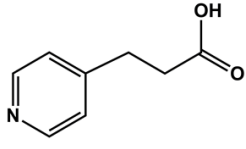
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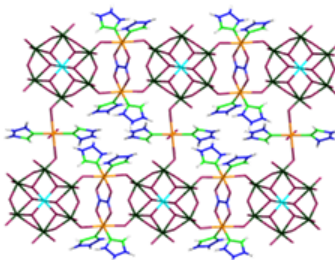
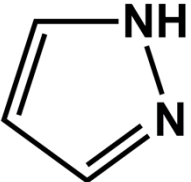
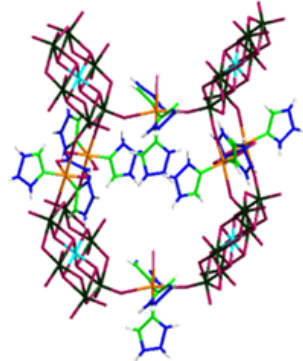
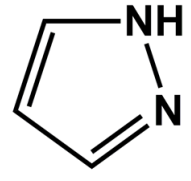
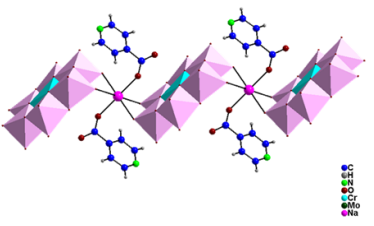
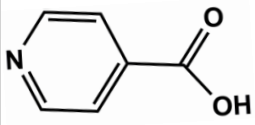
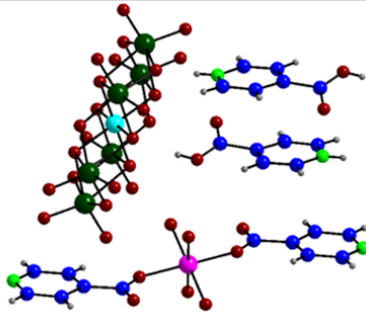
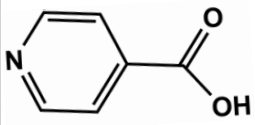
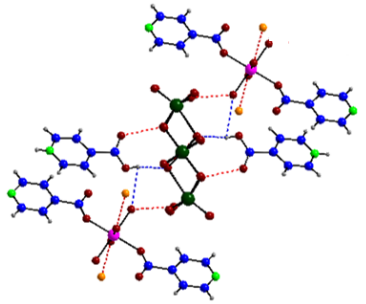
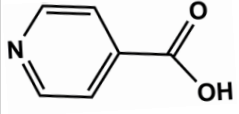
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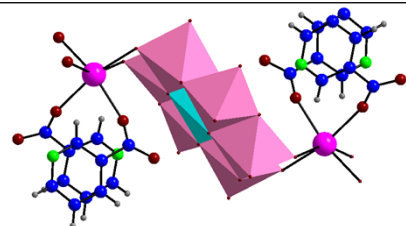
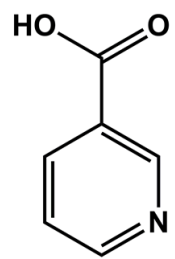
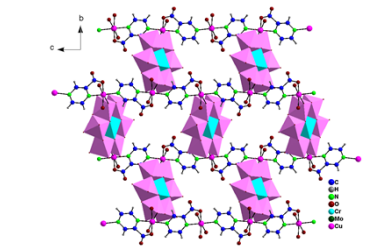
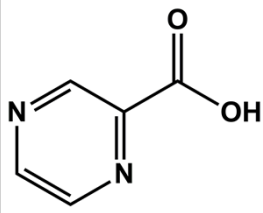
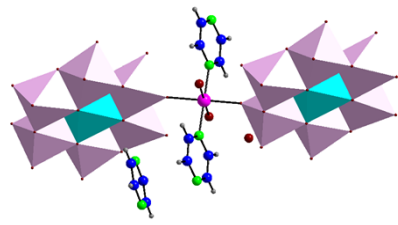
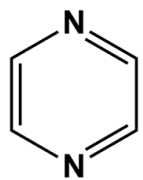
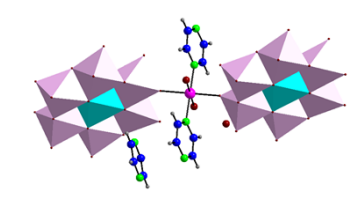
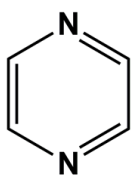
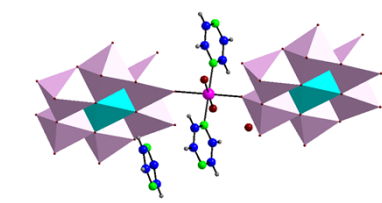
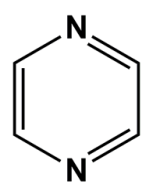
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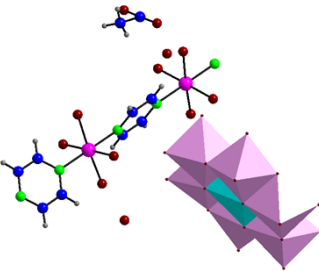
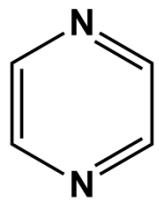
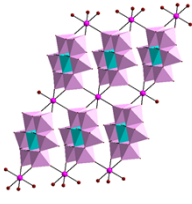
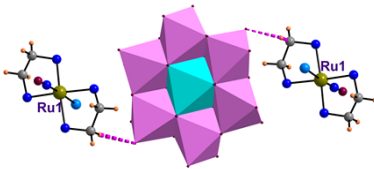
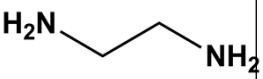
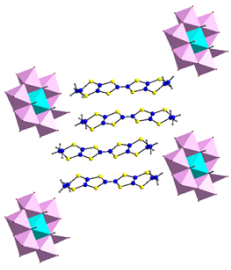
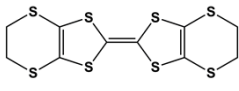
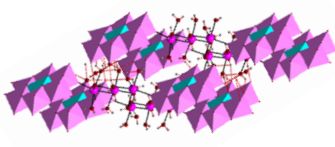
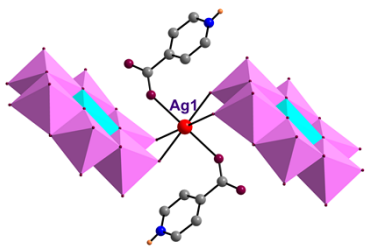
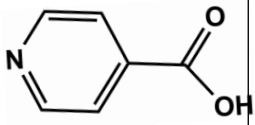
Table S1. Chromium Anderson–Evans cluster based solids reported in the literature

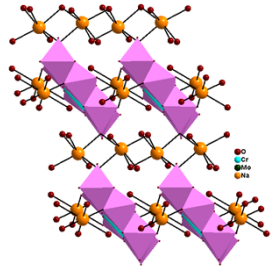
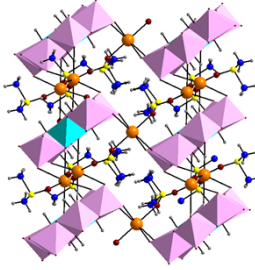
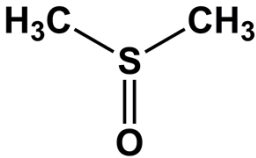
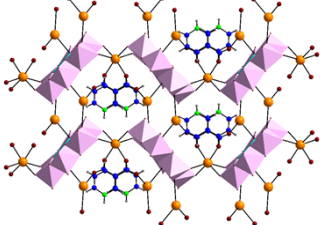
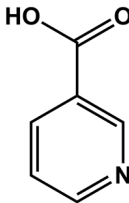
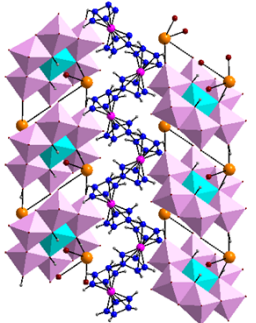
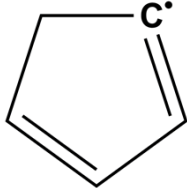
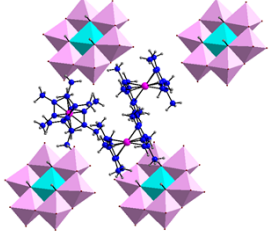
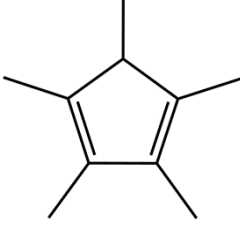
| S. No. | Compound | Cell parameters | Structural description | Organic | Reference |
|--------|---|---|--|---|--|
| 1. | $\text{Na}_3[\text{ZrEDTA}(\text{H}_2\text{O})_2]_2[\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 10\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 7.959(5)$ $b / \text{\AA} = 10.937(8)$ $c / \text{\AA} = 17.630(12)$ $\alpha / ^\circ = 74.772(8)$ $\beta / ^\circ = 81.772(9)$ $\gamma / ^\circ = 75.439(9)$ $Z = 1$ |  |  | <i>Solid State Sciences</i> , 2011 , <i>13</i> , 1122 |
| 2. | $[\text{Ce}_3(\text{HEDTA})_2(\text{H}_2\text{O})_9][\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 13\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 13.759(1)$ $b / \text{\AA} = 15.271(1)$ $c / \text{\AA} = 19.664(2)$ $\alpha / ^\circ = 72.386(1)$ $\beta / ^\circ = 71.489(1)$ $\gamma / ^\circ = 88.591(1)$ $Z = 2$ |  |  | <i>Solid State Sciences</i> , 2011 , <i>13</i> , 1122 |
| 3. | $[\{\text{Cu}(\text{C}_{12}\text{N}_2\text{H}_8)(\text{H}_2\text{O})_3\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}][\{\text{Cu}_2(\text{C}_2\text{O}_4)(\text{C}_{12}\text{N}_2\text{H}_8)_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 12\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 11.477(10)$ $b / \text{\AA} = 14.099(12)$ $c / \text{\AA} = 17.175(16)$ $\alpha / ^\circ = 76.829(10)$ $\beta / ^\circ = 72.209(10)$ $\gamma / ^\circ = 80.252(10)$ $Z = 1$ |  |  | <i>Inorg. Chem. Comm.</i> , 2011 , <i>14</i> , 384 |
| 4. | $[\text{Cu}(\text{phen})\text{H}_2\text{O}]_2[\text{H}_5\text{CrMo}_6\text{O}_2]_4 \cdot 5\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 8.385(5)$ $b / \text{\AA} = 9.236(5)$ $c / \text{\AA} = 14.762(8)$ $\alpha / ^\circ = 87.640(10)$ $\beta / ^\circ = 74.440(10)$ $\gamma / ^\circ = 72.427(10)$ $Z = 1$ |  |  | <i>J. Coord. Chem.</i> , 2011 , <i>64</i> , 2388 |
| 5. | $\beta - (4\text{-Hpya})_2[(4\text{-Hpya})_2(\text{H}_2\text{O})_4\text{Mn}][\text{H}_6\text{CrMo}_6\text{O}_{24}]\{[(4\text{-Hpya})(\text{H}_2\text{O})_3\text{Mn}]_2(\text{H}_6\text{CrMo}_6\text{O}_{24})\} \cdot 12\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 14.275(2)$ $b / \text{\AA} = 14.3852(2)$ $c / \text{\AA} = 15.755(2)$ $\alpha / ^\circ = 115.364(7)$ $\beta / ^\circ = 93.342(9)$ $\gamma / ^\circ = 112.530(7)$ $Z = 1$ |  |  | <i>CrystEngComm</i> , 2011 , <i>13</i> , 5384 |

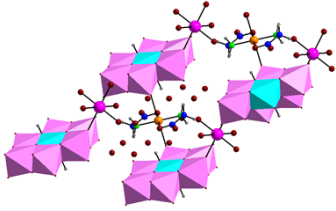
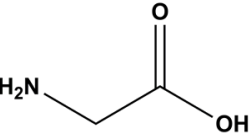
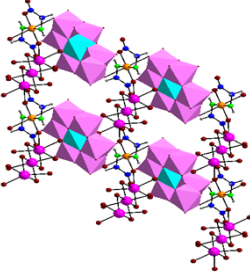
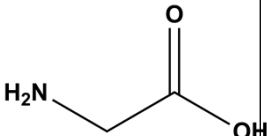
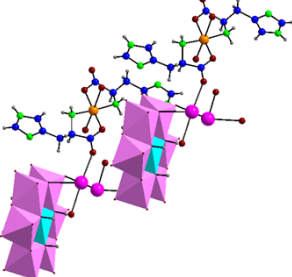
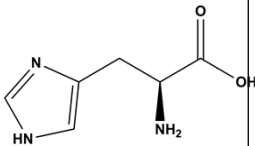
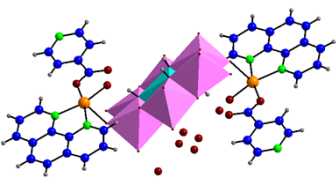
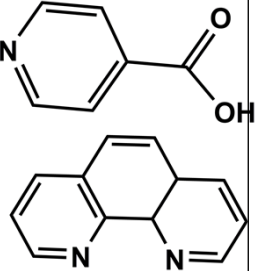
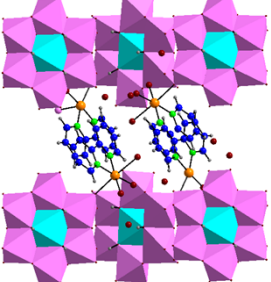
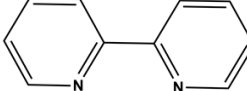
| | | | | | |
|-----|--|---|--|--|--|
| 6. | α -(4-Hpya) ₂ {[(4-Hpya) ₂ (H ₂ O) ₃ Mn] ₂ [(H ₂ O) ₄ Mn(H ₆ CrMo ₆ O ₂₄) ₂]}·12H ₂ O | $P2_1/c$ $a / \text{\AA} = 10.265(7)$ $b / \text{\AA} = 15.819(9)$ $c / \text{\AA} = 32.146(2)$ $\alpha / ^\circ = 90.00$ $\beta / ^\circ = 96.754(4)$ $\gamma / ^\circ = 90.00$ $Z = 2$ | | | <i>CrystEngComm</i> , 2011 , <i>13</i> , 5384 |
| 7. | [(3-Hpya) ₂ Na][(3-Hpya) ₂ Mn(H ₂ O) ₂][H ₆ CrMo ₆ O ₂₄]·4H ₂ O | $P\bar{1}$ $a / \text{\AA} = 10.6700(6)$ $b / \text{\AA} = 10.9118(7)$ $c / \text{\AA} = 11.7075(7)$ $\alpha / ^\circ = 106.238(3)$ $\beta / ^\circ = 94.151(3)$ $\gamma / ^\circ = 91.344(3)$ $Z = 1$ | | | <i>CrystEngComm</i> , 2011 , <i>13</i> , 5384 |
| 8. | {Mn(salen) ₂ (H ₂ O) ₂ }[H ₆ CrMo ₆ O ₂₄][arg]·11H ₂ O | $P\bar{1}$ $a / \text{\AA} = 12.997(3)$ $b / \text{\AA} = 13.642(3)$ $c / \text{\AA} = 19.196(4)$ $\alpha / ^\circ = 101.88(3)$ $\beta / ^\circ = 95.82(3)$ $\gamma / ^\circ = 93.48(3)$ $Z = 2$ | | | <i>Dalton Trans.</i> , 2011 , <i>40</i> , 56 |
| 9. | [{Cr ₃ O(CH ₃ COO) ₆ (H ₂ O) ₃ }] ₂ {H ₇ CrMo ₆ O ₂₄ }·24H ₂ O | $P\bar{1}$ $a / \text{\AA} = 10.134(14)$ $b / \text{\AA} = 14.688(2)$ $c / \text{\AA} = 15.442(2)$ $\alpha / ^\circ = 108.076(2)$ $\beta / ^\circ = 93.539(2)$ $\gamma / ^\circ = 92.825(2)$ $Z = 1$ | | | <i>Aust. J. Chem.</i> , 2011 , <i>64</i> , 68 |
| 10. | [{Cu ₂ (ox)(pz) ₄ }] ₂ {H ₇ CrMo ₆ O ₂₄ }·11H ₂ O | $P\bar{1}$ $a / \text{\AA} = 9.246(3)$ $b / \text{\AA} = 11.590(3)$ $c / \text{\AA} = 12.880(4)$ $\alpha / ^\circ = 78.061(5)$ $\beta / ^\circ = 80.244(5)$ $\gamma / ^\circ = 85.038(5)$ $Z = 1$ | | | <i>Aust. J. Chem.</i> , 2011 , <i>64</i> , 68 |

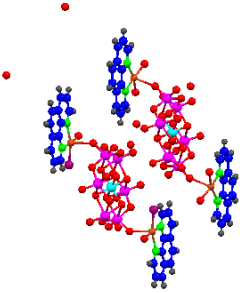
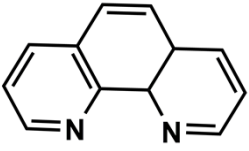
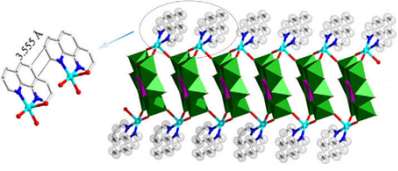
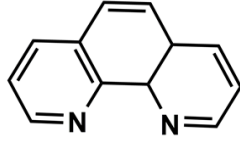
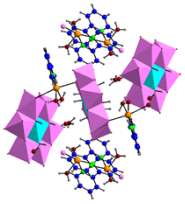
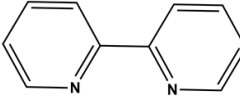
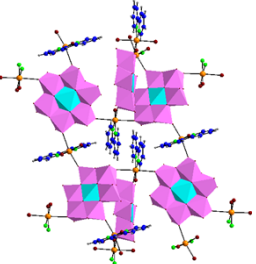
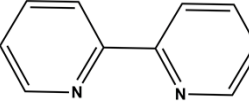
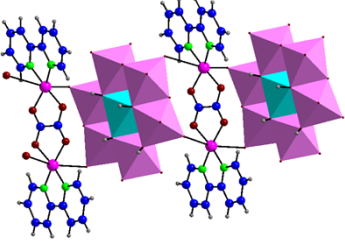
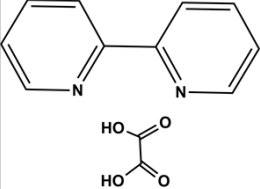
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| 11. | $[\{\text{Cu}(\text{pz})_2(\text{H}_2\text{O})_2\}\{\text{Cu}_2(\text{ox})(\text{pz})_4\}\{\text{H}_5\text{CrMo}_6\text{O}_{24}\}]\cdot 8\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 9.236(7)$ $b / \text{\AA} = 11.675(9)$ $c / \text{\AA} = 12.352(9)$ $\alpha / ^\circ = 93.103(15)$ $\beta / ^\circ = 98.542(17)$ $\gamma / ^\circ = 94.712(15)$ $Z = 1$ |  |  | <i>Aust. J. Chem.</i> 2011 , 64, 68 |
| 12. | $[\{\text{Cu}(\text{pz})_3\text{Cl}\}\{\text{Cu}_2(\text{ox})(\text{pz})_4\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 8\text{H}_2\text{O}$ | $P2/n$ $a / \text{\AA} = 13.396(3)$ $b / \text{\AA} = 11.557(3)$ $c / \text{\AA} = 18.981(5)$ $\alpha / ^\circ = 90.00$ $\beta / ^\circ = 97.367(5)$ $\gamma / ^\circ = 90.00$ $Z = 2$ |  |  | <i>Aust. J. Chem.</i> 2011 , 64, 68 |
| 13. | $(\text{H}_24\text{-pyc})_2[\{\text{Na}(4\text{-pyc})_2\}\{\text{H}_8\text{CrMo}_6\text{O}_{24}\}]\cdot 4\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.514(5)$ $b / \text{\AA} = 10.655(5)$ $c / \text{\AA} = 12.295(6)$ $\alpha / ^\circ = 97.351(9)$ $\beta / ^\circ = 112.286(8)$ $\gamma / ^\circ = 113.523(8)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2011 , 11, 3381 |
| 14. | $(\text{H}_24\text{-pyc})_2[\{\text{Ni}(4\text{-pyc})_2(\text{H}_2\text{O})_4\}\{\text{H}_7\text{CrMo}_6\text{O}_{24}\}]\cdot 12\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.599(12)$ $b / \text{\AA} = 11.843(14)$ $c / \text{\AA} = 13.142(16)$ $\alpha / ^\circ = 102.36(2)$ $\beta / ^\circ = 111.815(3)$ $\gamma / ^\circ = 107.759(2)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2011 , 11, 3381 |
| 15. | $(\text{H}_24\text{-pyc})_2[\{\text{Cu}(4\text{-pyc})_2(\text{H}_2\text{O})_4\}\{\text{H}_7\text{CrMo}_6\text{O}_{24}\}]\cdot 10\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.559(4)$ $b / \text{\AA} = 11.819(4)$ $c / \text{\AA} = 13.105(5)$ $\alpha / ^\circ = 102.202(6)$ $\beta / ^\circ = 111.925(5)$ $\gamma / ^\circ = 107.706(6)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2011 , 11, 3381 |

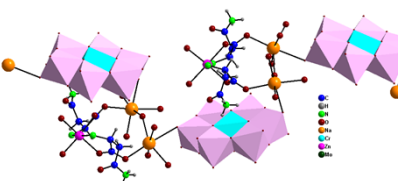
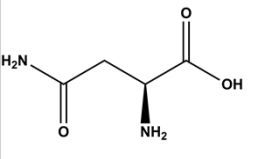
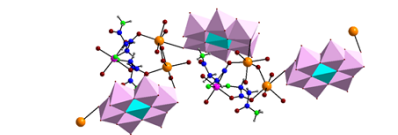
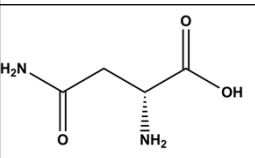
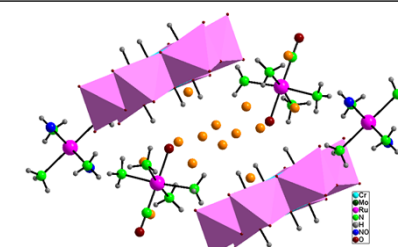
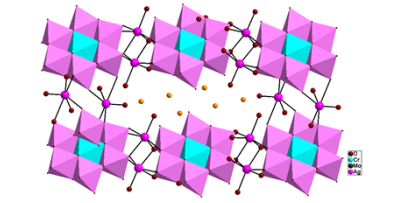
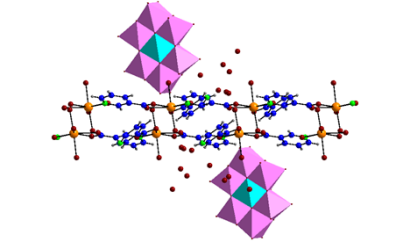
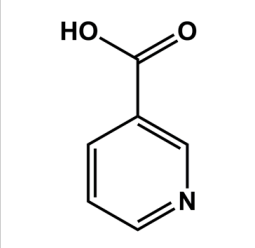
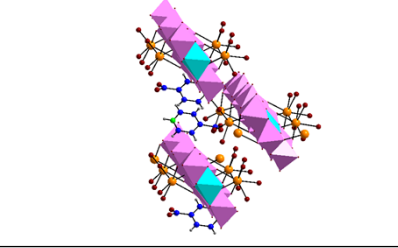
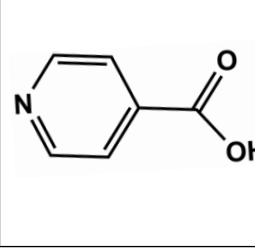
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| 16. | $(\text{H}_23\text{-pyc})_2[\{\text{Na}(3\text{-pyc})_2\}\{\text{H}_8\text{CrMo}_6\text{O}_{24}\}]\cdot 2\text{H}_2\text{O}$ | $C2/c$ $a / \text{\AA} = 22.084(3)$ $b / \text{\AA} = 9.4366(11)$ $c / \text{\AA} = 21.011(3)$ $\alpha / ^\circ = 90.00$ $\beta / ^\circ = 98.517(2)$ $\gamma / ^\circ = 90.00$ $Z = 4$ |  |  | <i>Cryst. Growth Des.</i> 2011 , <i>11</i> , 3381 |
| 17. | $[\{\text{Cu}_2(2\text{-pzc})_2(\text{H}_2\text{O})_4\}\{\text{H}_7\text{CrMo}_6\text{O}_{24}\}]\cdot 17\text{H}_2\text{O}$ | $P2_1/c$ $a / \text{\AA} = 10.880(17)$ $b / \text{\AA} = 17.084(3)$ $c / \text{\AA} = 13.590(2)$ $\alpha / ^\circ = 90.00$ $\beta / ^\circ = 107.703(3)$ $\gamma / ^\circ = 90.00$ $Z = 2$ |  |  | <i>Cryst. Growth Des.</i> 2011 , <i>11</i> , 3381 |
| 18. | $(\text{Hpyz})[\{\text{Co}(\text{pyz})_2(\text{H}_2\text{O})_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 2\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 8.1452(11)$ $b / \text{\AA} = 10.5171(15)$ $c / \text{\AA} = 11.6507(16)$ $\alpha / ^\circ = 101.448(2)$ $\beta / ^\circ = 98.692(3)$ $\gamma / ^\circ = 110.586(2)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2010 , <i>10</i> , 5105 |
| 19. | $(\text{Hpyz})[\{\text{Zn}(\text{pyz})_2(\text{H}_2\text{O})_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 2\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 8.161(2)$ $b / \text{\AA} = 10.483(3)$ $c / \text{\AA} = 11.595(3)$ $\alpha / ^\circ = 101.791(4)$ $\beta / ^\circ = 98.159(3)$ $\gamma / ^\circ = 110.274(4)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2010 , <i>10</i> , 5105 |
| 20. | $(\text{Hpyz})[\{\text{Ni}(\text{pyz})_2(\text{H}_2\text{O})_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 2\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 8.119(3)$ $b / \text{\AA} = 10.480(3)$ $c / \text{\AA} = 11.544(4)$ $\alpha / ^\circ = 101.758(5)$ $\beta / ^\circ = 98.320(6)$ $\gamma / ^\circ = 110.541(6)$ $Z = 1$ |  |  | <i>Cryst. Growth Des.</i> 2010 , <i>10</i> , 5105 |

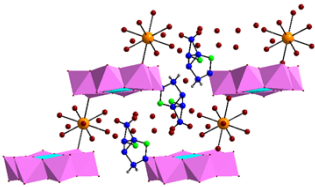
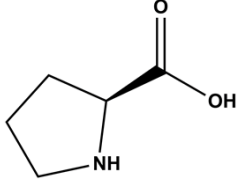

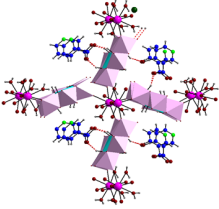
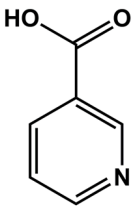
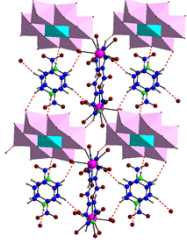
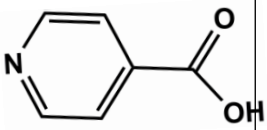
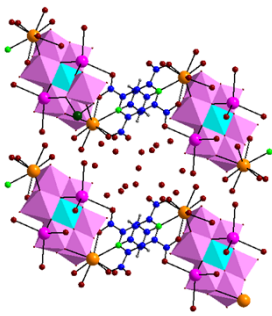
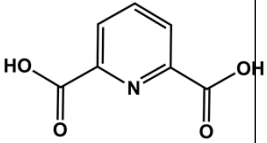
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| 21. | $[\{\text{Ni}(\text{pyz})(\text{H}_2\text{O})_4\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}](\text{CH}_3\text{COO})_2 \cdot 6\text{H}_2\text{O}$ | <i>Cmca</i> $a / \text{\AA} = 23.821(5)$ $b / \text{\AA} = 14.004(3)$ $c / \text{\AA} = 13.420(3)$ $Z = 4$ |  |  | <i>Cryst. Growth Des.</i> , 2010 , <i>10</i> , 5105 |
| 22. | $[\text{Na}(\text{H}_8\text{CrMo}_6\text{O}_{24})] \cdot 10\text{H}_2\text{O}$ | <i>P</i> $\bar{1}$ $a / \text{\AA} = 6.459(8)$ $b / \text{\AA} = 10.902(13)$ $c / \text{\AA} = 10.917(13)$ $\alpha / ^\circ = 108.95(2)$ $\beta / ^\circ = 106.590(4)$ $\gamma / ^\circ = 95.778(2)$ $Z = 1$ |  | - | <i>Cryst. Growth Des.</i> , 2010 , <i>10</i> , 5105 |
| 23. | $[\text{RuNO}(\text{en})_2\text{Cl}]_3[\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 17\text{H}_2\text{O}$ | <i>P</i> $\bar{1}$ $a / \text{\AA} = 7.994(0)$ $b / \text{\AA} = 12.898(0)$ $c / \text{\AA} = 22.499(1)$ $\alpha / ^\circ = 79.65(0)$ $\beta / ^\circ = 81.46(0)$ $\gamma / ^\circ = 87.53(0)$ $Z = 1$ |  |  | <i>Inorg. Chim. Acta</i> , 2009 , <i>362</i> , 2279 |
| 24. | $(\text{BEDT-TTF})_4[\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 2\text{H}_2\text{O}$ | <i>P</i> $\bar{1}$ $a / \text{\AA} = 5.954(2)$ $b / \text{\AA} = 16.376(6)$ $c / \text{\AA} = 21.864(6)$ $\alpha / ^\circ = 110.829(2)$ $\beta / ^\circ = 91.262(2)$ $\gamma / ^\circ = 98.129(1)$ $Z = 1$ |  |  | <i>J. Cluster Sci.</i> , 2003 , <i>14</i> , 193. |
| 25. | $[\{\text{Na}_3(\text{H}_2\text{O})_{11}\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 2\text{H}_2\text{O}$ | <i>P</i> $\bar{1}$ $a / \text{\AA} = 10.968(2)$ $b / \text{\AA} = 11.686(2)$ $c / \text{\AA} = 14.895(3)$ $\alpha / ^\circ = 72.10(3)$ $\beta / ^\circ = 70.99(3)$ $\gamma / ^\circ = 66.90(3)$ $Z = 2$ |  | - | <i>Acta Cryst. E.</i> , 2006 , <i>62</i> , i190. |
| 26. | $(\text{C}_6\text{NO}_2\text{H}_6)_2[(\text{C}_6\text{NO}_2\text{H}_5)_2\text{Ag}][\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 4\text{H}_2\text{O}$ | <i>P</i> $\bar{1}$ $a / \text{\AA} = 10.458(2)$ $b / \text{\AA} = 10.644(2)$ $c / \text{\AA} = 12.295(3)$ $\alpha / ^\circ = 97.40(3)$ $\beta / ^\circ = 112.38(3)$ $\gamma / ^\circ = 113.59(3)$ $Z = 1$ |  |  | <i>Inorg. Chem.</i> , 2005 , <i>44</i> , 6062 |

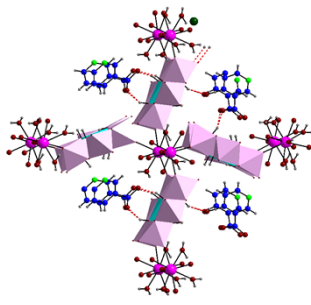
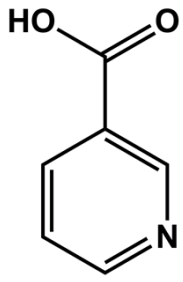
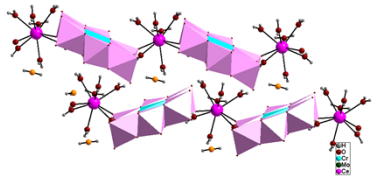
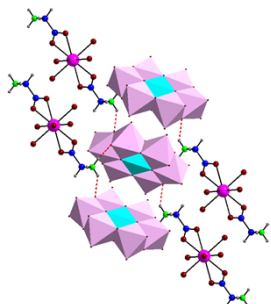
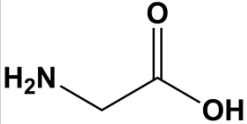
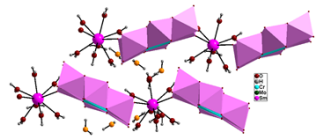
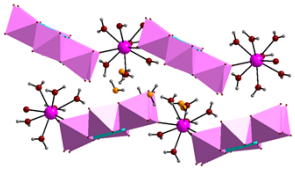
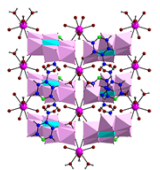
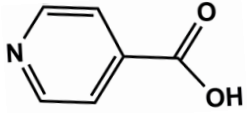
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| 27. | $[\text{Na}_3\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 8\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.908(4)$ $b / \text{\AA} = 10.980(4)$ $c / \text{\AA} = 6.467(2)$ $\alpha / ^\circ = 107.594(2)$ $\beta / ^\circ = 84.438(2)$ $\gamma / ^\circ = 112.465(3)$ $Z = 1$ |  | - | <i>Inorg. Chem.</i> , 1970 , <i>9</i> , 2228. |
| 28. | $[\text{Na}_3\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 6\text{DMSO}$ | $C2/c$ $a / \text{\AA} = 25.37(2)$ $b / \text{\AA} = 14.632(2)$ $c / \text{\AA} = 15.455(6)$ $\beta / ^\circ = 123.17(4)$ $Z = 4$ |  |  | <i>Inorg. Chem.</i> , 1998 , <i>37</i> , 1499. |
| 29. | $(\text{C}_6\text{H}_5\text{NO}_2)_2[\{\text{Na}_3(\text{C}_6\text{H}_5\text{NO}_2)_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]$ | $C2/c$ $a / \text{\AA} = 22.045(4)$ $b / \text{\AA} = 9.464(19)$ $c / \text{\AA} = 21.088(4)$ $\beta / ^\circ = 98.56(3)$ $Z = 4$ |  |  | <i>J. Mol. Struct.</i> , 2005 , <i>751</i> , 184. |
| 30. | $\{\text{Fe}(\text{C}_5\text{H}_5)_2\}_2[\text{Na}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]\cdot 3\text{H}_2\text{O}$ | $P2_1/n$ $a / \text{\AA} = 10.015(2)$ $b / \text{\AA} = 7.722(6)$ $c / \text{\AA} = 25.137(5)$ $\beta / ^\circ = 90.626(9)$ $Z = 2$ |  |  | <i>Inorg. Chem.</i> , 1998 , <i>37</i> , 1499. |
| 31. | $\{\text{Fe}(\text{C}_5\text{Me}_5)_2\}_3\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}\cdot 20\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 12.489(3)$ $b / \text{\AA} = 14.113(3)$ $c / \text{\AA} = 15.662(4)$ $\alpha / ^\circ = 101.55(2)$ $\beta / ^\circ = 105.82(2)$ $\gamma / ^\circ = 110.23(2)$ $Z = 1$ |  |  | <i>Inorg. Chem.</i> , 1998 , <i>37</i> , 1499. |

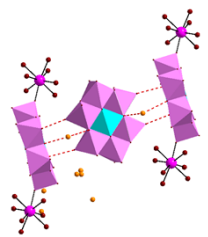
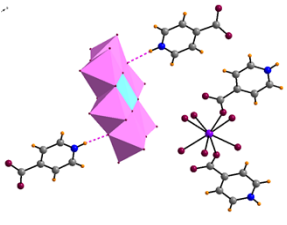
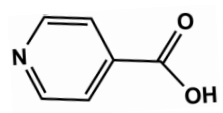
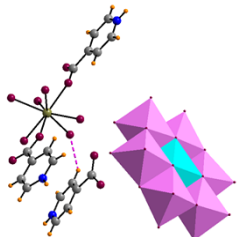
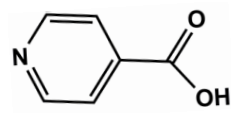
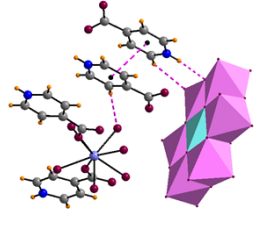
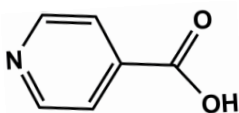
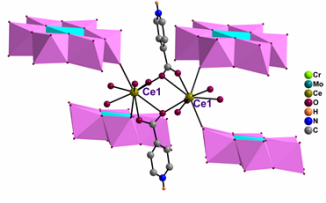
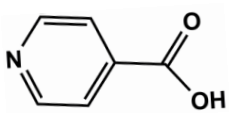
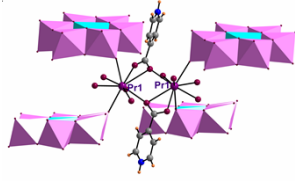
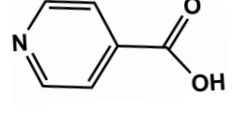
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| 32. | $[\{\text{Cu}(\text{Gly})_2\}\{\text{Na}(\text{H}_2\text{O})_4(\text{H}_6\text{CrMo}_6\text{O}_{24})\}].9.5\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.684(2)$ $b / \text{\AA} = 10.960(2)$ $c / \text{\AA} = 10.979(2)$ $\alpha / ^\circ = 60.42(3)$ $\beta / ^\circ = 63.10(3)$ $\gamma / ^\circ = 78.87(3)$ $Z = 1$ |  |  | <i>Inorg. Chem., Commun.</i> 2004 , 7, 521. |
| 33. | $[\text{Na}_3\{\text{Cu}(\text{Gly})_2\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}].13\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 10.577(2)$ $b / \text{\AA} = 10.852(2)$ $c / \text{\AA} = 10.955(2)$ $\alpha / ^\circ = 60.31(3)$ $\beta / ^\circ = 63.32(3)$ $\gamma / ^\circ = 78.95(3)$ $Z = 1$ |  |  | <i>J. Cluster Sci.</i> , 2008 19, 367. |
| 34. | $[\{\text{Cu}(\text{C}_6\text{H}_8\text{N}_3\text{O}_2)(\text{C}_6\text{H}_9\text{N}_3\text{O}_2)(\text{H}_2\text{O})_2\}\{\text{Na}(\text{H}_2\text{O})\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}].3\text{H}_2\text{O}$ | $P1$ $a / \text{\AA} = 10.205(16)$ $b / \text{\AA} = 11.209(18)$ $c / \text{\AA} = 11.804(19)$ $\alpha / ^\circ = 109.583(2)$ $\beta / ^\circ = 95.353(2)$ $\gamma / ^\circ = 109.081(2)$ $Z = 1$ |  |  | <i>J. Mol. Struct.</i> , 2009 , 931, 50. |
| 35. | $[\{\text{Cu}(4\text{-pyc}(\text{phen})(\text{H}_2\text{O})\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}](\text{H}_3\text{O}^+).5\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 9.941(9)$ $b / \text{\AA} = 9.945(9)$ $c / \text{\AA} = 14.249(12)$ $\alpha / ^\circ = 81.457(10)$ $\beta / ^\circ = 83.014(10)$ $\gamma / ^\circ = 77.224(10)$ $Z = 1$ |  |  | <i>J. Mol. Struct.</i> , 2009 , 920, 284. |
| 36. | $[\{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})_3\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}][\{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})\text{Cl}\}\{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})(\text{NO}_3)\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}].18\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 13.252(3)$ $b / \text{\AA} = 13.791(3)$ $c / \text{\AA} = 14.277(3)$ $\alpha / ^\circ = 90.71(3)$ $\beta / ^\circ = 108.34(3)$ $\gamma / ^\circ = 90.40(3)$ $Z = 1$ |  |  | <i>J. Solid State Chem.</i> , 2009 , 182, 49. |

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|-----|--|---|--|---|--|
| 37. | $[\{(\text{Cu}(\text{phen})(\text{H}_2\text{O})_2)_2(\text{H}_6\text{CrMo}_6\text{O}_{24})\} \{(\text{Cu}(\text{phen})(\text{H}_2\text{O})\text{Cl}(\text{H}_6\text{CrMo}_6\text{O}_{24})_2)\}_2] \cdot 5\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{Å} = 10.886(5)$ $b / \text{Å} = 15.250(7)$ $c / \text{Å} = 15.702(7)$ $\alpha / ^\circ = 64.985(10)$ $\beta / ^\circ = 83.043(10)$ $\gamma / ^\circ = 71.157(10)$ $Z = 1$ |  |  | <i>Inorg. Chem.</i> , 2005 , <i>44</i> , 8846. |
| 38. | $[\{\text{Cu}(\text{phen})\}_2 \{\text{H}_5\text{CrMo}_6\text{O}_{24}\}]$ | $P2_1/n$ $a / \text{Å} = 5.6671(10)$ $b / \text{Å} = 21.372(5)$ $c / \text{Å} = 14.709(3)$ $\beta / ^\circ = 98.10(10)$ $Z = 2$ |  |  | <i>J. Mol. Struct.</i> , 2010 , <i>967</i> , 15. |
| 39. | $[\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})_2\text{Cl}] [\{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})_2\} \{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 4\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{Å} = 11.244(2)$ $b / \text{Å} = 14.566(3)$ $c / \text{Å} = 15.330(3)$ $\alpha / ^\circ = 112.21(3)$ $\beta / ^\circ = 106.65(3)$ $\gamma / ^\circ = 93.90(3)$ $Z = 2$ |  |  | <i>J. Solid State Chem.</i> , 2009 , <i>182</i> , 49. |
| 40. | $(\text{H}_3\text{O})[\{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})_2\}_2 \{\text{Cu}(2,2'\text{-bpy})(\text{H}_2\text{O})_2\} \{\text{H}_6\text{CrMo}_6\text{O}_{24}\}]_3 \cdot 36\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{Å} = 14.189(13)$ $b / \text{Å} = 15.676(14)$ $c / \text{Å} = 16.226(15)$ $\alpha / ^\circ = 65.478(10)$ $\beta / ^\circ = 70.512(10)$ $\gamma / ^\circ = 80.586(10)$ $Z = 1$ |  |  | <i>J. Solid State Chem.</i> , 2009 , <i>182</i> , 49. |
| 41. | $[\{\text{Cu}_2(\text{bpy})_2(\mu\text{-ox})\} \{\text{H}_7\text{CrMo}_6\text{O}_{24}\}]$ | $Pna2$ $a / \text{Å} = 14.238(7)$ $b / \text{Å} = 26.331(13)$ $c / \text{Å} = 10.282(5)$ $Z = 4$ |  |  | <i>Inorg. Chem.</i> , 2007 , <i>46</i> , 3541. |

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|-----|--|--|--|---|--|
| 42. | $(\text{C}_4\text{NH}_7\text{O}_4)[\{(\text{Zn}(\text{L}-\text{C}_4\text{H}_8\text{N}_2\text{O}_3)_2)(\text{Na}_2(\text{H}_2\text{O})_9)\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}_2] \cdot 7\text{H}_2\text{O}$ | $P 2_1 2_1 2$ $a / \text{\AA} = 20.405(4)$ $b / \text{\AA} = 21.821(4)$ $c / \text{\AA} = 10.917(2)$ $Z = 4$ |  |  | <i>Inorg. Chem. Commun.</i> , 2008 , <i>11</i> , 914. |
| 43. | $(\text{C}_4\text{NH}_7\text{O}_4)[\{(\text{Zn}(\text{D}-\text{C}_4\text{H}_8\text{N}_2\text{O}_3)_2)(\text{Na}_2(\text{H}_2\text{O})_9)\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}_2] \cdot 7\text{H}_2\text{O}$ | $P 2_1 2_1 2$ $a / \text{\AA} = 20.454(4)$ $b / \text{\AA} = 21.822(4)$ $c / \text{\AA} = 10.918(2)$ $Z = 4$ |  |  | <i>Inorg. Chem. Commun.</i> , 2008 , <i>11</i> , 914. |
| 44. | $\{\text{RuNO}(\text{NH}_3)_4\text{OH}\}_3[\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}_2] \cdot 15\text{H}_2\text{O}$ | $P \bar{1}$ $a / \text{\AA} = 10.585(2)$ $b / \text{\AA} = 11.040(2)$ $c / \text{\AA} = 16.807(4)$ $\alpha / ^\circ = 76.919(1)$ $\beta / ^\circ = 73.774(1)$ $\gamma / ^\circ = 84.090(1)$ $Z = 1$ |  | — | <i>J. Cluster Sci.</i> , 2006 , <i>17</i> , 303. |
| 45. | $[\{\text{Ag}_3(\text{H}_2\text{O})_4\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 3\text{H}_2\text{O}$ | $P \bar{1}$ $a / \text{\AA} = 6.205(12)$ $b / \text{\AA} = 14.185(3)$ $c / \text{\AA} = 15.077(3)$ $\alpha / ^\circ = 90.68(3)$ $\beta / ^\circ = 90.08(3)$ $\gamma / ^\circ = 93.82(3)$ $Z = 2$ |  | — | <i>Cryst. Growth Des.</i> , 2006 , <i>6</i> , 1107. |
| 46. | $[\{(\text{H}_2\text{O})_2(\text{HC}_6\text{H}_4\text{NO}_2)\text{Cd}(\text{C}_6\text{H}_5\text{NO}_2)\}_2\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 9\text{H}_2\text{O}$ | $P \bar{1}$ $a / \text{\AA} = 7.992(16)$ $b / \text{\AA} = 13.861(3)$ $c / \text{\AA} = 14.357(3)$ $\alpha / ^\circ = 74.63(3)$ $\beta / ^\circ = 84.59(3)$ $\gamma / ^\circ = 82.96(3)$ $Z = 1$ |  |  | <i>J. Mol. Struct.</i> , 2009 , <i>933</i> , 86. |
| 47. | $[\{\text{Cd}_3(\text{H}_2\text{O})_{14}\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}_2](\text{C}_6\text{H}_5\text{NO}_2)_4$ | Pc $a / \text{\AA} = 12.639(3)$ $b / \text{\AA} = 10.761(2)$ $c / \text{\AA} = 13.777(3)$ $\beta / ^\circ = 104.29(3)$ $Z = 1$ |  |  | <i>J. Mol. Struct.</i> , 2009 , <i>933</i> , 86. |

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|-----|--|--|--|---|--|
| 48. | $(C_5H_9NO_2)_2[La(H_2O)_7\{H_6CrMo_6O_{24}\}].11H_2O$ | $C2/c$ $a / \text{\AA} = 26.257(5)$ $b / \text{\AA} = 11.526(2)$ $c / \text{\AA} = 19.890(4)$ $\beta / ^\circ = 127.44(3)$ $Z = 4$ |  |  | <i>Inorg. Chem. Commun.</i> 2004 , 7, 356. |
| 49. | $[Tm_2(H_2O)_{14}H_6CrMo_6O_{24}][H_6CrMo_6O_{24}].16H_2O$ | $P\bar{1}$ $a / \text{\AA} = 11.098(13)$ $b / \text{\AA} = 11.720(14)$ $c / \text{\AA} = 13.984(16)$ $\alpha / ^\circ = 74.993(2)$ $\beta / ^\circ = 84.548(2)$ $\gamma / ^\circ = 89.545(2)$ $Z = 1$ |  | — | <i>CrystEngComm</i> , 2008 , 10, 1318 |
| 50. | $(3-pyc)_2[La(H_2O)_5\{H_6CrMo_6O_{24}\}].0.5H_2O$ | $Pmn2_1$ $a / \text{\AA} = 15.080(3)$ $b / \text{\AA} = 11.630(2)$ $c / \text{\AA} = 23.096(5)$ $Z = 4$ |  |  | <i>Eur. J. Inorg. Chem.</i> , 2005 , 854. |
| 51. | $(4-pyc)[\{La(4-pyc)(H_2O)_7\}\{H_6CrMo_6O_{24}\}].10.5H_2O$ | $P\bar{1}$ $a / \text{\AA} = 11.071(2)$ $b / \text{\AA} = 13.252(3)$ $c / \text{\AA} = 17.318(4)$ $\alpha / ^\circ = 91.73(3)$ $\beta / ^\circ = 93.94(3)$ $\gamma / ^\circ = 94.46(3)$ $Z = 2$ |  |  | <i>J. Mol. Struct.</i> , 2005 , 743, 117. |
| 52. | $Na[\{Ce(dipic)(H_2O)_3\}_2\{H_6CrMo_6O_{24}\}].13H_2O$ | $P\bar{1}$ $a / \text{\AA} = 9.215(18)$ $b / \text{\AA} = 12.140(2)$ $c / \text{\AA} = 13.707(3)$ $\alpha / ^\circ = 70.99(3)$ $\beta / ^\circ = 75.04(3)$ $\gamma / ^\circ = 72.22(3)$ $Z = 1$ |  |  | <i>Trans. Metal Chem.</i> , 2006 , 31, 770. |

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|-----|---|---|--|---|--|
| 53. | $(3\text{-pyc})_2[\text{Ce}(\text{H}_2\text{O})_5\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 0.5\text{H}_2\text{O}$ | $Pmn2_1$ $a / \text{\AA} = 15.031(9)$ $b / \text{\AA} = 11.609(7)$ $c / \text{\AA} = 23.048(14)$ $Z = 4$ |  |  | <i>Eur. J. Inorg. Chem.</i> , 2005 , 854. |
| 54. | $[\text{Ce}(\text{H}_2\text{O})_7\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 4\text{H}_2\text{O}$ | $Pca2$ $a / \text{\AA} = 11.861(3)$ $b / \text{\AA} = 11.003(3)$ $c / \text{\AA} = 22.611(6)$ $Z = 4$ |  | — | <i>Z. Anorg. Allg. Chem.</i> , 2008 , 758. |
| 55. | $[\{\text{Nd}(\text{C}_2\text{H}_5\text{NO}_2)_2(\text{H}_2\text{O})_5\}\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 10\text{H}_2\text{O}$ | $C2/c$ $a / \text{\AA} = 33.202(7)$ $b / \text{\AA} = 10.733(2)$ $c / \text{\AA} = 11.910(2)$ $\beta / ^\circ = 106.38(3)$ $Z = 4$ |  |  | <i>J. Mol. Struct.</i> , 2005 , 743, 117. |
| 56. | $[\text{Sm}(\text{H}_2\text{O})_7\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 4\text{H}_2\text{O}$ | $Pca2$ $a / \text{\AA} = 11.828(4)$ $b / \text{\AA} = 10.969(4)$ $c / \text{\AA} = 22.437(7)$ $Z = 4$ |  | — | <i>Z. Anorg. Allg. Chem.</i> , 2008 , 758. |
| 57. | $[\text{Eu}(\text{H}_2\text{O})_7\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 4\text{H}_2\text{O}$ | $Pca2$ $a / \text{\AA} = 11.832(5)$ $b / \text{\AA} = 10.966(5)$ $c / \text{\AA} = 22.425(5)$ $Z = 4$ |  | — | <i>Z. Anorg. Allg. Chem.</i> , 2008 , 758. |
| 58. | $(\text{C}_6\text{H}_5\text{NO}_2)_2[\text{Dy}(\text{H}_2\text{O})_6\{\text{H}_6\text{CrMo}_6\text{O}_{24}\}] \cdot 4\text{H}_2\text{O}$ | $C2/c$ $a / \text{\AA} = 18.276(4)$ $b / \text{\AA} = 12.549(3)$ $c / \text{\AA} = 17.822(4)$ $\beta / ^\circ = 103.90(3)$ $Z = 4$ |  |  | <i>J. Mol. Struct.</i> , 2005 , 751, 184. |

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|-----|--|--|--|---|---|
| 59. | $[\{\text{Er}_2(\text{H}_2\text{O})_{14}(\text{H}_6\text{CrMo}_6\text{O}_{24})\} \{\text{H}_6\text{CrMo}_6\text{O}_{24}\} \cdot 14\text{H}_2\text{O}]$ | $P\bar{1}$ $a / \text{\AA} = 11.046(5)$ $b / \text{\AA} = 11.653(5)$ $c / \text{\AA} = 13.935(5)$ $\alpha / ^\circ = 75.006(5)$ $\beta / ^\circ = 84.497(5)$ $\gamma / ^\circ = 89.515(5)$ $Z = 1$ |  | - | <i>J. Chem. Crystallogr.</i> , 2008 , 38, 695. |
| 60. | $[(\text{C}_6\text{H}_5\text{NO}_2)_2\text{Er}(\text{H}_2\text{O})_6] (\text{H}_6\text{CrMo}_6\text{O}_{24}) \cdot 2\text{C}_6\text{H}_5\text{NO}_2 \cdot 6\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 12.797(5)$ $b / \text{\AA} = 12.927(5)$ $c / \text{\AA} = 18.190(7)$ $\alpha / ^\circ = 93.43(0)^\circ$ $\beta / ^\circ = 105.63(0)$ $\gamma / ^\circ = 113.06(0)$ $Z = 2$ |  |  | <i>J. Coord. Chem.</i> 2013 , 66, 1058, |
| 61. | $[(\text{C}_6\text{H}_5\text{NO}_2)_2\text{Dy}(\text{H}_2\text{O})_6] (\text{H}_6\text{CrMo}_6\text{O}_{24}) \cdot 2\text{C}_6\text{H}_5\text{NO}_2 \cdot 6\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 12.786(4)$ $b / \text{\AA} = 12.892(4)$ $c / \text{\AA} = 18.1606(3)$ $\alpha / ^\circ = 93.4270(3)$ $\beta / ^\circ = 105.60$ $\gamma / ^\circ = 112.76$ $Z = 2$ |  |  | <i>J. Coord. Chem.</i> , 2013 , 66, 1058 |
| 62. | $[(\text{C}_6\text{H}_5\text{NO}_2)_2\text{Sm}(\text{H}_2\text{O})_6] (\text{H}_6\text{CrMo}_6\text{O}_{24}) \cdot 2\text{C}_6\text{H}_5\text{NO}_2 \cdot 6\text{H}_2\text{O}$ | $P\bar{1}$ $a / \text{\AA} = 12.789(4)$ $b / \text{\AA} = 12.916(4)$ $c / \text{\AA} = 18.158(5)$ $\alpha / ^\circ = 93.46(3)$ $\beta / ^\circ = 105.61(3)$ $\gamma / ^\circ = 113.06(3)$ $Z = 2$ |  |  | <i>J. Coord. Chem.</i> , 2013 , 66, 1058 |
| 63. | $(\text{C}_6\text{NO}_2\text{H}_5)[(\text{H}_2\text{O})_4(\text{C}_6\text{NO}_2\text{H}_5)\text{Ce}(\text{H}_6\text{CrMo}_6\text{O}_{24})] \cdot 4\text{H}_2\text{O}$ | $C2/c$ $a / \text{\AA} = 23.616(5)$ $b / \text{\AA} = 13.384(3)$ $c / \text{\AA} = 24.746(5)$ $\beta / ^\circ = 103.06(3)$ $Z = 8$ |  |  | <i>New J. Chem.</i> , 2005 , 29, 667 |
| 64. | $(\text{C}_6\text{NO}_2\text{H}_5)[(\text{H}_2\text{O})_4(\text{C}_6\text{NO}_2\text{H}_5)\text{Pr}(\text{H}_6\text{CrMo}_6\text{O}_{24})] \cdot 4\text{H}_2\text{O}$ | $C2/c$ $a / \text{\AA} = 23.624(5)$ $b / \text{\AA} = 13.366(3)$ $c / \text{\AA} = 24.727(5)$ $\beta / ^\circ = 103.06(3)$ $Z = 8$ |  |  | <i>New J. Chem.</i> , 2005 , 29, 667 |

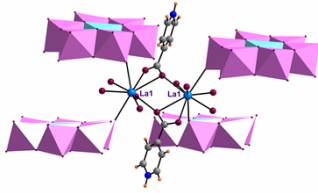
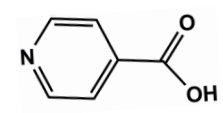
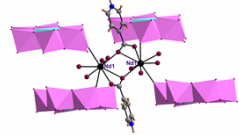
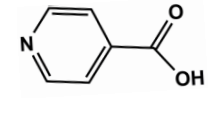
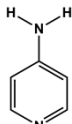
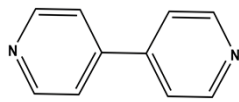
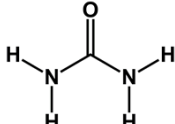
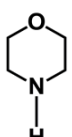
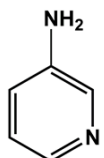
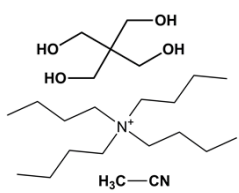
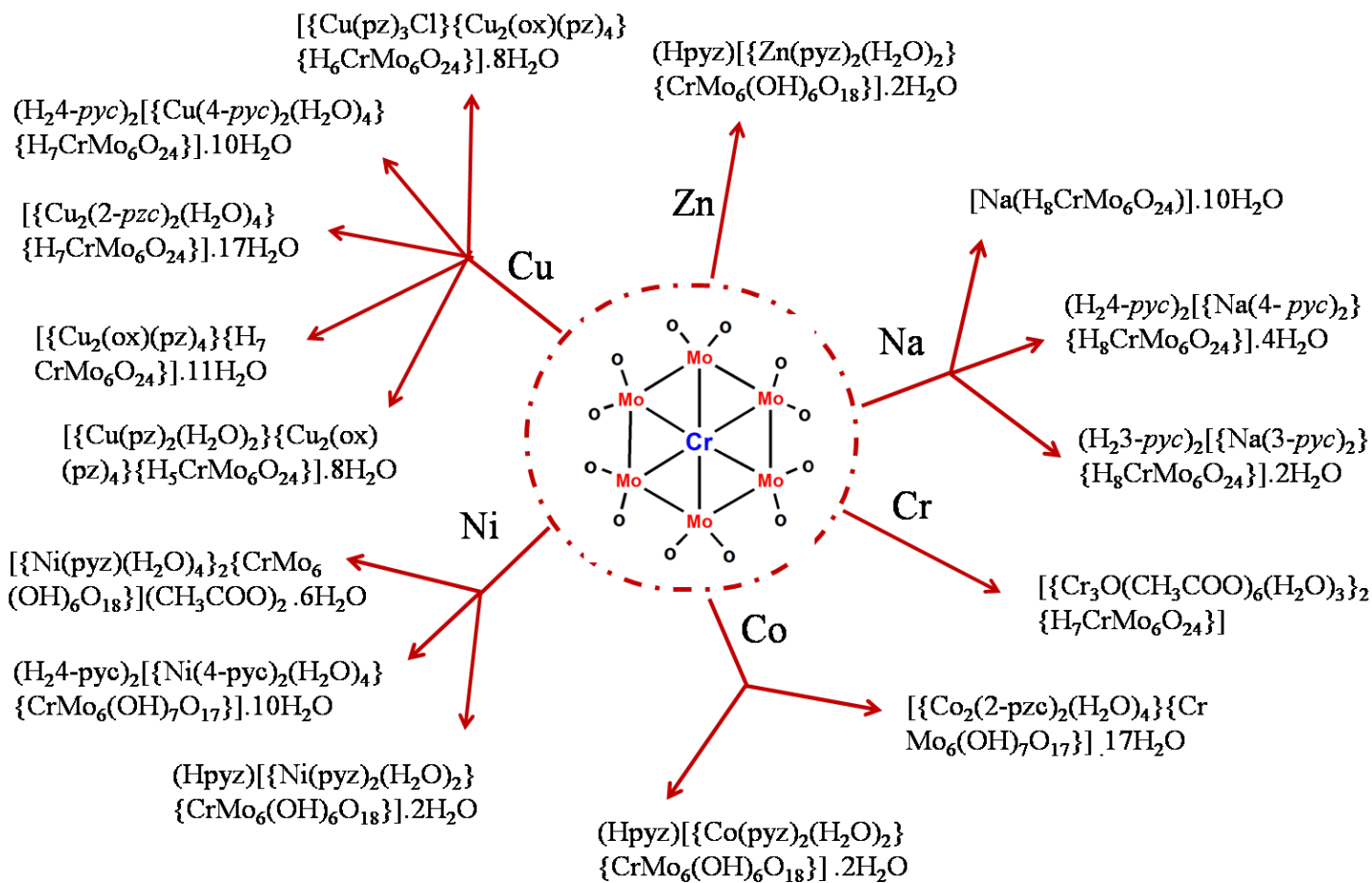
| | | | | | |
|-----|---|---|--|---|---|
| 65. | $(\text{C}_6\text{NO}_2\text{H}_5)(\text{H}_2\text{O})_4(\text{C}_6\text{NO}_2\text{H}_5)\text{La}(\text{H}_6\text{CrMo}_6\text{O}_{24}) \cdot 4\text{H}_2\text{O}$ | $C2/c$ $a / \text{Å} = 23.772(5)$ $b / \text{Å} = 13.440(3)$ $c / \text{Å} = 24.754(5)$ $\beta / ^\circ = 103.10(3)$ $Z = 8$ |  |  | <i>New J. Chem.</i> , 2005 , 29, 667 |
| 66. | $(\text{C}_6\text{NO}_2\text{H}_5)(\text{H}_2\text{O})_4(\text{C}_6\text{NO}_2\text{H}_5)\text{Nd}(\text{H}_6\text{CrMo}_6\text{O}_{24}) \cdot 4\text{H}_2\text{O}$ | $C2/c$ $a / \text{Å} = 23.564(5)$ $b / \text{Å} = 13.388(3)$ $c / \text{Å} = 24.787(5)$ $\beta / ^\circ = 103.00(3)$ $Z = 8$ |  |  | <i>New J. Chem.</i> , 2005 , 29, 667 |

Table S2. Chromium molybdate cluster and organic based salts

| S. No. | Composition | Organic | N-H...O [d (Å)] | Reference |
|--------|--|---|-------------------------|--|
| 1 | $(\text{C}_5\text{H}_7\text{N}_2)_2\{\text{H}_7\text{CrMo}_6\text{O}_{24}\} \cdot 2\text{H}_2\text{O}$ |  | 2.096 2.152 2.195 | <i>Z. Kristallogr. New Cryst. Struct.</i> , 2011 , 226, 387 |
| 2 | $(\text{C}_{10}\text{H}_{10}\text{N}_2)\{\text{H}_7\text{CrMo}_6\text{O}_{24}\} \cdot 3\text{H}_2\text{O}$ |  | 1.865 | <i>Z. Kristallogr. New Cryst. Struct.</i> , 2011 , 226, 387 |
| 3 | $\{(\text{N}_2\text{H}_5\text{CO})[(\text{CH}_3)_3\text{N}(\text{CH}_2)_2\text{OH}]_2\}[\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 4\text{H}_2\text{O}$ |  | 2.032 | <i>Inorg. Chim. Acta</i> , 2010 , 363, 1556 |
| 4 | $(\text{C}_4\text{H}_{10}\text{NO})_3[\text{H}_6\text{CrMo}_6\text{O}_{24}] \cdot 4\text{H}_2\text{O}$ |  | 1.86 1.94 2.19 2.53 | <i>Acta Cryst.</i> , 2011 , E67, m776 |
| 5 | $(\text{H}_3\text{O})[(3-\text{C}_5\text{H}_7\text{N}_2)_2(\text{H}_6\text{CrMo}_6\text{O}_{24})] \cdot 3\text{H}_2\text{O}$ |  | 1.91 2.21 2.17 | <i>J. Coord. Chem.</i> , 2011 , 64, 2848 |
| 6 | $[(\text{C}_4\text{H}_9)_4\text{N}]_5\{\text{H}_7[\text{HOCH}_2\text{C}(\text{CH}_2)_3(\text{CrMo}_6\text{O}_2)_4]_2\}$ |  | – | <i>Chem. Eur. J.</i> , 2011 , 17, 12002 |

| | | | | |
|---|---|--|-------------------------|--|
| 7 | $[(C_4H_9)_4N]_3 [(C_2H_5)_3NH] (CH_3CO_2H)Cl$ $\{H_3[(CrMo_6O_{24}(CH_2)_3 CCH_2OH)]\}$ | | — | <i>Chem. Eur. J.</i> , 2011 , 17, 12002 |
| 8 | $\{(Htemed)_3\}[\{H_6CrMo_6O_{24}\}_2].16H_2O$ | | 1.878 2.721 2.692 | <i>Proc. Natl. Acad. Sci., India, Sect. A Phys. Sci.</i> 2014 (DOI 10.1007/s40010-014-0144-6) |
| 9 | $\{Hpym\}_2[\{H_7CrMo_6O_{24}\}].2H_2O$ | | 1.897 2.071 | <i>Proc. Natl. Acad. Sci., India, Sect. A Phys. Sci.</i> 2014 (DOI 10.1007/s40010-014-0144-6) |



Cryst. Growth Desi. 2010, 10, 5105–5112

Cryst. Growth Des. 2011, 11, 3381–3394

Fig. S1 Chromium molybdate cluster, $[\text{H}_m\text{CrMo}_6\text{O}_{24}]^{n-}$ based solids reported earlier from our lab.

Table S3. Structural classification of Ln-[CrMo₆O₂₄]ⁿ⁻ system

| Class | Composition | Structural Description | Reference |
|-------|---|---|---|
| I | [Ln(H ₂ O) ₇ {CrMo ₆ (OH) ₆ O ₁₈ }]·4H ₂ O (Ln = Ce, Sm and Eu) | These solids forming 1-D chain between hydrated rare earth cation and cluster through the metal ligand coordination. | <i>Z. Anorg. Allg. Chem.</i> , 2008 , 758. |
| II | (C ₆ NO ₂ H ₅)[(H ₂ O) ₄ (C ₆ NO ₂ H ₅)Pr(H ₆ CrMo ₆ O ₂₄)]·4H ₂ O (Ln = La, Ce, Pr and Nd) | The structure is built of three main building blocks: A rare earth dimer bridged by a pair of 4-pyridine carboxylate, the chromium molybdate cluster and the zwitterionic 4-pyridine carboxylic acid. | <i>New J. Chem.</i> , 2005 , 29, 667 |
| III | (3- <i>pyc</i>) ₂ [Ce(H ₂ O) ₅ {H ₆ CrMo ₆ O ₂₄ }]. 0.5H ₂ O (Ln = La and Ce) | The structure of these having unique 3-D open framework constructed from chromium molybdate cluster building blocks and Ln ³⁺ cations, with 3-pyridine carboxylic acid molecules and lattice water molecules residing in the channels. | <i>Eur. J. Inorg. Chem.</i> , 2005 , 854 |
| IV | [(C ₆ H ₅ NO ₂) ₂ Ln(H ₂ O) ₆](H ₆ CrMo ₆ O ₂₄) ·2C ₆ H ₅ NO ₂ ·6H ₂ O (Ln = Sm, Dy and Er) | Single-crystal X-ray diffraction analysis reveals that these are made up of chromium molybdate cluster, lanthanum-4-pyridine carboxylic acid complexes as cations, discrete 4-pyridine carboxylic acid molecules and lattice water. | <i>J. Coord. Chem.</i> , 2013 , 66, 1058 |

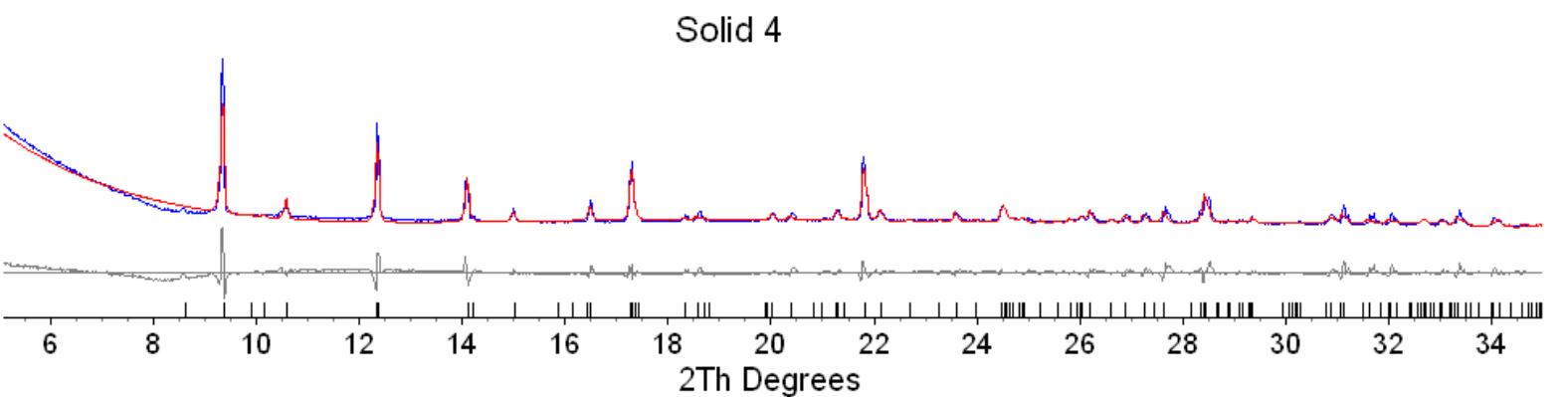
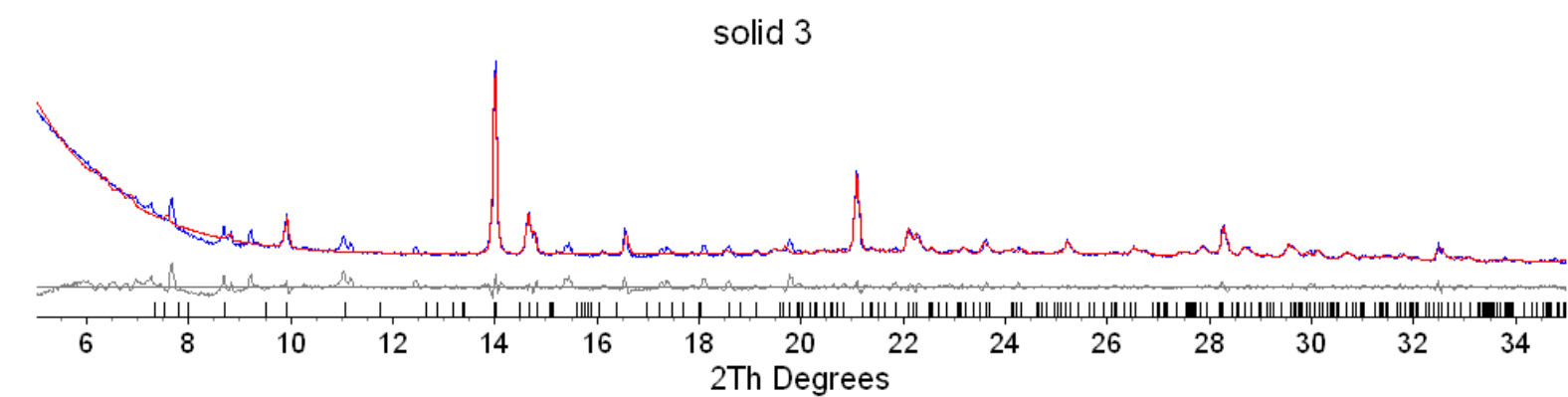
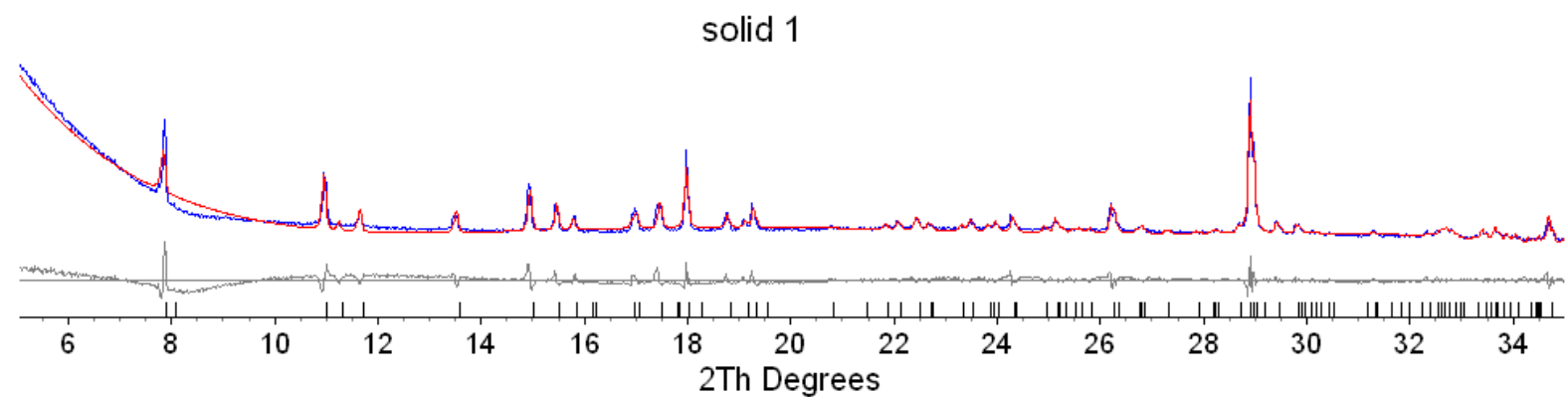


Fig. S2. Rietveld analysis of the powder diffraction data of **1**, **3** and **4**.

Red line – calculated intensity

Blue line – observed intensity

Grey line – difference ($I_{\text{obs}} - I_{\text{calc}}$)

Black bars – calculated Bragg reflections

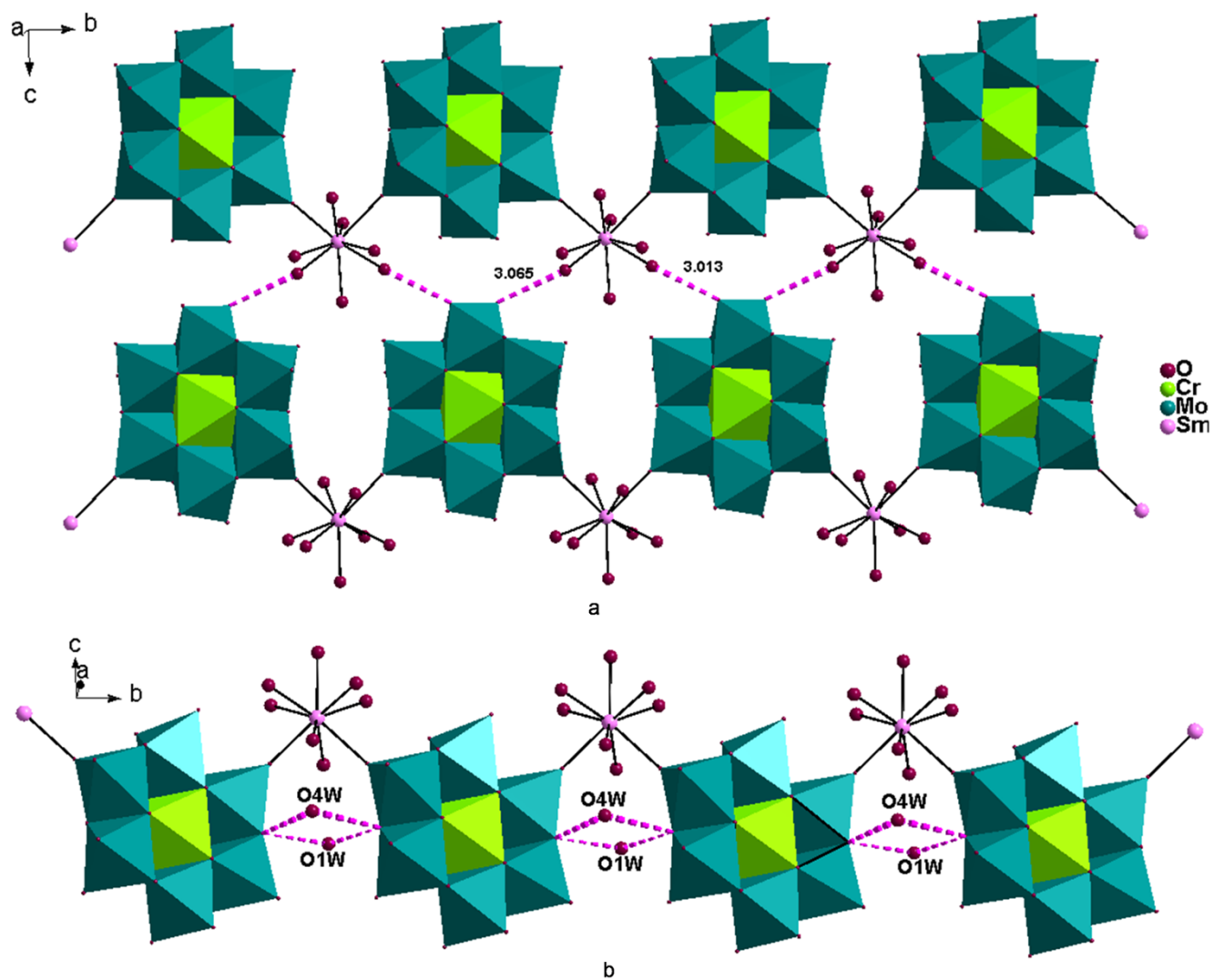


Fig. S3 (a) 2-D supramolecular sheet of **2** viewed along *bc* plane. Other atoms are omitted for clarity. (b) The 1-D chain incorporating a pair of water molecules through H-bonding.

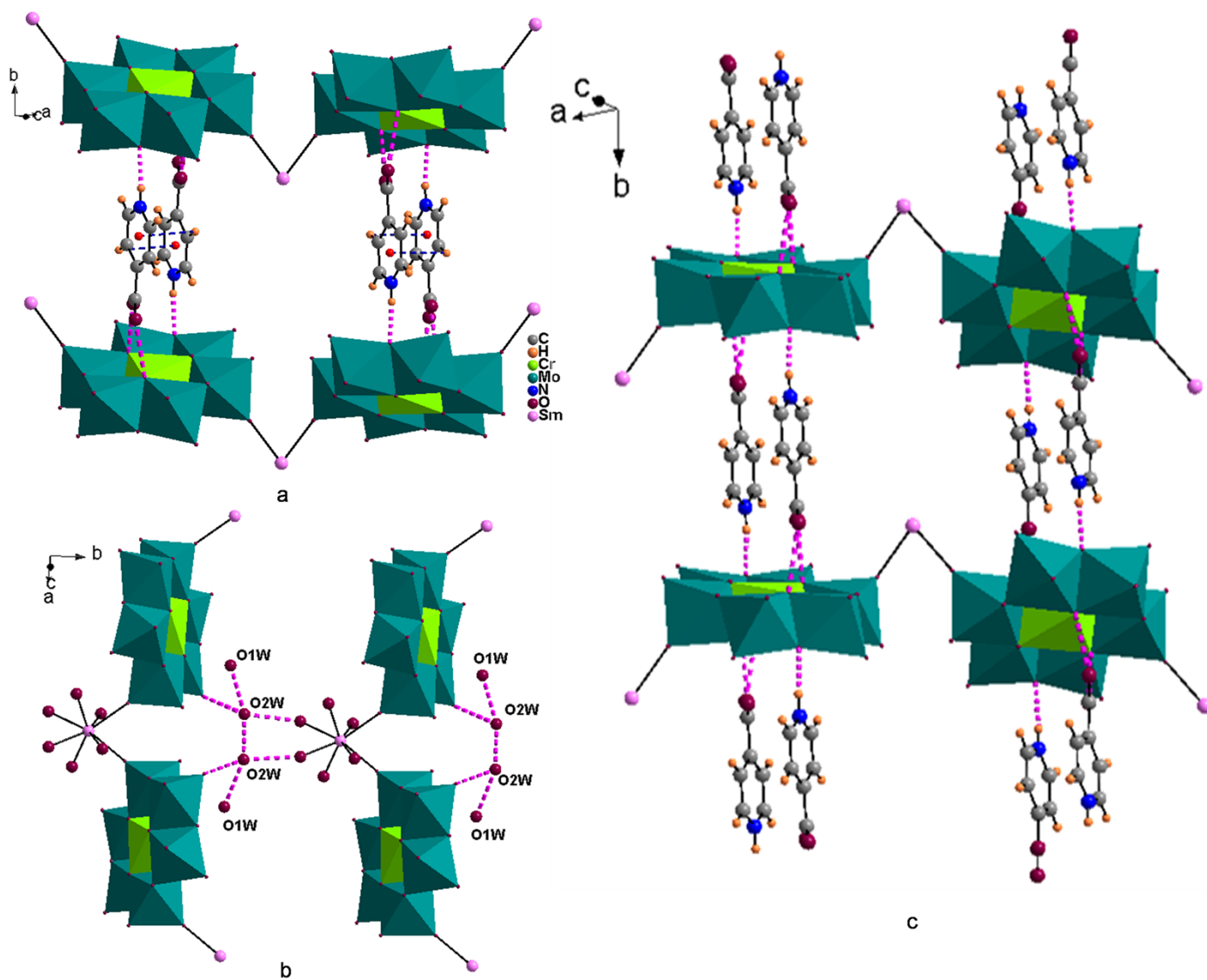


Fig. S4 (a) C–H···π interaction between two organic complex of solid **5**. (d) Two 1-D chain connected through the H–bonding with water molecules (c) 1-D chain connected through the organic cations through the H–bonding (N–H···O_t–Mo and O–H···O–C)

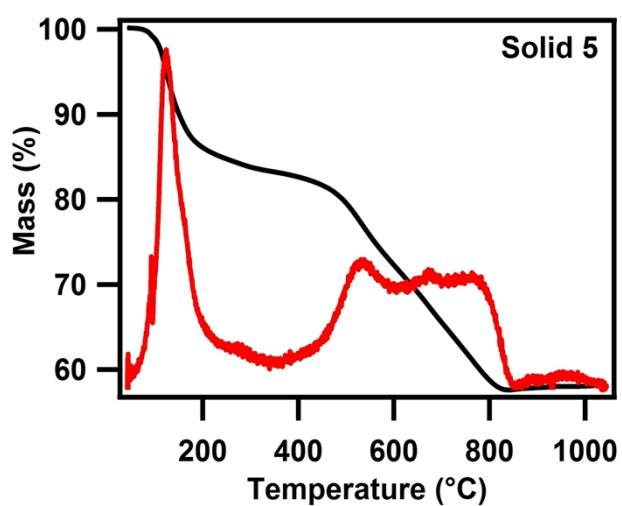
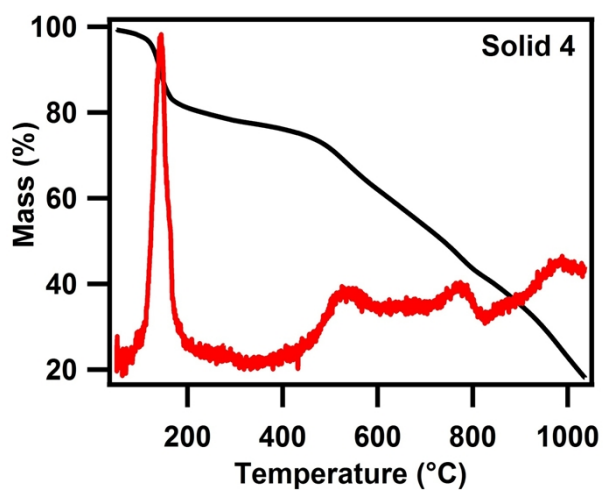
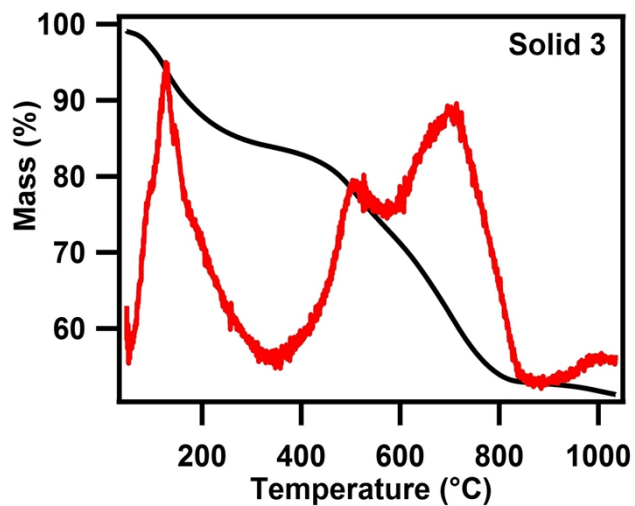
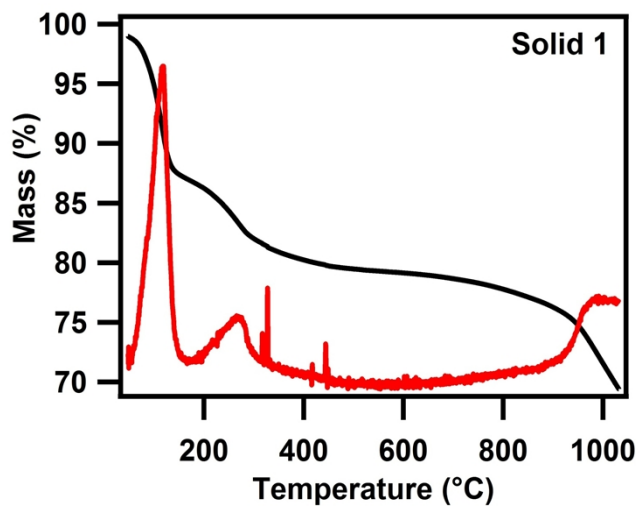
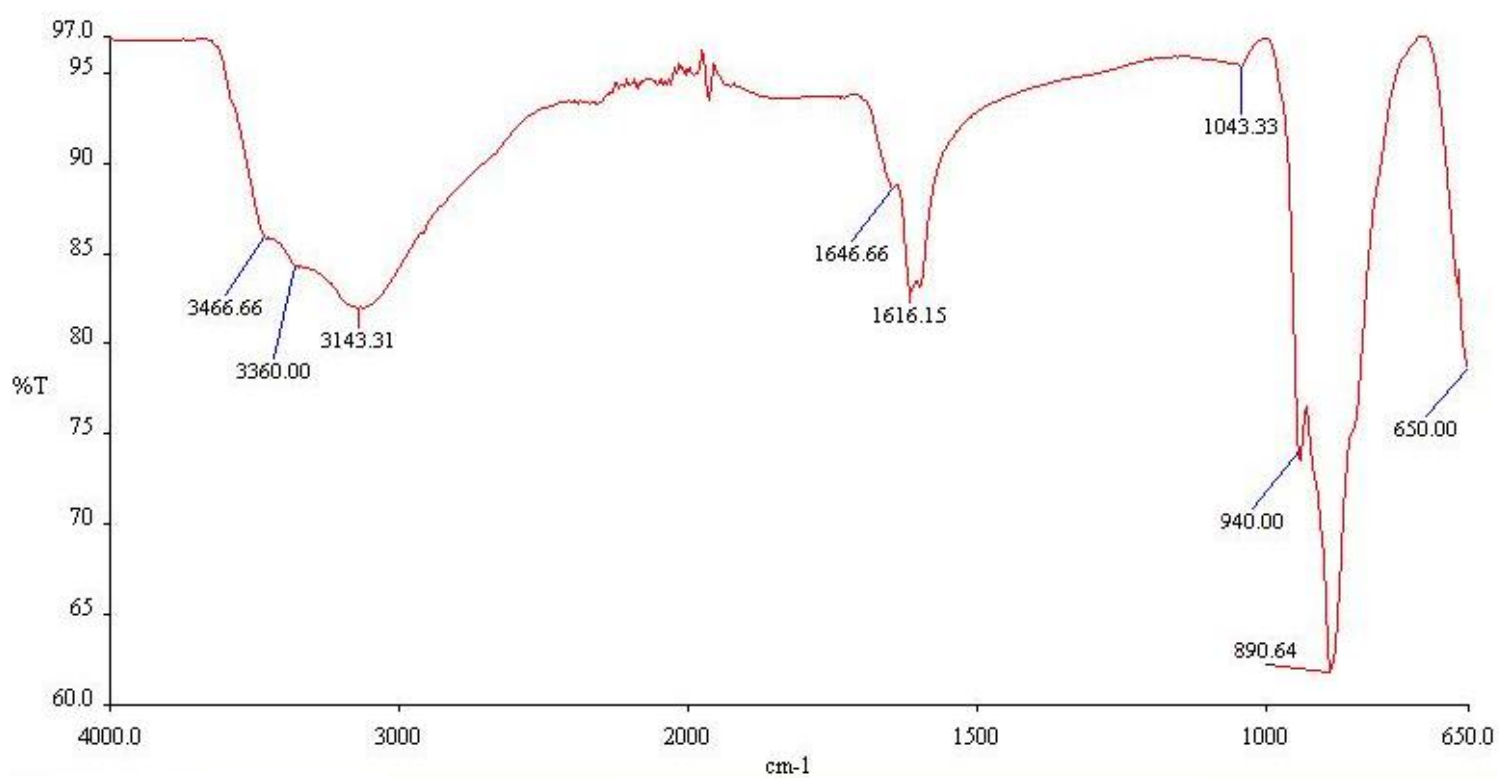
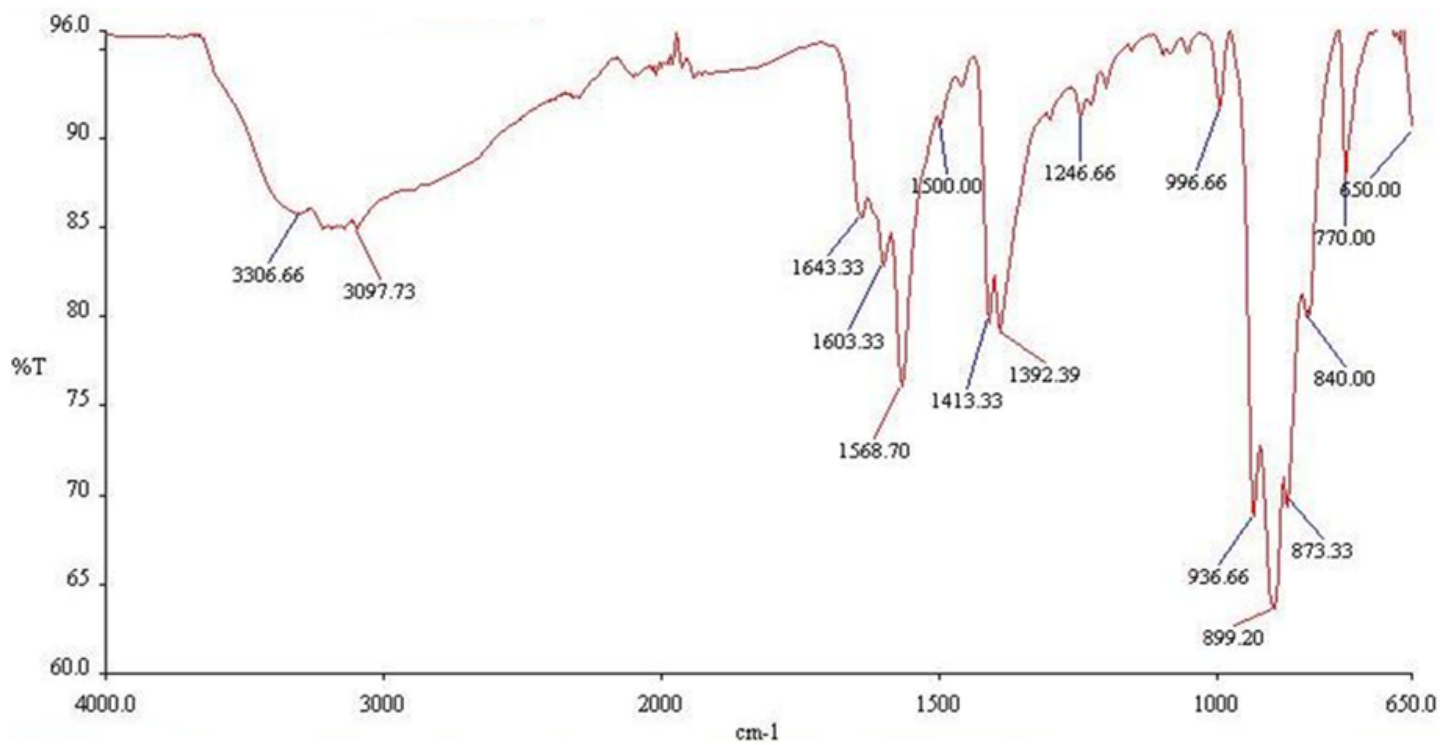


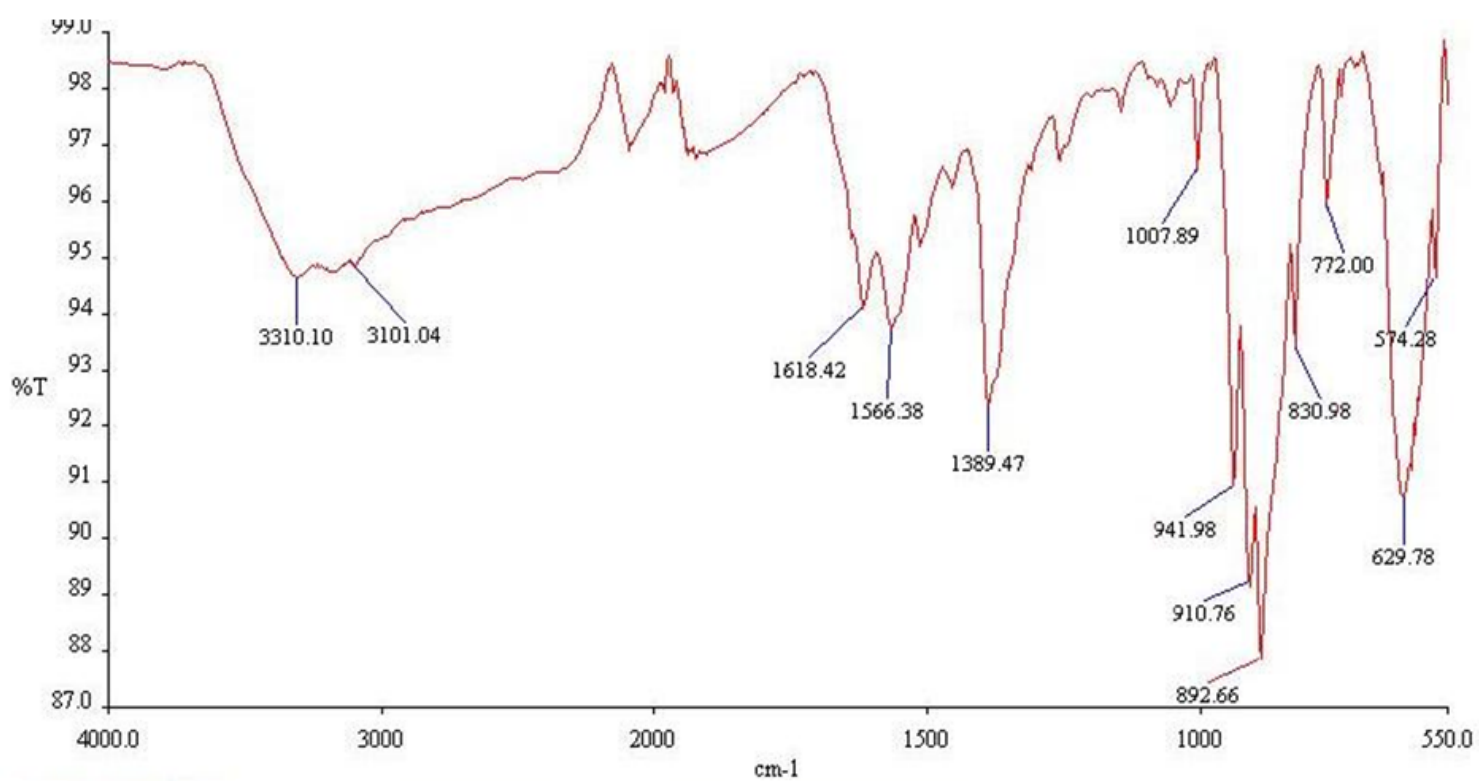
Fig. S5 TG/DT plots for solids 1, 3, 4 and 5 in nitrogen atmosphere.



ATR-FTIR of solid 1



ATR-FTIR of solid 3



ATR-FTIR of solid 4

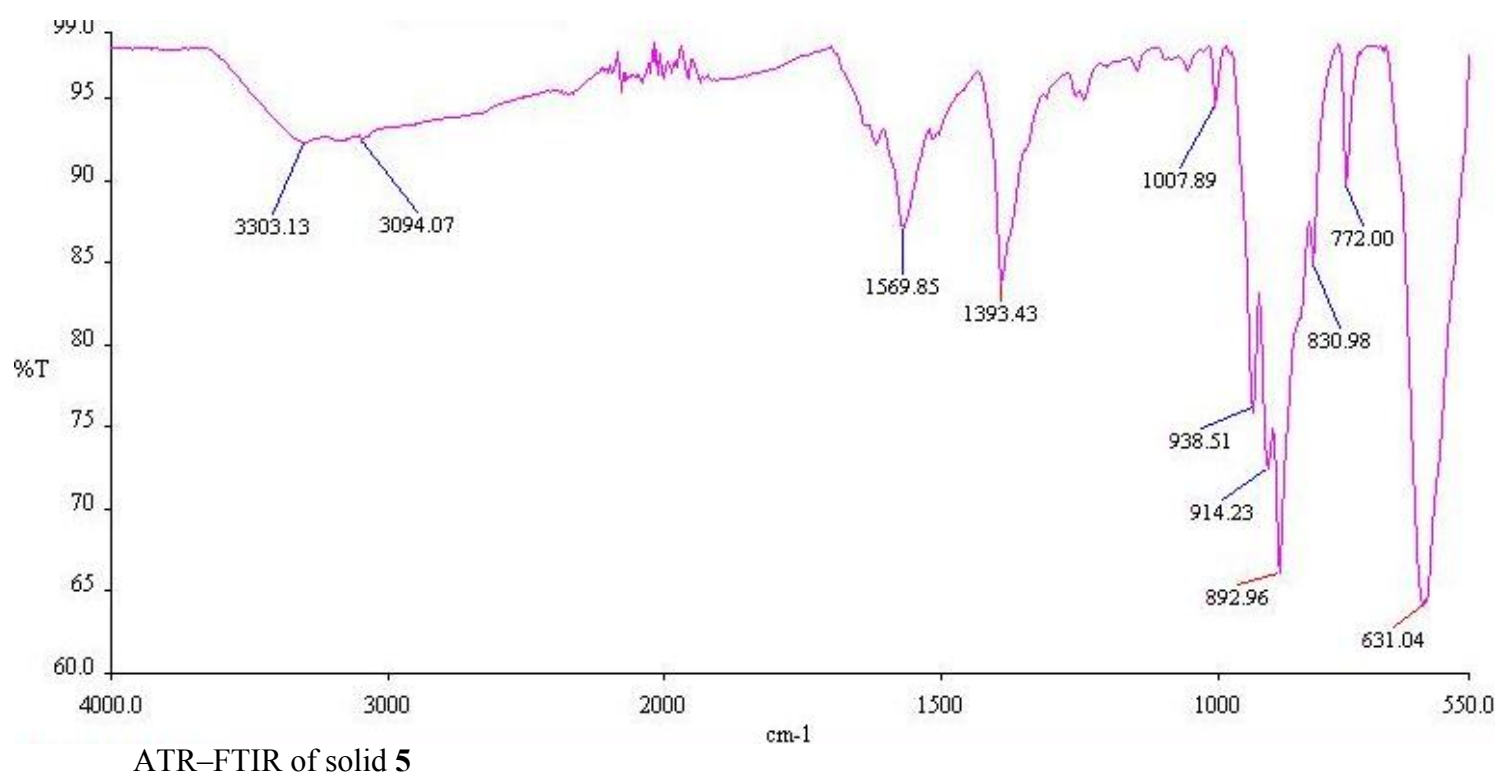


Fig. S6 ATR-FTIR of solids 1, 3, 4 and 5.

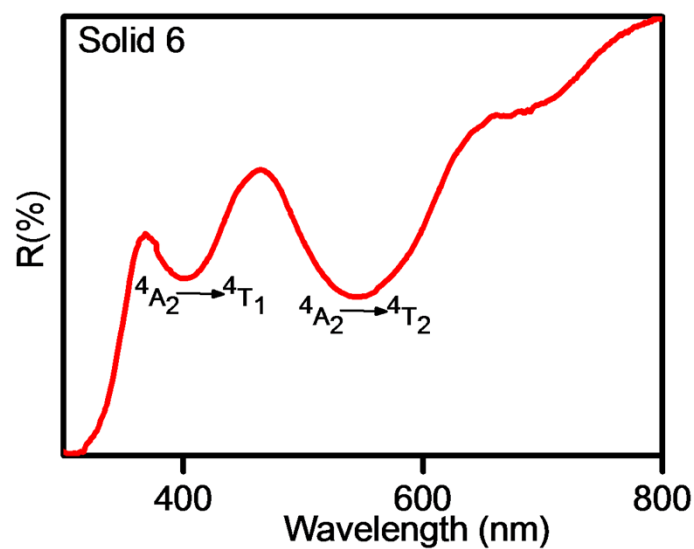
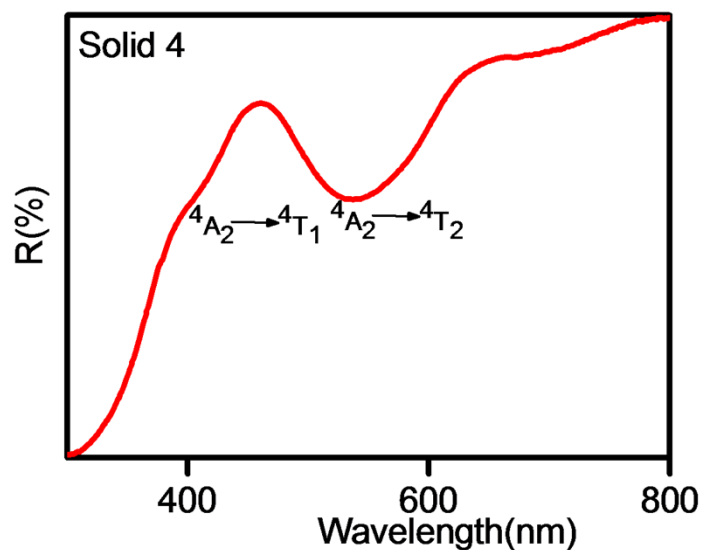
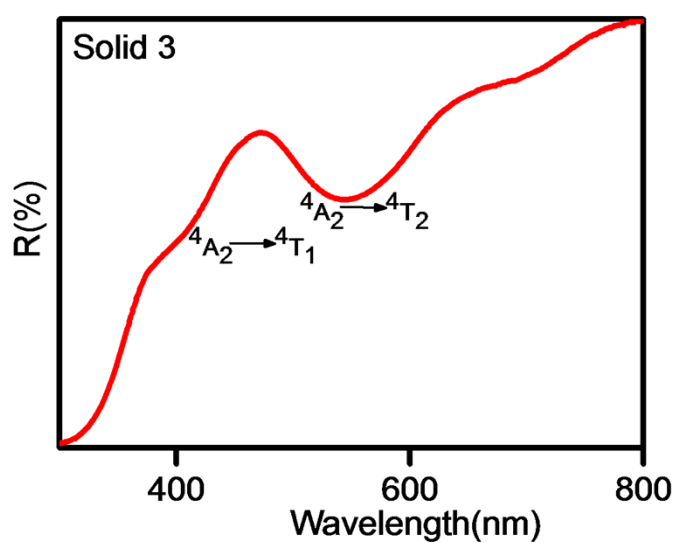
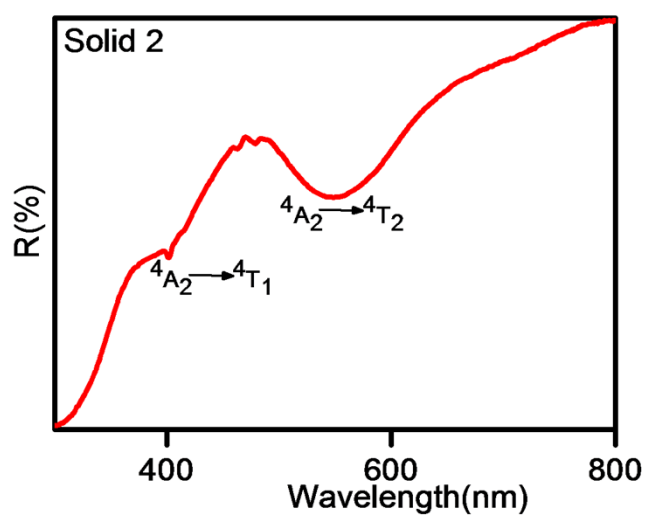
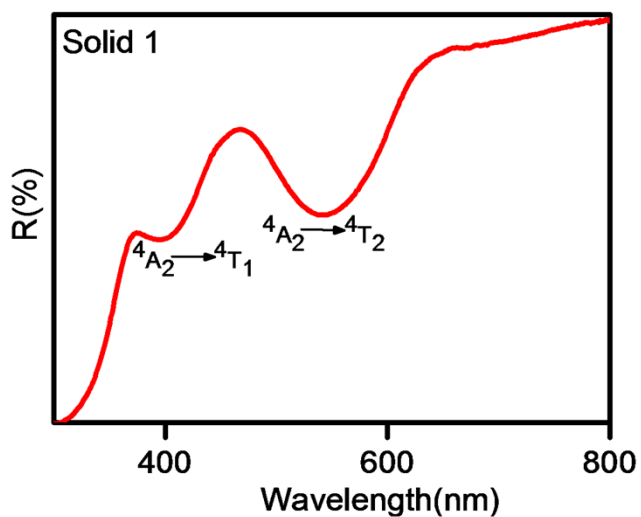


Fig. S7 Diffused reflectance of solids 1–4 and 6.