Electronic Supplementary Material (ESI) for Dalton Transactions


# Cage clusters built from uranyl ions bridged through peroxo and 1-hydroxyethane-1,1-diphosphonic acid ligands

*Zuolei Liao*[1], *Jie Ling*[1], *Laura R. Reinke*[1], *Jennifer E. S. Szymanowski*[1], *Ginger E. Sigmon*[1], *Peter C. Burns*[1,2]*

[1]Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, Indiana, 46556, USA.

[2]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana, 46556, USA

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Figure S1. UV-vis spectra for single crystals of $U24L_{12}$ (a) , $U40L_{20}$ (b), $U64L_{32}$ (c), $U20L_{10}$ (d), $U16L_8$ (e)and $U16L_8P_4$ (f).

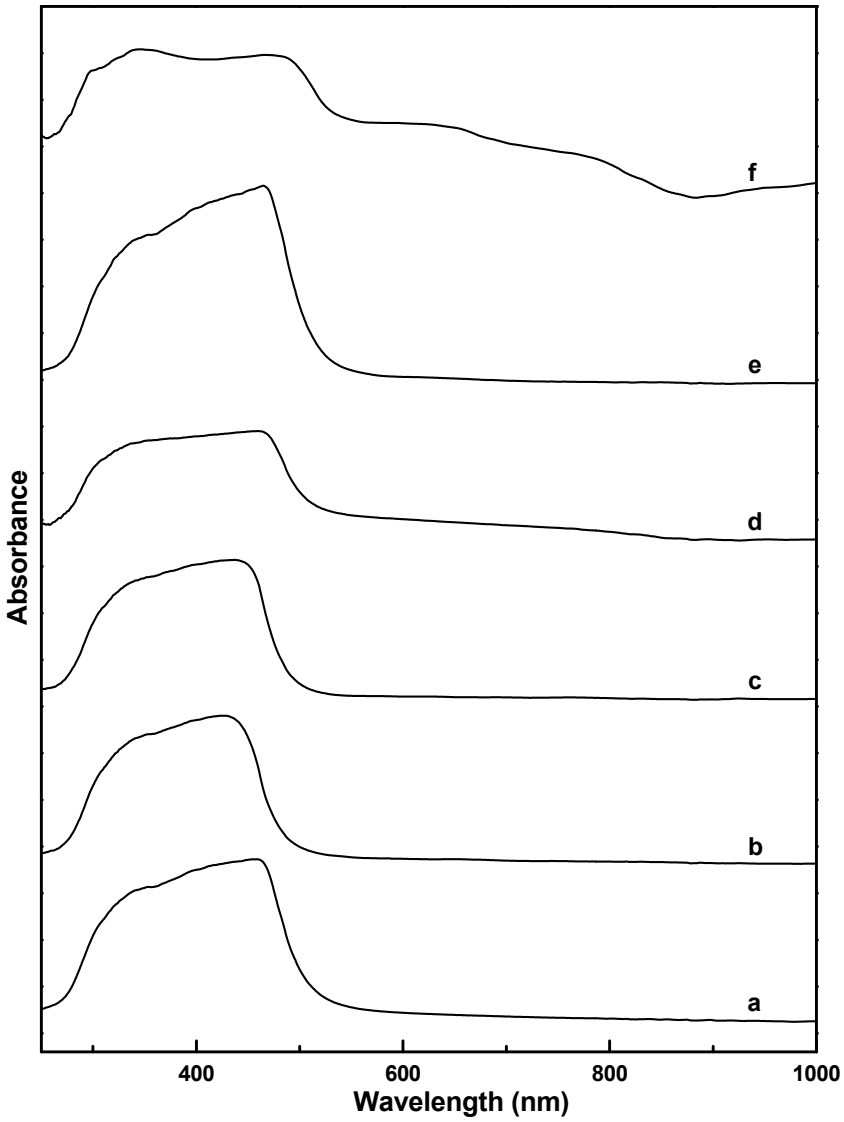

Figure S2. IR spectra for single crystals of $U24L_{12}$ (a) , $U40L_{20}$ (b), $U64L_{32}$ (c), $U20L_{10}$ (d), $U16L_8$ (e)and $U16L_8P_4$ (f).

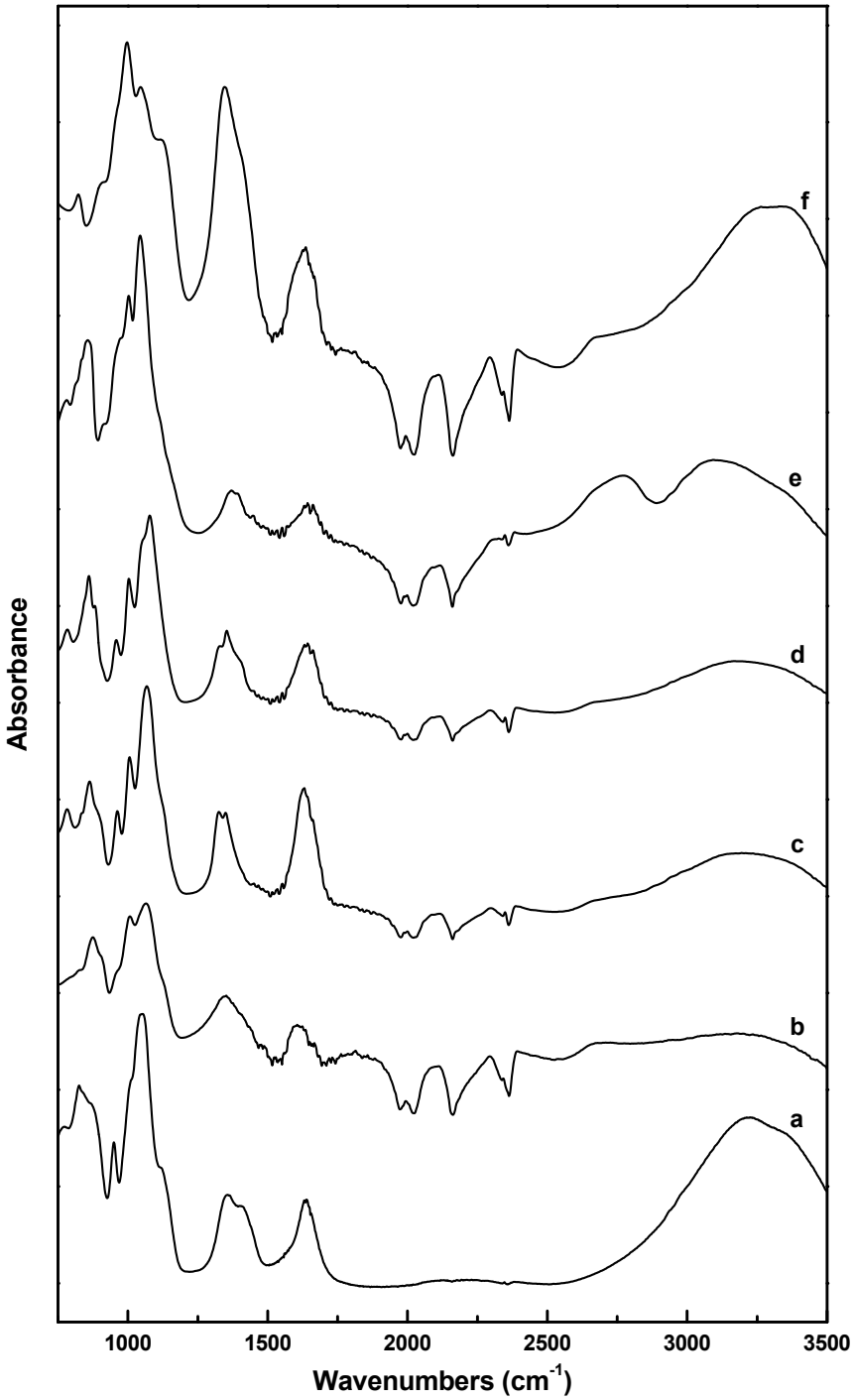

Table S1 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: $U24L_{12}$ P2/n R = 0.09

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0.74370(4) | 0.05956(3) | 0.12823(4) | 0.0383(3) |
| U2 | 0.44577(4) | 0.25226(3) | 0.11577(4) | 0.0287(3) |
| U3 | 0.62824(4) | 0.05954(3) | 0.24368(4) | 0.0384(3) |
| U4 | 0.61585(4) | 0.25233(3) | -0.05427(4) | 0.0287(3) |
| U5 | 0.63875(4) | 0.25023(4) | 0.54699(4) | 0.0364(3) |
| U6 | 0.44124(4) | 0.14525(3) | 0.23667(4) | 0.0342(3) |
| U7 | 0.73666(4) | 0.14522(3) | -0.05865(4) | 0.0344(3) |
| U8 | 0.74112(4) | 0.35917(4) | -0.04510(5) | 0.0406(3) |
| U9 | 0.45294(4) | 0.25020(4) | 0.36128(4) | 0.0363(3) |
| U10 | 0.45498(4) | 0.35913(4) | 0.24113(4) | 0.0402(3) |
| U11 | 0.74253(6) | 0.51807(4) | 0.12741(6) | 0.0816(6) |
| U12 | 0.62730(6) | 0.51811(4) | 0.24259(6) | 0.0814(6) |
| P1 | 0.4866(3) | 0.1966(2) | -0.0131(3) | 0.0297(19) |
| P2 | 0.4853(3) | 0.3060(2) | -0.0145(3) | 0.0296(19) |
| P3 | 0.4924(3) | 0.0314(2) | 0.1759(3) | 0.039(2) |
| P4 | 0.6757(3) | 0.0316(2) | -0.0076(3) | 0.041(3) |
| P5 | 0.7989(3) | 0.0306(3) | -0.0006(3) | 0.047(3) |
| P6 | 0.5011(3) | 0.2992(3) | 0.4988(3) | 0.048(3) |
| P7 | 0.5073(3) | 0.1909(3) | 0.4927(3) | 0.044(3) |
| P8 | 0.4993(3) | 0.0306(3) | 0.2991(3) | 0.048(3) |
| P9 | 0.6796(3) | 0.4768(2) | -0.0087(3) | 0.051(3) |
| P10 | 0.4913(3) | 0.4767(2) | 0.1793(3) | 0.049(3) |
| P11 | 0.8027(4) | 0.4761(3) | 0.0014(5) | 0.074(4) |
| P12 | 0.5015(5) | 0.4759(3) | 0.3025(4) | 0.075(4) |
| O1 | 0.6514(8) | 0.5347(8) | 0.1509(8) | 0.062(6) |
| O2 | 0.7358(14) | 0.5585(13) | -0.0218(14) | 0.132(12) |
| O3 | 0.4032(14) | 0.4910(12) | 0.2436(13) | 0.120(11) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.4825(15) | 0.5026(13) | 0.3505(15) | 0.138(12) |
| O5 | 0.6651(10) | 0.5284(9) | 0.3348(10) | 0.079(7) |
| O6 | 0.5606(11) | 0.4850(9) | 0.2973(11) | 0.086(8) |
| O7 | 0.7442(9) | 0.5762(8) | 0.0952(9) | 0.072(6) |
| O8 | 0.8516(14) | 0.5019(12) | -0.0207(14) | 0.126(11) |
| O9 | 0.7959(10) | 0.4851(9) | 0.0621(10) | 0.080(7) |
| O10 | 0.4720(8) | 0.3410(8) | 0.5274(8) | 0.060(6) |
| O11 | 0.4161(11) | 0.2405(9) | 0.5099(11) | 0.082(8) |
| O12 | 0.7339(10) | 0.0042(9) | -0.0917(10) | 0.074(7) |
| O13 | 0.5944(9) | 0.5765(8) | 0.2442(9) | 0.063(6) |
| O14 | 0.5495(9) | 0.4955(8) | 0.1806(9) | 0.066(6) |
| O15 | 0.3935(10) | 0.2509(7) | -0.0370(10) | 0.066(6) |
| O16 | 0.6945(9) | 0.5540(8) | 0.1935(9) | 0.066(6) |
| O17 | 0.4071(10) | 0.0050(9) | 0.2335(10) | 0.081(7) |
| O18 | 0.6809(9) | 0.4955(8) | 0.0500(9) | 0.064(6) |
| O19 | 0.8468(9) | 0.0036(8) | -0.0209(9) | 0.068(6) |
| O20 | 0.4801(9) | 0.0027(8) | 0.3467(9) | 0.061(6) |
| O21 | 0.6437(9) | 0.4512(8) | 0.2438(9) | 0.070(6) |
| O22 | 0.5609(8) | 0.0280(7) | 0.2986(8) | 0.049(5) |
| O23 | 0.5547(7) | 0.0275(7) | 0.1803(7) | 0.046(5) |
| O24 | 0.6249(8) | 0.0076(7) | -0.0353(8) | 0.052(5) |
| O25 | 0.6079(9) | 0.2504(7) | 0.6130(9) | 0.058(6) |
| O26 | 0.4850(8) | 0.1451(7) | 0.5160(8) | 0.059(6) |
| O27 | 0.3879(9) | 0.2506(6) | 0.3915(9) | 0.053(5) |
| O28 | 0.6513(6) | 0.0723(6) | 0.1514(6) | 0.033(4) |
| O29 | 0.6298(8) | 0.4936(7) | -0.0433(8) | 0.058(5) |
| O30 | 0.4650(8) | 0.0080(7) | 0.1252(8) | 0.054(5) |
| O31 | 0.7978(8) | 0.0272(7) | 0.0610(8) | 0.049(5) |
| O32 | 0.4563(8) | 0.4933(7) | 0.1291(8) | 0.055(5) |
| O33 | 0.7417(7) | 0.1178(6) | 0.0936(7) | 0.045(5) |

| | | | | |
|---|---|---|---|---|
| O34 | 0.6631(7) | 0.0741(6) | 0.3362(7) | 0.043(4) |
| O35 | 0.4904(7) | 0.4205(6) | 0.1863(7) | 0.041(4) |
| O36 | 0.8019(8) | 0.4235(7) | -0.0124(8) | 0.050(5) |
| O37 | 0.3757(7) | 0.1152(6) | 0.2325(7) | 0.039(4) |
| O38 | 0.7371(7) | 0.3903(6) | -0.1093(7) | 0.044(4) |
| O39 | 0.4868(8) | 0.4228(7) | 0.3013(8) | 0.050(5) |
| O40 | 0.6468(7) | 0.3345(6) | -0.0619(7) | 0.043(4) |
| O41 | 0.6796(7) | 0.0276(7) | 0.0549(7) | 0.048(5) |
| O42 | 0.4734(7) | 0.0850(6) | 0.1778(7) | 0.038(4) |
| O43 | 0.6917(7) | 0.0963(6) | 0.1919(7) | 0.039(4) |
| O44 | 0.7329(7) | 0.1153(6) | -0.1240(7) | 0.040(4) |
| O45 | 0.3901(7) | 0.3898(7) | 0.2365(8) | 0.048(5) |
| O46 | 0.5645(7) | 0.2986(6) | 0.5132(7) | 0.044(5) |
| O47 | 0.6996(9) | 0.5485(8) | 0.3013(9) | 0.071(6) |
| O48 | 0.4874(7) | 0.2985(6) | 0.4353(8) | 0.047(5) |
| O49 | 0.5175(8) | 0.2506(6) | 0.3310(8) | 0.045(5) |
| O50 | 0.6864(7) | 0.4214(6) | -0.0109(7) | 0.039(4) |
| O51 | 0.5941(7) | 0.1173(6) | 0.2421(7) | 0.043(4) |
| O52 | 0.4799(7) | 0.0835(6) | 0.2976(7) | 0.044(5) |
| O53 | 0.7429(7) | -0.0006(7) | 0.1572(8) | 0.050(5) |
| O54 | 0.5222(7) | 0.3318(6) | 0.2467(7) | 0.039(4) |
| O55 | 0.6579(7) | -0.0020(7) | 0.2429(8) | 0.050(5) |
| O56 | 0.3792(7) | 0.2552(5) | 0.0784(7) | 0.034(4) |
| O57 | 0.7465(6) | 0.3321(6) | 0.0216(7) | 0.036(4) |
| O58 | 0.7097(8) | 0.3002(7) | 0.5846(8) | 0.048(5) |
| O59 | 0.4376(7) | 0.3345(6) | 0.1469(7) | 0.043(4) |
| O60 | 0.6687(7) | 0.2500(6) | 0.4830(7) | 0.038(4) |
| O61 | 0.4607(8) | 0.1519(7) | -0.0392(8) | 0.050(5) |
| O62 | 0.5455(6) | 0.3038(5) | -0.0227(6) | 0.029(4) |
| O63 | 0.5694(7) | 0.1961(6) | 0.5087(7) | 0.041(4) |
| O64 | 0.6779(7) | 0.0848(6) | -0.0254(7) | 0.037(4) |

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|---|---|---|---|---|
| O65 | 0.4910(7) | 0.1967(6) | 0.4307(7) | 0.042(4) |
| O66 | 0.7984(7) | 0.0827(6) | -0.0201(7) | 0.041(4) |
| O67 | 0.6429(6) | 0.1724(6) | -0.0744(6) | 0.029(4) |
| O68 | 0.5052(6) | 0.1763(6) | 0.2403(6) | 0.033(4) |
| O69 | 0.5791(7) | 0.2554(6) | -0.1214(7) | 0.034(4) |
| O70 | 0.4151(7) | 0.3005(6) | 0.2899(7) | 0.041(4) |
| O71 | 0.4772(6) | 0.3032(6) | 0.0458(7) | 0.033(4) |
| O72 | 0.7094(7) | 0.2057(6) | 0.5933(7) | 0.044(5) |
| O73 | 0.4251(6) | 0.1721(6) | 0.1434(6) | 0.030(4) |
| O74 | 0.4061(7) | 0.2055(6) | 0.2908(7) | 0.042(4) |
| O75 | 0.5134(6) | 0.2490(5) | 0.1523(6) | 0.026(4) |
| O76 | 0.5477(6) | 0.2007(6) | -0.0225(6) | 0.031(4) |
| O77 | 0.4578(7) | 0.3495(6) | -0.0415(7) | 0.040(4) |
| O78 | 0.8322(7) | 0.3342(6) | -0.0591(7) | 0.042(4) |
| O79 | 0.7437(9) | 0.4535(8) | 0.1465(10) | 0.071(6) |
| O80 | 0.4312(7) | 0.1697(6) | 0.3296(7) | 0.039(4) |
| O81 | 0.6522(6) | 0.2479(5) | 0.0138(7) | 0.029(4) |
| O82 | 0.4029(7) | 0.2067(6) | 0.1796(7) | 0.037(4) |
| O83 | 0.7397(6) | 0.1757(5) | 0.0046(6) | 0.027(3) |
| O84 | 0.4403(7) | 0.3338(6) | 0.3316(7) | 0.041(4) |
| O85 | 0.4780(6) | 0.2008(5) | 0.0480(6) | 0.029(4) |
| O86 | 0.6705(7) | 0.1694(6) | 0.5681(7) | 0.036(4) |
| O87 | 0.4133(7) | 0.3005(6) | 0.1826(7) | 0.040(4) |
| O88 | 0.6826(7) | 0.2996(6) | -0.0860(7) | 0.039(4) |
| O89 | 0.6999(7) | 0.0954(6) | 0.3002(7) | 0.039(4) |
| O90 | 0.6798(7) | 0.2062(6) | -0.0968(7) | 0.034(4) |
| C1 | 0.4508(10) | 0.2511(8) | -0.0471(11) | 0.033(6) |
| C2 | 0.4753(13) | 0.2414(11) | 0.5254(14) | 0.056(8) |
| C3 | 0.4702(12) | 0.0013(11) | 0.2362(12) | 0.049(7) |
| C4 | 0.4636(11) | 0.2519(9) | -0.1068(11) | 0.036(6) |

| | | | | |
|---|---|---|---|---|
| C5 | 0.7354(11) | 0.0009(10) | -0.0299(12) | 0.047(7) |
| C6 | 0.4630(13) | 0.5049(12) | 0.2408(13) | 0.060(8) |
| C7 | 0.7401(13) | 0.5039(12) | -0.0364(13) | 0.061(8) |
| C8 | 0.4900(12) | 0.2398(10) | 0.5840(13) | 0.049(7) |
| C9 | 0.7359(12) | -0.0505(11) | -0.0118(12) | 0.050(7) |
| C10 | 0.4867(13) | -0.0521(12) | 0.2357(14) | 0.063(9) |
| C11 | 0.7438(13) | 0.4904(12) | -0.0963(14) | 0.061(9) |
| C12 | 0.4764(14) | 0.5572(12) | 0.2356(14) | 0.065(9) |
| *O1W | 0.6747(17) | 0.3898(16) | 0.1014(18) | 0.066(12) |
| Li4 | 0.707(2) | 0.3594(18) | 0.128(2) | 0.050(12) |
| *O2W | 0.301(2) | 0.3033(18) | 0.284(2) | 0.078(14) |
| *O3W | 0.714(2) | 0.3027(19) | 0.698(2) | 0.088(15) |
| *O4W | 0.8743(16) | -0.0963(15) | 0.0234(17) | 0.059(11) |
| *O5W | 0.7172(17) | 0.2690(15) | 0.2166(17) | 0.057(10) |
| *O6W | 0.6273(16) | 0.4274(14) | 0.3706(16) | 0.055(10) |
| *O7W | 0.5236(16) | -0.0967(15) | 0.3766(16) | 0.057(11) |
| *O8W | 0.6095(19) | -0.0372(18) | 0.1106(19) | 0.078(14) |
| *O10W | 0.5546(15) | 0.0439(14) | 0.0529(16) | 0.051(10) |
| *O11W | 0.4972(12) | 0.3959(11) | 0.4077(12) | 0.078(9) |
| *O12W | 3/4 | 0.3935(16) | 1/4 | 0.086(13) |
| *O13W | 0.9074(12) | 0.3954(11) | -0.0007(12) | 0.082(9) |
| *O14W | 0.5971(13) | 0.3969(12) | -0.1291(13) | 0.085(9) |
| *O15W | 0.6168(16) | 0.2871(14) | 0.3831(17) | 0.056(11) |
| *O16W | 0.5990(13) | 0.3806(12) | 0.0375(13) | 0.072(9) |
| *O17W | 0.3713(12) | 0.3973(11) | 0.0949(12) | 0.082(9) |
| *O18W | 0.5380(12) | 0.3821(11) | 0.1005(12) | 0.063(8) |
| O19W | 0.5534(10) | 0.1412(9) | 0.3611(10) | 0.080(7) |
| O20W | 0.8609(10) | 0.1420(9) | 0.0527(10) | 0.079(7) |
| *O21W | 0.8804(12) | -0.0208(11) | 0.1212(12) | 0.078(9) |
| *O22W | 3/4 | -0.077(3) | 1/4 | 0.10(2) |

| | | | | |
|---|---|---|---|---|
| O23W | 3/4 | 0.2068(14) | 1/4 | 0.098(12) |
| O24W | 0.9759(10) | 0.0307(9) | 0.0230(10) | 0.086(7) |
| O25W | 0.7484(9) | 0.2401(7) | 0.0995(9) | 0.060(6) |
| O26W | 0.6002(9) | 0.2400(7) | 0.2485(9) | 0.054(5) |
| O27W | 0.6632(7) | 0.1841(7) | 0.3371(8) | 0.050(5) |
| O28W | 0.6562(8) | 0.1869(7) | 0.1565(8) | 0.056(5) |
| O29W | 0.5438(8) | 0.1428(7) | 0.1236(8) | 0.050(5) |
| O30W | 0.6238(8) | 0.1435(7) | 0.0431(8) | 0.048(5) |
| O31W | 0.6115(7) | 0.2860(6) | 0.1111(7) | 0.039(4) |
| O32W | 0.5698(8) | 0.4917(7) | 0.0699(8) | 0.052(5) |
| *O9W | 0.490(3) | 0.403(3) | -0.116(3) | 0.07(2) |
| | | | | |
| Li1 | 0.302(3) | 0.280(3) | 0.174(3) | 0.09(2) |
| *Li2 | 0.827(3) | 0.281(3) | 0.699(3) | 0.06(2) |
| Li3 | 0.628(2) | 0.361(2) | 0.208(2) | 0.066(15) |
| Li5 | 0.298(2) | 0.2028(19) | 0.295(2) | 0.060(14) |
| Li6 | 0.704(2) | 0.2040(19) | 0.703(2) | 0.058(13) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S2 - (An)isotropic Displacement Parameters
for: $U24L_{12}$ P2/n R = 0.09

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0392(6) | 0.0276(5) | 0.0449(7) | -0.0036(4) | -0.0126(5) | 0.0050(4) |
| U2 | 0.0276(5) | 0.0245(5) | 0.0329(6) | 0.0016(4) | -0.0026(4) | 0.0003(4) |
| U3 | 0.0382(6) | 0.0282(5) | 0.0456(7) | 0.0052(4) | -0.0128(5) | -0.0035(4) |
| U4 | 0.0276(5) | 0.0252(5) | 0.0322(6) | -0.0001(4) | -0.0031(4) | 0.0014(4) |
| U5 | 0.0271(5) | 0.0484(6) | 0.0337(6) | 0.0041(4) | 0.0023(4) | -0.0023(4) |
| U6 | 0.0324(5) | 0.0332(6) | 0.0352(6) | 0.0056(4) | -0.0063(4) | -0.0115(4) |
| U7 | 0.0303(5) | 0.0332(6) | 0.0379(6) | -0.0116(4) | -0.0060(4) | 0.0054(4) |
| U8 | 0.0292(5) | 0.0330(6) | 0.0590(7) | 0.0121(5) | 0.0019(5) | -0.0010(4) |
| U9 | 0.0289(5) | 0.0477(6) | 0.0323(6) | 0.0024(4) | 0.0023(4) | -0.0038(4) |
| U10 | 0.0527(6) | 0.0329(6) | 0.0344(6) | -0.0007(4) | 0.0012(5) | 0.0125(5) |
| U11 | 0.0987(11) | 0.0309(7) | 0.0991(11) | -0.0091(6) | -0.0752(9) | 0.0124(6) |
| U12 | 0.0926(10) | 0.0312(7) | 0.1042(12) | 0.0118(6) | -0.0746(9) | -0.0088(6) |
| P1 | 0.031(3) | 0.024(3) | 0.033(4) | -0.004(3) | -0.003(3) | -0.001(3) |
| P2 | 0.029(3) | 0.029(3) | 0.029(4) | 0.001(3) | -0.006(3) | -0.001(3) |
| P3 | 0.036(4) | 0.030(4) | 0.047(4) | 0.000(3) | -0.012(3) | -0.016(3) |
| P4 | 0.044(4) | 0.030(4) | 0.045(5) | -0.014(3) | -0.016(3) | 0.001(3) |
| P5 | 0.044(4) | 0.044(4) | 0.051(5) | -0.019(4) | -0.013(4) | 0.022(3) |
| P6 | 0.034(4) | 0.072(6) | 0.036(4) | 0.001(4) | -0.008(3) | 0.000(4) |
| P7 | 0.035(4) | 0.058(5) | 0.037(4) | 0.016(3) | -0.008(3) | -0.013(3) |
| P8 | 0.048(4) | 0.041(4) | 0.050(5) | 0.022(3) | -0.013(4) | -0.018(3) |
| P9 | 0.057(5) | 0.027(4) | 0.061(5) | 0.009(3) | -0.031(4) | -0.001(3) |
| P10 | 0.055(5) | 0.022(4) | 0.062(5) | 0.002(3) | -0.029(4) | 0.005(3) |
| P11 | 0.058(5) | 0.035(5) | 0.123(9) | 0.030(5) | -0.028(5) | -0.023(4) |
| P12 | 0.114(8) | 0.036(5) | 0.066(6) | -0.025(4) | -0.030(6) | 0.025(5) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S3 - Bond Distances (Angstrom)
for: $U24L_{12}$ P2/n R = 0.09

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O28 | 2.405(15) | U4 | -O76 | 2.377(15) |
| U1 | -O31 | 2.38(2) | U4 | -O81 | 1.815(17) |
| U1 | -O33 | 1.815(17) | U4 | -O88 | 2.281(17) |
| U1 | -O41 | 2.432(17) | U4 | -O90 | 2.335(17) |
| U1 | -O43 | 2.333(17) | U5 | -O25 | 1.85(2) |
| U1 | -O53 | 1.805(19) | U5 | -O46 | 2.339(17) |
| U1 | -O34_a | 2.394(17) | U5 | -O58 | 2.34(2) |
| U1 | -O89_a | 2.342(17) | U5 | -O60 | 1.790(17) |
| U2 | -O56 | 1.791(17) | U5 | -O63 | 2.383(17) |
| U2 | -O59 | 2.407(17) | U5 | -O72 | 2.324(17) |
| U2 | -O71 | 2.396(17) | U5 | -O86 | 2.401(17) |
| U2 | -O73 | 2.380(16) | U5 | -O78_a | 2.433(17) |
| U2 | -O75 | 1.805(15) | U6 | -O37 | 1.798(17) |
| U2 | -O82 | 2.329(17) | U6 | -O42 | 2.381(17) |
| U2 | -O85 | 2.373(14) | U6 | -O52 | 2.398(17) |
| U2 | -O87 | 2.306(17) | U6 | -O68 | 1.777(15) |
| U3 | -O22 | 2.39(2) | U6 | -O73 | 2.396(15) |
| U3 | -O23 | 2.426(17) | U6 | -O74 | 2.338(17) |
| U3 | -O28 | 2.404(15) | U6 | -O80 | 2.406(17) |
| U3 | -O34 | 2.376(17) | U6 | -O82 | 2.335(17) |
| U3 | -O43 | 2.326(17) | U7 | -O44 | 1.794(17) |
| U3 | -O51 | 1.797(17) | U7 | -O64 | 2.392(17) |
| U3 | -O55 | 1.847(19) | U7 | -O66 | 2.423(17) |
| U3 | -O89 | 2.345(17) | U7 | -O67 | 2.407(15) |
| U4 | -O40 | 2.402(17) | U7 | -O83 | 1.756(14) |
| U4 | -O62 | 2.412(14) | U7 | -O90 | 2.321(17) |
| U4 | -O67 | 2.367(16) | U7 | -O72_a | 2.335(17) |
| U4 | -O69 | 1.797(17) | U7 | -O86_a | 2.397(17) |

| | | | | | |
|---|---|---|---|---|---|
| U8 | -O36 | 2.40(2) | U11 | -O18 | 2.39(2) |
| U8 | -O38 | 1.784(17) | U11 | -O79 | 1.84(2) |
| U8 | -O40 | 2.401(17) | U11 | -O5_a | 2.37(2) |
| U8 | -O50 | 2.376(17) | U11 | -O47_a | 2.30(2) |
| U8 | -O57 | 1.788(17) | U12 | -O1 | 2.42(2) |
| U8 | -O78 | 2.385(17) | U12 | -O5 | 2.37(2) |
| U8 | -O88 | 2.340(17) | U12 | -O6 | 2.39(3) |
| U8 | -O58_a | 2.290(19) | U12 | -O13 | 1.80(2) |
| U9 | -O27 | 1.82(2) | U12 | -O14 | 2.40(2) |
| U9 | -O48 | 2.340(18) | U12 | -O16 | 2.34(2) |
| U9 | -O49 | 1.81(2) | U12 | -O21 | 1.89(2) |
| U9 | -O65 | 2.372(17) | U12 | -O47 | 2.33(2) |
| U9 | -O70 | 2.350(17) | P1 | -O61 | 1.50(2) |
| U9 | -O74 | 2.330(17) | P1 | -O76 | 1.536(16) |
| U9 | -O80 | 2.395(17) | P1 | -O85 | 1.533(16) |
| U9 | -O84 | 2.429(17) | P1 | -C1 | 1.89(2) |
| U10 | -O35 | 2.374(17) | P2 | -O62 | 1.505(16) |
| U10 | -O39 | 2.38(2) | P2 | -O71 | 1.509(18) |
| U10 | -O45 | 1.791(18) | P2 | -O77 | 1.498(18) |
| U10 | -O54 | 1.801(17) | P2 | -C1 | 1.87(2) |
| U10 | -O59 | 2.402(17) | P3 | -O23 | 1.520(19) |
| U10 | -O70 | 2.282(17) | P3 | -O30 | 1.50(2) |
| U10 | -O84 | 2.380(17) | P3 | -O42 | 1.552(18) |
| U10 | -O87 | 2.330(17) | P3 | -C3 | 1.82(3) |
| U11 | -O1 | 2.40(2) | P4 | -O24 | 1.51(2) |
| U11 | -O7 | 1.79(2) | P4 | -O41 | 1.527(19) |
| U11 | -O9 | 2.34(2) | P4 | -O64 | 1.533(18) |
| U11 | -O16 | 2.31(2) | P4 | -C5 | 1.82(3) |
| P5 | -O19 | 1.51(2) | P12 | -O4 | 1.50(4) |
| P5 | -O31 | 1.51(2) | P12 | -O6 | 1.48(3) |
| P5 | -O66 | 1.514(18) | P12 | -O39 | 1.51(2) |

| | | | | | |
|---|---|---|---|---|---|
| P5 | -C5 | 1.84(3) | P12 | -C6 | 1.88(3) |
| P6 | -O10 | 1.56(2) | O1 | -O16 | 1.51(3) |
| P6 | -O46 | 1.556(19) | O2 | -C7 | 1.55(5) |
| P6 | -O48 | 1.56(2) | O3 | -C6 | 1.52(5) |
| P6 | -C2 | 1.86(3) | O5 | -O47 | 1.35(3) |
| P7 | -O26 | 1.51(2) | O11 | -C2 | 1.46(4) |
| P7 | -O63 | 1.538(19) | O12 | -C5 | 1.51(4) |
| P7 | -O65 | 1.539(19) | O15 | -C1 | 1.45(3) |
| P7 | -C2 | 1.82(3) | O17 | -C3 | 1.54(4) |
| P8 | -O20 | 1.51(2) | O28 | -O43 | 1.49(2) |
| P8 | -O22 | 1.51(2) | O34 | -O89 | 1.44(2) |
| P8 | -O52 | 1.534(19) | O40 | -O88 | 1.46(2) |
| P8 | -C3 | 1.82(3) | O58 | -O78_a | 1.48(3) |
| P9 | -O18 | 1.52(2) | O59 | -O87 | 1.45(2) |
| P9 | -O29 | 1.49(2) | O67 | -O90 | 1.44(2) |
| P9 | -O50 | 1.539(17) | O70 | -O84 | 1.46(2) |
| P9 | -C7 | 1.84(3) | O72 | -O86 | 1.48(2) |
| P10 | -O14 | 1.51(2) | O73 | -O82 | 1.44(2) |
| P10 | -O32 | 1.50(2) | O74 | -O80 | 1.46(2) |
| P10 | -O35 | 1.560(17) | O1W | -Li4 | 1.29(7) |
| P10 | -C6 | 1.88(3) | C1 | -C4 | 1.52(4) |
| P11 | -O8 | 1.53(4) | C2 | -C8 | 1.45(5) |
| P11 | -O9 | 1.53(3) | C3 | -C10 | 1.53(4) |
| P11 | -O36 | 1.49(2) | C5 | -C9 | 1.49(4) |
| P11 | -C7 | 1.88(3) | C6 | -C12 | 1.49(5) |
| C7 | -C11 | 1.52(5) | | | |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: u40l20 Imm2 R = 0.06

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0.13101(10) | 0.31764(8) | -0.19583(6) | 0.0287(9) |
| U2 | 0 | 0.31520(12) | -0.13240(8) | 0.0270(12) |
| U3 | 0.34954(16) | 1/2 | -0.13410(7) | 0.0247(12) |
| U4 | 0 | 0.31617(12) | -0.25993(7) | 0.0293(12) |
| U5 | 0 | 0.31568(12) | -0.00846(7) | 0.0243(12) |
| U6 | 0.13081(10) | 0.31742(8) | 0.05488(6) | 0.0266(9) |
| U7 | 0.34037(11) | 0.39568(7) | 0.05658(5) | 0.0254(8) |
| U8 | 0.34000(11) | 0.39589(7) | -0.19764(5) | 0.0246(8) |
| U9 | 0.34979(16) | 1/2 | -0.00699(7) | 0.0237(12) |
| U10 | 0.32870(16) | 1/2 | 0.12075(7) | 0.0236(11) |
| U11 | 0 | 0.39641(11) | 0.21960(7) | 0.0240(12) |
| U12 | 0.32942(17) | 1/2 | -0.26137(7) | 0.0253(12) |
| U13 | 0 | 0.39628(10) | -0.36019(8) | 0.0250(12) |
| U14 | 0.13158(15) | 1/2 | -0.35744(8) | 0.0260(12) |
| U15 | 0 | 0.31638(13) | 0.11899(7) | 0.0303(12) |
| U16 | 0.13139(15) | 1/2 | 0.21678(8) | 0.0239(11) |
| P1 | 0.2713(8) | 0.4466(5) | -0.3301(4) | 0.028(6) |
| P2 | 0.2711(8) | 0.4481(6) | 0.1885(3) | 0.028(5) |
| P3 | 0.0665(2) | 0.2503(2) | -0.0707(4) | 0.0287(17) |
| P4 | 0.2717(7) | 0.2872(5) | -0.2283(4) | 0.028(5) |
| P5 | 0.2724(7) | 0.2866(5) | 0.0889(3) | 0.027(5) |
| P6 | 0.0653(8) | 0.2881(6) | 0.1883(3) | 0.033(6) |
| P7 | 0.2757(3) | 0.4467(2) | -0.0713(5) | 0.0287(17) |
| P8 | 0.2740(6) | 0.2878(5) | -0.1646(3) | 0.024(5) |
| P9 | 0.0667(7) | 0.2866(6) | -0.3289(3) | 0.028(6) |
| P10 | 0.2764(8) | 0.2879(6) | 0.0224(3) | 0.041(6) |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: u40l20 Imm2 R = 0.06

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| *O1 | 0 | 0.244(2) | 0.2291(10) | 0.045(19) |
| O2 | 0 | 0.2566(12) | -0.3732(7) | 0.039(10) |
| O3 | 0.200(2) | 1/2 | -0.0995(10) | 0.071(17) |
| O4 | 0.3735(14) | 1/2 | 0.1978(8) | 0.044(10) |
| O5 | 0.2815(12) | 0.2056(8) | 0.0567(6) | 0.044(7) |
| O6 | 0 | 0.1804(12) | -0.0477(8) | 0.054(11) |
| O7 | 0.3958(19) | 1/2 | 0.1415(9) | 0.021(11) |
| O8 | 0.0684(12) | 0.2905(10) | 0.1539(6) | 0.045(9) |
| O9 | 0.393(3) | 1/2 | -0.2819(14) | 0.062(19) |
| O10 | 0.1683(19) | 1/2 | 0.2511(9) | 0.032(13) |
| O11 | 0.2314(7) | 0.4026(5) | -0.0694(12) | 0.054(5) |
| O12 | 0.0618(11) | 0.2815(8) | -0.2967(5) | 0.029(7) |
| O13 | 0.1772(17) | 1/2 | -0.3908(8) | 0.019(11) |
| O14 | 0.2033(14) | 0.2797(10) | 0.0846(6) | 0.051(10) |
| O15 | 0.3634(9) | 0.2589(7) | -0.1953(5) | 0.021(6) |
| O16 | 0.2043(9) | 0.2879(8) | -0.2285(5) | 0.014(6) |
| O17 | 0.2977(13) | 0.4019(9) | 0.2033(6) | 0.031(8) |
| O18 | 0.4050(10) | 0.3586(8) | 0.0601(5) | 0.019(7) |
| O19 | 0 | 0.3687(16) | -0.3943(6) | 0.054(17) |
| O20 | 0.2982(12) | 0.2578(9) | -0.0002(6) | 0.039(9) |
| O21 | 0.2058(10) | 0.2809(8) | 0.0227(5) | 0.027(6) |
| O22 | 0.2058(13) | 0.4528(9) | 0.1965(6) | 0.031(9) |
| O23 | 0.2981(14) | 0.2625(10) | -0.2566(6) | 0.029(9) |
| O24 | 0.3179(11) | 0.4498(9) | -0.0442(6) | 0.027(8) |
| O25 | 0.2988(12) | 0.2652(9) | -0.1363(6) | 0.035(8) |
| O26 | 0.2100(10) | 0.2939(8) | -0.1641(5) | 0.031(7) |

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: u40l20 Imm2 R = 0.06

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| O27 | 0.0943(11) | 0.2593(8) | -0.1974(5) | 0.017(6) |
| O28 | 0.3017(14) | 0.4088(10) | -0.3429(7) | 0.039(9) |
| O29 | 0.3655(11) | 0.4229(9) | 0.0084(6) | 0.017(7) |
| O30 | 0.0955(19) | 1/2 | -0.3216(9) | 0.044(9) |
| O31 | 0.2784(16) | 1/2 | -0.1483(7) | 0.018(10) |
| O32 | 0 | 0.3727(10) | 0.1372(7) | 0.006(8) |
| O33 | 0.2947(16) | 0.3380(11) | 0.0859(7) | 0.025(10) |
| O34 | 0.0966(13) | 0.2640(10) | 0.0531(7) | 0.035(9) |
| O35 | 0.0881(16) | 1/2 | 0.1840(7) | 0.0200 |
| O36 | 0.2963(11) | 0.3371(9) | -0.1653(5) | 0.021(7) |
| O37 | 0.1033(9) | 0.4189(7) | 0.2279(5) | 0.015(6) |
| O38 | 0 | 0.372(2) | -0.2798(14) | 0.070(19) |
| O39 | 0.1211(13) | 0.2631(10) | -0.3374(6) | 0.037(9) |
| O40 | 0.3073(11) | 0.4475(9) | -0.0984(6) | 0.027(8) |
| O41 | 0.2810(14) | 0.4505(10) | -0.2958(7) | 0.035(10) |
| O42 | 0.0991(12) | 0.4204(9) | -0.3627(6) | 0.038(8) |
| O43 | 0.3871(14) | 0.4569(10) | 0.0299(7) | 0.038(10) |
| O44 | 0.2043(13) | 0.4470(9) | -0.3345(6) | 0.026(8) |
| O45 | 0.3056(14) | 0.3383(11) | 0.0264(7) | 0.042(10) |
| O46 | 0.1655(14) | 0.3722(9) | 0.0550(8) | 0.028(9) |
| O47 | 0 | 0.2642(12) | 0.0093(7) | 0.018(10) |
| O48 | 0.2726(13) | 0.4289(9) | -0.1956(7) | 0.016(7) |
| O49 | 0.2972(18) | 0.3384(12) | -0.2275(8) | 0.033(11) |
| O50 | 0 | 0.2556(12) | 0.1023(8) | 0.028(10) |
| O51 | 0.1009(9) | 0.3266(7) | -0.1466(4) | 0.012(5) |
| O52 | 0.2735(19) | 1/2 | 0.0120(8) | 0.036(13) |

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Table S4 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: $U40L_{20}$ Imm2 R = 0.06

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| O53 | 0.2918(15) | 0.2605(11) | 0.1134(7) | 0.043(11) |
| O54 | 0.1226(12) | 0.2608(9) | 0.2017(6) | 0.030(8) |
| O55 | 0.1013(12) | 0.3354(9) | -0.2440(6) | 0.035(8) |
| O56 | 0.0999(10) | 0.3256(8) | 0.1047(5) | 0.015(6) |
| O57 | 0 | 0.3622(12) | 0.2537(5) | 0.015(9) |
| O58 | 0.3920(11) | 0.4512(9) | -0.1706(5) | 0.014(7) |
| O59 | 0.3614(14) | 0.4164(10) | -0.1497(7) | 0.033(9) |
| O60 | 0.2769(16) | 0.4284(12) | 0.0555(9) | 0.042(11) |
| O61 | 0.4213(12) | 1/2 | -0.1172(6) | 0.004(7) |
| O62 | 0 | 0.3788(11) | -0.1133(7) | 0.031(9) |
| O63 | 0 | 0.3653(9) | -0.0297(5) | 0.010(7) |
| O64 | 0.1706(15) | 0.3746(10) | -0.1965(9) | 0.036(10) |
| O65 | 0.0978(12) | 0.3378(9) | 0.0064(6) | 0.044(9) |
| O66 | 0.4118(12) | 0.3650(9) | -0.1987(6) | 0.033(8) |
| O67 | 0.0640(12) | 0.2832(9) | -0.0449(6) | 0.024(8) |
| O68 | 0.2861(12) | 0.4478(9) | 0.1572(6) | 0.019(8) |
| O69 | 0.0592(12) | 0.3472(9) | 0.0287(5) | 0.031(8) |
| O70 | 0.3465(12) | 0.4169(9) | 0.1045(6) | 0.025(8) |
| O71 | 0.0639(15) | 0.3389(11) | -0.3381(7) | 0.042(11) |
| O72 | 0.414(2) | 1/2 | -0.0269(11) | 0.072(18) |
| O73 | 0.0548(11) | 0.3548(8) | -0.1657(5) | 0.025(7) |
| O74 | 0 | 0.4235(14) | -0.3271(9) | 0.029(13) |
| O75 | 0.3797(12) | 0.4488(9) | 0.0861(6) | 0.027(8) |
| O76 | 0 | 0.2655(12) | -0.2418(8) | 0.028(11) |
| O77 | 0.0640(18) | 0.4510(13) | 0.2390(9) | 0.084(14) |
| O78 | 0.0628(11) | 0.3384(8) | 0.2010(5) | 0.011(7) |
| O79 | 0 | 0.4312(12) | 0.1863(7) | 0.012(10) |

| | | | | |
|---|---|---|---|---|
| O80 | 0.1208(6) | 0.2191(5) | -0.0704(12) | 0.032(3) |
| O81 | 0.2612(17) | 1/2 | 0.0986(8) | 0.017(10) |
| O82 | 0.0596(8) | 0.4543(6) | -0.3822(4) | 0.003(5) |
| O83 | 0.259(2) | 1/2 | -0.2433(9) | 0.039(14) |
| O84 | 0.3478(12) | 0.4233(9) | -0.2483(6) | 0.022(8) |
| O85 | 0 | 0.2564(14) | -0.1523(9) | 0.035(13) |
| O86 | 0.3804(11) | 0.4569(8) | -0.2291(5) | 0.019(7) |
| O87 | 0.0606(14) | 0.3503(10) | 0.0827(6) | 0.028(9) |
| O88 | 0.0590(14) | 0.3548(10) | -0.2264(7) | 0.032(9) |
| O89 | 0.0645(14) | 0.2781(11) | -0.0988(7) | 0.039(10) |
| O90 | 0.3698(18) | 1/2 | -0.3469(13) | 0.11(2) |
| C1 | 0 | 0.2139(9) | -0.070(2) | 0.022(6) |
| C2 | 0.2303(12) | 1/2 | -0.0727(12) | 0.030(8) |
| C3 | 0.308(3) | 1/2 | -0.3796(16) | 0.08(2) |
| C4 | 0 | 0.2608(13) | 0.2008(10) | 0.028(16) |
| C5 | 0.2971(13) | 0.2599(10) | -0.1967(7) | 0.0200 |
| C6 | 0.2978(16) | 1/2 | 0.2020(8) | 0.019(10) |
| C7 | 0.3085(18) | 1/2 | -0.3482(10) | 0.0200 |
| C8 | 0.3632(16) | 0.2476(13) | 0.0584(8) | 0.034(11) |
| C9 | 0 | 0.1915(14) | -0.1011(9) | 0.018(9) |
| C10 | 0.294(2) | 1/2 | 0.2367(10) | 0.0200 |
| C11 | 0.188(2) | 1/2 | -0.0437(10) | 0.021(12) |
| C12 | 0.300(2) | 0.2472(13) | 0.0565(10) | 0.056(12) |
| C13 | 0.266(2) | 0.2073(12) | -0.1939(10) | 0.066(15) |
| C14 | 0 | 0.2079(17) | -0.3255(11) | 0.037(16) |
| C15 | 0 | 0.2528(15) | -0.3416(11) | 0.033(17) |
| C16 | 0 | 0.2047(14) | 0.1925(10) | 0.026(13) |
| *O6W | 0.125(5) | 0.264(4) | -0.080(3) | 0.12(4) |
| Na6 | 0.2384(9) | 0.2049(7) | -0.0358(4) | 0.078(6) |
| O7W | 0.1560(14) | 0.1886(11) | -0.0370(7) | 0.103(10) |

| | | | | |
|---|---|---|---|---|
| *O10W | 0.019(2) | 0.1527(18) | 0.1110(12) | 0.072(19) |
| O1W | 0 | 1/2 | -0.2781(8) | 0.035(9) |
| O2W | 0.1278(5) | 0.3968(4) | 0.1605(3) | 0.050(3) |
| O3W | 0.1859(7) | 0.4432(5) | -0.2226(3) | 0.0200 |
| *O4W | 0.086(2) | 0.4382(17) | 0.0139(10) | 0.069(14) |
| *O5W | 0.1055(17) | 0.3763(13) | -0.0633(10) | 0.060(13) |
| O8W | 0.0972(9) | 0.4409(7) | -0.2435(4) | 0.045(5) |
| *O9W | 0.0354(18) | 0.1508(15) | 0.0265(9) | 0.055(12) |
| *O11W | 0.176(2) | 1/2 | 0.0497(12) | 0.042(14) |
| O12W | 0.2029(13) | 0.3010(10) | -0.2958(6) | 0.053(9) |
| O13W | 0.170(4) | 1/2 | -0.1886(17) | 0.12(3) |
| *O14W | 0.205(2) | 0.2927(18) | 0.1504(11) | 0.039(15) |
| *O15W | 0.1246(16) | 0.2057(13) | 0.0001(8) | 0.056(12) |
| *O16W | 0.1401(18) | 0.2128(14) | -0.1401(8) | 0.021(10) |
| *O17W | 0.1403(15) | 0.2208(12) | 0.1186(7) | 0.047(10) |
| *O18W | 0.150(2) | 0.2224(18) | -0.2676(11) | 0.050(15) |
| *O19W | 0.3982(18) | 0.3418(13) | 0.1296(8) | 0.068(13) |
| *O20W | 0.3966(17) | 0.3536(14) | -0.2773(9) | 0.026(10) |
| Na1 | 0 | 0.2180(4) | 0.0559(2) | 0.005(2) |
| *Na2 | 0.2161(12) | 0.3963(9) | 0.1156(6) | 0.023(7) |
| Na3 | 0.1824(5) | 0.3087(4) | -0.0377(3) | 0.048(3) |
| *Na4 | 1/2 | 1/2 | -0.072(3) | 0.072(12) |
| | | | | |
| *Na7 | 0.2202(12) | 0.3986(9) | -0.0063(5) | 0.042(7) |
| *Na8 | 0.2020(11) | 0.4102(8) | -0.1393(5) | 0.033(6) |
| *Na9 | 0.2229(12) | 0.3911(9) | -0.2603(6) | 0.072(9) |
| *Na10 | 0.0544(11) | 0.4419(8) | -0.2868(5) | 0.050(6) |
| *Na5 | 0.2413(19) | 0.2152(16) | -0.0985(9) | 0.020(11) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S4 - (An)isotropic Displacement Parameters
for: $U40L_{20}$ Imm2 R = 0.06

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0156(15) | 0.0436(16) | 0.0269(15) | 0.0067(14) | 0.0021(14) | -0.0004(12) |
| U2 | 0.018(2) | 0.043(2) | 0.020(2) | -0.0011(18) | 0 | 0 |
| U3 | 0.026(2) | 0.030(2) | 0.018(2) | 0.0000 | -0.0058(18) | 0 |
| U4 | 0.019(2) | 0.047(2) | 0.022(2) | 0.0074(18) | 0 | 0 |
| U5 | 0.018(2) | 0.039(2) | 0.016(2) | -0.0024(17) | 0 | 0 |
| U6 | 0.0175(16) | 0.0418(16) | 0.0205(14) | -0.0034(13) | -0.0003(14) | -0.0015(12) |
| U7 | 0.0239(15) | 0.0306(14) | 0.0216(14) | 0.0008(14) | 0.0000(13) | 0.0017(12) |
| U8 | 0.0225(15) | 0.0296(14) | 0.0218(14) | -0.0005(13) | -0.0011(13) | 0.0005(12) |
| U9 | 0.024(2) | 0.030(2) | 0.017(2) | 0 | 0.0034(18) | 0 |
| U10 | 0.021(2) | 0.0267(19) | 0.023(2) | 0.0000 | -0.0042(18) | 0 |
| U11 | 0.021(2) | 0.028(2) | 0.023(2) | 0.0036(17) | 0 | 0 |
| U12 | 0.023(2) | 0.032(2) | 0.021(2) | 0.0000 | -0.0008(18) | 0 |
| U13 | 0.022(2) | 0.025(2) | 0.028(2) | -0.0016(18) | 0 | 0 |
| U14 | 0.021(2) | 0.031(2) | 0.026(2) | 0.0000 | -0.0002(18) | 0 |
| U15 | 0.022(2) | 0.048(2) | 0.021(2) | -0.0066(18) | 0 | 0 |
| U16 | 0.018(2) | 0.0268(19) | 0.027(2) | 0.0000 | -0.0026(18) | 0 |
| P1 | 0.033(11) | 0.016(8) | 0.036(11) | 0.002(8) | -0.002(8) | 0.004(8) |
| P2 | 0.018(9) | 0.037(9) | 0.028(10) | 0.008(8) | -0.001(7) | -0.008(8) |
| P3 | 0.020(3) | 0.047(3) | 0.019(3) | -0.010(11) | -0.003(11) | 0.007(2) |
| P4 | 0.026(9) | 0.031(9) | 0.028(9) | -0.005(8) | 0.004(7) | 0.012(8) |
| P5 | 0.016(8) | 0.039(10) | 0.026(9) | 0.000(8) | -0.006(7) | -0.009(7) |
| P6 | 0.034(11) | 0.033(10) | 0.032(11) | 0.001(8) | 0.002(9) | 0.005(9) |
| P7 | 0.033(3) | 0.030(3) | 0.023(3) | -0.001(10) | -0.006(10) | -0.006(2) |
| P8 | 0.005(6) | 0.038(9) | 0.029(9) | 0.009(7) | -0.004(6) | -0.007(6) |
| P9 | 0.028(10) | 0.034(10) | 0.022(10) | 0.006(8) | 0.007(8) | 0.009(8) |
| P10 | 0.044(11) | 0.054(11) | 0.025(9) | -0.007(8) | -0.003(8) | 0.018(9) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S6 - Bond Distances (Angstrom)
for: $U40L_{20}$ Imm2 R = 0.06

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O16 | 2.40(2) | U4 | -O88 | 2.32(3) |
| U1 | -O26 | 2.41(2) | U4 | -O12_a | 2.41(2) |
| U1 | -O27 | 1.85(2) | U4 | -O55_a | 2.47(3) |
| U1 | -O51 | 2.397(19) | U4 | -O88_a | 2.32(3) |
| U1 | -O55 | 2.39(3) | U5 | -O47 | 1.67(3) |
| U1 | -O64 | 1.84(3) | U5 | -O63 | 1.72(2) |
| U1 | -O73 | 2.46(2) | U5 | -O65 | 2.40(3) |
| U1 | -O88 | 2.40(3) | U5 | -O67 | 2.41(3) |
| U2 | -O51 | 2.40(2) | U5 | -O69 | 2.36(3) |
| U2 | -O62 | 2.01(3) | U5 | -O65_a | 2.40(3) |
| U2 | -O73 | 2.28(2) | U5 | -O67_a | 2.41(3) |
| U2 | -O85 | 1.90(4) | U5 | -O69_a | 2.36(3) |
| U2 | -O89 | 2.38(3) | U6 | -O14 | 2.39(3) |
| U2 | -O51_a | 2.40(2) | U6 | -O21 | 2.49(2) |
| U2 | -O73_a | 2.28(2) | U6 | -O34 | 1.70(3) |
| U2 | -O89_a | 2.38(3) | U6 | -O46 | 1.74(3) |
| U3 | -O31 | 1.74(4) | U6 | -O56 | 2.43(2) |
| U3 | -O40 | 2.42(3) | U6 | -O65 | 2.44(3) |
| U3 | -O58 | 2.39(2) | U6 | -O69 | 2.19(3) |
| U3 | -O59 | 2.49(3) | U6 | -O87 | 2.25(3) |
| U3 | -O61 | 1.80(3) | U7 | -O18 | 1.81(2) |
| U3 | -O40_b | 2.42(3) | U7 | -O29 | 2.43(3) |
| U3 | -O58_b | 2.39(2) | U7 | -O33 | 2.36(3) |
| U3 | -O59_b | 2.49(3) | U7 | -O43 | 2.38(3) |
| U4 | -O12 | 2.41(2) | U7 | -O45 | 2.28(3) |
| U4 | -O38 | 1.83(6) | U7 | -O60 | 1.71(4) |
| U4 | -O55 | 2.47(3) | U7 | -O70 | 2.31(3) |
| U4 | -O76 | 1.66(4) | U7 | -O75 | 2.22(3) |

| | | | | | |
|---|---|---|---|---|---|
| U8 | -O36 | 2.45(2) | U11 | -O79 | 1.83(3) |
| U8 | -O48 | 1.79(3) | U11 | -O37_a | 2.45(2) |
| U8 | -O49 | 2.35(4) | U11 | -O77_a | 2.30(4) |
| U8 | -O58 | 2.33(2) | U11 | -O78_a | 2.34(2) |
| U8 | -O59 | 2.35(3) | U12 | -O9 | 1.73(7) |
| U8 | -O66 | 1.85(3) | U12 | -O41 | 2.39(3) |
| U8 | -O84 | 2.48(3) | U12 | -O83 | 1.80(4) |
| U8 | -O86 | 2.44(2) | U12 | -O84 | 2.29(3) |
| U9 | -O24 | 2.35(3) | U12 | -O86 | 2.25(2) |
| U9 | -O29 | 2.32(3) | U12 | -O41_b | 2.39(3) |
| U9 | -O43 | 2.27(3) | U12 | -O84_b | 2.29(3) |
| U9 | -O52 | 1.94(4) | U12 | -O86_b | 2.25(2) |
| U9 | -O72 | 1.72(5) | U13 | -O19 | 1.77(3) |
| U9 | -O24_b | 2.35(3) | U13 | -O42 | 2.35(3) |
| U9 | -O29_b | 2.32(3) | U13 | -O71 | 2.40(3) |
| U9 | -O43_b | 2.27(3) | U13 | -O74 | 1.72(4) |
| U10 | -O7 | 1.80(4) | U13 | -O82 | 2.357(18) |
| U10 | -O68 | 2.44(3) | U13 | -O42_a | 2.35(3) |
| U10 | -O70 | 2.50(3) | U13 | -O71_a | 2.40(3) |
| U10 | -O75 | 2.45(3) | U13 | -O82_a | 2.357(18) |
| U10 | -O81 | 1.84(4) | U14 | -O13 | 1.86(4) |
| U10 | -O68_b | 2.44(3) | U14 | -O30 | 1.85(4) |
| U10 | -O70_b | 2.50(3) | U14 | -O42 | 2.38(3) |
| U10 | -O75_b | 2.45(3) | U14 | -O44 | 2.47(3) |
| U11 | -O37 | 2.45(2) | U14 | -O82 | 2.376(18) |
| U11 | -O57 | 1.86(3) | U14 | -O42_b | 2.38(3) |
| U11 | -O77 | 2.30(4) | U14 | -O44_b | 2.47(3) |
| U11 | -O78 | 2.34(2) | U14 | -O82_b | 2.376(18) |
| U15 | -O8 | 2.36(3) | P3 | -O6W | 1.45(12) |
| U15 | -O32 | 1.80(3) | P4 | -O16 | 1.53(3) |
| U15 | -O50 | 1.89(3) | P4 | -O23 | 1.60(3) |

| | | | | | |
|---|---|---|---|---|---|
| U15 | -O56 | 2.37(2) | P4 | -O49 | 1.56(4) |
| U15 | -O87 | 2.37(3) | P4 | -C5 | 1.75(4) |
| U15 | -O8_a | 2.36(3) | P5 | -O14 | 1.59(4) |
| U15 | -O56_a | 2.37(2) | P5 | -O33 | 1.55(3) |
| U15 | -O87_a | 2.37(3) | P5 | -O53 | 1.43(4) |
| U16 | -O10 | 1.80(4) | P5 | -C12 | 1.97(5) |
| U16 | -O22 | 2.35(3) | P6 | -O8 | 1.60(3) |
| U16 | -O35 | 1.81(3) | P6 | -O54 | 1.63(3) |
| U16 | -O37 | 2.44(2) | P6 | -O78 | 1.54(3) |
| U16 | -O77 | 2.31(4) | P6 | -C4 | 1.77(3) |
| U16 | -O22_b | 2.35(3) | P7 | -O11 | 1.603(17) |
| U16 | -O37_b | 2.44(2) | P7 | -O24 | 1.58(3) |
| U16 | -O77_b | 2.31(4) | P7 | -O40 | 1.45(3) |
| P1 | -O28 | 1.40(3) | P7 | -C2 | 1.826(16) |
| P1 | -O41 | 1.61(4) | P8 | -O25 | 1.57(3) |
| P1 | -O44 | 1.53(3) | P8 | -O26 | 1.46(3) |
| P1 | -C7 | 1.92(3) | P8 | -O36 | 1.48(3) |
| P2 | -O17 | 1.60(3) | P8 | -C5 | 1.77(3) |
| P2 | -O22 | 1.53(3) | P9 | -O12 | 1.51(3) |
| P2 | -O68 | 1.49(3) | P9 | -O39 | 1.45(3) |
| P2 | -C6 | 1.71(3) | P9 | -O71 | 1.54(4) |
| P3 | -O67 | 1.52(3) | P9 | -C15 | 1.88(3) |
| P3 | -O80 | 1.513(15) | P10 | -O20 | 1.44(3) |
| P3 | -O89 | 1.52(4) | P10 | -O21 | 1.61(3) |
| P3 | -C1 | 1.824(16) | P10 | -O45 | 1.58(4) |
| P10 | -C12 | 2.03(5) | O56 | -O87 | 1.52(4) |
| Na6 | -O7W | 1.92(4) | O58 | -O59 | 1.55(4) |
| O1 | -C4 | 1.40(7) | O65 | -O69 | 1.38(4) |
| O2 | -C15 | 1.47(6) | O70 | -O75 | 1.45(4) |
| O3 | -C2 | 1.42(7) | O84 | -O86 | 1.50(4) |

| | | | | | |
|---|---|---|---|---|---|
| O4 | -C6 | 1.72(5) | O90 | -C7 | 1.39(6) |
| O5 | -C12 | 1.25(4) | O10W | -O10W_c | 0.86(6) |
| O6 | -C1 | 1.40(8) | C1 | -C9 | 1.58(10) |
| O6W | -O80 | 1.35(12) | C2 | -C11 | 1.65(7) |
| O6W | -O89 | 1.67(13) | C3 | -C7 | 1.46(9) |
| O15 | -C5 | 1.50(4) | C4 | -C16 | 1.63(5) |
| O29 | -O43 | 1.47(4) | C5 | -C13 | 1.65(5) |
| O37 | -O77 | 1.37(4) | C6 | -C10 | 1.61(6) |
| O42 | -O82 | 1.59(3) | C8 | -C12 | 1.43(6) |
| O51 | -O73 | 1.58(3) | C14 | -C15 | 1.47(7) |
| O55 | -O88 | 1.37(4) | | | |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: u64l32 I4/m R = 0.09

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0.67065(4) | 0.88558(4) | -0.07414(4) | 0.0381(6) |
| U2 | 0.88556(4) | 0.67065(4) | -0.07414(4) | 0.0379(6) |
| U3 | 0.58336(6) | 0.88545(6) | 0 | 0.0367(8) |
| U4 | 0.88548(6) | 0.58338(6) | 0 | 0.0367(8) |
| U5 | 0.75811(6) | 0.88527(6) | 0 | 0.0426(8) |
| U6 | 0.88526(6) | 0.75812(6) | 0 | 0.0427(8) |
| U7 | 0.74997(4) | 0.66301(4) | -0.14207(4) | 0.0444(6) |
| U8 | 0.66293(4) | 0.74994(4) | -0.14207(4) | 0.0444(6) |
| U9 | 0.66594(5) | 0.57881(5) | -0.17024(5) | 0.0612(7) |
| U10 | 0.57879(5) | 0.66588(5) | -0.17019(5) | 0.0614(7) |
| P1 | 0.6355(4) | 0.5001(4) | -0.2276(3) | 0.071(5) |
| P2 | 0.7219(4) | 0.4999(3) | -0.2120(3) | 0.061(5) |
| P3 | 0.7133(3) | 0.8457(3) | -0.1512(3) | 0.048(4) |
| P4 | 0.8458(3) | 0.7131(3) | -0.1513(3) | 0.049(4) |
| P5 | 0.8520(3) | 0.8520(3) | -0.0370(3) | 0.054(4) |
| P6 | 0.5000(3) | 0.8315(3) | -0.0375(3) | 0.043(4) |
| P7 | 0.8491(3) | 0.6244(3) | -0.1515(3) | 0.048(4) |
| P8 | 0.6245(3) | 0.8490(3) | -0.1515(3) | 0.047(4) |
| O1 | 0.6738(7) | 0.6104(7) | -0.2038(6) | 0.053(7) |
| O2 | 0.689(2) | 0.542(2) | -0.2646(19) | 0.24(3) |
| O3 | 0.5373(18) | 0.7753(18) | 0 | 0.13(2) |
| O4 | 0.5975(9) | 0.5976(9) | -0.1692(8) | 0.078(9) |
| O5 | 0.6584(9) | 0.5452(10) | -0.1365(8) | 0.086(10) |
| O6 | 0.5452(10) | 0.6586(10) | -0.1367(8) | 0.087(10) |
| O7 | 0.8713(12) | 0.8715(12) | -0.0689(10) | 0.118(13) |
| O8 | 0.7274(7) | 0.7274(7) | -0.1259(6) | 0.042(6) |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: u64l32 I4/m R = 0.09

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| O9 | 0.9178(18) | 0.8708(18) | 0 | 0.13(2) |
| O10 | 0.6314(10) | 0.5360(10) | -0.2075(8) | 0.090(10) |
| O11 | 0.5358(10) | 0.6316(10) | -0.2074(9) | 0.093(11) |
| O12 | 0.7639(10) | 0.5001(9) | -0.2262(9) | 0.088(10) |
| O13 | 0.8708(8) | 0.5900(8) | -0.1672(7) | 0.064(8) |
| O14 | 0.5905(8) | 0.8706(8) | -0.1671(7) | 0.062(8) |
| O15 | 0.5000(8) | 0.8051(8) | -0.0671(7) | 0.059(8) |
| O16 | 0.7339(10) | 0.8377(10) | 0 | 0.052(10) |
| O17 | 0.9110(7) | 0.6709(7) | -0.1684(6) | 0.046(7) |
| O18 | 0.9318(10) | 0.5557(10) | 0 | 0.049(10) |
| O19 | 0.8377(10) | 0.7340(10) | 0 | 0.051(10) |
| O20 | 0.6102(7) | 0.6737(7) | -0.2037(6) | 0.052(7) |
| O21 | 0.8588(9) | 0.7493(9) | -0.1707(8) | 0.079(10) |
| O22 | 0.6553(7) | 0.7659(7) | -0.1002(6) | 0.048(7) |
| O23 | 0.7082(7) | 0.8015(7) | -0.1532(6) | 0.051(7) |
| O24 | 0.8012(7) | 0.7082(7) | -0.1530(6) | 0.053(7) |
| O25 | 0.6705(7) | 0.9109(7) | -0.1685(6) | 0.048(7) |
| O26 | 0.6203(7) | 0.6962(7) | -0.1317(6) | 0.052(7) |
| O27 | 0.6070(14) | 0.5003(13) | -0.2572(12) | 0.135(15) |
| O28 | 0.7660(7) | 0.6553(7) | -0.1001(6) | 0.047(7) |
| O29 | 0.6965(7) | 0.6205(7) | -0.1322(6) | 0.043(6) |
| O30 | 0.5359(9) | 0.7143(9) | -0.1909(8) | 0.082(9) |
| O31 | 0.7139(9) | 0.5358(9) | -0.1915(8) | 0.077(9) |
| O32 | 0.5557(10) | 0.9309(10) | 0 | 0.045(9) |
| O33 | 0.8568(7) | 0.6291(7) | -0.1147(6) | 0.052(7) |
| O34 | 0.6709(7) | 0.7362(7) | -0.1845(6) | 0.045(7) |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: u64l32 I4/m R = 0.09

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| O35 | 0.6290(7) | 0.8568(7) | -0.1145(6) | 0.048(7) |
| O36 | 0.7360(7) | 0.6711(7) | -0.1847(6) | 0.044(7) |
| O37 | 0.8963(7) | 0.7375(7) | -0.0565(6) | 0.044(7) |
| O38 | 0.7272(9) | 0.5970(8) | -0.1472(7) | 0.070(9) |
| O39 | 0.6702(7) | 0.9307(7) | -0.0975(6) | 0.044(6) |
| O40 | 0.5970(8) | 0.7276(8) | -0.1469(7) | 0.069(8) |
| O41 | 0.7377(7) | 0.8965(7) | -0.0563(6) | 0.043(6) |
| O42 | 0.9308(7) | 0.6706(7) | -0.0974(6) | 0.045(7) |
| O43 | 0.7835(10) | 0.9329(10) | 0 | 0.046(9) |
| O44 | 0.6705(7) | 0.8393(7) | -0.0528(6) | 0.040(6) |
| O45 | 0.6945(7) | 0.6954(7) | -0.1198(6) | 0.042(6) |
| O46 | 0.8393(7) | 0.6699(7) | -0.0526(6) | 0.039(6) |
| O47 | 0.9325(10) | 0.7835(10) | 0 | 0.048(10) |
| O48 | 0.8081(7) | 0.8610(7) | -0.0354(6) | 0.054(7) |
| O49 | 0.8605(7) | 0.7125(7) | -0.1155(6) | 0.051(7) |
| O50 | 0.8611(7) | 0.8088(8) | -0.0352(6) | 0.055(7) |
| O51 | 0.7123(7) | 0.8606(7) | -0.1157(6) | 0.048(7) |
| O52 | 0.8049(7) | 0.6230(7) | -0.1587(6) | 0.048(7) |
| O53 | 0.8953(6) | 0.6045(6) | -0.0559(5) | 0.032(6) |
| O54 | 0.6228(7) | 0.8048(7) | -0.1587(6) | 0.048(7) |
| O55 | 0.6042(6) | 0.8953(6) | -0.0560(6) | 0.035(6) |
| O56 | 0.9146(7) | 0.7091(7) | -0.0336(6) | 0.042(6) |
| O57 | 0.7093(6) | 0.9149(6) | -0.0336(6) | 0.039(6) |
| O58 | 0.6206(8) | 0.6204(8) | -0.1454(7) | 0.064(8) |
| O59 | 0.8567(7) | 0.5364(7) | -0.0364(6) | 0.048(7) |
| O60 | 0.5365(7) | 0.8568(7) | -0.0362(6) | 0.049(7) |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table S7 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: $U64L_{32}$ I4/m R = 0.09

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| O61 | 0.6302(6) | 0.9160(6) | -0.0343(6) | 0.036(6) |
| O62 | 0.9161(6) | 0.6296(6) | -0.0340(5) | 0.033(6) |
| O63 | 0.8412(9) | 0.6097(9) | 0 | 0.031(8) |
| O64 | 0.6093(9) | 0.8409(9) | 0 | 0.035(8) |
| O65 | 0.7492(9) | 0.8591(9) | -0.1707(8) | 0.079(9) |
| C1 | 0.6856(19) | 0.4993(19) | -0.2445(17) | 0.12(2) |
| C2 | 0.8711(17) | 0.8713(17) | 0 | 0.058(17) |
| C3 | 0.5003(14) | 0.8038(14) | 0 | 0.030(13) |
| C4 | 0.8680(12) | 0.6695(12) | -0.1712(10) | 0.057(12) |
| C5 | 0.6699(12) | 0.8682(12) | -0.1712(10) | 0.057(12) |
| C6 | 0.8579(14) | 0.6688(14) | -0.2091(12) | 0.077(14) |
| C7 | 0.463(2) | 0.776(2) | 0 | 0.07(2) |
| C8 | 0.8724(19) | 0.9172(19) | 0 | 0.067(18) |
| C9 | 0.6690(14) | 0.8577(14) | -0.2097(12) | 0.077(14) |
| C10 | 0.688(2) | 0.456(2) | -0.2636(19) | 0.15(3) |
| *O1W | 0.7253(16) | 0.5645(16) | -0.0819(14) | 0.063(16) |
| *O2W | 0.7854(17) | 0.5400(17) | -0.1370(15) | 0.074(18) |
| *O3W | 0.5644(14) | 0.7267(14) | -0.0815(12) | 0.050(14) |
| *O4W | 0.5406(18) | 0.7858(18) | -0.1370(15) | 0.079(18) |
| *O5W | 0.5008(18) | 0.5812(18) | -0.1479(16) | 0.079(19) |
| *O6W | 0.5010(17) | 0.6634(17) | -0.0835(15) | 0.072(18) |
| *O7W | 0.5931(10) | 0.7721(10) | -0.2193(9) | 0.011(9) |
| *O8W | 0.933(2) | 0.429(2) | -0.1133(17) | 0.09(2) |
| *O9W | 0.9338(19) | 0.5706(19) | -0.1125(17) | 0.09(2) |
| *O10W | 1 | 1/2 | 0.036(2) | 0.08(3) |

| | | | | |
|---|---|---|---|---|
| *O11W | 0.6275(18) | 0.9998(18) | -0.1439(15) | 0.080(19) |
| *O12W | 0.7343(15) | 0.6512(15) | -0.2572(13) | 0.055(14) |
| *O13W | 0.6515(15) | 0.7337(15) | -0.2576(13) | 0.056(15) |
| *O14W | 0.736(2) | 0.999(2) | -0.1367(18) | 0.10(2) |
| *O15W | 0.6201(17) | 1.0007(17) | -0.0604(15) | 0.070(17) |
| *O16W | 0.7262(18) | 1.0002(18) | -0.0472(16) | 0.080(19) |
| O17W | 0.7720(9) | 0.5930(9) | -0.2192(8) | 0.084(10) |
| *O18W | 0.6317(12) | 0.7510(12) | 0.0248(10) | 0.030(11) |
| *O19W | 0.7512(12) | 0.6317(13) | -0.0251(11) | 0.036(12) |
| *O20W | 0.9276(12) | 0.5005(12) | -0.0640(10) | 0.028(11) |
| *O21W | 0.7443(12) | 0.7998(12) | -0.0770(10) | 0.030(11) |
| O22W | 0.7997(11) | 0.7440(11) | -0.0770(9) | 0.099(11) |
| O23W | 0.5909(7) | 0.5908(7) | -0.2449(6) | 0.042(6) |
| O24W | 0.7644(5) | 0.7644(5) | -0.1885(5) | 0.017(5) |
| K1 | 0.5930(3) | 0.8044(3) | -0.0688(3) | 0.065(4) |
| K2 | 0.8045(3) | 0.5929(3) | -0.0687(3) | 0.066(4) |
| Na1 | 0.8033(6) | 0.6717(6) | 0 | 0.045(5) |
| Na2 | 0.6723(6) | 0.8035(6) | 0 | 0.045(5) |
| Na3 | 0.6800(5) | 0.6799(5) | -0.2241(4) | 0.062(4) |
| Na4 | 0.6758(7) | 1.0002(7) | -0.1010(6) | 0.107(7) |
| *Na5 | 1.0000(13) | 0.5531(13) | 0 | 0.080(13) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S8 - (An)isotropic Displacement Parameters
for: $U64L_{32}$ I4/m R = 0.09

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0443(10) | 0.0331(9) | 0.0370(10) | -0.0003(7) | 0.0022(7) | -0.0005(7) |
| U2 | 0.0329(9) | 0.0436(10) | 0.0373(10) | 0.0021(7) | -0.0001(7) | -0.0005(7) |
| U3 | 0.0384(13) | 0.0370(13) | 0.0348(13) | 0 | 0 | 0.0024(10) |
| U4 | 0.0363(13) | 0.0392(13) | 0.0345(13) | 0 | 0 | 0.0022(10) |
| U5 | 0.0436(14) | 0.0344(13) | 0.0497(15) | 0 | 0.0000 | -0.0004(10) |
| U6 | 0.0347(13) | 0.0438(14) | 0.0496(15) | 0 | 0.0000 | -0.0002(10) |
| U7 | 0.0391(10) | 0.0446(10) | 0.0496(11) | -0.0010(8) | -0.0055(8) | 0.0062(7) |
| U8 | 0.0451(10) | 0.0390(10) | 0.0492(11) | -0.0061(8) | -0.0008(8) | 0.0065(7) |
| U9 | 0.0432(11) | 0.0382(10) | 0.1021(15) | -0.0053(9) | -0.0031(10) | 0.0017(8) |
| U10 | 0.0384(10) | 0.0436(11) | 0.1021(15) | -0.0033(10) | -0.0044(9) | 0.0020(8) |
| P1 | 0.079(9) | 0.061(8) | 0.074(9) | -0.001(7) | -0.032(8) | -0.002(7) |
| P2 | 0.065(8) | 0.042(7) | 0.076(9) | -0.002(6) | 0.024(7) | -0.003(6) |
| P3 | 0.057(7) | 0.043(7) | 0.045(7) | -0.007(5) | 0.016(6) | -0.006(5) |
| P4 | 0.043(7) | 0.058(7) | 0.045(7) | 0.015(6) | -0.006(5) | -0.004(5) |
| P5 | 0.051(7) | 0.053(7) | 0.059(8) | 0.011(6) | 0.012(6) | 0.001(6) |
| P6 | 0.036(6) | 0.044(7) | 0.048(7) | -0.018(5) | -0.001(5) | 0.000(5) |
| P7 | 0.040(7) | 0.049(7) | 0.055(8) | -0.009(6) | -0.003(6) | 0.002(5) |
| P8 | 0.047(7) | 0.038(7) | 0.057(8) | -0.002(6) | -0.010(6) | 0.004(5) |
| K1 | 0.064(7) | 0.047(6) | 0.085(8) | -0.012(5) | 0.025(6) | 0.010(5) |
| K2 | 0.047(6) | 0.069(7) | 0.082(7) | 0.027(6) | -0.010(5) | 0.010(5) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S9 - Bond Distances (Angstrom)
for: $U64L_{32}$ I4/m R = 0.09

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O35 | 2.36(2) | U4 | -O63 | 1.75(3) |
| U1 | -O39 | 1.80(2) | U4 | -O53_c | 2.37(2) |
| U1 | -O41 | 2.42(2) | U4 | -O59_c | 2.38(2) |
| U1 | -O44 | 1.79(2) | U4 | -O62_c | 2.33(2) |
| U1 | -O51 | 2.35(2) | U5 | -O16 | 1.82(3) |
| U1 | -O55 | 2.40(2) | U5 | -O41 | 2.39(2) |
| U1 | -O57 | 2.32(2) | U5 | -O43 | 1.84(3) |
| U1 | -O61 | 2.35(2) | U5 | -O48 | 2.36(2) |
| U2 | -O33 | 2.37(2) | U5 | -O57 | 2.36(2) |
| U2 | -O37 | 2.41(2) | U5 | -O41_c | 2.39(2) |
| U2 | -O42 | 1.80(2) | U5 | -O48_c | 2.36(2) |
| U2 | -O46 | 1.80(2) | U5 | -O57_c | 2.36(2) |
| U2 | -O49 | 2.35(2) | U6 | -O19 | 1.82(3) |
| U2 | -O53 | 2.39(2) | U6 | -O37 | 2.40(2) |
| U2 | -O56 | 2.31(2) | U6 | -O47 | 1.83(3) |
| U2 | -O62 | 2.37(2) | U6 | -O50 | 2.38(3) |
| U3 | -O32 | 1.81(3) | U6 | -O56 | 2.37(2) |
| U3 | -O55 | 2.38(2) | U6 | -O37_c | 2.40(2) |
| U3 | -O60 | 2.37(2) | U6 | -O50_c | 2.38(3) |
| U3 | -O61 | 2.35(2) | U6 | -O56_c | 2.37(2) |
| U3 | -O64 | 1.76(3) | U7 | -O8 | 2.41(2) |
| U3 | -O55_c | 2.38(2) | U7 | -O24 | 2.37(2) |
| U3 | -O60_c | 2.37(2) | U7 | -O28 | 1.79(2) |
| U3 | -O61_c | 2.35(2) | U7 | -O29 | 2.36(2) |
| U4 | -O18 | 1.84(3) | U7 | -O36 | 1.79(2) |
| U4 | -O53 | 2.37(2) | U7 | -O38 | 2.39(3) |
| U4 | -O59 | 2.38(2) | U7 | -O45 | 2.36(2) |
| U4 | -O62 | 2.33(2) | U7 | -O52 | 2.41(2) |

| | | | | | |
|---|---|---|---|---|---|
| U8 | -O8 | 2.41(2) | P2 | -O12 | 1.54(4) |
| U8 | -O22 | 1.78(2) | P2 | -O31 | 1.50(3) |
| U8 | -O23 | 2.38(2) | P2 | -C1 | 1.80(7) |
| U8 | -O26 | 2.37(2) | P2 | -O30_b | 1.51(3) |
| U8 | -O34 | 1.78(2) | P3 | -O23 | 1.52(3) |
| U8 | -O40 | 2.38(3) | P3 | -O51 | 1.51(3) |
| U8 | -O45 | 2.32(2) | P3 | -O65 | 1.52(3) |
| U8 | -O54 | 2.41(2) | P3 | -C5 | 1.85(4) |
| U9 | -O1 | 1.74(2) | P4 | -O21 | 1.52(3) |
| U9 | -O4 | 2.42(3) | P4 | -O24 | 1.53(3) |
| U9 | -O5 | 1.79(3) | P4 | -O49 | 1.52(3) |
| U9 | -O10 | 2.39(3) | P4 | -C4 | 1.85(4) |
| U9 | -O29 | 2.33(2) | P5 | -O7 | 1.58(4) |
| U9 | -O31 | 2.35(3) | P5 | -O48 | 1.53(3) |
| U9 | -O38 | 2.36(3) | P5 | -O50 | 1.51(3) |
| U9 | -O58 | 2.32(3) | P5 | -C2 | 1.75(3) |
| U10 | -O4 | 2.41(3) | P6 | -O15 | 1.49(3) |
| U10 | -O6 | 1.78(3) | P6 | -O60 | 1.51(3) |
| U10 | -O11 | 2.39(3) | P6 | -C3 | 1.77(3) |
| U10 | -O20 | 1.74(2) | P6 | -O59_a | 1.51(3) |
| U10 | -O26 | 2.33(2) | P7 | -O13 | 1.52(3) |
| U10 | -O30 | 2.35(3) | P7 | -O33 | 1.51(3) |
| U10 | -O40 | 2.38(3) | P7 | -O52 | 1.53(3) |
| U10 | -O58 | 2.33(3) | P7 | -C4 | 1.84(4) |
| P1 | -O10 | 1.47(4) | P8 | -O14 | 1.51(3) |
| P1 | -O27 | 1.53(5) | P8 | -O35 | 1.51(3) |
| P1 | -C1 | 1.84(7) | P8 | -O54 | 1.53(3) |
| P1 | -O11_b | 1.47(4) | P8 | -C5 | 1.86(4) |
| O2 | -C1 | 1.67(10) | O37 | -O56 | 1.47(3) |
| O3 | -C3 | 1.59(8) | O41 | -O57 | 1.47(3) |

| | | | | | |
|---|---|---|---|---|---|
| O4 | -O58 | 1.46(4) | O53 | -O62 | 1.41(3) |
| O8 | -O45 | 1.58(3) | O55 | -O61 | 1.43(3) |
| O9 | -C2 | 1.59(8) | C1 | -C10 | 1.66(10) |
| O17 | -C4 | 1.47(5) | C2 | -C8 | 1.56(9) |
| O25 | -C5 | 1.46(5) | C3 | -C7 | 1.58(8) |
| O26 | -O40 | 1.46(4) | C4 | -C6 | 1.56(6) |
| O29 | -O38 | 1.45(4) | C5 | -C9 | 1.58(6) |

Table S10 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: $U16L_8$ Immm R = 0.05

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0 | 0.38972(2) | 0.07873(2) | 0.0106(2) |
| U2 | 0.13557(3) | 1/2 | 0.07958(2) | 0.0108(2) |
| U3 | 0.09595(2) | 0.42185(2) | 0.42128(1) | 0.0107(1) |
| U4 | 0 | 0.32202(2) | 0.21826(2) | 0.0126(2) |
| U5 | 0.20548(3) | 1/2 | 0.21788(2) | 0.0135(2) |
| U6 | 0.14686(2) | 0.37590(2) | 0.28320(1) | 0.0131(2) |
| P1 | 0.25335(15) | 0.44351(12) | 0.13550(8) | 0.0137(9) |
| P2 | 0.13874(16) | 0.31276(12) | 0.36769(8) | 0.0151(9) |
| P3 | 0.22886(15) | 0.39893(12) | 0.36549(8) | 0.0131(9) |
| P4 | 0.06968(15) | 0.29149(12) | 0.13331(8) | 0.0131(9) |
| O1 | 0.1052(4) | 0.4155(3) | 0.0684(2) | 0.0178(19) |
| O2 | 0.1445(6) | 1/2 | 0.4319(3) | 0.016(3) |
| O3 | 0.0649(4) | 0.3157(3) | 0.1697(2) | 0.0185(19) |
| O4 | 0.1142(4) | 0.3318(3) | 0.3324(2) | 0.021(2) |
| O5 | 0.1224(7) | 1/2 | 0.2141(3) | 0.025(3) |
| O6 | 0.1275(4) | 0.3981(3) | 0.4611(2) | 0.0157(18) |
| O7 | 0.2153(4) | 0.4475(3) | 0.1693(2) | 0.0173(19) |
| O8 | 0.2084(4) | 0.4450(4) | 0.2662(2) | 0.022(2) |
| O9 | 0.1792(6) | 1/2 | 0.0395(3) | 0.015(3) |
| O10 | 0.1054(4) | 0.3397(3) | 0.3971(2) | 0.0165(18) |
| O11 | 0.0848(5) | 0.4199(4) | 0.2869(3) | 0.026(2) |
| O12 | 0.0622(4) | 0.4505(3) | 0.0508(2) | 0.0140(18) |
| O13 | 0.1957(4) | 0.4130(3) | 0.3316(2) | 0.0160(18) |
| O14 | 0 | 0.3532(5) | 0.0394(3) | 0.019(3) |
| O15 | 0.0843(6) | 1/2 | 0.4486(3) | 0.016(3) |
| O16 | 0.1946(4) | 0.4152(4) | 0.2344(2) | 0.022(2) |
| O17 | 0.0684(4) | 0.3319(3) | 0.1053(2) | 0.0189(19) |

| | | | | |
|---|---|---|---|---|
| O18 | 0.1044(4) | 0.3319(3) | 0.2352(2) | 0.019(2) |
| O19 | 0.2109(4) | 0.4440(3) | 0.1039(2) | 0.0178(19) |
| O20 | 0 | 0.3784(5) | 0.4312(3) | 0.014(3) |
| O21 | 0.1979(4) | 0.4223(3) | 0.3968(2) | 0.0158(19) |
| O22 | 0 | 0.2544(5) | 0.2200(3) | 0.018(3) |
| O23 | 0 | 0.4272(4) | 0.4489(3) | 0.015(3) |
| O24 | 0 | 0.3893(5) | 0.2151(3) | 0.018(3) |
| O25 | 0.0690(4) | 0.3191(3) | 0.2666(2) | 0.022(2) |
| O26 | 0.0670(4) | 0.4432(3) | 0.3796(2) | 0.0145(18) |
| O27 | 0.2889(6) | 1/2 | 0.2210(3) | 0.017(3) |
| O28 | 0.0964(6) | 1/2 | 0.1210(3) | 0.016(3) |
| O29 | 0.2098(4) | 0.3313(3) | 0.2812(2) | 0.0182(19) |
| O30 | 0 | 0.4237(5) | 0.1190(3) | 0.017(3) |
| O31 | 0.1352(5) | 0.2561(4) | 0.3700(3) | 0.027(2) |
| O32 | 0.2951(4) | 0.3980(3) | 0.1362(2) | 0.021(2) |
| O33 | 0.2964(4) | 0.4117(3) | 0.3639(2) | 0.0186(19) |
| O34 | 0.1251(4) | 0.2578(4) | 0.1293(2) | 0.022(2) |
| O35 | 0 | 0.2126(5) | 0.1519(3) | 0.019(3) |
| O36 | 0.2570(4) | 0.3052(3) | 0.3450(2) | 0.0182(19) |
| O37 | 0.3495(6) | 1/2 | 0.1585(3) | 0.020(3) |
| C1 | 0 | 0.2538(7) | 0.1267(5) | 0.019(4) |
| C2 | 0.2214(6) | 0.3313(5) | 0.3718(3) | 0.014(3) |
| C3 | 0 | 0.2316(7) | 0.0904(5) | 0.022(4) |
| C4 | 0.2454(6) | 0.3156(5) | 0.4070(3) | 0.020(3) |
| C5 | 0.3019(9) | 1/2 | 0.1313(5) | 0.018(4) |
| C6 | 0.3357(10) | 1/2 | 0.0963(5) | 0.025(4) |
| O38 | 0.3265(6) | 0.4286(5) | 0.2939(3) | 0.042(3) |
| O39 | 0 | 0.1605(7) | 0.2511(5) | 0.049(5) |
| O40 | 0.2758(7) | 0.4415(6) | 0.4521(4) | 0.061(4) |
| O41 | 0.2961(7) | 0.3657(5) | 0.2081(4) | 0.056(4) |
| O42 | 0.2454(10) | 0.3857(8) | 0.0467(5) | 0.095(6) |

| | | | | |
|---|---|---|---|---|
| O43 | 0.4006(9) | 0.2735(7) | 0.2040(5) | 0.089(6) |
| O44 | 0.3451(11) | 1/2 | 0.3893(6) | 0.075(7) |
| O45 | 0.2599(7) | 0.3022(6) | 0.1273(4) | 0.064(4) |
| O46 | 0.3923(7) | 0.3491(6) | 0.3722(4) | 0.059(4) |
| O47 | 0 | 1/2 | 0.3245(5) | 0.020(4) |
| O48 | 0.1716(4) | 0.3049(4) | 0.0674(2) | 0.022(2) |
| O49 | 0 | 1/2 | 0.1769(5) | 0.017(4) |
| O50 | 0.2912(4) | 0.2758(3) | 0.2388(2) | 0.0120(17) |
| *O51 | 1/2 | 0.3993(14) | 0.3587(9) | 0.046(9) |
| *O52 | 0.1998(10) | 0.2821(9) | 0.1998(6) | 0.036(5) |
| K1 | 0 | 1/2 | 1/2 | 0.014(2) |
| K2 | 0 | 1/2 | 0 | 0.017(2) |
| K3 | 0.1339(2) | 1/2 | 0.33227(11) | 0.0221(11) |
| K4 | 0.1482(3) | 0.4102(2) | 0 | 0.0447(19) |
| K5 | 0.09736(16) | 0.41495(13) | 0.16481(10) | 0.0359(11) |
| K6 | 0 | 0.3481(4) | 1/2 | 0.139(10) |
| K7 | 0 | 0.3710(3) | 0.34112(18) | 0.059(2) |
| K8 | 0 | 1/2 | 0.2519(2) | 0.065(4) |
| *K9 | 0.1846(5) | 1/2 | 1/2 | 0.070(5) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S11 - (An)isotropic Displacement Parameters
for: $U16L_8$ Immm R = 0.05

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0106(3) | 0.0102(3) | 0.0109(3) | -0.0004(2) | 0 | 0 |
| U2 | 0.0104(3) | 0.0115(3) | 0.0106(3) | 0 | 0.0010(2) | 0 |
| U3 | 0.0103(2) | 0.0113(2) | 0.0105(2) | 0.0004(2) | -0.0002(2) | 0.0005(2) |
| U4 | 0.0133(3) | 0.0111(3) | 0.0134(3) | -0.0009(2) | 0 | 0 |
| U5 | 0.0132(3) | 0.0138(3) | 0.0136(3) | 0 | 0.0007(2) | 0 |
| U6 | 0.0134(3) | 0.0137(3) | 0.0121(2) | -0.0009(2) | -0.0007(2) | 0.0022(2) |
| P1 | 0.0126(16) | 0.0124(15) | 0.0160(16) | -0.0007(12) | -0.0003(12) | 0.0007(13) |
| P2 | 0.0184(17) | 0.0118(16) | 0.0151(16) | -0.0008(12) | 0.0015(13) | -0.0014(13) |
| P3 | 0.0124(16) | 0.0128(16) | 0.0141(15) | -0.0012(12) | -0.0006(12) | 0.0015(12) |
| P4 | 0.0117(15) | 0.0123(15) | 0.0152(15) | -0.0003(12) | -0.0003(12) | 0.0027(12) |
| K1 | 0.015(4) | 0.015(4) | 0.013(4) | 0 | 0 | 0 |
| K2 | 0.018(4) | 0.019(4) | 0.014(4) | 0 | 0 | 0 |
| K3 | 0.023(2) | 0.0133(19) | 0.030(2) | 0 | 0.0074(18) | 0 |
| K4 | 0.053(4) | 0.054(3) | 0.027(3) | 0 | 0 | 0.017(3) |
| K5 | 0.0279(18) | 0.0357(19) | 0.044(2) | 0.0188(16) | -0.0178(15) | -0.0173(15) |
| K6 | 0.37(3) | 0.030(5) | 0.016(4) | 0 | 0 | 0 |
| K7 | 0.014(2) | 0.096(5) | 0.068(4) | -0.047(4) | 0 | 0 |
| K8 | 0.040(5) | 0.124(9) | 0.031(4) | 0 | 0 | 0 |
| K9 | 0.036(6) | 0.154(14) | 0.019(5) | 0 | 0 | 0 |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S12 - Bond Distances (Angstrom)
for: $U16L_8$ Immm R = 0.05

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O1 | 2.412(9) | U4 | -O25 | 2.385(8) |
| U1 | -O12 | 2.365(8) | U4 | -O3_a | 2.341(8) |
| U1 | -O14 | 1.798(12) | U4 | -O18_a | 2.367(9) |
| U1 | -O17 | 2.370(8) | U4 | -O25_a | 2.385(8) |
| U1 | -O30 | 1.793(12) | U5 | -O5 | 1.804(15) |
| U1 | -O1_a | 2.412(9) | U5 | -O7 | 2.343(8) |
| U1 | -O12_a | 2.365(8) | U5 | -O8 | 2.367(9) |
| U1 | -O17_a | 2.370(8) | U5 | -O16 | 2.362(10) |
| U2 | -O1 | 2.388(8) | U5 | -O27 | 1.810(13) |
| U2 | -O9 | 1.806(12) | U5 | -O7_b | 2.343(8) |
| U2 | -O12 | 2.343(8) | U5 | -O8_b | 2.367(9) |
| U2 | -O19 | 2.401(8) | U5 | -O16_b | 2.362(10) |
| U2 | -O28 | 1.803(12) | U6 | -O4 | 2.336(8) |
| U2 | -O1_b | 2.388(8) | U6 | -O8 | 2.367(10) |
| U2 | -O12_b | 2.343(8) | U6 | -O11 | 1.790(11) |
| U2 | -O19_b | 2.401(8) | U6 | -O13 | 2.357(8) |
| U3 | -O2 | 2.371(6) | U6 | -O16 | 2.384(9) |
| U3 | -O6 | 1.791(8) | U6 | -O18 | 2.371(8) |
| U3 | -O10 | 2.390(8) | U6 | -O25 | 2.355(8) |
| U3 | -O15 | 2.348(5) | U6 | -O29 | 1.811(8) |
| U3 | -O20 | 2.409(7) | P1 | -O7 | 1.541(9) |
| U3 | -O21 | 2.399(9) | P1 | -O19 | 1.523(9) |
| U3 | -O23 | 2.337(5) | P1 | -O32 | 1.514(9) |
| U3 | -O26 | 1.812(8) | P1 | -C5 | 1.845(12) |
| U4 | -O3 | 2.341(8) | P2 | -O4 | 1.542(8) |
| U4 | -O18 | 2.367(9) | P2 | -O10 | 1.521(9) |
| U4 | -O22 | 1.806(13) | P2 | -O31 | 1.516(11) |
| U4 | -O24 | 1.799(13) | P2 | -C2 | 1.863(13) |

| | | | | | |
|---|---|---|---|---|---|
| P3 | -O13 | 1.533(9) | O8 | -O16 | 1.488(12) |
| P3 | -O21 | 1.512(9) | O18 | -O25 | 1.469(11) |
| P3 | -O33 | 1.502(9) | O20 | -O23 | 1.469(17) |
| P3 | -C2 | 1.828(14) | O35 | -C1 | 1.47(2) |
| P4 | -O3 | 1.543(8) | O36 | -C2 | 1.463(15) |
| P4 | -O17 | 1.524(8) | O37 | -C5 | 1.47(2) |
| P4 | -O34 | 1.507(10) | C1 | -C3 | 1.52(3) |
| P4 | -C1 | 1.831(11) | C2 | -C4 | 1.508(17) |
| O1 | -O12 | 1.482(12) | C5 | -C6 | 1.53(3) |
| O2 | -O15 | 1.453(18) | | | |

Table S13 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: $U20L_{10}$ Pmna R = 0.08

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0.10675(3) | 0.32007(6) | 0.43861(6) | 0.0278(4) |
| U2 | 0 | 0.36139(8) | 0.55676(8) | 0.0284(5) |
| U3 | 0.10912(3) | -0.02124(6) | 0.28034(6) | 0.0351(4) |
| U4 | 0 | 0.15224(9) | 0.72635(9) | 0.0364(6) |
| U5 | 0.17427(4) | 0.09158(6) | 0.55033(6) | 0.0383(4) |
| U6 | 0.06563(3) | 0.24384(6) | 0.25170(6) | 0.0276(3) |
| P1 | 0.0471(2) | 0.3151(4) | 0.7135(4) | 0.036(3) |
| P2 | 0.0863(2) | 0.1002(4) | 0.1545(4) | 0.033(3) |
| P3 | 0.1803(2) | 0.2693(4) | 0.5640(4) | 0.034(3) |
| P4 | 0.2040(2) | 0.2189(4) | 0.4319(4) | 0.032(3) |
| P5 | 0.1598(2) | 0.1356(4) | 0.2379(4) | 0.028(3) |
| O1 | 0.1210(7) | 0.0796(10) | 0.5200(10) | 0.044(6) |
| O2 | 0.2271(6) | 0.1067(10) | 0.5771(10) | 0.039(5) |
| O3 | 0.1662(7) | -0.0365(11) | 0.3497(11) | 0.048(6) |
| O4 | 0.1462(8) | -0.1012(12) | 0.3441(12) | 0.064(7) |
| O5 | 0 | 0.4487(15) | 0.5676(15) | 0.044(8) |
| O6 | 0 | 0.1727(14) | 0.8133(14) | 0.037(7) |
| O7 | 0.0437(7) | 0.2410(10) | 0.7024(10) | 0.041(5) |
| O8 | 0.1988(8) | 0.2948(12) | 0.6274(12) | 0.055(6) |
| O9 | 0.1383(7) | -0.0475(10) | 0.2119(10) | 0.044(6) |
| O10 | 0.0761(6) | 0.0555(10) | 0.2116(10) | 0.038(5) |
| O11 | 0.0439(6) | 0.3748(9) | 0.4653(9) | 0.034(5) |
| O12 | 0.0710(8) | 0.1174(12) | 0.7291(12) | 0.057(7) |
| O13 | -0.0447(7) | 0.0669(11) | 0.7591(11) | 0.050(6) |
| O14 | 0.0802(8) | 0.0079(12) | 0.3504(12) | 0.058(7) |
| O15 | 0.1077(6) | 0.2951(9) | 0.3291(9) | 0.031(5) |
| O16 | 0.1905(6) | 0.1516(10) | 0.4541(10) | 0.037(5) |

| | | | | |
|---|---|---|---|---|
| O17 | 0.1949(7) | 0.0161(10) | 0.4702(10) | 0.044(6) |
| O18 | 0.0848(6) | 0.3034(10) | 0.1942(10) | 0.037(5) |
| O19 | 0.1309(6) | 0.3972(9) | 0.4196(9) | 0.033(5) |
| O20 | 0.0742(7) | 0.0698(11) | 0.0898(11) | 0.045(6) |
| O21 | 0.1515(6) | 0.0746(10) | 0.2799(10) | 0.036(5) |
| O22 | 0.0482(6) | 0.1823(9) | 0.3087(9) | 0.030(5) |
| O23 | 0.1495(6) | 0.3170(9) | 0.5344(9) | 0.034(5) |
| O24 | 0.1660(6) | 0.2580(9) | 0.4081(9) | 0.031(5) |
| O25 | 0.0450(6) | 0.3508(9) | 0.6483(9) | 0.034(5) |
| O26 | 0.2380(6) | 0.2163(10) | 0.3803(10) | 0.037(5) |
| O27 | 0.0857(7) | 0.3325(10) | 0.7532(11) | 0.046(6) |
| O28 | 0.1600(7) | 0.2015(11) | 0.5706(11) | 0.047(6) |
| O29 | 0.2053(6) | 0.1544(9) | 0.2389(9) | 0.030(5) |
| O30 | 0 | 0.1204(13) | 0.6476(13) | 0.030(7) |
| O31 | 0.0663(6) | 0.1671(9) | 0.1651(9) | 0.029(5) |
| O32 | 0.0826(6) | 0.2432(9) | 0.4575(9) | 0.033(5) |
| O33 | 0.1321(6) | 0.1923(8) | 0.2584(9) | 0.026(4) |
| O34 | 0.0701(6) | 0.3693(9) | 0.5237(9) | 0.030(5) |
| O35 | 0 | 0.2444(13) | 0.1999(13) | 0.029(7) |
| O36 | 0.0657(6) | 0.3234(9) | 0.3393(9) | 0.031(5) |
| O37 | 0 | 0.2953(13) | 0.2538(13) | 0.033(7) |
| O38 | 0 | 0.2734(14) | 0.5505(14) | 0.037(7) |
| O39 | 0.1664(7) | 0.0592(10) | 0.1312(10) | 0.042(5) |
| O40 | 0.2583(7) | 0.2259(10) | 0.5323(10) | 0.045(6) |
| O41 | 0 | 0.3147(14) | 0.8234(14) | 0.039(7) |
| C1 | 0.2233(9) | 0.2631(14) | 0.5041(14) | 0.029(7) |
| C2 | 0.1424(9) | 0.1146(14) | 0.1545(14) | 0.031(7) |
| C3 | 0 | 0.342(2) | 0.757(3) | 0.052(13) |
| C4 | 0.2388(9) | 0.3306(14) | 0.4860(14) | 0.032(7) |
| C5 | 0.1534(11) | 0.1735(17) | 0.1027(17) | 0.048(9) |
| C6 | 0 | 0.421(3) | 0.762(3) | 0.067(16) |

| | | | | |
|---|---|---|---|---|
| *O42 | 0.2347(10) | 0.0630(15) | 0.3451(15) | 0.013(7) |
| *O43 | 0 | 0.108(4) | 0.459(4) | 0.07(2) |
| *O44 | 0 | 0.098(3) | 0.031(3) | 0.031(13) |
| *O45 | 0.3407(11) | 0.2536(17) | 0.5600(17) | 0.027(9) |
| *O46 | 0.1983(12) | 0.1947(19) | 0.7160(19) | 0.034(10) |
| *O47 | 0.1632(11) | 0.4511(17) | 0.5562(17) | 0.026(9) |
| *O48 | 0.0885(10) | 0.4702(16) | 0.6431(16) | 0.018(8) |
| *O49 | 0.0521(11) | -0.0635(16) | 0.1056(16) | 0.020(8) |
| *O50 | 0.0463(13) | 0.249(2) | 0.063(2) | 0.038(10) |
| *O51 | 0.2245(14) | 0.060(2) | 0.042(2) | 0.047(12) |
| *O52 | 0 | 0.370(4) | 0.128(4) | 0.07(2) |
| *O53 | 0.0465(13) | 0.438(2) | 0.285(2) | 0.041(11) |
| *O54 | 0.1224(19) | 0 | 0 | 0.045(16) |
| *O55 | 0.2336(14) | 0.346(2) | 0.178(2) | 0.045(11) |
| *O56 | 0.1134(13) | 0.211(2) | 0.813(2) | 0.041(11) |
| *O57 | 0.062(2) | 0 | 1/2 | 0.053(18) |
| *O58 | 0.2937(10) | 0.3041(15) | 0.3457(15) | 0.014(8) |
| K1 | 0.0721(3) | 0.1948(5) | 0.5837(4) | 0.068(4) |
| K2 | 0.1871(2) | 0.2954(4) | 0.2830(4) | 0.054(3) |
| K3 | 0 | 0.0679(6) | 0.2821(7) | 0.060(5) |
| K4 | 0.0777(3) | 1/2 | 1/2 | 0.051(4) |
| K5 | 0 | 0.2439(6) | 0.4101(5) | 0.047(4) |
| K6 | 0.11205(19) | 0.1339(3) | 0.3910(3) | 0.035(2) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S14 - (An)isotropic Displacement Parameters
for: $U20L_{10}$ Pmna R = 0.08

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0095(5) | 0.0358(7) | 0.0381(7) | -0.0002(5) | 0.0000(5) | -0.0003(5) |
| U2 | 0.0129(7) | 0.0327(9) | 0.0395(10) | -0.0011(8) | 0 | 0 |
| U3 | 0.0227(6) | 0.0399(7) | 0.0428(7) | 0.0020(6) | -0.0010(5) | -0.0078(5) |
| U4 | 0.0297(9) | 0.0392(10) | 0.0402(10) | -0.0026(8) | 0 | 0 |
| U5 | 0.0232(6) | 0.0473(8) | 0.0443(8) | 0.0111(6) | 0.0022(5) | 0.0061(5) |
| U6 | 0.0071(5) | 0.0410(7) | 0.0347(6) | 0.0049(6) | 0.0000(5) | 0.0003(5) |
| P1 | 0.024(4) | 0.041(5) | 0.042(5) | 0.003(4) | -0.005(4) | 0.000(4) |
| P2 | 0.017(4) | 0.051(5) | 0.032(5) | -0.007(4) | -0.002(3) | -0.002(4) |
| P3 | 0.022(4) | 0.046(5) | 0.035(5) | -0.001(4) | -0.003(4) | 0.003(4) |
| P4 | 0.011(4) | 0.049(5) | 0.036(5) | 0.002(4) | -0.003(3) | 0.000(3) |
| P5 | 0.005(3) | 0.042(5) | 0.036(5) | 0.000(4) | 0.003(3) | -0.003(3) |
| K1 | 0.043(5) | 0.115(8) | 0.046(5) | 0.020(5) | 0.017(4) | 0.033(5) |
| K2 | 0.038(4) | 0.067(5) | 0.056(5) | 0.002(4) | 0.008(4) | -0.002(4) |
| K3 | 0.013(5) | 0.069(8) | 0.097(10) | -0.011(7) | 0 | 0 |
| K4 | 0.036(6) | 0.033(6) | 0.083(9) | 0.007(6) | 0 | 0 |
| K5 | 0.010(5) | 0.086(8) | 0.044(6) | -0.020(6) | 0 | 0 |
| K6 | 0.021(3) | 0.047(4) | 0.036(4) | 0.004(3) | -0.001(3) | 0.002(3) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S15 - Bond Distances (Angstrom)
for: $U20L_{10}$ Pmna R = 0.08

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O11 | 2.362(19) | U4 | -O30 | 1.74(3) |
| U1 | -O15 | 2.294(18) | U4 | -O7_c | 2.34(2) |
| U1 | -O19 | 1.796(19) | U4 | -O12_c | 2.38(3) |
| U1 | -O23 | 2.387(19) | U4 | -O13_c | 2.35(2) |
| U1 | -O24 | 2.362(19) | U5 | -O1 | 1.83(2) |
| U1 | -O32 | 1.791(19) | U5 | -O2 | 1.801(19) |
| U1 | -O34 | 2.324(19) | U5 | -O16 | 2.37(2) |
| U1 | -O36 | 2.416(19) | U5 | -O17 | 2.34(2) |
| U2 | -O5 | 1.80(3) | U5 | -O28 | 2.33(2) |
| U2 | -O11 | 2.352(19) | U5 | -O3_a | 2.35(2) |
| U2 | -O25 | 2.368(19) | U5 | -O4_a | 2.34(2) |
| U2 | -O34 | 2.345(19) | U5 | -O17_a | 2.33(2) |
| U2 | -O38 | 1.80(3) | U6 | -O15 | 2.324(19) |
| U2 | -O11_c | 2.352(19) | U6 | -O18 | 1.80(2) |
| U2 | -O25_c | 2.368(19) | U6 | -O22 | 1.801(18) |
| U2 | -O34_c | 2.345(19) | U6 | -O31 | 2.363(18) |
| U3 | -O3 | 2.33(2) | U6 | -O33 | 2.375(19) |
| U3 | -O4 | 2.40(2) | U6 | -O35 | 2.349(12) |
| U3 | -O9 | 1.76(2) | U6 | -O36 | 2.417(18) |
| U3 | -O10 | 2.35(2) | U6 | -O37 | 2.346(12) |
| U3 | -O14 | 1.80(2) | P1 | -O7 | 1.53(2) |
| U3 | -O21 | 2.38(2) | P1 | -O25 | 1.52(2) |
| U3 | -O12_a | 2.32(2) | P1 | -O27 | 1.52(2) |
| U3 | -O13_b | 2.40(2) | P1 | -C3 | 1.83(3) |
| U4 | -O6 | 1.82(3) | P2 | -O10 | 1.52(2) |
| U4 | -O7 | 2.34(2) | P2 | -O20 | 1.51(2) |
| U4 | -O12 | 2.38(3) | P2 | -O31 | 1.52(2) |
| U4 | -O13 | 2.35(2) | P2 | -C2 | 1.82(3) |

| | | | | | |
|---|---|---|---|---|---|
| P3 | -O8 | 1.52(3) | O3 | -O4 | 1.47(3) |
| P3 | -O23 | 1.51(2) | O11 | -O34 | 1.46(3) |
| P3 | -O28 | 1.54(2) | O12 | -O13_c | 1.47(3) |
| P3 | -C1 | 1.84(3) | O15 | -O36 | 1.48(3) |
| P4 | -O16 | 1.51(2) | O17 | -O17_a | 1.38(3) |
| P4 | -O24 | 1.53(2) | O35 | -O37 | 1.51(4) |
| P4 | -O26 | 1.51(2) | O39 | -C2 | 1.45(4) |
| P4 | -C1 | 1.84(3) | O40 | -C1 | 1.47(4) |
| P5 | -O21 | 1.54(2) | O41 | -C3 | 1.47(7) |
| P5 | -O29 | 1.50(2) | C1 | -C4 | 1.51(4) |
| P5 | -O33 | 1.516(19) | C2 | -C5 | 1.64(5) |
| P5 | -C2 | 1.84(3) | C3 | -C6 | 1.62(7) |

Table S16 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: $U16L_8P_4$ P1 R = 0.05

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| U1 | 0.70383(8) | 0.48799(8) | 0.85083(8) | 0.0127(4) |
| U2 | 0.51788(8) | 0.24655(8) | 0.75411(8) | 0.0138(4) |
| U3 | 0.56043(8) | 0.61424(8) | 0.56965(8) | 0.0140(4) |
| U4 | 0.66845(8) | 0.50964(9) | 1.05180(8) | 0.0156(4) |
| U5 | 0.06479(8) | 0.42755(9) | 0.50566(8) | 0.0144(4) |
| U6 | 0.02946(8) | 0.44953(9) | 0.70575(8) | 0.0139(4) |
| U7 | 0.21562(9) | 0.69101(8) | 0.80299(8) | 0.0137(4) |
| U8 | 0.45001(8) | 0.66946(9) | 1.12262(8) | 0.0146(4) |
| U9 | 0.28405(9) | 0.26819(9) | 0.43488(8) | 0.0142(4) |
| U10 | 0.17292(9) | 0.32293(9) | 0.98774(8) | 0.0139(4) |
| U11 | 0.25321(9) | 0.66643(9) | 0.60189(8) | 0.0166(4) |
| U12 | 0.47988(9) | 0.27080(9) | 0.95483(8) | 0.0158(4) |
| U13 | 0.60032(9) | 0.82376(9) | 1.05995(8) | 0.0163(4) |
| U14 | 0.64448(9) | 0.78175(9) | 0.76779(9) | 0.0190(5) |
| U15 | 0.13319(9) | 0.11371(9) | 0.49733(9) | 0.0171(5) |
| U16 | 0.08886(10) | 0.15561(9) | 0.78897(9) | 0.0196(5) |
| P1 | 0.7294(5) | 0.5626(6) | 0.6933(6) | 0.014(3) |
| P2 | 0.1063(6) | 0.3263(7) | 0.3587(6) | 0.018(3) |
| P3 | 0.0038(7) | 0.3748(6) | 0.8644(6) | 0.015(3) |
| P4 | 0.6248(7) | 0.6078(6) | 1.1988(6) | 0.015(3) |
| P5 | 0.4421(6) | 0.1951(6) | 0.5374(6) | 0.016(3) |
| P6 | 0.2911(6) | 0.7437(7) | 1.0167(6) | 0.016(3) |
| P7 | -0.0112(7) | 0.2110(7) | 0.4110(6) | 0.020(3) |
| P8 | 0.2695(7) | 0.1146(7) | 0.9001(6) | 0.018(3) |
| P9 | 0.3262(7) | 0.0763(7) | 0.5900(6) | 0.019(3) |
| P10 | 0.3431(6) | 0.2517(6) | 1.0558(6) | 0.014(2) |
| P11 | 0.2635(6) | 0.5215(6) | 1.1337(5) | 0.016(3) |

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|---|---|---|---|---|
| P12 | 0.4073(6) | 0.8597(6) | 0.9634(6) | 0.014(3) |
| P13 | 0.3898(7) | 0.6868(7) | 0.5021(6) | 0.020(2) |
| P14 | 0.7450(7) | 0.7280(7) | 1.1471(7) | 0.020(3) |
| P15 | -0.0626(6) | 0.2411(7) | 0.7082(6) | 0.019(3) |
| P16 | 0.4698(6) | 0.4167(6) | 0.4251(6) | 0.015(3) |
| P17 | 0.4641(6) | 0.8242(6) | 0.6517(6) | 0.016(3) |
| P18 | 0.8001(6) | 0.6958(7) | 0.8472(6) | 0.016(3) |
| P19 | 0.0358(8) | 0.0103(8) | 0.6083(8) | 0.044(3) |
| P20 | 0.6952(9) | 0.9263(7) | 0.9469(7) | 0.037(3) |
| O1 | 0.5416(16) | 0.7266(16) | 0.6295(15) | 0.0212(2) |
| O2 | 0.2424(14) | 0.3943(14) | 0.9553(14) | 0.0212(2) |
| O3 | 0.1905(17) | 0.2099(17) | 0.9255(16) | 0.0212(2) |
| O4 | 0.0535(15) | 0.4308(16) | 0.8290(14) | 0.0212(2) |
| O5 | 0.1331(12) | 0.3918(13) | 0.4340(12) | 0.0212(2) |
| O6 | 0.4961(14) | 0.5473(15) | 0.5992(14) | 0.0212(2) |
| O7 | 0.4145(12) | 0.5949(14) | 1.0311(14) | 0.0212(2) |
| O8 | 0.6793(16) | 0.5067(16) | 0.7236(14) | 0.0212(2) |
| O9 | 0.0599(16) | 0.2577(16) | 0.8504(15) | 0.0212(2) |
| O10 | 0.0928(16) | 0.5801(15) | 0.7973(15) | 0.0212(2) |
| O11 | 0.5558(14) | 0.7485(13) | 0.9731(13) | 0.0212(2) |
| O12 | 0.5369(15) | 0.6059(15) | 1.1963(15) | 0.0212(2) |
| O13 | 0.1947(16) | 0.3346(16) | 0.3589(15) | 0.0212(2) |
| O14 | 0.6112(12) | 0.5468(14) | 1.1310(12) | 0.0212(2) |
| O15 | 0.4349(13) | 0.6310(14) | 0.4829(13) | 0.0212(2) |
| O16 | 0.6579(15) | 0.3456(15) | 0.8381(15) | 0.0212(2) |
| O17 | 0.1837(14) | 0.1984(13) | 0.5902(13) | 0.0212(2) |
| O18 | 0.5054(14) | 0.8917(14) | 0.9895(14) | 0.0212(2) |
| O19 | 0.8089(13) | 0.5447(13) | 0.7009(13) | 0.0212(2) |
| O20 | -0.0832(14) | 0.3838(13) | 0.8521(14) | 0.0212(2) |
| O21 | 0.2716(13) | 0.7492(14) | 0.7249(11) | 0.0212(2) |
| O22 | 0.1450(16) | 0.2175(16) | 0.4282(16) | 0.0212(2) |

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|---|---|---|---|---|
| O23 | 0.4583(15) | 0.7712(15) | 1.0605(14) | 0.0212(2) |
| O24 | 0.5904(17) | 0.7214(17) | 1.1304(16) | 0.0212(2) |
| O25 | 0.1727(12) | 0.6887(13) | 0.6701(13) | 0.0212(2) |
| O26 | 0.3280(13) | 0.3417(14) | 0.5269(14) | 0.0212(2) |
| O27 | 0.0751(16) | 0.5866(15) | 0.7170(15) | 0.0212(2) |
| O28 | 0.6296(14) | 0.3736(12) | 1.0223(14) | 0.0212(2) |
| O29 | -0.0122(15) | 0.3078(13) | 0.6884(14) | 0.0212(2) |
| O30 | 0.6719(16) | 0.6774(16) | 0.7050(16) | 0.0212(2) |
| O31 | 0.3316(12) | 0.1702(14) | 0.8828(12) | 0.0212(2) |
| O32 | 0.1565(11) | 0.5529(12) | 0.4955(12) | 0.0212(2) |
| O33 | 0.4346(13) | 0.3355(14) | 0.9002(13) | 0.0212(2) |
| O34 | 0.4285(11) | 0.8845(12) | 0.6183(11) | 0.0212(2) |
| O35 | 0.0086(13) | 0.4704(14) | 0.5853(13) | 0.0212(2) |
| O36 | 0.2223(14) | 0.0490(15) | 0.5642(14) | 0.0212(2) |
| O37 | 0.2719(15) | 0.1625(15) | 0.4986(15) | 0.0212(2) |
| O38 | -0.0222(15) | 0.3783(15) | 0.5693(15) | 0.0212(2) |
| O39 | 0.3776(13) | 0.9303(14) | 0.9663(12) | 0.0212(2) |
| O40 | 0.6677(16) | 0.5529(15) | 0.6080(15) | 0.0212(2) |
| O41 | 0.5509(12) | 0.2510(14) | 0.8835(13) | 0.0212(2) |
| O42 | 0.4673(14) | 0.1889(14) | 0.8420(11) | 0.0212(2) |
| O43 | 0.1094(14) | 0.5734(13) | 0.5358(14) | 0.0212(2) |
| O44 | 0.2921(13) | 0.6014(15) | 0.6604(13) | 0.0212(2) |
| O45 | 0.4611(15) | 0.3149(15) | 0.7482(14) | 0.0212(2) |
| O46 | 0.3072(13) | 0.3118(15) | 1.0795(14) | 0.0212(2) |
| O47 | 0.7521(16) | 0.5547(16) | 0.9848(15) | 0.0212(2) |
| O48 | 0.2682(15) | 0.6193(16) | 0.8034(14) | 0.0212(2) |
| O49 | 0.3921(13) | 0.7613(14) | 0.6668(12) | 0.0212(2) |
| O50 | 0.3783(16) | 0.1441(17) | 0.6704(16) | 0.0212(2) |
| O51 | 0.7093(13) | 0.6488(13) | 1.0738(11) | 0.0212(2) |
| O52 | 0.0666(16) | 0.3805(15) | 0.9505(15) | 0.0212(2) |

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|---|---|---|---|---|
| O53 | 0.3769(14) | 0.3765(14) | 0.4060(14) | 0.0212(2) |
| O54 | 0.3630(14) | 0.0112(15) | 0.5996(12) | 0.0212(2) |
| O55 | 0.2917(11) | 0.0453(13) | 0.9294(11) | 0.0212(2) |
| O56 | 0.6386(16) | 0.3525(15) | 0.7580(15) | 0.0212(2) |
| O57 | 0.3789(11) | 0.2136(14) | 1.1225(13) | 0.0212(2) |
| O58 | 0.1119(14) | 0.2582(15) | 1.0261(12) | 0.0212(2) |
| O59 | 0.7666(16) | 0.5194(16) | 1.1371(14) | 0.0212(2) |
| O60 | 0.2516(11) | 0.6892(12) | 0.9344(11) | 0.0212(2) |
| O61 | 0.7331(13) | 0.4678(15) | 0.9785(13) | 0.0212(2) |
| O62 | 0.3573(17) | 0.7931(17) | 0.8866(16) | 0.0212(2) |
| O63 | -0.0830(15) | 0.4418(15) | 0.6782(13) | 0.0212(2) |
| O64 | 0.0403(13) | 0.3278(11) | 0.2807(13) | 0.0212(2) |
| O65 | 0.7290(14) | 0.7961(15) | 1.1075(13) | 0.0212(2) |
| O66 | 0.6275(14) | 0.6803(15) | 0.5383(13) | 0.0212(2) |
| O67 | 0.6400(11) | 0.8999(13) | 1.1465(12) | 0.0212(2) |
| O68 | 0.0166(13) | 0.2821(14) | 0.4718(11) | 0.0212(2) |
| O69 | 0.3432(12) | 0.7205(14) | 0.4341(13) | 0.0212(2) |
| O70 | 0.7458(15) | 0.6231(14) | 0.8675(15) | 0.0212(2) |
| O71 | 0.2324(14) | 0.4332(12) | 1.1062(13) | 0.0212(2) |
| O72 | 0.3275(14) | 0.6411(14) | 0.5311(13) | 0.0212(2) |
| O73 | 0.5896(12) | 0.3944(12) | 1.0707(12) | 0.0212(2) |
| O74 | 0.8145(15) | 0.4919(16) | 0.8726(13) | 0.0212(2) |
| O75 | -0.0340(16) | 0.4171(16) | 0.4154(14) | 0.0212(2) |
| O76 | 0.6889(14) | 0.5976(11) | 1.2759(13) | 0.0212(2) |
| O77 | 0.5040(14) | 0.5144(12) | 0.4560(13) | 0.0212(2) |
| O78 | 0.5011(11) | 0.1525(11) | 0.5285(9) | 0.0212(2) |
| O79 | 0.5244(11) | 0.2035(13) | 1.0139(12) | 0.0212(2) |
| O80 | -0.0016(14) | 0.1380(15) | 0.4430(13) | 0.0212(2) |
| O81 | 0.3631(14) | 0.5680(14) | 1.1520(14) | 0.0212(2) |
| O82 | -0.0361(14) | 0.1732(12) | 0.6964(13) | 0.0212(2) |
| O83 | 0.4827(14) | 0.7386(14) | 1.2094(12) | 0.0212(2) |

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|---|---|---|---|---|
| O84 | 0.2440(14) | 0.1940(15) | 0.3393(12) | 0.0212(2) |
| O85 | 0.1617(15) | 0.7646(16) | 0.8025(15) | 0.0212(2) |
| O86 | 0.7745(14) | 0.7740(13) | 0.8643(14) | 0.0212(2) |
| O87 | 0.5702(16) | 0.1759(16) | 0.7541(15) | 0.0212(2) |
| O88 | 0.1632(16) | 0.4347(16) | 0.5884(15) | 0.0212(2) |
| O89 | 0.4954(11) | 0.2439(12) | 0.6247(12) | 0.0212(2) |
| O90 | 0.4099(15) | 0.2930(15) | 1.0314(13) | 0.0212(2) |
| O91 | 0.5899(13) | 0.4790(12) | 0.8210(13) | 0.0212(2) |
| O92 | 0.1363(13) | 0.4478(12) | 0.7322(13) | 0.0212(2) |
| O93 | 0.2471(11) | 0.7880(11) | 1.0460(9) | 0.0212(2) |
| O94 | 0.3138(14) | 0.6846(12) | 1.0699(13) | 0.0212(2) |
| O96 | 0.4194(14) | 0.2437(13) | 0.4814(13) | 0.0212(2) |
| O98 | 0.4747(11) | 0.3885(12) | 0.3459(9) | 0.0212(2) |
| O99 | 0.5715(16) | 0.5050(16) | 0.9662(15) | 0.0212(2) |
| O100 | 0.5599(12) | 0.8592(13) | 0.7364(12) | 0.0212(2) |
| O101 | 0.1727(10) | 0.2431(10) | 0.7800(10) | 0.0212(2) |
| O102 | -0.1041(12) | 0.1855(12) | 0.3376(10) | 0.0212(2) |
| O103 | 0.8370(12) | 0.7478(12) | 1.2052(10) | 0.0212(2) |
| O104 | 0.0799(11) | 0.0325(13) | 0.4048(12) | 0.0212(2) |
| O105 | 0.5782(10) | 0.7104(10) | 0.7894(10) | 0.0212(2) |
| O106 | 0.1839(12) | 0.0755(13) | 0.8286(12) | 0.0212(2) |
| O109 | 0.2210(11) | 0.7321(13) | 0.5486(12) | 0.0212(2) |
| O110 | 0.8905(11) | 0.7123(11) | 0.8915(12) | 0.0212(2) |
| O111 | 0.2443(11) | 0.5452(12) | 1.1954(9) | 0.0212(2) |
| O112 | 0.5230(12) | 0.3863(14) | 0.4961(13) | 0.0212(2) |
| O113 | -0.1696(11) | 0.2122(11) | 0.6649(12) | 0.0212(2) |
| O114 | 0.2008(13) | 0.5457(14) | 1.0597(14) | 0.0212(2) |
| O115 | 0.0427(11) | 0.0274(12) | 0.5313(9) | 0.0212(2) |
| O117 | 0.6789(11) | 0.9023(12) | 1.0094(9) | 0.0212(2) |
| O119 | 0.0108(11) | 0.0729(11) | 0.7935(9) | 0.0212(2) |

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|---|---|---|---|---|
| O120 | 0.7175(11) | 0.8569(11) | 0.7445(9) | 0.0212(2) |
| O130 | 0.6493(10) | 0.8346(9) | 0.8840(9) | 0.0212(2) |
| O131 | 0.0517(10) | 0.0724(9) | 0.6721(9) | 0.0212(2) |
| O132 | 0.6739(10) | 0.9894(9) | 0.9212(9) | 0.0212(2) |
| O144 | -0.0699(9) | -0.0098(9) | 0.5783(8) | 0.0212(2) |
| O151 | 0.7910(9) | 0.9964(9) | 0.9860(8) | 0.0212(2) |
| O152 | 0.1032(10) | -0.0345(9) | 0.6468(9) | 0.0212(2) |
| C1 | 0.757(2) | 0.671(2) | 0.7434(18) | 0.0167(10) |
| C2 | 0.0703(19) | 0.227(2) | 0.3748(16) | 0.0167(10) |
| C3 | -0.023(2) | 0.269(2) | 0.8207(18) | 0.0167(10) |
| C4 | 0.669(2) | 0.713(2) | 1.1919(16) | 0.0167(10) |
| C5 | 0.3257(16) | 0.1188(19) | 0.5096(17) | 0.0167(10) |
| C6 | 0.3959(17) | 0.814(2) | 1.0413(18) | 0.0167(10) |
| C7 | 0.2496(18) | 0.172(2) | 0.9694(18) | 0.0167(10) |
| C8 | 0.4925(18) | 0.768(2) | 0.5854(19) | 0.0167(10) |
| C9 | 0.7062(16) | 0.7681(14) | 1.2678(15) | 0.0167(10) |
| C10 | 0.2020(14) | 0.1158(16) | 1.0096(13) | 0.0167(10) |
| C11 | 0.8197(18) | 0.7246(18) | 0.7130(13) | 0.0167(10) |
| C12 | 0.0249(17) | 0.1532(14) | 0.2930(15) | 0.0167(10) |
| C13 | -0.0914(18) | 0.2080(18) | 0.8300(13) | 0.0167(10) |
| C14 | 0.5482(15) | 0.8309(16) | 0.5643(13) | 0.0167(10) |
| C15 | 0.4363(17) | 0.8911(15) | 1.1241(15) | 0.0167(10) |
| C16 | 0.2972(17) | 0.0597(15) | 0.4406(16) | 0.0167(10) |
| O95 | 0.9666(14) | 0.5852(14) | 0.8365(12) | 0.0212(2) |
| O97 | 0.5050(10) | 0.5979(12) | 0.3456(11) | 0.0212(2) |
| O107 | -0.2306(14) | 0.3509(14) | 0.7127(12) | 0.0212(2) |
| O108 | 0.2444(10) | 0.3410(12) | 1.2196(11) | 0.0212(2) |
| O116 | 0.4420(11) | 0.4347(12) | 1.2214(11) | 0.0212(2) |
| O118 | 0.3053(11) | 0.5099(13) | 0.3461(11) | 0.0212(2) |
| O121 | -0.1956(9) | 0.3044(9) | 0.9073(8) | 0.0212(2) |
| O122 | 0.0784(11) | 0.7101(11) | 1.0015(9) | 0.0212(2) |

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| O123 | 0.2263(9) | -0.0771(9) | 0.7849(8) | 0.0212(2) |
| O124 | 0.6592(11) | 0.2268(11) | 0.5379(9) | 0.0212(2) |
| O125 | 0.2105(9) | 0.9163(9) | 0.9980(9) | 0.0212(2) |
| O126 | 0.4955(10) | 0.0057(9) | 0.5266(9) | 0.0212(2) |
| O127 | 0.6838(9) | 0.6708(9) | 1.4060(8) | 0.0212(2) |
| O128 | 0.3391(10) | 0.8725(9) | 0.4391(9) | 0.0212(2) |
| O129 | 0.4289(10) | 0.0817(9) | 1.1140(9) | 0.0212(2) |
| O133 | 0.2703(9) | -0.1006(9) | 0.6584(9) | 0.0212(2) |
| O134 | 0.4334(9) | 1.0394(9) | 0.8611(9) | 0.0212(2) |
| O135 | 0.0638(9) | 0.7894(9) | 0.8703(8) | 0.0212(2) |
| O136 | -0.1824(9) | 0.2536(9) | 0.5140(8) | 0.0212(2) |
| O137 | 0.1520(9) | -0.1151(9) | 0.5424(8) | 0.0212(2) |
| O138 | 0.8403(9) | 0.8148(9) | 1.0354(8) | 0.0212(2) |
| O139 | 0.7425(9) | 0.5768(9) | 1.5066(8) | 0.0212(2) |
| O140 | 0.2859(9) | 0.2105(9) | 1.2085(8) | 0.0212(2) |
| O141 | 0.2991(9) | 0.4165(9) | 0.8451(8) | 0.0212(2) |
| O142 | 0.3929(10) | 0.6969(9) | 1.3178(9) | 0.0212(2) |
| O143 | 0.8675(9) | 0.6752(9) | 1.3304(8) | 0.0212(2) |
| O145 | 0.6713(9) | 0.1724(9) | 0.9485(8) | 0.0212(2) |
| O146 | 0.8800(9) | 0.4447(10) | 1.0551(8) | 0.0212(2) |
| O147 | -0.1761(9) | 0.4437(10) | 0.4875(8) | 0.0212(2) |
| O148 | 0.4596(9) | 0.5445(9) | 0.2342(8) | 0.0212(2) |
| O149 | 0.7987(9) | 0.1245(9) | 1.0916(8) | 0.0212(2) |
| O150 | 0.4435(9) | 0.5837(9) | 0.8755(8) | 0.0212(2) |
| K1 | 0.2282(5) | 0.5271(6) | 0.9103(5) | 0.028(3) |
| K2 | 0.3049(4) | 0.4887(4) | 0.5353(6) | 0.044(3) |
| K3 | 0.4301(7) | 0.4478(7) | 1.0250(6) | 0.048(3) |
| K4 | 0.0879(8) | 0.2756(8) | 0.6306(7) | 0.056(3) |
| K5 | 0.6501(8) | 0.6721(8) | 0.9316(6) | 0.053(4) |

| | | | | |
|---|---|---|---|---|
| K6 | 0.4556(8) | 0.7624(10) | 0.8215(7) | 0.072(4) |
| K7 | 0.2814(7) | 0.1867(10) | 0.7360(6) | 0.070(5) |
| K8 | 0.4314(4) | 0.4430(3) | 0.8133(3) | 0.0351(17) |
| K9 | 0.5029(6) | 0.4077(5) | 0.6459(5) | 0.021(3) |
| K10 | 0.7087(6) | 0.3932(6) | 0.5541(6) | 0.086(3) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S17 - (An)isotropic Displacement Parameters
for: $U16L_8P_4$ P1 R = 0.05

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| U1 | 0.0138(6) | 0.0154(8) | 0.0129(7) | 0.0038(6) | 0.0081(5) | 0.0085(6) |
| U2 | 0.0188(6) | 0.0127(8) | 0.0161(7) | 0.0055(6) | 0.0117(6) | 0.0086(6) |
| U3 | 0.0195(6) | 0.0132(8) | 0.0154(7) | 0.0063(6) | 0.0096(6) | 0.0117(6) |
| U4 | 0.0177(7) | 0.0189(9) | 0.0126(7) | 0.0045(6) | 0.0089(6) | 0.0077(6) |
| U5 | 0.0185(7) | 0.0145(8) | 0.0139(7) | 0.0042(6) | 0.0102(6) | 0.0076(6) |
| U6 | 0.0173(7) | 0.0156(8) | 0.0154(7) | 0.0064(6) | 0.0114(6) | 0.0087(6) |
| U7 | 0.0206(7) | 0.0109(8) | 0.0140(7) | 0.0040(6) | 0.0108(6) | 0.0079(6) |
| U8 | 0.0167(6) | 0.0146(8) | 0.0147(7) | 0.0060(6) | 0.0082(6) | 0.0072(6) |
| U9 | 0.0191(7) | 0.0128(8) | 0.0155(8) | 0.0062(6) | 0.0096(6) | 0.0097(6) |
| U10 | 0.0178(7) | 0.0144(8) | 0.0151(7) | 0.0071(6) | 0.0102(6) | 0.0090(6) |
| U11 | 0.0247(7) | 0.0151(8) | 0.0156(7) | 0.0059(6) | 0.0130(6) | 0.0094(7) |
| U12 | 0.0235(7) | 0.0128(8) | 0.0168(8) | 0.0061(6) | 0.0129(6) | 0.0088(7) |
| U13 | 0.0209(7) | 0.0155(8) | 0.0178(7) | 0.0060(6) | 0.0116(6) | 0.0099(6) |
| U14 | 0.0241(7) | 0.0211(9) | 0.0183(8) | 0.0074(7) | 0.0105(6) | 0.0161(7) |
| U15 | 0.0200(7) | 0.0149(9) | 0.0220(8) | 0.0074(7) | 0.0130(6) | 0.0089(7) |
| U16 | 0.0271(8) | 0.0175(9) | 0.0197(8) | 0.0040(7) | 0.0130(7) | 0.0137(7) |
| P1 | 0.006(4) | 0.023(6) | 0.016(5) | 0.006(4) | 0.007(4) | 0.008(4) |
| P2 | 0.012(4) | 0.024(6) | 0.016(5) | 0.007(4) | 0.003(4) | 0.010(4) |
| P3 | 0.028(5) | 0.012(5) | 0.016(5) | 0.009(4) | 0.014(4) | 0.014(4) |
| P4 | 0.028(5) | 0.015(5) | 0.015(5) | 0.008(4) | 0.018(4) | 0.012(4) |
| P5 | 0.018(4) | 0.012(5) | 0.014(5) | -0.001(4) | 0.008(4) | 0.004(4) |
| P6 | 0.021(5) | 0.017(6) | 0.023(5) | 0.015(4) | 0.014(4) | 0.017(4) |
| P7 | 0.019(5) | 0.017(6) | 0.022(5) | 0.009(5) | 0.009(4) | 0.006(4) |
| P8 | 0.030(5) | 0.018(5) | 0.014(4) | 0.007(4) | 0.013(4) | 0.014(4) |
| P9 | 0.025(5) | 0.014(5) | 0.022(5) | 0.003(4) | 0.015(4) | 0.009(4) |
| P11 | 0.020(4) | 0.028(6) | 0.004(4) | 0.009(4) | 0.005(3) | 0.015(4) |
| P12 | 0.019(4) | 0.010(5) | 0.016(5) | 0.007(4) | 0.009(4) | 0.009(4) |
| P13 | 0.034(4) | 0.021(4) | 0.021(3) | 0.013(2) | 0.017(3) | 0.025(3) |
| P14 | 0.018(5) | 0.016(6) | 0.026(6) | 0.001(5) | 0.012(5) | 0.008(5) |
| P15 | 0.021(4) | 0.019(6) | 0.018(5) | 0.004(4) | 0.011(4) | 0.009(4) |
| P16 | 0.018(4) | 0.004(5) | 0.030(6) | 0.005(4) | 0.018(4) | 0.005(4) |
| P17 | 0.016(4) | 0.011(5) | 0.026(5) | 0.010(4) | 0.012(4) | 0.008(4) |
| P18 | 0.018(4) | 0.016(6) | 0.019(5) | 0.006(4) | 0.009(4) | 0.013(4) |
| P20 | 0.067(6) | 0.019(4) | 0.024(4) | -0.001(3) | 0.038(4) | -0.008(3) |
| K1 | 0.018(4) | 0.035(5) | 0.029(5) | 0.025(4) | 0.002(3) | 0.015(4) |
| K2 | 0.008(2) | -0.006(2) | 0.115(7) | -0.002(3) | 0.018(3) | 0.0040(17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| K4 | 0.092(6) | 0.083(6) | 0.063(6) | 0.051(5) | 0.062(5) | 0.076(5) |
| K5 | 0.098(7) | 0.098(8) | 0.028(4) | 0.045(4) | 0.048(4) | 0.087(6) |
| K6 | 0.056(5) | 0.162(11) | 0.037(6) | 0.047(6) | 0.033(5) | 0.070(7) |
| K7 | 0.060(6) | 0.183(12) | 0.029(5) | 0.060(6) | 0.038(4) | 0.092(7) |
| K8 | 0.040(3) | 0.035(3) | 0.040(3) | 0.015(3) | 0.024(2) | 0.018(3) |
| K9 | 0.024(4) | 0.005(4) | 0.025(5) | 0.002(3) | 0.009(4) | -0.001(3) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S18 - Bond Distances (Angstrom)
for: $U16L_8P_4$ P1 R = 0.05

| | | | | | |
|---|---|---|---|---|---|
| U1 | -O8 | 2.40(2) | U4 | -O61 | 2.36(3) |
| U1 | -O16 | 2.39(3) | U4 | -O73 | 2.31(2) |
| U1 | -O47 | 2.38(3) | U4 | -O99 | 1.80(3) |
| U1 | -O56 | 2.45(3) | U5 | -O5 | 2.35(2) |
| U1 | -O61 | 2.40(2) | U5 | -O32 | 2.45(2) |
| U1 | -O70 | 2.26(3) | U5 | -O35 | 2.34(3) |
| U1 | -O74 | 1.82(3) | U5 | -O38 | 2.41(3) |
| U1 | -O91 | 1.82(3) | U5 | -O43 | 2.42(2) |
| U2 | -O16 | 2.31(3) | U5 | -O68 | 2.40(2) |
| U2 | -O41 | 2.31(2) | U5 | -O75 | 1.83(3) |
| U2 | -O42 | 2.45(2) | U5 | -O88 | 1.77(3) |
| U2 | -O45 | 1.79(3) | U6 | -O4 | 2.33(2) |
| U2 | -O50 | 2.33(3) | U6 | -O10 | 2.38(3) |
| U2 | -O56 | 2.39(3) | U6 | -O27 | 2.30(3) |
| U2 | -O87 | 1.78(3) | U6 | -O29 | 2.37(2) |
| U2 | -O89 | 2.36(2) | U6 | -O35 | 2.30(2) |
| U3 | -O1 | 2.38(3) | U6 | -O38 | 2.43(3) |
| U3 | -O6 | 1.74(3) | U6 | -O63 | 1.81(3) |
| U3 | -O15 | 2.31(2) | U6 | -O92 | 1.77(3) |
| U3 | -O30 | 2.39(3) | U7 | -O10 | 2.45(3) |
| U3 | -O40 | 2.39(3) | U7 | -O21 | 2.33(2) |
| U3 | -O66 | 1.78(3) | U7 | -O25 | 2.35(2) |
| U3 | -O77 | 2.28(2) | U7 | -O27 | 2.36(3) |
| U4 | -O14 | 2.31(2) | U7 | -O48 | 1.80(3) |
| U4 | -O28 | 2.26(2) | U7 | -O60 | 2.358(19) |
| U4 | -O47 | 2.40(3) | U7 | -O62 | 2.35(3) |
| U4 | -O51 | 2.32(2) | U7 | -O85 | 1.85(3) |
| U4 | -O59 | 1.78(3) | U8 | -O7 | 1.82(2) |

| | | | | | |
|---|---|---|---|---|---|
| U8 | -O12 | 2.31(3) | U12 | -O28 | 2.42(3) |
| U8 | -O23 | 2.31(3) | U12 | -O31 | 2.39(2) |
| U8 | -O24 | 2.35(3) | U12 | -O33 | 1.81(2) |
| U8 | -O81 | 2.33(3) | U12 | -O41 | 2.30(2) |
| U8 | -O83 | 1.72(2) | U12 | -O42 | 2.37(2) |
| U8 | -O94 | 2.33(3) | U12 | -O73 | 2.52(2) |
| U9 | -O13 | 2.39(3) | U12 | -O79 | 1.88(2) |
| U9 | -O22 | 2.33(3) | U12 | -O90 | 2.38(3) |
| U9 | -O26 | 1.78(2) | U13 | -O11 | 1.73(2) |
| U9 | -O37 | 2.39(3) | U13 | -O18 | 2.43(3) |
| U9 | -O53 | 2.45(3) | U13 | -O23 | 2.45(3) |
| U9 | -O84 | 1.86(2) | U13 | -O24 | 2.43(3) |
| U9 | -O96 | 2.40(3) | U13 | -O65 | 2.33(3) |
| U10 | -O2 | 1.87(3) | U13 | -O67 | 1.75(2) |
| U10 | -O3 | 2.40(3) | U13 | -O117 | 2.30(2) |
| U10 | -O9 | 2.42(3) | U14 | -O1 | 2.39(3) |
| U10 | -O46 | 2.40(3) | U14 | -O30 | 2.39(3) |
| U10 | -O52 | 2.32(3) | U14 | -O86 | 2.35(3) |
| U10 | -O58 | 1.80(3) | U14 | -O100 | 2.29(2) |
| U10 | -O71 | 2.43(2) | U14 | -O105 | 1.699(19) |
| U11 | -O21 | 2.49(2) | U14 | -O120 | 1.83(2) |
| U11 | -O25 | 2.41(2) | U14 | -O130 | 2.291(17) |
| U11 | -O32 | 2.30(2) | U15 | -O17 | 1.88(2) |
| U11 | -O43 | 2.29(3) | U15 | -O22 | 2.44(3) |
| U11 | -O44 | 1.81(3) | U15 | -O36 | 2.30(3) |
| U11 | -O49 | 2.25(2) | U15 | -O37 | 2.37(3) |
| U11 | -O72 | 2.37(3) | U15 | -O80 | 2.39(3) |
| U11 | -O109 | 1.73(2) | U15 | -O104 | 1.83(2) |
| U15 | -O115 | 2.27(2) | P6 | -O60 | 1.51(2) |
| U16 | -O3 | 2.36(3) | P6 | -O93 | 1.49(2) |

| | | | | | |
|---|---|---|---|---|---|
| U16 | -O9 | 2.36(3) | P6 | -O94 | 1.59(2) |
| U16 | -O82 | 2.35(2) | P6 | -C6 | 1.75(4) |
| U16 | -O101 | 1.913(19) | P7 | -O68 | 1.43(2) |
| U16 | -O106 | 2.48(2) | P7 | -O80 | 1.54(3) |
| U16 | -O119 | 1.76(2) | P7 | -O102 | 1.55(2) |
| U16 | -O131 | 2.265(16) | P7 | -C2 | 1.84(4) |
| P1 | -O8 | 1.49(3) | P8 | -O31 | 1.45(3) |
| P1 | -O19 | 1.50(3) | P8 | -O55 | 1.52(3) |
| P1 | -O40 | 1.51(3) | P8 | -O106 | 1.45(2) |
| P1 | -C1 | 1.88(4) | P8 | -C7 | 1.81(4) |
| P2 | -O5 | 1.55(2) | P9 | -O36 | 1.61(3) |
| P2 | -O13 | 1.55(3) | P9 | -O50 | 1.56(3) |
| P2 | -O64 | 1.49(2) | P9 | -O54 | 1.50(3) |
| P2 | -C2 | 1.82(4) | P9 | -C5 | 1.82(3) |
| P3 | -O4 | 1.56(3) | P10 | -O46 | 1.52(3) |
| P3 | -O20 | 1.54(3) | P10 | -O57 | 1.53(3) |
| P3 | -O52 | 1.54(3) | P10 | -O90 | 1.50(3) |
| P3 | -C3 | 1.81(4) | P10 | -C7 | 1.82(3) |
| P4 | -O12 | 1.55(3) | P11 | -O71 | 1.46(2) |
| P4 | -O14 | 1.49(2) | P11 | -O81 | 1.59(3) |
| P4 | -O76 | 1.53(3) | P11 | -O111 | 1.43(2) |
| P4 | -C4 | 1.87(4) | P11 | -O114 | 1.61(3) |
| P5 | -O78 | 1.53(2) | P12 | -O18 | 1.51(3) |
| P5 | -O89 | 1.53(2) | P12 | -O39 | 1.51(3) |
| P5 | -O96 | 1.47(3) | P12 | -O62 | 1.51(3) |
| P5 | -C5 | 1.93(3) | P12 | -C6 | 1.86(3) |
| P13 | -O15 | 1.56(3) | P20 | -O117 | 1.45(2) |
| P13 | -O69 | 1.54(3) | P20 | -O130 | 1.66(2) |
| P13 | -O72 | 1.53(3) | P20 | -O132 | 1.38(2) |
| P13 | -C8 | 1.86(4) | P20 | -O151 | 1.59(2) |
| P14 | -O51 | 1.63(2) | O1 | -C8 | 1.40(5) |

| | | | | | |
|---|---|---|---|---|---|
| P14 | -O65 | 1.55(3) | O3 | -C7 | 1.45(5) |
| P14 | -O103 | 1.45(2) | O9 | -C3 | 1.44(5) |
| P14 | -C4 | 1.88(4) | O10 | -O27 | 1.48(4) |
| P15 | -O29 | 1.47(3) | O16 | -O56 | 1.47(4) |
| P15 | -O82 | 1.46(3) | O21 | -O25 | 1.57(3) |
| P15 | -O113 | 1.62(3) | O22 | -C2 | 1.38(4) |
| P15 | -C3 | 1.93(3) | O23 | -C6 | 1.48(5) |
| P16 | -O53 | 1.46(3) | O24 | -C4 | 1.48(5) |
| P16 | -O77 | 1.62(2) | O28 | -O73 | 1.47(4) |
| P16 | -O98 | 1.60(2) | O30 | -C1 | 1.44(5) |
| P16 | -O112 | 1.58(3) | O32 | -O43 | 1.46(4) |
| P17 | -O34 | 1.49(2) | O35 | -O38 | 1.53(4) |
| P17 | -O49 | 1.60(3) | O37 | -C5 | 1.38(4) |
| P17 | -O100 | 1.67(2) | O41 | -O42 | 1.39(3) |
| P17 | -C8 | 1.86(4) | O47 | -O61 | 1.47(4) |
| P18 | -O70 | 1.58(3) | C1 | -C11 | 1.61(5) |
| P18 | -O86 | 1.64(3) | C2 | -C12 | 1.64(4) |
| P18 | -O110 | 1.39(3) | C3 | -C13 | 1.48(5) |
| P18 | -C1 | 1.77(3) | C4 | -C9 | 1.42(4) |
| P19 | -O115 | 1.61(2) | C5 | -C16 | 1.39(4) |
| P19 | -O131 | 1.43(2) | C6 | -C15 | 1.71(4) |
| P19 | -O144 | 1.64(2) | C7 | -C10 | 1.61(4) |
| P19 | -O152 | 1.62(2) | C8 | -C14 | 1.50(5) |