**Table S1.** Atomic coordinates (·104) and equivalent isotropic displacement parameters (A2·103) for compound 1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | *x* | *y* | *z* | U(eq) |
| Pr(1) | 5501(1) | 8877(1) | -652(1) | 41(1) |
| N(1) | 4549(4) | 7118(4) | 109(4) | 48(1) |
| N(2) | 4081(4) | 8874(4) | -1985(4) | 50(1) |
| O(1) | 6126(3) | 10220(3) | -47(3) | 48(1) |
| O(2) | 7469(4) | 8961(5) | -381(5) | 85(2) |
| O(3) | 5798(3) | 7864(3) | 1327(3) | 54(1) |
| O(4) | 5191(3) | 9091(3) | 2081(3) | 52(1) |
| O(5) | 6734(4) | 7141(3) | -827(3) | 63(1) |
| O(6) | 6634(3) | 8798(4) | -2296(3) | 58(1) |
| C(1) | 7155(5) | 9793(6) | -143(5) | 55(1) |
| C(2) | 7938(5) | 10320(6) | 54(6) | 60(2) |
| C(3) | 8059(6) | 11350(7) | -756(7) | 77(2) |
| C(4) | 8769(7) | 11859(8) | -531(10) | 106(3) |
| C(5) | 9312(7) | 11305(12) | 507(12) | 131(5) |
| C(6) | 9179(7) | 10297(11) | 1268(10) | 119(4) |
| C(7) | 8501(6) | 9789(8) | 1066(7) | 80(2) |
| C(8) | 7510(8) | 11900(8) | -1865(7) | 111(3) |
| C(9) | 8390(7) | 8653(10) | 1948(8) | 120(3) |
| C(10) | 5583(4) | 8080(5) | 2144(4) | 47(1) |
| C(11) | 5824(5) | 7051(5) | 3262(4) | 53(2) |
| C(12) | 6737(6) | 6056(6) | 3440(6) | 75(2) |
| C(13) | 6953(8) | 5108(6) | 4518(8) | 99(3) |
| C(14) | 6251(11) | 5156(8) | 5328(7) | 114(4) |
| C(15) | 5387(8) | 6094(7) | 5138(6) | 89(2) |
| C(16) | 5137(6) | 7071(6) | 4129(5) | 63(2) |
| C(17) | 7535(7) | 5935(7) | 2596(8) | 111(3) |
| C(18) | 4120(7) | 8087(7) | 4007(6) | 87(2) |
| C(19) | 7004(5) | 7705(5) | -1774(5) | 52(1) |
| C(20) | 7796(6) | 6981(6) | -2279(6) | 65(2) |
| C(21) | 7389(8) | 6937(8) | -3160(8) | 95(3) |
| C(22) | 8108(11) | 6163(12) | -3577(11) | 139(5) |
| C(23) | 9159(11) | 5516(11) | -3063(12) | 145(5) |
| C(24) | 9525(9) | 5617(10) | -2236(11) | 141(4) |
| C(25) | 8852(7) | 6348(7) | -1794(8) | 93(3) |
| C(26) | 6247(9) | 7653(9) | -3678(7) | 110(3) |
| C(27) | 9278(7) | 6496(9) | -889(7) | 113(3) |
| C(28) | 4789(6) | 6235(6) | 1113(5) | 64(2) |
| C(29) | 4401(7) | 5281(6) | 1504(6) | 86(2) |
| C(30) | 3691(7) | 5239(6) | 831(6) | 82(2) |
| C(31) | 3439(5) | 6118(5) | -217(5) | 61(2) |
| C(32) | 3875(5) | 7045(5) | -549(5) | 49(1) |
| C(33) | 3618(5) | 7976(5) | -1657(5) | 53(1) |
| C(34) | 2912(6) | 7942(6) | -2358(6) | 69(2) |
| C(35) | 2669(7) | 8835(7) | -3382(7) | 90(2) |
| C(36) | 3113(7) | 9741(7) | -3724(6) | 93(3) |
| C(37) | 3826(6) | 9709(6) | -2995(5) | 75(2) |
| C(38) | 2733(7) | 6103(7) | -964(7) | 85(2) |
| C(39) | 2475(6) | 6961(8) | -1959(7) | 84(2) |

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

**Table S2.** Atomic coordinates (·104) and equivalent isotropic displacement parameters (A2·103) for compound 2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | *x* | *y* | *z* | U(eq) |
| Sm(1) | 4534(1) | 3450(1) | 5879(1) | 42(1) |
| N(1) | 5365(5) | 2062(4) | 4797(4) | 52(1) |
| N(2) | 6081(4) | 1680(5) | 6630(4) | 54(1) |
| O(1) | 2610(4) | 4522(4) | 6502(4) | 71(1) |
| O(2) | 3920(3) | 5651(4) | 5446(3) | 48(1) |
| O(3) | 3833(3) | 4330(4) | 4253(3) | 52(1) |
| O(4) | 4468(4) | 6003(4) | 3172(3) | 51(1) |
| O(5) | 3241(4) | 2031(4) | 6471(4) | 60(1) |
| O(6) | 3635(4) | 2221(4) | 7824(3) | 55(1) |
| C(1) | 2902(6) | 5490(6) | 6035(5) | 49(2) |
| C(2) | 2094(5) | 6522(6) | 6137(5) | 55(2) |
| C(3) | 1412(6) | 7180(7) | 5370(6) | 71(2) |
| C(4) | 731(7) | 8155(8) | 5486(9) | 100(3) |
| C(5) | 710(8) | 8474(9) | 6294(10) | 109(4) |
| C(6) | 1358(8) | 7821(8) | 7042(8) | 89(3) |
| C(7) | 2072(6) | 6818(6) | 6993(6) | 68(2) |
| C(8) | 1421(7) | 6852(8) | 4468(7) | 95(3) |
| C(9) | 2787(8) | 6114(7) | 7834(6) | 91(3) |
| C(10) | 3921(5) | 5190(5) | 3385(5) | 47(2) |
| C(11) | 3372(6) | 5209(6) | 2523(5) | 58(2) |
| C(12) | 2341(7) | 4720(7) | 2837(7) | 79(2) |
| C(13) | 1860(10) | 4762(10) | 2011(10) | 128(4) |
| C(14) | 2365(12) | 5248(12) | 969(10) | 150(5) |
| C(15) | 3387(11) | 5699(9) | 658(8) | 116(4) |
| C(16) | 3891(7) | 5735(6) | 1417(6) | 70(2) |
| C(17) | 1726(7) | 4139(9) | 3964(8) | 106(3) |
| C(18) | 4991(7) | 6267(7) | 996(6) | 79(2) |
| C(19) | 3143(6) | 1755(5) | 7464(5) | 50(2) |
| C(20) | 2457(6) | 774(6) | 8213(5) | 59(2) |
| C(21) | 3017(8) | -229(7) | 8930(6) | 71(2) |
| C(22) | 2389(10) | -1140(8) | 9555(7) | 101(3) |
| C(23) | 1311(12) | -1098(11) | 9477(9) | 118(4) |
| C(24) | 733(9) | -147(11) | 8820(8) | 109(4) |
| C(25) | 1326(8) | 836(9) | 8145(7) | 83(3) |
| C(26) | 4235(8) | -317(7) | 8991(7) | 105(3) |
| C(27) | 706(7) | 1881(10) | 7429(8) | 117(4) |
| C(28) | 5048(6) | 2233(6) | 3907(6) | 64(2) |
| C(29) | 5442(7) | 1516(7) | 3329(6) | 77(2) |
| C(30) | 6191(7) | 554(7) | 3721(6) | 77(2) |
| C(31) | 6545(6) | 326(6) | 4657(6) | 66(2) |
| C(32) | 6110(6) | 1111(6) | 5191(5) | 53(2) |
| C(33) | 6461(5) | 893(6) | 6153(6) | 54(2) |
| C(34) | 7216(6) | -117(6) | 6604(7) | 66(2) |
| C(35) | 7525(7) | -290(7) | 7555(7) | 86(3) |
| C(36) | 7161(7) | 501(7) | 8013(7) | 86(3) |
| C(37) | 6428(6) | 1475(6) | 7514(6) | 70(2) |
| C(38) | 7282(7) | -682(7) | 5158(8) | 84(3) |
| C(39) | 7588(7) | -903(7) | 6073(8) | 86(3) |

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

**Table S3.** Atomic coordinates (·104) and equivalent isotropic displacement parameters (A2·103) for compound 3.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | *x* | *y* | *z* | U(eq) |
| Er(1) | 4838(1) | 6004(1) | 6049(1) | 53(1) |
| N(1) | 6323(14) | 6563(13) | 6613(13) | 62(5) |
| N(2) | 4427(13) | 8206(11) | 6036(13) | 59(5) |
| O(1) | 3812(14) | 4696(12) | 6217(12) | 75(5) |
| O(2) | 3921(13) | 3485(13) | 5270(11) | 66(4) |
| O(3) | 3572(13) | 6773(12) | 5073(10) | 66(4) |
| O(4) | 3531(15) | 5695(14) | 4071(11) | 74(4) |
| O(5) | 3321(16) | 6711(13) | 7283(11) | 76(5) |
| O(6) | 4734(15) | 5244(16) | 7637(12) | 84(5) |
| O(7) | 890(30) | 1520(40) | 1740(20) | 208(15) |
| O(8) | 8630(20) | 1350(20) | 2213(18) | 140(8) |
| C(1) | 3527(18) | 3884(17) | 6013(14) | 54(5) |
| C(2) | 2530(20) | 3480(20) | 6640(18) | 74(5) |
| C(3) | 2670(20) | 2970(20) | 7520(20) | 86(5) |
| C(4) | 1810(20) | 2540(20) | 8110(20) | 91(6) |
| C(5) | 800(30) | 2640(20) | 7810(20) | 96(6) |
| C(6) | 660(20) | 3120(20) | 6942(19) | 83(5) |
| C(7) | 1550(20) | 3530(20) | 6337(19) | 80(5) |
| C(8) | 3750(30) | 2850(30) | 7873(19) | 101(10) |
| C(9) | 1420(30) | 3950(30) | 5380(20) | 111(11) |
| C(10) | 3148(18) | 6551(18) | 4463(16) | 61(6) |
| C(11) | 2008(17) | 7434(17) | 4227(19) | 66(7) |
| C(12) | 1065(17) | 7742(18) | 4970(20) | 70(7) |
| C(13) | 110(20) | 8590(20) | 4740(20) | 113(11) |
| C(14) | 70(30) | 9140(30) | 3897(18) | 96(9) |
| C(15) | 970(20) | 8880(20) | 3160(20) | 86(9) |
| C(16) | 2020(30) | 7920(20) | 3370(20) | 80(8) |
| C(17) | 1010(30) | 7270(30) | 5880(20) | 101(10) |
| C(18) | 2970(30) | 7630(20) | 2600(20) | 89(8) |
| C(19) | 3810(20) | 5979(19) | 7895(17) | 64(6) |
| C(20) | 3280(30) | 6100(30) | 8850(20) | 107(6) |
| C(21) | 2200(40) | 5890(30) | 9200(20) | 115(7) |
| C(22) | 1690(40) | 5960(30) | 10170(20) | 122(7) |
| C(23) | 2280(30) | 6280(30) | 10690(20) | 123(7) |
| C(24) | 3340(30) | 6440(30) | 10318(19) | 118(7) |
| C(25) | 3930(30) | 6310(30) | 9459(18) | 116(7) |
| C(26) | 1540(30) | 5560(30) | 8630(30) | 143(16) |
| C(27) | 5000(30) | 6670(30) | 9020(20) | 123(13) |
| C(28) | 7280(20) | 5710(20) | 6908(19) | 83(8) |
| C(29) | 8080(30) | 6050(30) | 7230(20) | 100(9) |
| C(30) | 8000(30) | 7150(30) | 7167(18) | 95(9) |
| C(31) | 7010(20) | 8100(20) | 6857(16) | 71(7) |
| C(32) | 6260(20) | 7658(18) | 6589(15) | 65(6) |
| C(33) | 5221(19) | 8545(14) | 6309(16) | 62(6) |
| C(34) | 5050(30) | 9800(20) | 6306(18) | 92(10) |
| C(35) | 4060(20) | 10568(18) | 6012(19) | 80(8) |
| C(36) | 3290(20) | 10178(15) | 5761(19) | 83(8) |
| C(37) | 3475(17) | 9025(14) | 5782(17) | 78(7) |
| C(38) | 6880(30) | 9400(20) | 6810(20) | 107(12) |
| C(39) | 5990(30) | 10120(30) | 6560(20) | 101(10) |
| C(40) | 1310(40) | 1610(70) | 820(20) | 240(20) |
| C(41) | 2620(40) | 1240(70) | 620(40) | 240(20) |
| C(42) | 8160(40) | 650(40) | 1890(30) | 170(14) |
| C(43) | 8510(40) | 640(40) | 900(30) | 174(14) |

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

**Table S4.** Bond length (Å) of the organic group in compounds 1-3

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound 1 | Bond length | Compound 2 | Bond length | Compound 3 | Bond length |
| N(1)-C(32) | 1.361(7) | N(1)-C(32) | 1.369(8) | N(1)-C(32) | 1.36(3) |
| N(2)-C(37) | 1.319(8) | N(2)-C(37) | 1.330(8) | N(2)-C(37) | 1.395(10) |
| N(2)-C(33) | 1.383(7) | N(2)-C(33) | 1.392(8) | N(2)-C(33) | 1.39(3) |
| O(1)-C(1) | 1.277(7) | O(1)-C(1) | 1.244(7) | O(1)-C(1) | 1.31(3) |
| O(2)-C(1) | 1.241(7) | O(2)-C(1) | 1.302(7) | O(2)-C(1) | 1.29(2) |
| O(3)-C(10) | 1.268(6) | O(3)-C(10) | 1.268(7) | O(3)-C(10) | 1.32(3) |
| O(4)-C(10) | 1.253(6) | O(4)-C(10) | 1.274(7) | O(4)-C(10) | 1.25(3) |
| O(5)-C(19) | 1.254(6) | O(5)-C(19) | 1.271(7) | O(5)-C(19) | 1.32(3) |
| O(6)-C(19) | 1.252(7) | O(6)-C(19) | 1.261(7) | O(6)-C(19) | 1.27(3) |
| C(1)-C(2) | 1.498(8) | C(1)-C(2) | 1.521(9) | C(1)-C(2) | 1.57(3) |
| C(2)-C(3) | 1.371(10) | C(2)-C(7) | 1.410(9) | C(2)-C(7) | 1.41(4) |
| C(2)-C(7) | 1.391(10) | C(2)-C(3) | 1.413(9) | C(2)-C(3) | 1.45(4) |
| C(3)-C(4) | 1.422(10) | C(3)-C(4) | 1.407(11) | C(3)-C(4) | 1.43(4) |
| C(3)-C(8) | 1.491(11) | C(3)-C(8) | 1.503(11) | C(3)-C(8) | 1.56(4) |
| C(4)-C(5) | 1.406(15) | C(4)-C(5) | 1.363(13) | C(4)-C(5) | 1.43(4) |
| C(4)-H(4) | 0.9300 | C(4)-H(4) | 0.9300 | C(4)-H(4) | 0.9300 |
| C(5)-C(6) | 1.336(15) | C(5)-C(6) | 1.368(13) | C(5)-C(6) | 1.42(4) |
| C(5)-H(5) | 0.9300 | C(5)-H(5) | 0.9300 | C(5)-H(5) | 0.9300 |
| C(6)-C(7) | 1.371(11) | C(6)-C(7) | 1.421(10) | C(6)-C(7) | 1.45(3) |
| C(6)-H(6) | 0.9300 | C(6)-H(6) | 0.9300 | C(6)-H(6) | 0.9300 |
| C(7)-C(9) | 1.498(12) | C(7)-C(9) | 1.519(10) | C(7)-C(9) | 1.54(4) |
| C(8)-H(8A) | 0.9600 | C(8)-H(8A) | 0.9600 | C(8)-H(8A) | 0.9600 |
| C(8)-H(8B) | 0.9600 | C(8)-H(8B) | 0.9600 | C(8)-H(8B) | 0.9600 |
| C(8)-H(8C) | 0.9600 | C(8)-H(8C) | 0.9600 | C(8)-H(8C) | 0.9600 |
| C(9)-H(9A) | 0.9600 | C(9)-H(9A) | 0.9600 | C(9)-H(9A) | 0.9600 |
| C(9)-H(9B) | 0.9600 | C(9)-H(9B) | 0.9600 | C(9)-H(9B) | 0.9600 |
| C(9)-H(9C) | 0.9600 | C(9)-H(9C) | 0.9600 | C(9)-H(9C) | 0.9600 |
| C(10)-C(11) | 1.506(7) | C(10)-C(11) | 1.533(8) | C(10)-C(11) | 1.59(3) |
| C(11)-C(12) | 1.407(9) | C(11)-C(12) | 1.423(10) | C(11)-C(16) | 1.38(3) |
| C(11)-C(16) | 1.414(9) | C(11)-C(16) | 1.439(10) | C(11)-C(12) | 1.47(3) |
| C(12)-C(13) | 1.430(11) | C(12)-C(13) | 1.421(11) | C(12)-C(13) | 1.398(10) |
| C(12)-C(17) | 1.499(11) | C(12)-C(17) | 1.506(11) | C(12)-C(17) | 1.44(4) |
| C(13)-C(14) | 1.372(13) | C(13)-C(14) | 1.359(14) | C(13)-C(14) | 1.394(10) |
| C(13)-H(13) | 0.9300 | C(13)-H(13) | 0.9300 | C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.322(13) | C(14)-C(15) | 1.387(14) | C(14)-C(15) | 1.43(4) |
| C(14)-H(14) | 0.9300 | C(14)-H(14) | 0.9300 | C(14)-H(14) | 0.9300 |
| C(15)-C(16) | 1.385(9) | C(15)-C(16) | 1.397(11) | C(15)-C(16) | 1.54(4) |
| C(15)-H(15) | 0.9300 | C(15)-H(15) | 0.9300 | C(15)-H(15) | 0.9300 |
| C(16)-C(18) | 1.513(10) | C(16)-C(18) | 1.515(10) | C(16)-C(18) | 1.49(4) |
| C(17)-H(17A) | 0.9600 | C(17)-H(17A) | 0.9600 | C(17)-H(17A) | 0.9600 |
| C(17)-H(17B) | 0.9600 | C(17)-H(17B) | 0.9600 | C(17)-H(17B) | 0.9600 |
| C(17)-H(17C) | 0.9600 | C(17)-H(17C) | 0.9600 | C(17)-H(17C) | 0.9600 |
| C(18)-H(18A) | 0.9600 | C(18)-H(18A) | 0.9600 | C(18)-H(18A) | 0.9600 |
| C(18)-H(18B) | 0.9600 | C(18)-H(18B) | 0.9600 | C(18)-H(18B) | 0.9600 |
| C(18)-H(18C) | 0.9600 | C(18)-H(18C) | 0.9600 | C(18)-H(18C) | 0.9600 |
| C(19)-C(20) | 1.517(8) | C(19)-C(20) | 1.530(9) | C(19)-C(20) | 1.52(4) |
| C(20)-C(25) | 1.386(11) | C(20)-C(25) | 1.396(10) | C(20)-C(21) | 1.43(5) |
| C(20)-C(21) | 1.395(11) | C(20)-C(21) | 1.440(10) | C(20)-C(25) | 1.52(5) |
| C(21)-C(22) | 1.444(12) | C(21)-C(22) | 1.399(11) | C(21)-C(22) | 1.53(4) |
| C(21)-C(26) | 1.500(12) | C(21)-C(26) | 1.492(11) | C(21)-C(26) | 1.55(5) |
| C(22)-C(23) | 1.394(16) | C(22)-C(23) | 1.340(13) | C(22)-C(23) | 1.42(5) |
| C(22)-H(22) | 0.9300 | C(22)-H(22) | 0.9300 | C(22)-H(22) | 0.9300 |
| C(23)-C(24) | 1.346(15) | C(23)-C(24) | 1.379(14) | C(23)-C(24) | 1.392(10) |
| C(23)-H(23) | 0.9300 | C(23)-H(23) | 0.9300 | C(23)-H(23) | 0.9300 |
| C(24)-C(25) | 1.406(12) | C(24)-C(25) | 1.453(13) | C(24)-C(25) | 1.396(10) |
| C(24)-H(24) | 0.9300 | C(24)-H(24) | 0.9300 | C(24)-H(24) | 0.9300 |
| C(25)-C(27) | 1.518(12) | C(25)-C(27) | 1.503(12) | C(25)-C(27) | 1.53(5) |
| C(26)-H(26A) | 0.9600 | C(26)-H(26A) | 0.9600 | C(26)-H(26A) | 0.9600 |
| C(26)-H(26B) | 0.9600 | C(26)-H(26B) | 0.9600 | C(26)-H(26B) | 0.9600 |
| C(26)-H(26C) | 0.9600 | C(26)-H(26C) | 0.9600 | C(26)-H(26C) | 0.9600 |
| C(27)-H(27A) | 0.9600 | C(27)-H(27A) | 0.9600 | C(27)-H(27A) | 0.9600 |
| C(27)-H(27B) | 0.9600 | C(27)-H(27B) | 0.9600 | C(27)-H(27B) | 0.9600 |
| C(27)-H(27C) | 0.9600 | C(27)-H(27C) | 0.9600 | C(27)-H(27C) | 0.9600 |
| C(28)-C(29) | 1.379(9) | C(28)-C(29) | 1.418(9) | C(28)-C(29) | 1.44(4) |
| C(28)-H(28) | 0.9300 | C(28)-H(28) | 0.9300 | C(28)-H(28) | 0.9300 |
| C(29)-C(30) | 1.386(10) | C(29)-C(30) | 1.380(11) | C(29)-C(30) | 1.35(4) |
| C(29)-H(29) | 0.9300 | C(29)-H(29) | 0.9300 | C(29)-H(29) | 0.9300 |
| C(30)-C(31) | 1.372(10) | C(30)-C(31) | 1.395(10) | C(30)-C(31) | 1.53(4) |
| C(30)-H(30) | 0.9300 | C(30)-H(30) | 0.9300 | C(30)-H(30) | 0.9300 |
| C(31)-C(32) | 1.393(7) | C(31)-C(38) | 1.443(11) | C(31)-C(32) | 1.42(3) |
| C(31)-C(38) | 1.440(10) | C(31)-C(32) | 1.450(9) | C(31)-C(38) | 1.58(3) |
| C(32)-C(33) | 1.451(8) | C(32)-C(33) | 1.431(9) | C(32)-C(33) | 1.52(3) |
| C(33)-C(34) | 1.406(8) | C(33)-C(34) | 1.439(9) | C(33)-C(34) | 1.52(3) |
| C(34)-C(35) | 1.356(10) | C(34)-C(35) | 1.408(10) | C(34)-C(35) | 1.43(4) |
| C(34)-C(39) | 1.448(9) | C(34)-C(39) | 1.444(10) | C(34)-C(39) | 1.53(4) |
| C(35)-C(36) | 1.374(10) | C(35)-C(36) | 1.376(11) | C(35)-C(36) | 1.396(10) |
| C(35)-H(35) | 0.9300 | C(35)-H(35) | 0.9300 | C(35)-H(35) | 0.9300 |
| C(36)-C(37) | 1.395(9) | C(36)-C(37) | 1.415(10) | C(36)-C(37) | 1.393(10) |
| C(36)-H(36) | 0.9300 | C(36)-H(36) | 0.9300 | C(36)-H(36) | 0.9300 |
| C(37)-H(37) | 0.9300 | C(37)-H(37) | 0.9300 | C(37)-H(37) | 0.9300 |
| C(38)-C(39) | 1.315(10) | C(38)-C(39) | 1.341(11) | C(38)-C(39) | 1.29(4) |
| C(38)-H(38) | 0.9300 | C(38)-H(38) | 0.9300 | C(38)-H(38) | 0.9300 |
| C(39)-H(39) | 0.9300 | C(39)-H(39) | 0.9300 | C(39)-H(39) | 0.9300 |
|  |  |  |  | O(7)-C(40) | 1.427(10) |
|  |  |  |  | O(7)-H(7) | 0.8200 |
|  |  |  |  | O(8)-C(42) | 1.435(10) |
|  |  |  |  | O(8)-H(8) | 0.8200 |
|  |  |  |  | C(40)-C(41) | 1.527(10) |
|  |  |  |  | C(40)-H(40A) | 0.9700 |
|  |  |  |  | C(40)-H(40B) | 0.9700 |
|  |  |  |  | C(41)-H(41A) | 0.9600 |
|  |  |  |  | C(41)-H(41B) | 0.9600 |
|  |  |  |  | C(41)-H(41C) | 0.9600 |
|  |  |  |  | C(42)-C(43) | 1.528(10) |
|  |  |  |  | C(42)-H(42A) | 0.9700 |
|  |  |  |  | C(42)-H(42B) | 0.9700 |
|  |  |  |  | C(43)-H(43A) | 0.9600 |
|  |  |  |  | C(43)-H(43B) | 0.9600 |
|  |  |  |  | C(43)-H(43C) | 0.9600 |

**Table S5.** Experimental and smoothed isobaric molar heat capacities of compounds 1 and 2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **T(K)** | **Compound 1**  ***C*p.m(J·mol-1·K-1)** | | **Compound 2**  ***C*p.m(J·mol-1·K-1)** | |
| **Exp.** | **smoothed** | **Exp.** | **smoothed** |
| 293.15 | 1510.81 | 1510.40 | 1503.49 | 1503.78 |
| 296.15 | 1522.92 | 1523.46 | 1517.99 | 1517.91 |
| 299.15 | 1535.88 | 1536.65 | 1532.59 | 1532.07 |
| 302.15 | 1549.03 | 1549.95 | 1545.61 | 1546.27 |
| 305.15 | 1564.00 | 1563.36 | 1561.42 | 1560.5 |
| 308.15 | 1578.03 | 1576.87 | 1576.09 | 1574.77 |
| 311.15 | 1590.99 | 1590.47 | 1588.16 | 1589.06 |
| 314.15 | 1604.80 | 1604.16 | 1603.55 | 1603.38 |
| 317.15 | 1618.86 | 1617.93 | 1616.92 | 1617.72 |
| 320.15 | 1632.14 | 1631.77 | 1632.02 | 1632.08 |
| 323.15 | 1646.13 | 1645.67 | 1644.39 | 1646.46 |
| 326.15 | 1657.52 | 1659.63 | 1660.20 | 1660.85 |
| 329.15 | 1671.51 | 1673.63 | 1674.20 | 1675.25 |
| 332.15 | 1686.99 | 1687.68 | 1689.77 | 1689.66 |
| 335.15 | 1702.30 | 1701.76 | 1705.18 | 1704.08 |
| 338.15 | 1715.94 | 1715.87 | 1720.02 | 1718.50 |
| 341.15 | 1730.28 | 1730.00 | 1734.04 | 1732.92 |
| 344.15 | 1744.57 | 1744.14 | 1749.24 | 1747.33 |
| 347.15 | 1758.61 | 1758.29 | 1762.26 | 1761.75 |
| 350.15 | 1772.12 | 1772.43 | 1776.15 | 1776.15 |
| 353.15 | 1787.13 | 1786.56 | 1790.58 | 1790.55 |
| 356.15 | 1800.95 | 1800.68 | 1803.68 | 1804.93 |
| 359.15 | 1815.30 | 1814.77 | 1817.90 | 1819.30 |
| 362.15 | 1828.92 | 1828.83 | 1832.56 | 1833.64 |
| 365.15 | 1843.15 | 1842.85 | 1847.13 | 1847.97 |
| 368.15 | 1855.03 | 1856.82 | 1862.18 | 1862.27 |
| 371.15 | 1871.27 | 1870.74 | 1877.27 | 1876.54 |
| 374.15 | 1884.68 | 1884.60 | 1891.73 | 1890.79 |

**Table S6.** Thermodynamical function values of compound 1 and compound 2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **T(K)** | **HT-H298.15/(kJ·mol-1)** | | **ST-S298.15/(kJ·mol-1)** | |
| **Compound 1** | **Compound 2** | **Compound 1** | **Compound 2** |
| 293.15 | -7.62 | -7.59 | -25.78 | -25.68 |
| 296.15 | -3.07 | -3.06 | -10.33 | -10.30 |
| 299.15 | 1.55 | 1.54 | 5.19 | 5.17 |
| 302.15 | 6.18 | 6.163 | 20.59 | 20.53 |
| 305.15 | 10.85 | 10.82 | 35.97 | 35.88 |
| 308.15 | 15.56 | 15.52 | 51.33 | 51.22 |
| 311.15 | 20.31 | 20.27 | 66.67 | 66.54 |
| 314.15 | 25.103 | 25.06 | 82.00 | 81.86 |
| 317.15 | 29.93 | 29.89 | 97.31 | 97.16 |
| 320.15 | 34.81 | 34.76 | 112.61 | 112.46 |
| 323.15 | 39.72 | 39.68 | 127.89 | 127.75 |
| 326.15 | 44.68 | 44.64 | 143.16 | 143.03 |
| 329.15 | 49.68 | 49.65 | 158.42 | 158.31 |
| 332.15 | 54.72 | 54.69 | 173.67 | 173.57 |
| 335.15 | 59.81 | 59.78 | 188.91 | 188.83 |
| 338.15 | 64.93 | 64.92 | 204.14 | 204.08 |
| 341.15 | 70.10 | 70.09 | 219.36 | 219.32 |
| 344.15 | 75.31 | 75.32 | 234.56 | 234.56 |
| 347.15 | 80.57 | 80.58 | 249.76 | 249.78 |
| 350.15 | 85.86 | 85.89 | 264.95 | 265 |
| 353.15 | 91.20 | 91.24 | 280.14 | 280.22 |
| 356.15 | 96.58 | 96.63 | 295.31 | 295.43 |
| 359.15 | 102.01 | 102.07 | 310.47 | 310.63 |
| 362.15 | 107.47 | 107.55 | 325.63 | 325.82 |
| 365.15 | 112.98 | 113.07 | 340.77 | 341.01 |
| 368.15 | 118.53 | 118.63 | 355.91 | 356.18 |
| 371.15 | 124.12 | 124.24 | 371.03 | 371.36 |
| 374.15 | 129.75 | 129.89 | 386.15 | 386.52 |