Supporting Information

Improved NMR transfer of magnetization from protons to half-integer spin quadrupolar nuclei at moderate and high MAS frequencies

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Figure S1: ¹H MAS spectrum of AlPO₄-14. The spectrum was acquired at $B_0 = 18.8$ T and $v_R = 20$ kHz by averaging 16 transients separated by a recycle interval of 1 s, using the DEPTH pulse sequence for probe background suppression, with $v_1 \approx 208$ kHz.



Figure S2: Variation at $v_R = 20$ kHz of ²⁷AlO₄ signal of AlPO₄-14 as function of v_1 or $v_{1,max}$ of the recoupling for PRESTO-R22⁷₂(180₀) and -R18⁵₂(180₀) as well as RINEPT-SR4²₁ (tt), -SR4²₁ (270₀90₁₈₀) and -R12⁵₃ (270₀90₁₈₀). For each curve τ was fixed to its optimum value given in Table 6.



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65 Figure S3: Variation at $v_R = 20$ kHz of ²⁷AlO4 signal of AlPO4-14 as function of offset of the recoupling for PRESTO-R22⁷₂(180₀) and -R18⁵₂(180₀) as well as RINEPT-SR4²₁ (tt), -SR4²₁ (270₀90₁₈₀) and -R12⁵₃ (270₀90₁₈₀). For each curve τ and v_1 or $v_{1,max}$ were fixed to their optimum values given in Table 5.



Figure S4: Variation at $v_R = 62.5$ kHz of 27 AlO₄ signal of AlPO₄-14 as function of v_1 or $v_{1,max}$ of the recoupling for PRESTO-R16 ${}^6_7(270_090_{180})$ and -R14 ${}^5_6(270_090_{180})$ as well as RINEPT-SR4 2_1 (tt), -SR4 2_1 (270 ${}^0_090_{180}$) and -R12 5_3 (270 ${}^0_090_{180}$). For each curve τ was fixed to its optimum value given in Table 8.



100 Figure S5: Variation at $v_R = 62.5$ kHz of ²⁷AlO₄ signal of AlPO₄-14 as function of offset of the recoupling for PRESTO-R16⁶₇(270₀90₁₈₀) and -R14⁵₆(270₀90₁₈₀) as well as RINEPT-SR4²₁ (tt), -SR4²₁ (270₀90₁₈₀) and -R12⁵₃ (270₀90₁₈₀). For each curve τ and v_1 or $v_{1,max}$ were fixed to their optimum values given in Table 8.

Table S1. Distances between the different hydrogen atoms and their closest Al neighbours in the structure of isopropylamine templated AlPO₄-14 determined from X-ray diffraction. (Broach et al., 2003) The H and Al atoms are numbered according to the cif file.

| | Н | Al | $r_{ m HAl}/{ m \AA}$ |
|--|-------------------------------------|-------------------|-----------------------|
| | H1 (OH) | Al4O ₆ | 2.496 |
| | | Al4O ₆ | 2.499 |
| | | Al1O ₅ | 2.503 |
| | | Al2O ₄ | 4.299 |
| | H2 (NH ₃) | Al4O ₆ | 3.069 |
| | | Al2O ₄ | 3.779 |
| | | A13O ₄ | 3.778 |
| | 113 (1113) | Al4O ₆ | 3.960 |
| | H4 (NH ₃) | Al2O ₄ | 3.479 |
| | | Al1O ₅ | 3.801 |
| | H5 (CH) | Al2O ₄ | 3.737 |
| | III5 (CII) | Al1O ₅ | 4.850 |
| | H6 (CH _a), | Al1O ₅ | 3.655 |
| | | A13O ₄ | 4.594 |
| | | A13O ₄ | 4.082 |
| | | Al105 | 4.320 |
| | H8 (CH ₃) ₁ | Al2O ₄ | 3.772 |
| | | A13O ₄ | 4.651 |
| | H9 (CH ₃) ₂ | Al4O ₆ | 3.888 |
| | | A13O ₄ | 4.124 |
| | H10 (CH ₂) ₂ | Al4O ₆ | 3.509 |
| | | A13O ₄ | 4.502 |
| | H11 (CH ₃) ₂ | Al4O ₆ | 3.970 |
| | | A13O ₄ | 4.048 |

Broach, R. W., Wilson, S. T. and Kirchner, R. M.: Corrected crystallographic tables and figure for as-synthesized AlPO₄-14, Microporous and Mesoporous Materials, 57(2), 211–214, https://doi.org/10.1016/S1387-1811(02)00563-2, 2003.