Supporting Information

A Double Quantum ^{129}Xe NMR Experiment for Probing Xenon in Multiply Occupied Cavities of Solid-State Inclusion Compounds

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Physical Chemistry Chemical Physics

Table S1. Lennard-Jones interaction parameters used for Dianin's compound (4-*p*-hydroxyphenyl-2,2,4-trimethyl-chroman) and xenon guests in the MD simulations. The AMBER force field atom types for the atoms of the compound are given. The intermolecular potential parameters between unlike atoms are determined from standard combination rules.

Atom (assignment)	σ_{ii}^0 (Å)	ε_{ii}^0 (kcal/mol)
OH (hydroxyl oxygen)	3.0665	0.2104
OS (ether oxygen)	3.0000	0.7128
C3 (alkyl carbons)	3.3997	0.1094
CA (aromatic carbons)	3.3997	0.0860
HC (alkyl hydrogens)	2.6494	0.0157
HA (aromatic hydrogens)	2.5996	0.0150
Xe	4.0990	1.8480

Table S2. Cartesian coordinates (from X-ray structure analysis) and electrostatic point charges determined from CHELPG calculations at the HF/6-31G* level for Dianin's compound.

Atom	Cartesian coordinates (Å)	CHELPG charges (*e*)
H	-0.773 2.680 11.000	0.438817
O	0.126 2.764 10.704	-0.657397
O	-1.180 6.097 4.088	-0.598939
C	0.200 3.740 9.732	0.466222
C	1.409 4.066 9.126	-0.265853
C	1.447 5.023 8.135	-0.119218
C	0.293 5.690 7.690	-0.079688
C	-0.903 5.354 8.343	-0.011125
C	-0.948 4.406 9.339	-0.386271
C	0.379 6.699 6.549	0.528714
C	0.938 6.073 5.258	-0.346496
C	-0.040 5.243 4.446	0.855634
C	-1.658 6.950 5.046	0.399179
C	-0.982 7.308 6.215	-0.229518
C	-1.584 8.248 7.056	-0.033620
C	-2.811 8.824 6.753	-0.213864
C	-3.465 8.448 5.591	-0.055530
C	-2.900 7.542 4.725	-0.279596
C	-0.577 4.014 5.150	-0.304210

C	0.578 4.875 3.115	-0.448283
C	1.355 7.839 6.956	-0.465786
H	2.324 3.557 9.437	0.162460
H	2.392 5.266 7.678	0.132127
H	-1.797 5.874 8.082	0.074718
H	-1.892 4.166 9.819	0.159561
H	1.297 6.880 4.631	0.059247
H	1.797 5.453 5.854	0.022817
H	-1.094 8.542 7.995	0.076860
H	-3.283 9.572 7.438	0.122090
H	-4.432 8.893 5.374	0.107283
H	-3.405 7.302 3.790	0.159057
H	-1.135 3.417 4.533	0.088767
H	-1.257 4.376 5.920	0.039978
H	0.324 3.510 5.592	0.017328
H	1.486 4.259 3.288	0.062264
H	0.865 5.570 2.490	0.151320
H	-0.270 4.212 2.643	0.067197
H	1.581 8.402 6.182	0.136813
H	1.081 8.519 7.831	0.099152
H	2.256 7.278 7.263	0.067787