

Electronic Supporting Information for

Properties of CB7CB-D₄ as derived from ¹²⁹Xe and ²H NMR experiments and computations

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Table S1. Optimised geometry (in Å) of 5CB in the .xyz format at the PBE0+D4/def2-TZVP level.

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N	-8.8217392	0.4787990	-0.5914383
C	2.9521194	0.0885639	-0.1476724
C	2.1759280	-0.6780437	0.9206281
C	4.4572243	-0.0317606	0.0126594
C	0.6928141	-0.5492852	0.7530972
C	5.2385075	0.7287099	-1.0459869
C	-0.0224140	-1.4512849	-0.0283154
C	-0.0057398	0.5037843	1.3356480
C	-2.0816966	-0.2503414	0.3585461
C	6.7425079	0.6022235	-0.8774655
C	-1.3846000	-1.3088954	-0.2214223
C	-1.3666209	0.6548873	1.1412463
C	-3.5298707	-0.0946770	0.1546538
C	-4.3684376	-1.2088036	0.0870705
C	-4.1015253	1.1722473	0.0232562
C	-5.7280450	-1.0684913	-0.1046048
C	-5.4595725	1.3264452	-0.1684882
C	-6.2840587	0.2037499	-0.2339304
C	-7.6873501	0.3558233	-0.4316918
H	2.6587342	1.1441983	-0.1146643
H	2.6542211	-0.2760046	-1.1375432
H	2.4677439	-0.3096905	1.9095715
H	2.4603273	-1.7345942	0.8826394
H	4.7476155	0.3300559	1.0071505
H	4.7431427	-1.0908243	-0.0168411
H	4.9514059	1.7861049	-1.0149521
H	4.9466348	0.3663050	-2.0384187
H	0.4998353	-2.2792451	-0.4970540
H	0.5261228	1.2123860	1.9625140
H	7.0589519	-0.4429788	-0.9368547
H	7.2820423	1.1564488	-1.6486884
H	7.0636861	0.9874372	0.0944231
H	-1.9119852	-2.0151638	-0.8526721
H	-1.8897933	1.4686326	1.6306944
H	-3.9490606	-2.1997270	0.2129998
H	-3.4650781	2.0486592	0.0464664
H	-6.3706647	-1.9391284	-0.1462464
H	-5.8913127	2.3134781	-0.2783138

Table S2. Optimised geometry (in Å) of CB7CB in the .xyz format at the PBE0+D4/def2-TZVP level.

65

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N -13.3705334 -0.5307434 2.2333518
C -1.5984603 -1.1472871 2.1400103
C -2.3333067 -1.7815629 3.3184342
C -0.0896731 -1.2864151 2.2392562
C -3.8204926 -1.6359303 3.2106734
C 0.6499356 -0.6562675 1.0716957
C -4.5914154 -2.5995267 2.5683391
C -4.4682332 -0.5097023 3.7088587
C -6.6053110 -1.3148331 2.9232642
C 2.1589854 -0.7983825 1.1716229
C -5.9589206 -2.4461692 2.4283325
C -5.8342769 -0.3478288 3.5664897
C -8.0590084 -1.1473536 2.7754581
C -8.9204474 -2.2414938 2.8734470
C -8.6127034 0.1110576 2.5330728
C -10.2853243 -2.0899805 2.7351351
C -9.9757527 0.2762506 2.3928715
C -10.8232828 -0.8264704 2.4932711
C -12.2319116 -0.6629552 2.3495375
H -1.8700229 -0.0872191 2.0773571
H -1.9525706 -1.6042537 1.2087947
H -1.9849907 -1.3204859 4.2484937
H -2.0708102 -2.8428447 3.3766606
H 0.2567378 -0.8324011 3.1761409
H 0.1740638 -2.3494255 2.3049696
H 0.3882388 0.4070608 1.0066605
H 0.3032715 -1.1089497 0.1345579
H -4.1094049 -3.4855743 2.1676157
H -3.8916510 0.2492252 4.2280668
C 2.9001313 -0.1682460 0.0056488
H 2.5050015 -0.3464549 2.1096705
H -6.5313857 -3.2035113 1.9047488
H -6.3165761 0.5261541 3.9895663
H -8.5137292 -3.2225497 3.0874370
H -7.9596211 0.9689950 2.4274827
H -10.9455091 -2.9439485 2.8221867
H -10.3941693 1.2554228 2.1958374
H 2.4199917 -1.8621343 1.2363563
H 2.6484759 0.8964078 -0.0620433
H 2.5620119 -0.6178306 -0.9350538
C 4.4158201 -0.3169037 0.1136576
H 5.3215773 2.2343685 -0.1172626
C 5.5104717 1.6491092 -1.0115652
C 5.1362826 0.3093174 -1.0410815
C 5.4109635 -0.4181557 -2.1947374
H 5.1256866 -1.4642193 -2.2441539
C 6.0370615 0.1688130 -3.2793852
H 6.2199350 -0.4169745 -4.1731718
C 6.4068080 1.5124022 -3.2499127
C 6.1313331 2.2431629 -2.0952276
H 6.4378227 3.2813305 -2.0335273
H 6.0594394 4.0211330 -4.1897309
C 6.7943306 3.4612964 -4.7556173
C 7.0726314 2.1400495 -4.4013075
C 7.9985939 1.4305006 -5.1679738
H 8.2485363 0.4125579 -4.8940942
C 8.6262653 2.0141100 -6.2497375
H 9.3499465 1.4577414 -6.8323301
C 8.3376955 3.3348273 -6.5910604
C 8.9825666 3.9436390 -7.7069927
C 7.4150934 4.0567518 -5.8348698
H 7.1852464 5.0794474 -6.1068535
N 9.5038989 4.4356727 -8.6090123
H 4.6692470 -1.3804314 0.1720396
H 4.7553961 0.1386122 1.0496313
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Table S3. Optimised geometry (in Å) of CB7CB in the .xyz format at the PBE0+D4/def2-SVP level.

65

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N 0.17178851 -3.74452000 12.89604795
C -0.08529369 1.87866446 2.53823693
C -0.12857594 2.72614158 3.80744814
C -0.12698498 2.71117468 1.26905067
C -0.08933459 1.89398889 5.05264899
C -0.08635989 1.87591940 0.00098018
C 1.11968380 1.55507502 5.65168595
C -1.25881312 1.39683366 5.61948463
C -0.01090549 0.24860201 7.33901552
C -0.12591671 2.71055179 -1.26757705
C 1.16123427 0.75009579 6.77572902
C -1.22327896 0.58650636 6.73959817
C 0.02896202 -0.60860358 8.53347829
C 0.95898906 -0.38020352 9.54920703
C -0.86302210 -1.67246533 8.68007309
C 1.00100390 -1.18181058 10.67198764
C -0.83165260 -2.48150336 9.79780380
C 0.10334055 -2.24066071 10.80386721
C 0.14120966 -3.07228226 11.96084741
H -0.92594521 1.17537493 2.54846830
H 0.82186184 1.26357483 2.54866147
H -1.03817061 3.33566693 3.80088304
H 0.71609866 3.42265001 3.80362735
H -1.03413959 3.32838798 1.26840506
H 0.71506090 3.41461137 1.26761124
H -0.92917900 1.17375290 0.00083477
H 0.81982552 1.25773483 0.00148733
H 2.04638467 1.92715144 5.22650557
H -2.21599252 1.65953542 5.18040556
C -0.08623733 1.87716845 -2.53634126
H -1.03190668 3.32948702 -1.26698175
H 2.11912544 0.48526920 7.20901254
H -2.15173105 0.23676247 7.17675760
H 1.64276536 0.45613712 9.46755898
H -1.57534797 -1.88288564 7.89137956
H 1.72038356 -0.99023177 11.45841866
H -1.52207509 -3.30980713 9.89731636
H 0.71746886 3.41239426 -1.26686474
H -0.92945936 1.17697677 -2.54676206
H 0.81864195 1.25871722 -2.54550560
C -0.12506320 2.72405456 -3.80612628
H -2.21493861 1.68550486 -5.19772441
C -1.25751945 1.41025129 -5.62850357
C -0.08663242 1.89142622 -5.05107391
C 1.12308451 1.53668220 -5.63957222
H 2.05087263 1.89616753 -5.20592090
C 1.16378311 0.73207113 -6.76382150
H 2.12179444 0.45470929 -7.18894372
C -0.00996820 0.24692315 -7.33806218
C -1.22294900 0.60040554 -6.74906041
H -2.15213300 0.26359925 -7.19483319
H -1.59747451 -1.86307123 -7.90850137
C -0.87518078 -1.66061646 -8.69017480
C 0.02931072 -0.60894746 -8.53343433
C 0.97155061 -0.39111713 -9.54010079
H 1.66543063 0.43603689 -9.45046086
C 1.01342904 -1.19120378 -10.66388528
H 1.74250891 -1.00787205 -11.44331241
C 0.10316957 -2.23777484 -10.80595830
C 0.14085232 -3.06773781 -11.96421422
C -0.84413934 -2.46797761 -9.80905993
H -1.54444710 -3.28694507 -9.91663513
N 0.17136958 -3.73853280 -12.90049766
H 0.72205732 3.41766064 -3.80140777
H -1.03251696 3.33671968 -3.80138432
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Table S4. Computational data used in conformational averaging the magnetizability (susceptibility) tensor in CB7CB, obtained at the PBE0+D4/def2-SVP level.

ϕ_1	ϕ_2	$E/\text{a.u.}$	E/J	$\exp(-E/k_B T)$	weight	$\Delta\xi$	$\Delta\xi \times \text{weight}$	ξ_{iso}	$\xi_{\text{iso}} \times \text{weight}$
90	90	-1382.4046	5.84E-24	0.99859216	0.0375	-54.37	-2.04	-5159.90	-193.56
90	120	-1382.4040	2.89E-21	0.49732892	0.0187	433.24	8.09	-5153.86	-96.29
90	150	-1382.4031	6.84E-21	0.19169251	0.0072	801.09	5.77	-5160.46	-37.16
90	180	-1382.4032	6.35E-21	0.21569985	0.0081	819.09	6.64	-5164.92	-41.85
90	210	-1382.4030	6.98E-21	0.18546569	0.0070	522.58	3.64	-5163.16	-35.97
90	240	-1382.4039	3.06E-21	0.47788301	0.0180	72.31	1.30	-5156.22	-92.56
90	270	-1382.4046	3.72E-23	0.99106956	0.0372	-78.55	-2.92	-5158.10	-192.03
90	300	-1382.4040	2.81E-21	0.50725247	0.0191	392.23	7.47	-5153.88	-98.21
90	330	-1382.4031	6.87E-21	0.19058217	0.0072	807.36	5.78	-5161.31	-36.95
90	360	-1382.4032	6.35E-21	0.21577710	0.0081	819.02	6.64	-5164.61	-41.86
90	390	-1382.4030	7.00E-21	0.18471224	0.0069	538.32	3.74	-5163.05	-35.83
90	420	-1382.4040	2.97E-21	0.48775668	0.0183	15.34	0.28	-5155.16	-94.46
120	90	-1382.4039	3.03E-21	0.48152557	0.0181	398.11	7.20	-5157.27	-93.29
120	120	-1382.4033	5.90E-21	0.24054370	0.0090	428.66	3.87	-5157.27	-46.60
120	150	-1382.4024	9.87E-21	0.09228579	0.0035	935.68	3.24	-5155.61	-17.87
120	180	-1382.4025	9.39E-21	0.10351331	0.0039	925.54	3.60	-5160.98	-20.07
120	210	-1382.4023	1.00E-20	0.08879371	0.0033	617.51	2.06	-5159.19	-17.21
120	240	-1382.4032	6.10E-21	0.22930056	0.0086	211.66	1.82	-5152.00	-44.38
120	270	-1382.4039	3.05E-21	0.47893826	0.0180	60.62	1.09	-5153.86	-92.72
120	300	-1382.4033	5.82E-21	0.24544400	0.0092	514.60	4.74	-5149.46	-47.48
120	330	-1382.4024	9.90E-21	0.09168893	0.0034	942.99	3.25	-5156.44	-17.76
120	360	-1382.4025	9.39E-21	0.10358743	0.0039	925.09	3.60	-5160.73	-20.08
120	390	-1382.4023	1.00E-20	0.08848158	0.0033	630.89	2.10	-5158.86	-17.15
120	420	-1382.4033	6.02E-21	0.23402052	0.0088	154.92	1.36	-5151.03	-45.28
150	90	-1382.4030	6.95E-21	0.18654913	0.0070	-53.86	-0.38	-5159.90	-36.16
150	120	-1382.4024	9.83E-21	0.09328674	0.0035	974.37	3.41	-5152.58	-18.06
150	150	-1382.4015	1.38E-20	0.03558657	0.0013	1307.13	1.75	-5157.90	-6.90
150	180	-1382.4016	1.33E-20	0.04006921	0.0015	1251.33	1.88	-5162.35	-7.77
150	210	-1382.4014	1.40E-20	0.03430499	0.0013	936.52	1.21	-5162.26	-6.65
150	240	-1382.4023	1.00E-20	0.08896411	0.0033	610.19	2.04	-5153.94	-17.22
150	270	-1382.4030	6.96E-21	0.18612258	0.0070	514.89	3.60	-5157.79	-36.06
150	300	-1382.4024	9.74E-21	0.09518643	0.0036	944.63	3.38	-5152.04	-18.42
150	330	-1382.4015	1.38E-20	0.03540687	0.0013	1313.54	1.75	-5158.79	-6.86
150	360	-1382.4016	1.33E-20	0.04007078	0.0015	1251.02	1.88	-5162.44	-7.77
150	390	-1382.4014	1.40E-20	0.03413843	0.0013	950.13	1.22	-5163.39	-6.62
150	420	-1382.4024	9.93E-21	0.09093177	0.0034	559.84	1.91	-5153.64	-17.60
180	90	-1382.4032	6.33E-21	0.21683890	0.0081	845.02	6.88	-5170.10	-42.11
180	120	-1382.4025	9.23E-21	0.10764055	0.0040	1251.45	5.06	-5161.85	-20.87
180	150	-1382.4016	1.32E-20	0.04106344	0.0015	1563.90	2.41	-5166.48	-7.97
180	180	-1382.4017	1.28E-20	0.04602470	0.0017	1547.41	2.68	-5173.44	-8.94
180	210	-1382.4016	1.34E-20	0.03974334	0.0015	1263.09	1.89	-5171.78	-7.72

ϕ_1	ϕ_2	$E/\text{a.u.}$	E/J	$\exp(-E/k_B T)$	weight	$\Delta\xi$	$\Delta\xi \times \text{weight}$	ξ_{iso}	$\xi_{\text{iso}} \times \text{weight}$
180	240	-1382.4025	9.39E-21	0.10354626	0.0039	928.55	3.61	-5164.02	-20.09
180	270	-1382.4032	6.35E-21	0.21577989	0.0081	822.83	6.67	-5166.11	-41.88
180	300	-1382.4025	9.15E-21	0.10979736	0.0041	1220.81	5.04	-5161.89	-21.29
180	330	-1382.4016	1.33E-20	0.04080060	0.0015	1569.90	2.41	-5167.16	-7.92
180	360	-1382.4017	1.27E-20	0.04605638	0.0017	1545.81	2.67	-5172.69	-8.95
180	390	-1382.4016	1.34E-20	0.03957467	0.0015	1275.85	1.90	-5171.56	-7.69
180	420	-1382.4025	9.31E-21	0.10565075	0.0040	887.75	3.52	-5162.93	-20.49
210	90	-1382.4031	6.84E-21	0.19194280	0.0072	827.83	5.97	-5161.19	-37.21
210	120	-1382.4024	9.77E-21	0.09463726	0.0036	1237.48	4.40	-5159.33	-18.34
210	150	-1382.4015	1.38E-20	0.03613966	0.0014	1531.22	2.08	-5162.59	-7.01
210	180	-1382.4016	1.33E-20	0.04054448	0.0015	1571.52	2.39	-5172.11	-7.88
210	210	-1382.4015	1.39E-20	0.03524911	0.0013	1319.65	1.75	-5164.01	-6.84
210	240	-1382.4024	9.92E-21	0.09111185	0.0034	943.45	3.23	-5158.60	-17.66
210	270	-1382.4031	6.90E-21	0.18903720	0.0071	810.70	5.76	-5161.49	-36.65
210	300	-1382.4024	9.69E-21	0.09634193	0.0036	1201.81	4.35	-5159.85	-18.67
210	330	-1382.4015	1.38E-20	0.03595599	0.0014	1536.55	2.08	-5163.19	-6.97
210	360	-1382.4016	1.33E-20	0.04057240	0.0015	1570.97	2.39	-5171.78	-7.88
210	390	-1382.4015	1.39E-20	0.03512266	0.0013	1329.16	1.75	-5163.89	-6.81
210	420	-1382.4024	9.83E-21	0.09312110	0.0035	902.09	3.16	-5157.30	-18.04
240	90	-1382.4040	2.86E-21	0.50143577	0.0188	466.83	8.79	-5157.61	-97.15
240	120	-1382.4033	5.77E-21	0.24839193	0.0093	921.47	8.60	-5152.27	-48.08
240	150	-1382.4024	9.73E-21	0.09536329	0.0036	1230.71	4.41	-5158.21	-18.48
240	180	-1382.4025	9.21E-21	0.10833538	0.0041	1254.29	5.10	-5162.80	-21.01
240	210	-1382.4024	9.81E-21	0.09364955	0.0035	985.35	3.47	-5161.83	-18.16
240	240	-1382.4033	5.89E-21	0.24146348	0.0091	566.40	5.14	-5153.24	-46.74
240	270	-1382.4040	2.87E-21	0.50014175	0.0188	444.41	8.35	-5155.54	-96.86
240	300	-1382.4033	5.68E-21	0.25352492	0.0095	879.59	8.38	-5152.20	-49.07
240	330	-1382.4024	9.76E-21	0.09477969	0.0036	1233.49	4.39	-5159.13	-18.37
240	360	-1382.4025	9.20E-21	0.10840603	0.0041	1254.30	5.11	-5162.70	-21.02
240	390	-1382.4024	9.83E-21	0.09323168	0.0035	999.43	3.50	-5161.83	-18.08
240	420	-1382.4033	5.80E-21	0.24649559	0.0093	520.75	4.82	-5152.20	-47.71
270	90	-1382.4046	0.00E+00	1.00000000	0.0376	-28.96	-1.09	-5159.82	-193.83
270	120	-1382.4040	2.89E-21	0.49789844	0.0187	459.63	8.60	-5153.92	-96.40
270	150	-1382.4031	6.84E-21	0.19181978	0.0072	819.71	5.91	-5160.45	-37.18
270	180	-1382.4032	6.35E-21	0.21611864	0.0081	839.97	6.82	-5164.96	-41.93
270	210	-1382.4030	6.97E-21	0.18589101	0.0070	546.62	3.82	-5163.30	-36.06
270	240	-1382.4039	3.05E-21	0.47882582	0.0180	93.85	1.69	-5156.11	-92.74
270	270	-1382.4046	2.96E-23	0.99288279	0.0373	-55.84	-2.08	-5157.97	-192.38
270	300	-1382.4040	2.81E-21	0.50782597	0.0191	413.52	7.89	-5153.93	-98.32
270	330	-1382.4031	6.86E-21	0.19074762	0.0072	826.02	5.92	-5161.23	-36.98
270	360	-1382.4032	6.34E-21	0.21628291	0.0081	839.35	6.82	-5164.60	-41.96
270	390	-1382.4030	6.98E-21	0.18524485	0.0070	560.93	3.90	-5163.20	-35.93

ϕ_1	ϕ_2	$E/\text{a.u.}$	E/J	$\exp(-E/k_B T)$	weight	$\Delta\xi$	$\Delta\xi \times \text{weight}$	ξ_{iso}	$\xi_{\text{iso}} \times \text{weight}$
270	420	-1382.4040	2.96E-21	0.48886987	0.0184	36.30	0.67	-5154.91	-94.67
300	90	-1382.4040	2.94E-21	0.49148339	0.0185	35.22	0.65	-5156.19	-95.20
300	120	-1382.4033	5.82E-21	0.24557807	0.0092	515.12	4.75	-5149.74	-47.51
300	150	-1382.4024	9.79E-21	0.09415998	0.0035	896.74	3.17	-5155.85	-18.24
300	180	-1382.4025	9.30E-21	0.10576701	0.0040	882.70	3.51	-5161.82	-20.51
300	210	-1382.4024	9.94E-21	0.09071176	0.0034	568.05	1.94	-5159.95	-17.58
300	240	-1382.4033	6.01E-21	0.23406425	0.0088	163.23	1.44	-5152.51	-45.30
300	270	-1382.4040	2.96E-21	0.48923627	0.0184	10.79	0.20	-5154.53	-94.73
300	300	-1382.4033	5.73E-21	0.25055478	0.0094	474.67	4.47	-5149.88	-48.47
300	330	-1382.4024	9.81E-21	0.09356906	0.0035	904.69	3.18	-5156.68	-18.13
300	360	-1382.4025	9.30E-21	0.10584296	0.0040	881.72	3.51	-5161.41	-20.52
300	390	-1382.4024	9.96E-21	0.09038066	0.0034	580.68	1.97	-5159.74	-17.52
300	420	-1382.4033	5.93E-21	0.23896255	0.0090	101.13	0.91	-5151.53	-46.24
330	90	-1382.4030	6.98E-21	0.18540278	0.0070	551.09	3.84	-5161.74	-35.95
330	120	-1382.4024	9.85E-21	0.09281319	0.0035	986.88	3.44	-5152.73	-17.97
330	150	-1382.4015	1.38E-20	0.03538307	0.0013	1315.53	1.75	-5158.52	-6.86
330	180	-1382.4016	1.33E-20	0.03983785	0.0015	1261.06	1.89	-5162.46	-7.73
330	210	-1382.4014	1.40E-20	0.03412518	0.0013	947.91	1.22	-5162.40	-6.62
330	240	-1382.4023	1.00E-20	0.08854906	0.0033	621.64	2.07	-5154.38	-17.15
330	270	-1382.4030	6.99E-21	0.18508348	0.0070	534.74	3.72	-5158.09	-35.86
330	300	-1382.4024	9.76E-21	0.09471303	0.0036	957.95	3.41	-5152.29	-18.33
330	330	-1382.4015	1.39E-20	0.03521698	0.0013	1323.56	1.75	-5159.21	-6.83
330	360	-1382.4016	1.33E-20	0.03985466	0.0015	1261.00	1.89	-5162.53	-7.73
330	390	-1382.4014	1.40E-20	0.03396962	0.0013	958.24	1.22	-5163.52	-6.59
330	420	-1382.4024	9.95E-21	0.09049510	0.0034	575.30	1.96	-5154.11	-17.52
360	90	-1382.4032	6.33E-21	0.21691025	0.0081	844.89	6.88	-5169.76	-42.12
360	120	-1382.4025	9.23E-21	0.10763443	0.0040	1251.22	5.06	-5161.73	-20.87
360	150	-1382.4016	1.32E-20	0.04107432	0.0015	1564.23	2.41	-5166.57	-7.97
360	180	-1382.4017	1.28E-20	0.04602666	0.0017	1547.08	2.67	-5173.20	-8.94
360	210	-1382.4016	1.34E-20	0.03974908	0.0015	1263.06	1.89	-5171.81	-7.72
360	240	-1382.4025	9.39E-21	0.10351987	0.0039	928.56	3.61	-5163.82	-20.08
360	270	-1382.4032	6.35E-21	0.21584633	0.0081	821.53	6.66	-5166.12	-41.89
360	300	-1382.4025	9.15E-21	0.10979683	0.0041	1220.78	5.04	-5161.85	-21.29
360	330	-1382.4016	1.33E-20	0.04080159	0.0015	1570.30	2.41	-5167.16	-7.92
360	360	-1382.4017	1.27E-20	0.04605656	0.0017	1545.71	2.67	-5172.61	-8.95
360	390	-1382.4016	1.34E-20	0.03957669	0.0015	1275.80	1.90	-5171.57	-7.69
360	420	-1382.4025	9.31E-21	0.10566100	0.0040	887.80	3.52	-5162.95	-20.49
390	90	-1382.4031	6.86E-21	0.19067698	0.0072	833.36	5.97	-5161.25	-36.97
390	120	-1382.4024	9.79E-21	0.09411837	0.0035	1243.27	4.40	-5159.86	-18.24
390	150	-1382.4015	1.38E-20	0.03591645	0.0013	1535.65	2.07	-5163.08	-6.97
390	180	-1382.4016	1.33E-20	0.04030149	0.0015	1577.33	2.39	-5172.59	-7.83
390	210	-1382.4015	1.39E-20	0.03504915	0.0013	1324.31	1.74	-5164.37	-6.80

ϕ_1	ϕ_2	$E/\text{a.u.}$	E/J	$\exp(-E/k_B T)$	weight	$\Delta\xi$	$\Delta\xi \times \text{weight}$	ξ_{iso}	$\xi_{\text{iso}} \times \text{weight}$
390	240	-1382.4024	9.95E-21	0.09057027	0.0034	950.02	3.23	-5159.10	-17.55
390	270	-1382.4031	6.92E-21	0.18797570	0.0071	815.73	5.76	-5161.86	-36.45
390	300	-1382.4024	9.72E-21	0.09579774	0.0036	1208.30	4.35	-5160.35	-18.57
390	330	-1382.4015	1.38E-20	0.03572812	0.0013	1541.70	2.07	-5163.77	-6.93
390	360	-1382.4016	1.33E-20	0.04031934	0.0015	1576.84	2.39	-5172.26	-7.83
390	390	-1382.4015	1.39E-20	0.03490953	0.0013	1334.66	1.75	-5164.18	-6.77
390	420	-1382.4024	9.86E-21	0.09255646	0.0035	908.54	3.16	-5157.83	-17.93
420	90	-1382.4040	2.78E-21	0.51085638	0.0192	423.36	8.12	-5157.27	-98.97
420	120	-1382.4033	5.69E-21	0.25339842	0.0095	155.35	1.48	-5151.03	-49.03
420	150	-1382.4024	9.65E-21	0.09727624	0.0037	1193.18	4.36	-5158.18	-18.85
420	180	-1382.4025	9.12E-21	0.11048465	0.0042	1226.49	5.09	-5162.59	-21.43
420	210	-1382.4024	9.73E-21	0.09550361	0.0036	957.07	3.43	-5161.62	-18.52
420	240	-1382.4033	5.81E-21	0.24614275	0.0092	529.74	4.90	-5153.34	-47.65
420	270	-1382.4040	2.79E-21	0.50972085	0.0191	398.44	7.63	-5155.48	-98.72
420	300	-1382.4034	5.60E-21	0.25860832	0.0097	839.38	8.15	-5152.01	-50.05
420	330	-1382.4024	9.68E-21	0.09667446	0.0036	1198.18	4.35	-5159.07	-18.74
420	360	-1382.4025	9.12E-21	0.11054140	0.0042	1226.24	5.09	-5162.41	-21.44
420	390	-1382.4024	9.75E-21	0.09508901	0.0036	971.18	3.47	-5161.52	-18.44
420	420	-1382.4033	5.72E-21	0.25136557	0.0094	480.50	4.54	-5152.43	-48.65

Table S5. ^{129}Xe chemical shift relative to gaseous external xenon reference and linewidth (full width at half maximum).

T (K)	^{129}Xe chemical shift (ppm)	Linewidth $\nu_{1/2}$ (Hz)
393.102	202.09	19.49
387.598	203.81	23.42
386.4972	211.6	74.75
385.3964	213.57	46.6
384.2956	214.86	47.58
383.1948	215.9	39.7
380.9932	217.5	31.8
378.7916	218.81	29.02
376.59	219.94	24.58
374.3884	220.98	19.36
374.3884	222.19	16.82
373.2876	222.98	36.7
372.1868	223.68	31.99
371.086	224.28	27.07
369.9852	224.84	26.31
367.7836	225.83	23.06
365.582	226.73	22.52
363.3804	227.56	22.92
361.1788	228.37	22.84
358.9772	229.13	22.32
356.7756	229.86	23.62
354.574	230.57	24.64
352.3724	231.26	29.67
350.1708	231.91	28.19
347.9692	232.58	31.19
345.7676	233.23	36.6
343.566	233.85	36.23
341.3644	234.48	42.15
339.1628	235.1	43.69
336.9612	235.68	54.2
334.7596	236.56	62.69
332.558	237.12	71.5
330.3564	237.67	81.72
328.1548	238.26	89.64

Table S6. ^2H quadrupole splittings.

T (K)	Quadrupole splitting (kHz)	
388	26.4	
387	30.5	
386	33.5	
385	35.6	
384	37.1	
383	38.5	
382	39.5	
380	41.1	
379	41.7	
378	42.1	
377	42.7	
376	43.1	47.2
375	42.7	47.3
374	42.3	48.1
372	42.1	49.3
371	41.9	49.8
370	41.8	50.2
369	41.7	50.6
368	41.6	50.9
367	41.5	51.2
366	41.5	51.5
365	41.3	51.8
363	41.2	52.3
361	41.0	52.8
359	40.9	53.2
357	40.7	53.6
355	40.6	53.9
353	40.4	54.2
351	40.3	54.6
349	40.1	54.9
347	40.0	55.2
345	39.8	55.4
343	39.6	55.6
341	39.4	55.9
339	39.2	56.2
337	39.2	56.4
335	39.0	56.6
330	38.6	57.0
325	38.1	57.4
320	37.6	57.8
315	37.2	58.2
310	36.8	58.4
305	36.7	58.7