ChemistrySelect

Supporting Information

VT-NMR Analysis of Rotation-Inversion of *N*-(4-hydroxybutyl)-*N*-(2,2,2-trifluoroethyl) *tert*-butyl Carbamate: Utilizing the $-CH_2CF_3$ Appendage as a Reporter on *E*/*Z*-Isomerization

Brian Jameson and Rainer Glaser*

Supporting Information

VT-NMR Analysis of Rotation-Inversion of *N*-(4-hydroxybutyl)-*N*-(2,2,2-trifluoroethyl) *tert*-butyl carbamate: The $-CH_2CF_3$ Appendage as a Reporter on *E*/*Z*-Isomerization

Brian Jameson and Rainer Glaser[a]*

[a] Prof. Dr. Rainer Glaser*

Department of Chemistry, Missouri University of Science and Technology, Rolla, Missouri 65409, United States.

Table of Content

Table S1. Temperature Dependence of Lorentzian Parameters: ^{13}C Spectra of **1**[a],[b]

Temp.	$\omega_E(1)$	$\omega_Z(1)$	$\omega(1)$	$p_o(1)$	$I_L(1)$	$\langle\Delta I\rangle_1$	$\omega_E(2)$	$\omega_Z(2)$	$\omega(2)$	$p_o(2)$	$I_L(2)$	$\langle\Delta I\rangle_2$	$\langle\Delta I\rangle_S$
288	0.06	0.07	0.07	122.30	78.97	15.43	0.06	0.05	0.06	125.07	81.00	11.65	13.54
289	0.08	0.06	0.07	122.29	73.19	12.94	0.07	0.06	0.07	125.08	77.81	13.54	13.24
290	0.07	0.06	0.07	122.32	76.11	12.79	0.07	0.06	0.07	125.12	82.27	13.76	13.28
291	0.09	0.08	0.09	122.28	77.73	13.99	0.09	0.13	0.12	125.14	78.93	12.68	13.33
292	0.09	0.08	0.08	122.34	78.83	13.81	0.09	0.07	0.08	125.19	82.56	13.04	13.42
293	0.11	0.09	0.10	122.29	76.03	13.68	0.16	0.14	0.15	125.04	83.94	13.44	13.56
294	0.12	0.09	0.10	122.34	73.99	12.41	0.11	0.09	0.11	125.14	83.93	13.92	13.17
295	0.14	0.11	0.12	122.29	78.44	13.05	0.16	0.11	0.12	125.09	75.18	13.69	13.37
296	0.12	0.10	0.11	122.36	77.16	12.60	0.09	0.10	0.10	125.16	79.69	14.12	13.36
297	0.10	0.12	0.11	122.32	74.03	13.26	0.16	0.17	0.17	125.11	73.31	13.70	13.48
298	0.12	0.15	0.14	122.37	77.82	10.83	0.12	0.10	0.11	125.17	82.06	14.96	12.90
299	0.12	0.10	0.11	122.37	79.99	12.24	0.15	0.16	0.15	125.17	83.48	12.44	12.34
300	0.16	0.12	0.13	122.31	77.70	10.32	0.13	0.07	0.10	125.12	83.96	14.40	12.36
301	0.15	0.10	0.12	122.24	72.87	12.16	0.15	0.13	0.14	125.12	76.49	9.75	10.96
302	0.19	0.15	0.17	122.33	75.46	9.47	0.23	0.09	0.16	125.09	80.38	12.78	11.13
303	0.16	0.10	0.13	122.33	76.10	11.28	0.23	0.13	0.18	125.10	89.28	8.92	10.10
304	0.20	0.13	0.16	122.33	79.75	6.68	0.25	0.09	0.25	125.09	99.99	10.43	8.55
305	0.12	0.13	0.12	122.36	80.18	7.99	0.25	0.16	0.19	125.11	87.40	6.63	7.31
306	0.22	0.11	0.15	122.35	77.38	6.31	0.28	0.12	0.20	125.12	92.29	5.93	6.12
307	0.16	0.11	0.13	122.36	88.85	5.22	0.16	0.07	0.11	125.13	96.98	6.50	5.86
308	0.16	0.15	0.15	122.34	89.69	4.09	0.17	0.12	0.15	125.12	87.89	4.82	4.46
309	0.15	0.14	0.14	122.40	93.11	3.69	0.17	0.15	0.17	125.19	90.08	4.06	3.87
310	0.15	0.12	0.13	122.35	91.60	3.07	0.13	0.13	0.13	125.14	95.00	3.39	3.23
311	~	~	0.14	122.41	93.25	2.29	~	~	0.13	125.20	100.00	3.11	2.70
312	~	~	0.12	122.41	90.55	1.43	~	~	0.12	125.20	99.99	1.75	1.59
313	~	~	0.10	122.39	89.95	1.95	~	~	0.09	125.18	99.99	2.21	2.08
314	~	~	0.10	122.42	89.05	1.13	~	~	0.09	125.21	99.99	1.56	1.34
315	~	~	0.08	122.39	89.86	1.71	~	~	0.08	125.18	99.99	2.14	1.92
316	~	~	0.08	122.42	91.68	1.12	~	~	0.08	125.22	100.00	1.60	1.36
317	~	~	0.08	122.43	90.97	1.18	~	~	0.07	125.22	100.00	1.13	1.16
318	~	~	0.08	122.42	94.11	1.31	~	~	0.07	125.22	99.99	1.12	1.21
319	~	~	0.07	122.43	90.00	1.06	~	~	0.06	125.22	99.99	1.24	1.15
320	~	~	0.07	122.43	97.21	1.06	~	~	0.07	125.23	99.99	1.38	1.22
321	~	~	0.06	122.43	99.37	0.92	~	~	0.05	125.22	100.00	1.16	1.04
322	~	~	0.05	122.44	99.95	0.90	~	~	0.05	125.23	99.99	1.22	1.06
323	~	~	0.05	122.44	99.38	0.99	~	~	0.05	125.24	99.99	1.43	1.21

[a] Maximum intensities, I_o, and chemical shifts at maximum intensity, p_o, were calculated using the intensities and chemical shifts of the *E*- and *Z*-signals below 310 K (Eq. 11-12). The full spectral widths at half maximum intensity of the Lorentzian function ω_L are weighted values determined by the ω_E and ω_Z of the E- and Z-signals, respectively (Eq. 13). [b] The Lorentzian quality-of-fit parameters $\langle\Delta I\rangle_1$ and $\langle\Delta I\rangle_2$ of the two inner peaks of the ^{13}C quartet **1** and **2**, respectively, were calculated using ω_L, p_o, and I_o (Eq. 9) and were averaged to generate $\langle\Delta I\rangle_S$ (Eq. 10).

Table S2. Temperature Dependence of Lorentzian Parameters: ^{19}F Spectra of **1**[a],[b]

Temp.	$\omega_E(1)$	$\omega_Z(1)$	$\omega(1)$	$p_o(1)$	$I_L(1)$	$\langle\Delta I\rangle_1$
288	0.02	0.02	0.02	-71.20	86.08	4.06
289	0.02	0.02	0.02	-71.21	85.87	4.03
290	0.02	0.01	0.02	-71.20	84.77	4.07
291	0.02	0.02	0.02	-71.20	84.39	4.02
292	0.02	0.02	0.02	-71.19	83.76	4.10
293	0.03	0.02	0.02	-71.19	84.28	4.00
294	0.03	0.02	0.02	-71.19	85.72	3.89
295	0.03	0.02	0.02	-71.19	85.20	3.84
296	0.04	0.02	0.02	-71.20	86.83	3.53
297	0.03	0.02	0.03	-71.19	86.83	3.60
298	0.05	0.03	0.04	-71.16	90.31	3.23
299	0.04	0.04	0.04	-71.18	90.08	2.87
300	0.04	0.03	0.04	-70.97	93.30	2.79
301	0.06	0.02	0.05	-70.93	93.62	2.30
302	0.03	0.03	0.03	-70.94	94.44	2.25
303	0.04	0.03	0.04	-70.91	94.98	1.60
304	0.04	0.04	0.04	-70.95	97.04	1.66
305	~	~	0.03	-70.90	100.00	1.21
306	~	~	0.03	-70.89	100.00	0.84
307	~	~	0.03	-70.88	99.99	0.56
308	~	~	0.03	-70.92	100.00	0.78
309	~	~	0.03	-70.91	100.00	0.88
310	~	~	0.03	-70.91	99.99	0.66
311	~	~	0.02	-70.90	99.99	0.52
312	~	~	0.02	-70.90	99.99	0.78
313	~	~	0.02	-70.89	99.99	0.53
314	~	~	0.02	-70.88	99.99	0.42
315	~	~	0.01	-70.87	99.90	0.28
316	~	~	0.01	-70.87	99.99	0.34
317	~	~	0.01	-70.86	100.00	0.22
318	~	~	0.01	-70.83	99.99	0.35
319	~	~	0.01	-70.83	99.99	0.40
320	~	~	0.01	-70.82	99.99	0.31
321	~	~	0.01	-70.81	100.00	0.25
322	~	~	0.01	-70.81	99.99	0.28
323	~	~	0.01	-70.80	100.00	0.28

[a] Maximum intensities, I_o, and chemical shifts at maximum intensity, p_o, were calculated using the intensities and chemical shifts of the *E*- and *Z*-signals below 304 K (Eq. 11-12). The full spectral widths at half maximum intensity of the Lorentzian function ω_L are weighted values determined by the ω_E and ω_Z of the E- and Z-signals, respectively (Eq. 13). [b] The Lorentzian quality-of-fit parameters $\langle\Delta I\rangle_1$ was calculated using ω_L, p_o, and I_o (Eq. 9) and were averaged to generate $\langle\Delta I\rangle_S$ (Eq. 10).