Supplementary Material (ESI) for New Journal of Chemistry

Experimental determination of the conformational free energies (A Values) of fluorinated substituents in cyclohexane by dynamic ^{19}F NMR spectroscopy, Part 2: extension to fluoromethyl, difluoromethyl, pentafluoroethyl, trifluoromethylthio and trifluoromethoxy groups.

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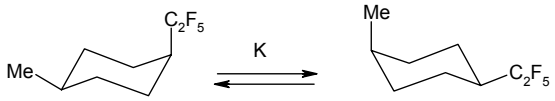
Chemical shifts must be read with one digit after the comma, but all the numbers are required and are given by the software of simulated spectra.

Table 1: ^{19}F chemical shifs [a] of 4-methyl-1-pentafluoroethylcyclohexane (4a)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-124.000**	**-122.969**	*-116.083*	*-124.551*
293	**-124.035**	**-123.020**	*-116.057*	*-124.568*
288	**-124.070**	**-123.078**	*-116.031*	*-124.585*
283	**-124.105**	**-123.134**	*-116.005*	*-124.601*
278	**-124.139**	**-123.192**	*-115.979*	*-124.618*
273	**-124.174**	**-123.251**	*-115.953*	*-124.635*
268	**-124.208**	**-123.311**	*-115.928*	*-124.651*
263	**-124.240**	**-123.368**	*-115.902*	*-124.668*
258	**-124.274**	**-123.433**	*-115.876*	*-124.685*
253	**-124.307**	-	-	-
248	**-124.339**	-	-	-
243	**-124.372**	-	-	-
238	**-124.404**	-	-	-
233	**-124.435**	-	-	-
228	**-124.466**	-	-	-
223	**-124.496**	-	-	-
218	**-124.523**	-	-	-
213	**-124.552**	-	-	-
208	**-124.579**	-	-	-
203	**-124.605**	-	-	-
198	**-124.631**	-	-	-
193	**-124.656**	-	**(-124.896)**	**-115.537**
188	**-124.679**	-	**-124.918**	**-115.515**
183	**-124.702**	-	**-124.935**	**-115.492**
178	**-124.724**	-	**-124.953**	**-115.464**
173	**-124.744**	-	**-124.969**	**-115.438**
168	**-124.764**	-	**-124.985**	**-115.408**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -114.542 - 5.17.10^{-3}\ T$
$\delta_{eq} = -125.547 + 3.34.10^{-3}\ T$

Table 2: Thermodynamic parameters of *cis*-4-methyl-1-pentafluoroethylcyclohexane



T / K	K[a]	ΔG° / J.mol^{-1}
298	4.352	-3643.8
293	4.499	-3663.3
288	4.676	-3693.2
283	4.859	-3719.6
278	5.057	-3746.0
273	5.274	-3774.0
268	5.509	-3802.2
263	5.745	-3822.8
258	6.035	-3855.7

[a] Equilibrium constants were calculated from the values of the chemical shifts :

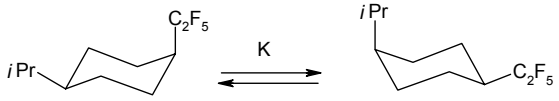
$$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$$

Table 3: ^{19}F chemical shifs [a] of 4-*iso*propyl-1-pentafluoroethylcyclohexane (4b)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-121.307**	**-119.520**	*-113.507*	*-122.028*
293	**-121.344**	**-119.603**	*-113.476*	*-122.043*
288	**-121.378**	**-119.681**	*-113.445*	*-122.059*
283	**-121.415**	**-119.764**	*-113.414*	*-122.074*
278	**-121.453**	**-119.855**	*-113.384*	*-122.089*
273	**-121.489**	**-119.945**	*-113.353*	*-122.105*
268	**-121.526**	**-120.037**	*-113.322*	*-122.120*
263	**-121.563**	**-120.133**	*-113.291*	*-122.135*
258	**-121.598**	**-120.227**	*-113.260*	*-122.151*
238	**-121.735**	-	-	-
218	**-121.855**	-	-	-
198	**-121.957**	-	-	-
193	**-121.984**	-	-	-
188	**-122.008**	-	**-122.365**	**-112.830**
183	**-122.030**	-	**-122.383**	**-112.798**
178	**-122.052**	-	**-122.397**	**-112.765**
173	**-122.074**	-	**-122.412**	**-112.739**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -111.671 - 6.16.10^{-3}\ T$
$\delta_{eq} = -122.923 + 3.07.10^{-3}\ T$

Table 4: Thermodynamic parameters of *cis*-4-*iso*propyl-1-pentafluoroethylcyclohexane



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	2.398	-2167.0
293	2.511	-2242.6
288	2.622	-2308.1
283	2.749	-2379.4
278	2.897	-2458.3
273	3.053	-2533.2
268	3.224	-2608.3
263	3.416	-2686.0
258	3.622	-2760.5

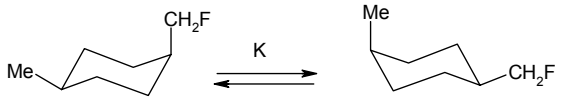
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 5: ^{19}F chemical shifs [a] of 4-methyl-1-fluoromethylcyclohexane (9a)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-223.819**	**-223.485**	*-222.710*	*-224.539*
293	**-223.782**	**-223.460**	*-222.694*	*-224.482*
288	**-223.744**	**-223.435**	*-222.679*	*-224.425*
283	**-223.706**	**-223.409**	*-222.663*	*-224.368*
278	**-223.668**	**-223.383**	*-222.647*	*-224.311*
273	**-223.628**	**-223.357**	*-222.632*	*-224.254*
268	**-223.589**	**-223.330**	*-222.616*	*-224.197*
263	**-223.549**	**-223.302**	*-222.601*	*-224.140*
258	**-223.508**	**-223.275**	*-222.585*	*-224.083*
253	**-223.466**	**-223.247**	*-222.569*	*-224.026*
248	**-223.425**	-	-	-
243	**-223.382**	-	-	-
238	**-223.339**	-	-	-
233	**-223.294**	-	-	-
228	**-223.249**	-	-	-
223	**-223.203**	-	-	-
218	**-223.158**	-	-	-
213	**-223.112**	-	-	-
208	**-223.066**	-	-	-
203	**-223.021**	-	-	-
198	**-222.975**	-	-	-
193	**-222.927**	-	**-222.382**	**-223.345**
188	**-222.877**	-	**-222.367**	**-223.289**
183	**-222.823**	-	**-222.349**	**-223.230**
178	**-222.771**	-	**-222.333**	**-223.172**
173	**-222.720**	-	**-222.317**	**-223.113**
168	**-222.667**	-	**-222.302**	**-223.052**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -221.777 - 3.13.10^{-3}\ T$
$\delta_{eq} = -221.142 + 1.14.10^{-2}\ T$

Table 6: Thermodynamic parameters of *cis*-4-methyl-1-fluoromethylcyclohexane



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	0.735	762.7
293	0.749	704.4
288	0.764	645.6
283	0.778	592.0
278	0.792	537.9
273	0.808	483.3
268	0.823	433.9
263	0.837	389.6
258	0.854	339.0
253	0.870	293.5

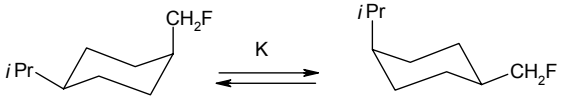
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 7: ^{19}F chemical shifs [a] of 4-*iso*propyl-1-fluoromethylcyclohexane (9b)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-222.867**	**-222.423**	*-222.003*	*-223.569*
293	**-222.824**	**-222.405**	*-221.983*	*-223.521*
288	**-222.780**	**-222.385**	*-221.964*	*-223.474*
283	**-222.735**	**-222.365**	*-221.944*	*-223.426*
278	**-222.690**	**-222.345**	*-221.924*	*-223.378*
273	**-222.644**	**-222.323**	*-221.904*	*-223.330*
268	**-222.597**	**-222.302**	*-221.885*	*-223.283*
263	**-222.550**	**-222.280**	*-221.865*	*-223.235*
258	**-222.503**	**-222.258**	*-221.845*	*-223.187*
253	**-222.455**	**-222.236**	*-221.825*	*-223.139*
233	**-222.274**	-	-	-
213	**-222.074**	-	-	-
193	**-221.890**	-	**-221.590**	**-222.565**
188	**-221.835**	-	**-221.569**	**-222.519**
183	**-221.777**	-	**-221.549**	**-222.471**
178	**-221.720**	-	**-221.529**	**-222.422**
173	**-221.661**	-	**-221.511**	**-222.375**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -220.826 - 3.95.10^{-3}\ T$
$\delta_{eq} = -220.723 - 9.55.10^{-3}\ T$

Table 8: Thermodynamic parameters of *cis*-4-*iso*propyl-1-fluoromethylcyclohexane



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	0.367	2485.2
293	0.377	2373.3
288	0.387	2272.4
283	0.396	2178.3
278	0.407	2078.4
273	0.416	1990.6
268	0.425	1906.1
263	0.435	1821.2
258	0.444	1740.3
253	0.454	1659.7

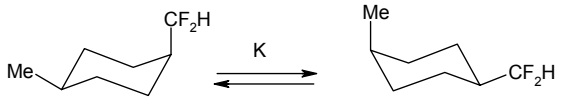
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 9: ^{19}F chemical shifs [a] of 4-methyl-1-difluoromethylcyclohexane (10a)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-125.879**	**-125.462**	*-124.069*	*-126.684*
293	**-125.876**	**-125.480**	*-124.128*	*-126.652*
288	**-125.873**	**-125.497**	*-124.187*	*-126.621*
283	**-125.868**	**-125.513**	*-124.246*	*-126.590*
278	**-125.864**	**-125.530**	*-124.305*	*-126.559*
273	**-125.859**	**-125.547**	*-124.364*	*-126.528*
268	**-125.853**	**-125.563**	*-124.423*	*-126.496*
263	**-125.845**	**-125.579**	*-124.482*	*-126.465*
258	**-125.840**	**-125.595**	*-124.541*	*-126.434*
253	**-125.832**	**-125.610**	*-124.600*	*-126.403*
248	**-125.824**	-	-	-
243	**-125.814**	-	-	-
238	**-125.804**	-	-	-
233	**-125.794**	-	-	-
228	**-125.782**	-	-	-
223	**-125.770**	-	-	-
218	**-125.755**	-	-	-
213	**-125.741**	-	-	-
208	**-125.720**	-	-	-
203	**-125.704**	-	**-125.186**	**-126.085**
198	**-125.685**	-	**-125.248**	**-126.059**
193	**-125.664**	-	**-125.307**	**-126.031**
188	**-125.641**	-	**-125.367**	**-126.003**
183	**-125.617**	-	**-125.426**	**-125.971**
178	**-125.590**	-	**-125.485**	**-125.938**
173	**-125.561**	-	**-125.561**	**-125.903**
168	**-125.534**	-	**-125.599**	**-125.866**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -127.582 + 1.18.10^{-2}\ T$
$\delta_{eq} = -124.824 - 6.24.10^{-3}\ T$

Table 10: Thermodynamic parameters of *cis*-4-methyl-1-difluoromethylcyclohexane



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	1.141	-326.7
293	1.153	-346.3
288	1.164	-364.3
283	1.177	-383.2
278	1.191	-404.9
273	1.206	-424.9
268	1.220	-443.7
263	1.237	-465.3
258	1.257	-490.4
253	1.275	-511.5

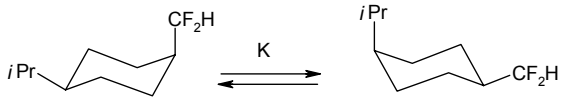
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 11: ^{19}F chemical shifs [a] of 4-*iso*propyl-1-difluoromethylcyclohexane (10b)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-123.097**	**-122.355**	*-121.425*	*-123.961*
293	**-123.092**	**-122.385**	*-121.480*	*-123.927*
288	**-123.087**	**-122.413**	*-121.534*	*-123.894*
283	**-123.081**	**-122.443**	*-121.589*	*-123.860*
278	**-123.075**	**-122.472**	*-121.644*	*-123.826*
273	**-123.068**	**-122.501**	*-121.698*	*-123.793*
268	**-123.061**	**-122.530**	*-121.753*	*-123.759*
263	**-123.053**	**-122.559**	*-121.808*	*-123.725*
258	**-123.043**	**-122.588**	*-121.862*	*-123.692*
253	**-123.034**	**-122.617**	*-121.917*	*-123.658*
233	**-122.984**	-	-	-
213	**-122.913**	-	-	-
203	**-122.867**	-	**-**	**-**
193	**-122.819**	-	**-**	**-**
188	**-122.785**	-	**-122.570**	**-123.250**
183	**-122.753**	-	**-122.627**	**-123.222**
178	**-122.719**	-	**-122.685**	**-123.190**
173	**-122.682**	-	**-122.79**	**-123.12**
168	**-122.641**	-	**-122.843**	**-123.083**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -124.682 + 1.09.10^{-2}\ T$
$\delta_{eq} = -121.955 - 6.73.10^{-3}\ T$

Table 12: Thermodynamic parameters of *cis*-4-*iso*propyl-1-difluoromethylcyclohexane



T / K	K[a]	ΔG° / J.mol^{-1}
298	0.579	1352.0
293	0.586	1300.0
288	0.594	1247.9
283	0.602	1192.4
278	0.612	1136.4
273	0.621	1080.8
268	0.633	1020.2
263	0.645	960.1
258	0.658	897.9
253	0.673	832.7

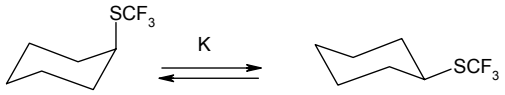
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 13: ^{19}F chemical shifs [a] of cyclohexyl trifluoromethyl sulfur (15a)

T / K	δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-38.804**	*-39.980*	*-38.645*
293	**-38.798**	*-39.971*	*-38.631*
288	**-38.790**	*-39.961*	*-38.618*
283	**-38.782**	*-39.951*	*-38.605*
278	**-38.773**	*-39.940*	*-38.591*
273	**-38.763**	*-39.929*	*-38.578*
268	**-38.753**	*-39.917*	*-38.564*
263	**-38.741**	*-39.905*	*-38.551*
258	**-38.727**	*-39.892*	*-38.538*
253	-	-	-
248	-	-	-
243	-	-	-
238	-	-	-
233	-	-	-
228	-	-	**-38.455**
223	-	**-39.790**	**-38.441**
218	-	**-39.774**	**-38.431**
213	-	**-39.756**	**-38.419**
208	-	**-39.740**	**-38.408**
203	-	**-39.721**	**-38.393**
198	-	**-39.704**	**-38.381**
193	-	**-39.685**	**-38.366**
188	-	**-39.664**	**-38.350**
183	-	**-39.645**	**-38.335**
178	-	**-39.626**	**-38.321**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -38.608 - 7.37.10^{-3}\ T + 9.27.10^{-6}\ T^2$
$\delta_{eq} = -37.847 - 2.68.10^{-3}\ T$

Table 14: Thermodynamic parameters of cyclohexyl trifluoromethyl sulfur



T / K	K [a]	$\Delta G°$ / J.mol^{-1}
298	7.371	-4949.1
293	7.058	-4760.2
288	6.820	-4596.9
283	6.598	-4439.5
278	6.433	-4302.2
273	6.295	-4175.8
268	6.188	-4060.9
263	6.145	-3969.9
258	6.171	-3903.6

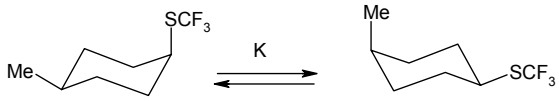
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 15: ^{19}F chemical shifs [a] of 4-methylcyclohexyl trifluoromethyl sulfur (15b)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-41.600**	**-42.655**	*-43.072*	*-41.559*
293	**-41.595**	**-42.656**	*-43.051*	*-41.551*
288	**-41.589**	**-42.655**	*-43.030*	*-41.544*
283	**-41.584**	**-42.655**	*-43.008*	*-41.536*
278	**-41.578**	**-42.654**	*-42.987*	*-41.528*
273	**-41.571**	**-42.651**	*-42.965*	*-41.5230*
268	**-41.563**	**-42.649**	*-42.944*	*-41.512*
263	**-41.555**	**-42.647**	*-42.923*	*-41.504*
258	**-41.546**	**-42.645**	*-42.901*	*-41.496*
253	**-41.537**	**-42.645**	*-42.880*	*-41.488*
248	**-41.527**	-	-	-
243	**-41.516**	-	-	-
238	**-41.505**	-	-	-
233	**-41.492**	-	-	-
228	**-41.479**	-	-	-
223	**-41.465**	-	-	-
218	**-41.451**	-	-	-
213	**-41.437**	-	-	-
208	**-41.422**	-	**-42.684**	**-**
203	**-41.407**	-	**-42.665**	**-**
198	**-41.392**	-	**-42.646**	**-**
193	**-41.375**	-	**-42.626**	**-**
188	**-41.357**	-	**-42.604**	**-41.386**
183	**-41.339**	-	**-42.582**	**-41.378**
178	**-41.322**	-	**-42.559**	**-41.370**
173	**-41.303**	-	**-42.536**	**-41.362**
168	**-41.286**	-	**-42.514**	**(-41.355)**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -41.797 - 4.28.10^{-3}\ T$
$\delta_{eq} = -41.088 - 1.58.10^{-3}\ T$

Table 16: Thermodynamic parameters of 4-methylcyclohexyl trifluoromethyl sulfur



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	0.381	2393.9
293	0.358	2504.6
288	0.337	2607.1
283	0.316	2711.8
278	0.296	2812.8
273	0.278	2906.4
268	0.259	3008.6
263	0.241	3108.7
258	0.223	3218.1
253	0.203	3353.6

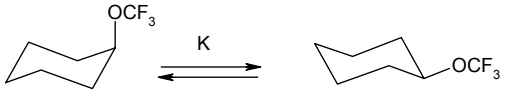
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 17: ^{19}F chemical shifs [a] of trifluoromethoxycyclohexane (19a)

T / K	δ_{obs} [b]	δ_{ax} [b,c]	δ_{eq} [b,c]
298	**-60.177**	*-60.500*	*-60.093*
293	**-60.175**	*-60.487*	*-60.093*
288	**-60.172**	*-60.474*	*-60.092*
283	**-60.169**	*-60.461*	*-60.091*
278	**-60.166**	*-60.448*	*-60.090*
273	**-60.163**	*-60.434*	*-60.089*
268	**-60.159**	*-60.421*	*-60.087*
263	**-60.155**	*-60.408*	*-60.085*
258	**-60.150**	*-60.395*	*-60.082*
253	**-60.145**	*-60.382*	*-60.079*
248	**-60.140**	*-60.368*	*-60.076*
243	-	-	-
238	-	-	-
228	-	-	-
218	-	**-60.290**	**-60.055**
208	-	**-60.262**	**-60.041**
198	-	**-60.238**	**-60.027**
193	-	**-60.225**	**-60.020**
188	-	**-60.211**	**-60.013**
183	-	**-60.198**	**-60.006**
178	-	**-60.183**	**-59.998**
173	-	**-60.176**	**-59.996**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -59.713 - 2.64.10^{-3}\ T$
$\delta_{eq} = -59.514 - 3.88.10^{-3}\ T + 6.50.10^{-6}\ T^2$

Table 18: Thermodynamic parameters of trifluoromethoxycyclohexane



T / K	K [a]	$\Delta G°$ / J.mol^{-1}
298	3.824	-3323.4
293	3.813	-3260.6
288	3.792	-3191.5
283	3.766	-3119.8
278	3.729	-3041.7
273	3.686	-2960.7
268	3.669	-2896.7
263	3.629	-2818.2
258	3.616	-2757.1
253	3.605	-2697.6
248	3.590	-2635.7

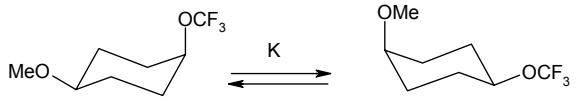
[a] Equilibrium constants were calculated from the values of the chemical shifts :
$K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 19: ^{19}F chemical shifs [a] of 4-methoxy-1-trifluoromethoxycyclohexane (19d)

T / K	*trans* isomer[b]	*cis* isomer		
		δ_{obs} [b]	δ_{ax} [b.c]	δ_{eq} [b.c]
298	**-60.392**	**-60.236**	*-60.439*	*-60.112*
293	**-60.388**	**-60.232**	*-60.435*	*-60.109*
288	**-60.384**	**-60.228**	*-60.431*	*-60.105*
283	**-60.379**	**-60.224**	*-60.426*	*-60.101*
278	**-60.375**	**-60.220**	*-60.421*	*-60.097*
273	**-60.369**	**-60.215**	*-60.415*	*-60.093*
268	**-60.364**	**-60.210**	*-60.409*	*-60.088*
263	**-60.358**	-	-	-
258	**-60.351**	-	-	-
253	**-60.343**	-	-	-
248	**-60.336**	-	-	-
243	**-60.329**	-	-	-
238	**-60.320**	-	-	-
233	**-60.312**	-	-	-
228	**-60.302**	-	-	-
223	-	-	-	-
218	-	-	-	-
213	-	-	-	-
208	-	-	-	-
203	-	-	-	-
198	-	-	-	-
193	-	-	-	-
188	-	-	**-60.007**	**-60.246**
183	-	-	**-60.001**	**-60.231**
178	-	-	**-59.995**	**-60.216**
173	-	-	**-59.990**	**-60.200**
168	-	-	**-59.984**	**-60.182**

[a] Chemical shifts are in ppm and were measured in THF-d^8 relative to $CFCl_3$.
[b] Shifts in bold are experimental values.
[c] Shifts in italic were calculated by linear regression : $\delta_{ax} = -59.371 - 6.46.10^{-3}\ T + 9.65.10^{-6}\ T^2$
$\delta_{eq} = -59.731 - 1.81.10^{-3}\ T + 1.77.10^{-6}\ T^2$

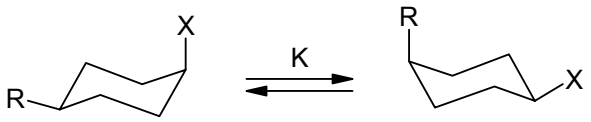
Table 20: Thermodynamic parameters of 4-methoxy-1-trifluoromethoxycyclohexane



T / K	K[a]	$\Delta G°$ / J.mol^{-1}
298	1.652	-1243.0
293	1.649	-1219.1
288	1.640	-1184.7
283	1.634	-1155.8
278	1.628	-1126.0
273	1.631	-1110.2
268	1.635	-1096.1
263	1.652	-1243.0

[a] Equilibrium constants were calculated from the values of the chemical shifts : $K = (\delta_{ax} - \delta_{obs}) / (\delta_{obs} - \delta_{eq})$

Table 21. Thermodynamic parameters of 4-substituted-1-fluorinated cyclohexanes.



	R	X	$\Delta H°$ / kJ.mol^{-1} ($\Delta H°$ / kcal.mol^{-1})[a]	$\Delta S°$ / J. mol^{-1}.K^{-1} ($\Delta S°$ / cal.mol^{-1}.K^{-1})[b]	$\Delta G°_{298K}$ / kJ.mol^{-1} ($\Delta G°_{298K}$ / kcal.mol^{-1})
1a	Me	C_2F_5	-5.23 ± 0.02 (-1.25 ± 0.01)	-5.33 ± 0.07 (-1.27 ± 0.02)	-3.64 (-0.87)
1b	*i*Pr	C_2F_5	-6.59 ± 0.03 (-1.58 ± 0.01)	-14.86 ± 0.11 (-3.55 ± 0,04)	-2.17 (-0.52)
2a	Me	CH_2F	2.35 ± 0.04 (-0.56 ± 0.01)	-10.41 ± 0.15 (-2.49 ± 0,05)	0.76 (0.18)
2b	*i*Pr	CH_2F	2.97 ± 0.09 (-0.71 ± 0.02)	-18.21 ± 0.33 (-4.35 ± 0.08)	2.49 (0.59)
3a	Me	CF_2H	-1.54 ± 0.02 (-0.37 ± 0.01)	-4.10 ± 0.06 (-0.98 ± 0,02)	-0.33 (-0.08)
3b	*i*Pr	CF_2H	-2.07 ± 0.04 (-0.50 ± 0.01)	-11.51 ± 0.14 (-2.75 ± 0,04)	1.35 (0.32)
4a	H	SCF_3	2.96 ± 0.37 (0.71 ± 0.09)	26.30 ± 1.34 (6.28 ± 0.32)	-4.95 (-1.18)
4b	Me	SCF_3	8.47 ± 0.07 (2.02 ± 0.02)	20.36 ± 0.25 (4.86 ± 0,05)	2.39 (0.57)
5a	H	OCF_3	0.87 ± 0.05 (0.21 ± 0.01)	14.08 ± 0.20 (3.36 ± 0,05)	-3.32 (-0.79)
5d	OMe	OCF_3	0.23 ± 0.07 (0.05 ± 0.02)	4.92 ± 0.26 (1.18 ± 0,06)	-1.24 (-0.30)