Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary material

Microwave survey of the conformational landscape exhibited by the propeller molecule triethyl amine

Ha Vinh Lam Nguyen, Raphaela Kannengießer, and Wolfgang Stahl

Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, D-52074 Aachen, Germany

Table S-1

Cartesian nuclear coordinates of 7 stable conformers of triethyl amine in the principal axes of inertia as calculated at the MP2/6-311++G(d,p) level of theory.

	Conformer I			Conformer II		
	a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
N1	–0.025346	–0.323840	0.580016	–0.174363	0.020183	0.392375
C2	–0.199295	1.119037	0.752136	0.253764	1.117371	–0.475894
H3	0.588598	1.451659	1.437939	–0.599315	1.791841	–0.591073
H4	–1.149774	1.289321	1.273328	0.508366	0.757177	–1.491363
C5	–0.183514	1.997897	–0.509110	1.423501	1.910470	0.098585
H6	–1.009583	1.748752	–1.181472	2.355552	1.339377	0.086685
H7	–0.303073	3.046849	–0.216550	1.583033	2.815417	–0.495635
H8	0.748820	1.905574	–1.069618	1.207830	2.204312	1.129969
C9	–0.851757	–0.918473	–0.462254	0.898701	–0.931283	0.699021
H10	–0.605416	–1.986681	–0.490667	0.470921	–1.678452	1.377282
H11	–0.633795	–0.518743	–1.468839	1.668471	–0.404276	1.271489
C12	–2.341837	–0.760590	–0.169732	1.548307	–1.643282	–0.495769
H13	–2.930022	–1.314243	–0.908374	2.302187	–2.350871	–0.135112
H14	–2.570297	–1.148980	0.826747	0.812469	–2.205656	–1.078101
H15	–2.656415	0.285872	–0.212579	2.048307	–0.937774	–1.165926
C16	1.358650	–0.788064	0.566542	–1.357160	–0.651227	–0.149074
H17	1.830998	–0.433411	1.490797	–1.224981	–0.919190	–1.214391
H18	1.321614	–1.882727	0.633784	–1.477516	–1.589981	0.403819
C19	2.242300	–0.399211	–0.629927	–2.629957	0.177669	0.011574
H20	3.197145	–0.933004	–0.567907	–2.612307	1.082154	–0.601316
H21	1.770068	–0.665939	–1.580253	–3.499415	–0.412152	–0.296380
H22	2.461034	0.671435	–0.639252	–2.754023	0.469112	1.057932

Table S-1 continued

	Conformer III			Conformer IV		
	a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
N1	0.000042	–0.000034	–0.026249	–0.000046	–0.409887	–0.274148
C2	–0.644863	1.233365	0.434748	–0.000004	1.007500	–0.649776
H3	–0.402276	1.423763	1.498352	–0.871533	1.180605	–1.287838
H4	–1.727923	1.089413	0.381951	0.871435	1.180466	–1.288006
C5	–0.273824	2.440354	–0.421518	0.000205	2.022552	0.501673
H6	–0.565999	2.262101	–1.459577	0.886148	1.917970	1.135220
H7	–0.788992	3.335318	–0.057307	0.000313	3.038656	0.093498
H8	0.800441	2.641628	–0.398527	–0.885660	1.918215	1.135356
C9	–0.745677	–1.175277	0.434559	1.194863	–0.813362	0.468367
H10	–1.031548	–1.060710	1.498297	1.102475	–1.892104	0.640239
H11	–0.079570	–2.041293	0.381301	1.238699	–0.340598	1.468242
C12	–1.976730	–1.457141	–0.421469	2.493520	–0.541625	–0.284084
H13	–2.493807	–2.351144	–0.057628	3.324442	–1.039780	0.224694
H14	–2.688431	–0.627683	–0.397702	2.426083	–0.930818	–1.304205
H15	–1.676552	–1.620296	–1.459730	2.728972	0.524807	–0.331811
C16	1.390622	–0.058295	0.434785	–1.194962	–0.813140	0.468476
H17	1.807453	0.951659	0.382140	–1.102608	–1.891840	0.640605
H18	1.434200	–0.363723	1.498356	–1.238724	–0.340120	1.468222
C19	2.250436	–0.982971	–0.421591	–2.493600	–0.541509	–0.284081
H20	3.283029	–0.984445	–0.057247	–2.426026	–0.930789	–1.304156
H21	1.887535	–2.013925	–0.398875	–3.324551	–1.039638	0.224664
H22	2.242311	–0.640578	–1.459575	–2.729102	0.524904	–0.331946

Table S-1 continued

	Conformer V			Conformer VI		
	a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
N1	–0.000256	–0.287941	–0.066036	0.073814	–0.009432	0.374452
C2	0.000384	0.976562	0.689094	–0.463659	–1.046339	–0.517106
H3	0.876351	1.010685	1.351755	0.317939	–1.788309	–0.723708
H4	–0.876017	1.011888	1.351081	–0.735928	–0.612240	–1.492058
C5	0.001426	2.198366	–0.226126	–1.668020	–1.761084	0.094333
H6	–0.882205	2.191969	–0.869695	–2.477141	–1.056728	0.299869
H7	0.002298	3.124038	0.361020	–2.042681	–2.538076	–0.582194
H8	0.884888	2.190477	–0.869904	–1.380934	–2.228605	1.040416
C9	–1.208132	–1.073226	0.185244	–0.201458	1.347150	–0.090185
H10	–1.345146	–1.266133	1.267974	0.168905	1.515068	–1.119198
H11	–1.073604	–2.045837	–0.300337	0.348221	2.032864	0.566006
C12	–2.456772	–0.405753	–0.382343	–1.687748	1.687490	–0.038303
H13	–3.331529	–1.043658	–0.219891	–1.842914	2.734092	–0.320197
H14	–2.654550	0.557215	0.096614	–2.263271	1.068440	–0.732257
H15	–2.335682	–0.238921	–1.456187	–2.076434	1.530493	0.971558
C16	1.207055	–1.074199	0.184898	1.486742	–0.211165	0.701919
H17	1.343800	–1.267811	1.267527	1.735451	0.471946	1.523374
H18	1.071899	–2.046418	–0.301293	1.586351	–1.228251	1.098718
C19	2.456241	–0.407272	–0.382123	2.484104	–0.007354	–0.447072
H20	2.654803	0.555194	0.097489	2.482091	1.028209	–0.798297
H21	3.330451	–1.046050	–0.220129	3.498275	–0.244275	–0.108557
H22	2.335398	–0.239650	–1.455870	2.252288	–0.657110	–1.296885

Table S-1 continued

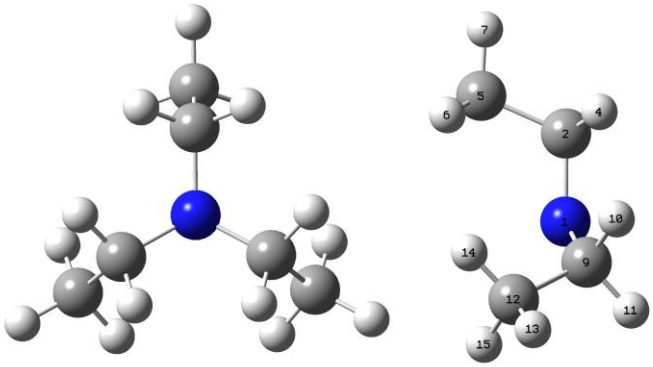
	Conformer VII		
	a /Å	b /Å	c /Å
N1	0.073814	–0.009432	0.374452
C2	–0.463659	–1.046339	–0.517106
H3	0.317939	–1.788309	–0.723708
H4	–0.735928	–0.612240	–1.492058
C5	–1.668020	–1.761084	0.094333
H6	–2.477141	–1.056728	0.299869
H7	–2.042681	–2.538076	–0.582194
H8	–1.380934	–2.228605	1.040416
C9	–0.201458	1.347150	–0.090185
H10	0.168905	1.515068	–1.119198
H11	0.348221	2.032864	0.566006
C12	–1.687748	1.687490	–0.038303
H13	–1.842914	2.734092	–0.320197
H14	–2.263271	1.068440	–0.732257
H15	–2.076434	1.530493	0.971558
C16	1.486742	–0.211165	0.701919
H17	1.735451	0.471946	1.523374
H18	1.586351	–1.228251	1.098718
C19	2.484104	–0.007354	–0.447072
H20	2.482091	1.028209	–0.798297
H21	3.498275	–0.244275	–0.108557
H22	2.252288	–0.657110	–1.296885

Table S-2

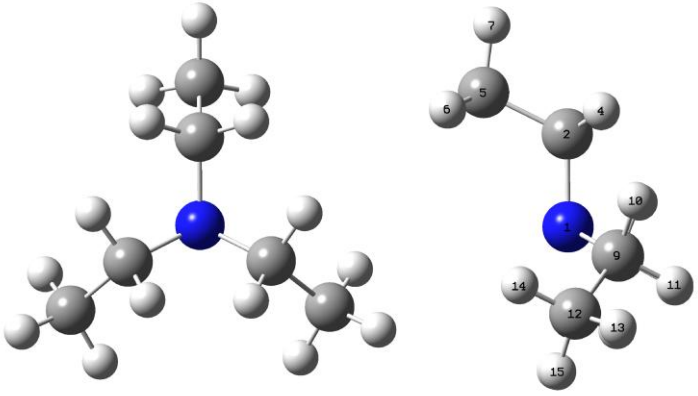
Fourier coefficients of the potential function for the transition state calculated at the MP2/6-311++G(d,p) level of theory. The potential is expanded as $V(\varphi) = a_0 + \sum_{n=1}^{5} a_{3n}\cos(3n\varphi) + \sum_{n=1}^{5} b_{3n}\sin(3n\varphi)$.

	kJ/mol
a_0	21.50(85)
a_3	–32.1(12)
a_6	6.83(34)
a_9	–0.97(32)
a_{12}	0.36(32)
a_{15}	1.07(11)
b_3	–18.75(95)
b_6	13.0(12)
b_9	–4.78(70)
b_{12}	–1.12(21)
b_{15}	–0.306(56)

Figure S-1



Transtition state (C_{3v})



$\beta_1 = \beta_2 = \beta_3 = 70.5$ (C_1)

Table S-3

Cartesian nuclear coordinates of the transition state of triethyl amine in in the principal axes of inertia as calculated at the MP2/6-311++G(d,p) level of theory.

	a /Å	b /Å	c /Å
N1	0.000000	0.000000	0.375230
C2	0.000000	1.434889	0.614542
H3	0.882031	1.702527	1.214379
H4	–0.882031	1.702527	1.214379
C5	0.000000	2.270746	–0.669197
H6	–0.885462	2.046297	–1.270710
H7	0.000000	3.342098	–0.434941
H8	0.885462	2.046297	–1.270710
C9	–1.242650	–0.717445	0.614542
H10	–1.915447	–0.087402	1.214379
H11	–1.033416	–1.615125	1.214379
C12	–1.966523	–1.135373	–0.669197
H13	–2.894342	–1.671049	–0.434941
H14	–2.214877	–0.256316	–1.270710
H15	–1.329414	–1.789982	–1.270710
C16	1.242650	–0.717445	0.614542
H17	1.915447	–0.087402	1.214379
H18	1.033416	–1.615125	1.214379
C19	1.966523	–1.135373	–0.669197
H20	2.214877	–0.256316	–1.270710
H21	2.894342	–1.671049	–0.434941
H22	1.329414	–1.789982	–1.270710

Table S-4

The energy values, dipole moments, and rotational constants of the stable conformers of related molecules as calculated at the MP2/6–311++G(d,p) level of theory.

A. Triethyl phosphine

Conf.	rel. E kJ/mol	μ_a / D	μ_b / D	μ_c / D	α_1 / °	α_2 / °	α_3 / °	A / GHz	B / GHz	C / GHz	Freq. calc.
I	12.8898	–0.490	0.585	1.314	80.5	176.5	56.2	2.314	1.608	1.299	0
II	1.9084	–0.288	–0.525	1.336	–167.2	54.1	–178.8	2.344	1.590	1.159	0
III	0.0000	0.000	0.000	1.407	67.0	168.0	67.0	1.892	1.892	1.040	0
IV	0.4886	0.000	0.715	1.273	50.7	–168.9	168.9	2.778	1.468	1.157	0
V	6.0054	0.000	–0.319	1.394	129.4	176.0	–176.0	2.364	1.545	1.033	1
VI	6.7048	–0.611	0.111	1.344	155.4	175.4	–50.8	2.263	1.607	1.151	0
VII	27.3810	0.000	0.000	1.558	–77.9	30.3	–77.9	1.862	1.862	1.551	0

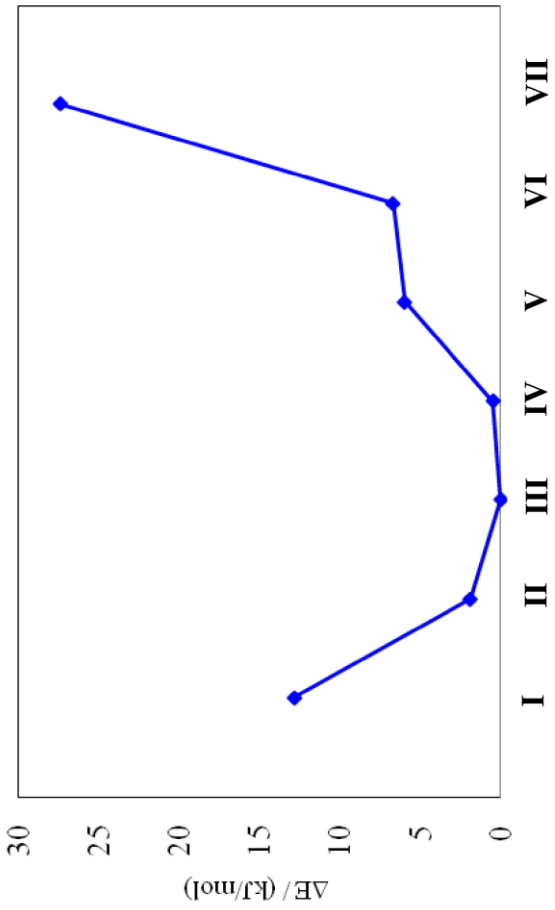


Fig. S-2 Stable conformers of triethyl phosphine. The energy values are relative to the most stable conformer III (–577.8018180 Hartree).

Table S-4/A continued

Cartesian nuclear coordinates of conformer III (most stable) in *Gaussian03* internal coordinate system (called standard orientation)

Number	Atomic number	a /Å	b /Å	c /Å
1	6	–0.966140	–1.315831	0.299141
2	1	–0.784949	–1.246439	1.380952
3	1	–0.583746	–2.286420	–0.034972
4	6	–2.467839	–1.238127	0.001931
5	1	–2.654105	–1.254363	–1.076749
6	1	–2.997439	–2.085318	0.448260
7	1	–2.910051	–0.323319	0.405783
8	6	1.622539	–0.178783	0.299018
9	1	1.471852	–0.057020	1.380882
10	1	2.271654	0.637980	–0.034811
11	6	2.306431	–1.517855	0.001273
12	1	3.304885	–1.552889	0.447683
13	1	1.735439	–2.358540	0.404687
14	1	2.413751	–1.670532	–1.077466
15	6	–0.656558	1.494595	0.298692
16	1	–1.688249	1.648633	–0.035650
17	1	–0.687265	1.303251	1.380546
18	6	0.161616	2.756195	0.001322
19	1	–0.307412	3.638546	0.447290
20	1	1.174875	2.681913	0.405433
21	1	0.240936	2.925322	–1.077388
22	15	–0.000031	–0.000132	–0.584849

Table S-4 continued

B. Triisopropyl amine

Conf.	rel. E kJ/mol	μ_a / D	μ_b / D	μ_c / D	A / GHz	B / GHz	C / GHz	Freq. calc.
I	27.7414	–0.071	–0.383	0.747	1.474	1.068	0.855	0
II	8.8007	0.292	0.165	0.747	1.310	1.194	0.867	0
III	18.8596	0.000	0.000	0.194	1.265	1.265	0.890	0
IV	20.9184	–0.117	0.263	0.647	1.400	1.144	0.844	0
V	22.3288	0.269	–0.112	0.336	1.430	1.076	0.902	1
VI	29.8116	–0.077	–0.280	–0.839	1.352	1.183	0.814	0
VII	0.0000	0.000	0.000	0.555	1.186	1.186	0.953	0
VIII	15.6744	0.105	–0.356	0.392	1.387	1.087	0.911	0

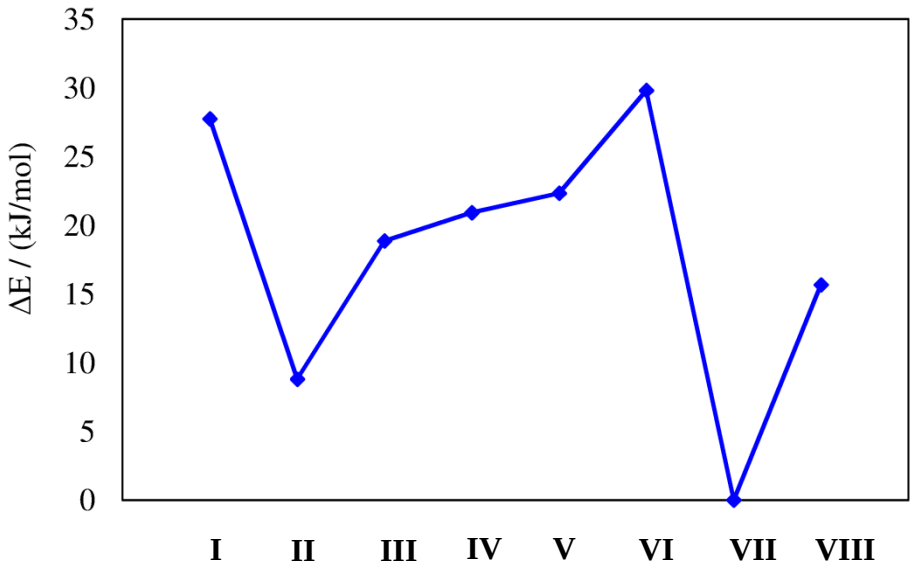


Fig. S-3 Stable conformers of triisopropyl amine. The energy values are relative to the most stable conformer VII (–409.1508669 Hartree).

Table S-4/B. continued

Cartesian nuclear coordinates of conformer VII (most stable) in *Gaussian03* internal coordinate system (called standard orientation)

Number	Atomic number	a /Å	b /Å	c /Å
1	7	0.000039	–0.000007	–0.325707
2	6	–0.932943	1.098862	–0.067962
3	1	–1.937174	0.662320	–0.125409
4	6	–0.485187	–1.357397	–0.067945
5	1	0.394971	–2.008852	–0.125149
6	6	1.418161	0.258503	–0.067800
7	1	1.542213	1.346474	–0.125029
8	6	–0.805949	1.778119	1.306973
9	1	–1.582844	2.543757	1.415116
10	1	–0.917011	1.062408	2.125124
11	1	0.163780	2.276900	1.410066
12	6	–0.837931	2.145389	–1.184491
13	1	0.152950	2.612528	–1.201232
14	1	–1.010388	1.674039	–2.155787
15	1	–1.578218	2.939755	–1.035391
16	6	–1.438803	–1.798433	–1.184626
17	1	–0.944170	–1.712222	–2.155828
18	1	–1.756677	–2.836695	–1.035494
19	1	–2.338767	–1.173835	–1.201608
20	6	–1.137260	–1.586863	1.306868
21	1	–0.462085	–1.325125	2.125145
22	1	–2.054079	–0.996390	1.409685
23	1	–1.411946	–2.642469	1.415066
24	6	1.942831	–0.191388	1.307080
25	1	1.889955	–1.280614	1.409925
26	1	2.994324	0.098614	1.415367
27	1	1.378464	0.262443	2.125291
28	6	2.277069	–0.346797	–1.184390
29	1	1.955134	0.038393	–2.155635
30	1	3.335132	–0.102849	–1.035185
31	1	2.186240	–1.438496	–1.201339

Table S-4 continued

C. Tri-n-propyl amine

Conf.	E_{MP2} / Hartree	μ_a / D	μ_b / D	μ_c / D	A / GHz	B / GHz	C / GHz	Freq. calc.
chain	–409.1473522	0.000	0.000	0.547	0.913	0.913	0.485	0
ring	–409.1413649	0.000	0.000	0.674	1.121	1.121	0.656	0

Table S-4/C. continued

Cartesian nuclear coordinates of the *chain* tri-n-propyl amine and the *ring* tri-n-propyl amine in *Gaussian03* internal coordinate system (called standard orientation)

Nr.	Atomic number	*chain* tri-n-propyl amine			*ring* tri-n-propyl amine		
		a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
1	7	–0.000003	–0.000013	–0.057498	0.000078	–0.000067	0.366425
2	6	1.269563	–0.571150	0.399921	1.400942	0.145269	0.790525
3	1	1.192267	–0.903324	1.454912	1.575865	–0.387183	1.744228
4	1	2.030052	0.217381	0.376346	1.589456	1.203905	0.991907
5	6	1.751648	–1.724021	–0.477117	2.414207	–0.321330	–0.256693
6	1	1.879708	–1.344519	–1.496632	2.262952	0.272093	–1.165707
7	1	0.984890	–2.505383	–0.523539	3.416925	–0.081637	0.122757
8	6	–0.140197	1.385038	0.399878	–0.826205	1.140343	0.790842
9	1	0.185973	1.484206	1.454915	–0.452492	1.557841	1.744620
10	1	–1.203320	1.649393	0.376141	–1.837249	0.774221	0.992202
11	6	0.617308	2.378945	–0.477079	–0.928812	2.251397	–0.256115
12	1	1.677368	2.105581	–0.523365	–1.637813	2.999785	0.123500
13	1	0.224746	2.300091	–1.496643	–1.367049	1.823881	–1.165242
14	6	–1.129406	–0.813961	0.399832	–0.574384	–1.285950	0.790570
15	1	–0.826773	–1.866828	0.376032	0.248221	–1.978575	0.991570
16	1	–1.378366	–0.581130	1.454885	–1.122612	–1.171311	1.744488
17	6	–2.368916	–0.654879	–0.477105	–1.485504	–1.929987	–0.256411
18	1	–2.662208	0.399841	–0.523395	–1.779118	–2.918288	0.122969
19	1	–2.104385	–0.955437	–1.496673	–0.896303	–2.095532	–1.165680
20	6	3.061252	–2.319544	0.042423	2.351851	–1.807536	–0.608746
21	1	3.414123	–3.128123	–0.604134	2.494493	–2.431936	0.280401
22	1	3.845820	–1.556504	0.084871	1.390853	–2.064629	–1.061094
23	1	2.933513	–2.725810	1.051196	3.137245	–2.064482	–1.326478
24	6	0.478205	3.810868	0.042421	0.389427	2.940673	–0.607956

Table S-4/C. continued

Nr.	Atomic number	*chain* tri-n-propyl amine			*ring* tri-n-propyl amine		
		a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
25	1	1.002108	4.520734	–0.604086	0.858793	3.376188	0.281330
26	1	–0.574891	4.108823	0.084740	1.092635	2.237137	–1.060472
27	1	0.893794	3.903385	1.051242	0.219237	3.749503	–1.325474
28	6	–3.539448	–1.491282	0.042442	–2.741572	–1.132843	–0.607829
29	1	–4.416162	–1.392526	–0.604068	–3.353280	–0.944330	0.281600
30	1	–3.270942	–2.552267	0.084803	–2.483930	–0.171966	–1.060126
31	1	–3.827354	–1.177586	1.051249	–3.357075	–1.684435	–1.325398

Table S-4 continued

D. Tri-*tert*-butyl amine

Conf.	E_{MP2} / Hartree	μ_a / D	μ_b / D	μ_c / D	A / GHz	B / GHz	C / GHz	Freq. calc.
I	–526.694531	0.000	0.000	0.521	0.840	0.840	0.5848	0

Table S-4/D. continued

Cartesian nuclear coordinates of tri-*tert*-butyl amine in *Gaussian03* internal coordinate system (called standard orientation)

Number	Atomic number	a /Å	b /Å	c /Å
1	7	–0.000005	–0.000008	–0.304005
2	6	–1.389865	–0.541522	–0.029630
3	6	–1.771151	–1.630607	–1.075898
4	1	–1.491757	–2.643440	–0.796632
5	1	–2.858229	–1.632924	–1.207805
6	1	–1.312923	–1.385318	–2.038238
7	6	0.225952	1.474413	–0.029621
8	6	1.687607	1.934757	–0.241193
9	1	1.708829	3.002692	–0.003396
10	1	2.415483	1.454755	0.407625
11	1	1.995941	1.824767	–1.282662
12	6	1.163904	–0.932896	–0.029627
13	6	2.297704	–0.718556	–1.075913
14	1	2.843217	–1.658845	–1.207888
15	1	1.856155	–0.444294	–2.038228
16	1	3.035178	0.029783	–0.796615
17	6	–2.519349	0.494151	–0.241214
18	1	–3.454848	–0.021464	–0.003580
19	1	–2.467681	1.364440	0.407704
20	1	–2.578138	0.816283	–1.282657
21	6	–1.613606	–1.084873	1.402331
22	1	–2.625030	–1.505085	1.467932
23	1	–0.917375	–1.873525	1.683383
24	1	–1.534954	–0.286823	2.145549
25	6	–0.132754	1.939833	1.402345
26	1	–1.163846	1.731137	1.683407
27	1	0.519088	1.472731	2.145554
28	1	0.008971	3.025867	1.467953
29	6	–0.526544	2.349156	–1.075908
30	1	–1.543365	2.613666	–0.796640
31	1	0.015031	3.291724	–1.207852
32	1	–0.543265	1.829642	–2.038230
33	6	1.746349	–0.854956	1.402328
34	1	2.081199	0.142337	1.683366
35	1	1.015909	–1.185879	2.145555
36	1	2.615997	–1.520740	1.467928
37	6	0.831751	–2.428902	–0.241182
38	1	0.052177	–2.819278	0.407693
39	1	0.582254	–2.640919	–1.282636
40	1	1.746025	–2.981238	–0.003462

Table S-5

Fitted parameters and their values from the *.par file of the *spfit* program

A. Main isotopologue

```
6   48   30    0    0.0000E+000    1.0000E+006    1.0000E+000 1.0000000000
's'  -3 -1  0   30   0   6   2   2     0    1   0
        10000  2.314873978171599E+003 1.00000000E+037 /A
       -20000  2.314873978171599E+003 1.00000000E-037 /B
        30000  1.326200000000000E+003 1.00000000E-037 /C
    110030000 -7.866604626405583E+000 1.00000000E+037 /1.5eqQ
          200 -9.619265665507071E-004 1.00000000E+037 /-DJ
         1100  1.588482320026774E-003 1.00000000E+037 /-DJK
```

B. $^{13}C_2$ isotopologue

```
6   16   30    0    0.0000E+000    1.0000E+006    1.0000E+000 1.0000000000
'a'  3  -2  0 ,,,,,,,,
        10000  2.312933148388725E+003 1.00000000E+037 /A
        20000  2.292833008304470E+003 1.00000000E+037 /B
        30000  1.326805735176605E+003 1.00000000E+037 /C
    110030000 -7.899035842546669E+000 1.00000000E+037 /1.5eqQ
          200 -9.693832871525565E-004 1.00000000E+037 /-DJ
         1100  3.594275012304982E-002 1.00000000E+037 /-DJK
```

C. $^{13}C_5$ isotopologue

```
7   10   30    0    0.0000E+000    1.0000E+006    1.0000E+000 1.0000000000
'a'  3  -2  0 ,,,,,,,,
        10000  2.313028148094109E+003 1.00000000E+037 /A
        20000  2.251267851743531E+003 1.00000000E+037 /B
        30000  1.329893199268403E+003 1.00000000E+037 /C
    110030000 -8.920996876517142E+000 1.00000000E+037 /1.5eqQ
    110040000 -5.641992532481138E-001 1.00000000E+036 /0.25X-
          200 -1.369036407949056E-003 1.00000000E+037 /-DJ
         1100 -1.987760643678322E-002 1.00000000E+037 /-DJK
```

Table S-6

Observed frequencies ($\nu_{Obs.}$) of the main isotopologue of triethyl amine. $\nu_{Calc.}$ is the calculated value; $\nu_{Obs.} - \nu_{Calc.}$ values obtained after a fit with the program *spfit*. J and K_c are the symmetric top rotational quantum numbers, F is the total angular momentum in the coupled basis with $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$.

Upper level			Lower level			$\nu_{Obs.}$	$\nu_{Obs.} - \nu_{Calc.}$
J	K_c	F	J	K_c	F	MHz	kHz
2	0	3	1	0	2	9259.5790	1.5
2	0	2	1	0	1	9259.4630	–2.1
2	0	2	1	0	2	9257.8925	0.5
2	0	1	1	0	1	9262.0870	–0.6
2	0	1	1	0	2	9260.5150	0.6
2	1	1	1	1	0	9261.4380	–0.6
2	1	2	1	1	1	9258.1610	0.2
2	1	3	1	1	2	9259.7895	–0.5
2	1	2	1	1	2	9258.9470	–0.2
2	1	1	1	1	2	9260.2590	0.3
3	0	4	2	0	3	13889.2020	–0.4
3	0	3	2	0	2	13889.1370	–3.0
3	0	2	2	0	1	13888.8760	–1.7
3	0	3	2	0	3	13887.4530	–1.4
3	0	2	2	0	2	13891.5010	0.9
3	1	4	2	1	3	13889.2920	2.0
3	1	3	2	1	2	13888.8225	0.8
3	1	3	2	1	3	13887.9805	1.5
3	1	2	2	1	2	13890.5930	1.1
3	2	2	2	2	2	13887.8685	1.0
3	2	2	2	2	1	13890.4890	–0.5
3	2	3	2	2	3	13889.5535	0.7
4	0	4	3	0	3	18518.7440	–1.6
4	0	5	3	0	4	18518.7830	–2.3
4	0	4	3	0	4	18516.9990	1.5
4	0	3	3	0	3	18520.9940	0.7
4	1	5	3	1	4	18518.8370	1.2
4	1	4	3	1	3	18518.6245	–2.7
4	1	4	3	1	4	18517.3195	3.3
4	1	3	3	1	3	18520.5395	1.7
4	2	5	3	2	4	18518.9895	2.4
4	2	4	3	2	3	18518.2705	–1.5
4	2	3	3	2	2	18519.1690	–1.9
4	3	5	3	3	4	18519.2390	–0.4
4	3	4	3	3	3	18517.6805	0.4
4	3	3	3	3	2	18519.8430	–0.4
4	3	3	3	3	3	18516.8930	–0.6
5	0	5	4	0	4	23148.2570	–1.8

Table S-6 continued

Upper level			Lower level			$\nu_{Obs.}$ MHz	$\nu_{Obs.} - \nu_{Calc.}$ kHz
J	K_c	F	J	K_c	F		
5	1	6	4	1	5	23148.3220	–1.3
5	1	5	4	1	4	23148.2130	3.9
5	1	5	4	1	5	23146.6885	–1.0
5	3	6	4	3	5	23148.6180	–1.1
5	3	5	4	3	4	23147.8115	–0.3
5	3	4	4	3	3	23148.8185	1.6
5	3	5	4	3	5	23148.4380	0.4
5	4	6	4	4	5	23148.8770	–0.9
5	4	5	4	4	4	23147.4645	0.3
5	4	4	4	4	3	23149.3000	0.3

Table S-7

Observed frequencies ($\nu_{Obs.}$) of the $^{13}C_2$ isotopologue of triethyl amine. For $\nu_{Calc.}$, $\nu_{Obs.} - \nu_{Calc.}$, and F see Table S–6, J, K_a, and K_c are the asymmetric top rotational quantum numbers.

Upper level				Lower level				$\nu_{Obs.}$ MHz	$\nu_{Obs.} - \nu_{Calc.}$ kHz
J	K_a	K_c	F	J	K_a	K_c	F		
2	1	1	2	1	0	1	2	9191.0185	0.0
2	2	0	3	1	1	0	2	9211.9245	–0.1
2	2	1	2	1	1	1	1	9230.4292	0.1
2	2	1	1	1	1	1	1	9231.7460	–0.1
2	2	1	3	1	1	1	2	9232.0648	–0.2
3	3	0	2	2	2	0	1	13818.1711	–0.9
3	3	0	3	2	2	0	2	13818.4359	0.0
3	3	0	4	2	2	0	3	13818.4991	0.9
3	3	1	3	2	2	1	2	13847.4235	0.3
3	3	1	4	2	2	1	3	13847.8932	–0.1
4	4	0	3	3	3	0	2	18425.8052	–0.5
4	4	0	4	3	3	0	3	18425.9203	1.0
4	4	0	5	3	3	0	4	18425.9581	–0.5
4	4	1	4	3	3	1	3	18463.7852	0.0
4	4	1	3	3	3	1	2	18463.9261	0.1
4	4	1	5	3	3	1	4	18463.9943	–0.2

Table S-8

Observed frequencies ($\nu_{Obs.}$) of the $^{13}C_5$ isotopologue of triethyl amine. For $\nu_{Calc.}$, $\nu_{Obs.} - \nu_{Calc.}$, J, K_a, K_c, and F see Table S-7.

Upper level				Lower level				$\nu_{Obs.}$	$\nu_{Obs.} - \nu_{Calc.}$
J	K_a	K_c	F	J	K_a	K_c	F	MHz	kHz
2	1	1	3	1	0	1	2	9067.0450	–0.4
3	2	1	4	2	1	1	3	13602.0519	0.4
3	1	2	2	2	0	2	1	13681.7775	0.0
3	3	0	2	2	2	0	1	13704.4148	–0.6
3	3	0	3	2	2	0	2	13704.6741	0.6
3	3	1	3	2	2	1	2	13786.7173	0.3
3	3	1	2	2	2	1	1	13787.1890	–0.4
3	3	1	2	2	2	1	3	13787.9226	0.1
4	3	1	4	3	2	1	3	18139.2802	0.2
4	3	1	3	3	2	1	2	18139.4766	–0.3