Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplemental material

Substituent steering of dihedral angles around single bonds: The case of succinonitrile

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S1: Rotational transitions of the main isotopologue of succinonitrile

J	K_a	K_c	F_1	F	J'	K_a	K_c	F_1	F	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	0	4	3	2	3	1	3	2	1	13242.96841	13242.96822	0.00019
4	0	4	3	4	3	1	3	2	3	13243.11094	13243.11106	-0.00012
4	0	4	5	4	3	1	3	4	3	13243.16023	13243.15978	0.00045
4	0	4	5	6	3	1	3	4	5	13243.25850	13243.25891	-0.00041
4	0	4	5	5	3	1	3	4	4	13243.50145	13243.50119	0.00026
4	0	4	4	5	3	1	3	3	4	13243.69998	13243.69983	0.00015
4	0	4	4	4	3	1	3	3	3	13243.89825	13243.89839	-0.00014
4	2	2	5	6	4	1	3	5	6	12548.10396	12548.10246	0.00150
4	2	2	4	4	4	1	3	4	4	12547.52780	12547.52781	-0.00001
4	2	2	4	5	4	1	3	4	5	12547.74799	12547.74787	0.00012
4	2	2	4	3	4	1	3	4	3	12547.78855	12547.78970	-0.00115
4	2	2	5	5	4	1	3	5	5	12547.86677	12547.86584	0.00093
4	2	2	3	3	4	1	3	3	3	12547.97526	12547.97586	-0.00060
4	2	2	5	4	4	1	3	5	4	12548.16093	12548.16137	-0.00044
2	2	0	2	2	2	1	1	2	2	13660.35472	13660.35399	0.00073
2	2	0	2	3	2	1	1	2	3	13660.57925	13660.57878	0.00047
2	2	0	2	2	2	1	1	2	3	13660.61168	13660.61260	-0.00092
2	2	0	3	3	2	1	1	3	3	13660.89714	13660.89771	-0.00057
2	2	0	3	4	2	1	1	3	4	13661.21045	13661.21082	-0.00037
2	2	0	3	2	2	1	1	3	2	13661.36752	13661.36794	-0.00042
2	2	0	1	2	2	1	1	1	2	13661.48469	13661.48573	-0.00104
2	2	0	1	1	2	1	1	1	0	13661.79908	13661.79978	-0.00070
2	1	2	2	2	1	0	1	1	1	12608.35779	12608.35850	-0.00071
2	1	2	2	3	1	0	1	2	3	12608.59861	12608.59923	-0.00062
2	1	2	2	3	1	0	1	1	2	12608.63158	12608.63028	0.00130
2	1	2	2	1	1	0	1	1	0	12608.70430	12608.70468	-0.00038
2	1	2	3	3	1	0	1	2	2	12608.99710	12608.99460	0.00250
2	1	2	3	4	1	0	1	2	3	12609.37088	12609.36914	0.00174
2	1	2	1	1	1	0	1	0	1	12609.52393	12609.52411	-0.00018
2	1	2	3	2	1	0	1	2	1	12609.55178	12609.55202	-0.00024
2	1	2	1	2	1	0	1	0	1	12609.66497	12609.66440	0.00057
2	1	2	1	2	1	0	1	1	1	12609.72915	12609.73017	-0.00102
5	2	3	5	5	5	1	4	5	5	12110.80847	12110.80826	0.00021
5	2	3	5	6	5	1	4	5	6	12110.93674	12110.93552	0.00122
5	2	3	5	4	5	1	4	5	4	12110.95467	12110.95558	-0.00091
5	2	3	6	6	5	1	4	6	6	12110.98911	12110.98833	0.00078
5	2	3	4	4	5	1	4	4	4	12111.03347	12111.03273	0.00074
5	2	3	6	7	5	1	4	6	7	12111.12201	12111.12130	0.00071
5	2	3	6	5	5	1	4	6	5	12111.14634	12111.14740	-0.00106
8	2	6	7	6	8	1	7	7	6	12762.06527	12762.06520	0.00007
8	2	6	7	8	8	1	7	7	8	12762.09840	12762.09907	-0.00067
8	2	6	9	10	8	1	7	9	10	12762.13297	12762.13302	-0.00005
8	2	6	7	7	8	1	7	7	7	12762.33024	12762.33002	0.00022
8	2	6	9	9	8	1	7	9	9	12762.37312	12762.37196	0.00116

J	K_a	K_c	F_1	F	J'	K_a	K_c	F_1	F	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
8	2	6	8	7	8	1	7	8	7	12762.40490	12762.40575	-0.00085
8	2	6	8	9	8	1	7	8	9	12762.43182	12762.43166	0.00016
8	2	6	8	8	8	1	7	8	8	12762.66698	12762.66670	0.00028
6	1	5	5	4	6	0	6	5	4	11472.56982	11472.56950	0.00032
6	1	5	5	6	6	0	6	5	6	11472.73164	11472.73253	-0.00089
6	1	5	7	6	6	0	6	7	6	11472.75900	11472.75796	0.00104
6	1	5	7	8	6	0	6	7	8	11472.89450	11472.89617	-0.00167
6	1	5	5	5	6	0	6	5	5	11473.51147	11473.51153	-0.00006
6	1	5	7	7	6	0	6	7	7	11473.72617	11473.72515	0.00102
6	1	5	6	5	6	0	6	6	5	11473.89032	11473.88838	0.00194
6	1	5	6	7	6	0	6	6	7	11474.00019	11474.00146	-0.00127
6	1	5	6	6	6	0	6	6	6	11474.80524	11474.80567	-0.00043
3	1	3	3	3	2	0	2	2	3	16176.96852	16176.96973	-0.00121
3	1	3	3	3	2	0	2	2	2	16177.00598	16177.00592	0.00006
3	1	3	3	4	2	0	2	2	3	16177.37733	16177.37685	0.00048
3	1	3	3	2	2	0	2	2	1	16177.46018	16177.46102	-0.00084
3	1	3	4	4	2	0	2	3	3	16177.63664	16177.63525	0.00139
3	1	3	2	2	2	0	2	1	2	16177.87985	16177.87953	0.00032
3	1	3	2	2	2	0	2	1	1	16177.89877	16177.89877	0.00000
3	1	3	4	5	2	0	2	3	4	16178.05236	16178.04946	0.00290
3	1	3	4	3	2	0	2	3	2	16178.17887	16178.17788	0.00099
3	1	3	2	3	2	0	2	1	2	16178.22416	16178.22420	-0.00004
3	1	3	2	1	2	0	2	1	0	16178.39388	16178.39539	-0.00151
3	1	3	2	1	2	0	2	1	1	16178.45543	16178.45815	-0.00272
3	2	1	2	2	3	1	2	3	3	13107.74684	13107.74926	-0.00242
3	2	1	3	4	3	1	2	3	3	13107.90187	13107.90037	0.00150
3	2	1	3	3	3	1	2	3	3	13107.99451	13107.99438	0.00013
3	2	1	2	3	3	1	2	3	4	13108.02562	13108.02648	-0.00086
3	2	1	3	4	3	1	2	3	4	13108.25811	13108.25720	0.00091
3	2	1	3	2	3	1	2	3	2	13108.32144	13108.32309	-0.00165
3	2	1	4	4	3	1	2	4	4	13108.46206	13108.46234	-0.00028
3	2	1	2	3	3	1	2	2	2	13108.60774	13108.60542	0.00232
3	2	1	2	2	3	1	2	2	2	13108.68339	13108.68504	-0.00165
3	2	1	4	5	3	1	2	4	5	13108.76649	13108.76522	0.00127
3	2	1	4	3	3	1	2	4	3	13108.87160	13108.87225	-0.00065
3	2	1	2	3	3	1	2	2	3	13108.91305	13108.91252	0.00053
3	2	1	2	1	3	1	2	2	1	13109.05988	13109.06035	-0.00047
3	2	1	2	2	3	1	2	2	1	13109.19043	13109.18954	0.00089
3	2	1	4	4	3	1	2	4	3	13109.01823	13109.01649	0.00174
4	0	4	4	3	3	1	3	3	2	13243.64498	13243.64688	-0.00190
4	2	2	3	2	4	1	3	3	2	12548.25214	12548.25406	-0.00192
4	4	1	5	6	3	3	0	4	5	50560.68070	50560.69071	-0.01001
4	4	0	5	6	3	3	1	4	5	50562.43790	50562.44782	-0.00992
5	4	2	6	7	4	3	1	5	6	54838.07960	54838.08881	-0.00921
5	4	1	6	7	4	3	2	5	6	54850.46830	54850.47744	-0.00914

J	K_a	K_c	F_1	F	J'	K_a	K_c	F_1	F	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
6	4	3	7	8	5	3	2	6	7	59092.39440	59092.40474	-0.01034
6	4	2	7	8	5	3	3	6	7	59142.21450	59142.22458	-0.01008
6	5	2	7	8	5	4	1	6	7	68675.01540	68674.98963	0.02577
7	6	1	8	9	7	5	2	8	9	52455.09070	52455.05780	0.03290
7	6	2	8	8	7	5	3	8	8	52455.24200	52455.20913	0.03287
7	4	4	8	9	6	3	3	7	8	63297.00000	63297.01348	-0.01348
7	4	3	8	8	6	3	4	7	7	63446.74580	63446.75907	-0.01327
7	3	4	8	9	6	2	5	7	8	54981.27530	54981.27247	0.00283
8	6	2	9	9	8	5	3	9	9	52419.27110	52419.24594	0.02516
8	6	3	9	9	8	5	4	9	9	52419.92080	52419.89570	0.02510
8	4	5	9	10	7	3	4	8	9	67410.18970	67410.20803	-0.01833
8	4	4	9	10	7	3	5	8	9	67783.23660	67783.26043	-0.02383
9	4	6	10	11	8	3	5	9	10	71373.36190	71373.38567	-0.02377
9	6	3	10	11	9	5	4	10	11	52366.21390	52366.19721	0.01669
9	6	4	10	11	9	5	5	10	11	52368.46140	52368.44513	0.01627
10	6	4	11	12	10	5	5	11	12	52290.53620	52290.52862	0.00758
10	6	5	11	12	10	5	6	11	12	52297.18210	52297.17565	0.00645
11	6	6	12	13	11	5	7	12	13	52202.61420	52202.61851	-0.00431
11	2	10	12	13	10	1	9	11	12	50040.98130	50040.98711	-0.00581
11	6	5	12	13	11	5	6	12	13	52185.20540	52185.20668	-0.00128
12	6	6	13	14	12	5	7	13	14	52040.68550	52040.69409	-0.00859
12	6	7	13	14	12	5	8	13	14	52082.04750	52082.06375	-0.01625
12	2	11	13	14	11	1	10	12	13	52884.01780	52883.99752	0.02028
13	0	13	14	14	12	1	12	13	13	50783.46980	50783.47165	-0.00185
13	1	13	14	15	12	0	12	13	14	50956.21170	50956.22252	-0.01082
13	6	7	14	15	13	5	8	14	15	51843.70680	51843.71895	-0.01215
13	6	8	14	15	13	5	9	14	15	51934.31430	51934.34409	-0.02979
13	2	12	14	15	12	1	11	13	14	55900.54830	55900.50095	0.04735
14	2	12	15	16	13	3	11	14	15	51722.74260	51722.76628	-0.02368
14	6	9	15	16	14	5	10	15	16	51760.80550	51760.85140	-0.04590
14	1	14	15	16	13	0	13	14	15	54711.36870	54711.37765	-0.00895
14	0	14	15	16	13	1	13	14	15	54607.87820	54607.88137	-0.00317
15	2	13	16	16	14	3	12	15	15	57605.94880	57605.99537	-0.04657
16	0	16	17	18	15	1	15	16	17	62220.82300	62220.82762	-0.00462
16	1	16	17	18	15	0	15	16	17	62257.01020	62257.01706	-0.00686
17	0	17	18	19	16	1	16	17	18	66017.63060	66017.63576	-0.00516
17	1	17	18	19	16	0	16	17	18	66038.80630	66038.81283	-0.00653
18	0	18	19	20	17	1	17	18	19	69811.02130	69811.02703	-0.00573
18	1	18	19	20	17	0	17	18	19	69823.34280	69823.34936	-0.00656
6	3	4	7	7	5	2	3	6	6	48812.92810	48812.95623	-0.02813
7	3	5	8	9	6	2	4	7	8	52370.51980	52370.55813	-0.03833
13	1	12	14	15	12	2	11	13	14	52197.92360	52197.83836	0.08524
14	1	13	15	16	13	2	12	14	15	56576.88140	56576.79121	0.09019
7	2	5	6	6	6	1	6	5	5	53043.99760	53043.88803	0.10957

S2: Rotational transitions of $^{13}CH_2$ isotopologue of succinonitrile

J	K_a	K_c	J'	K_a	K_c	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	4	1	3	3	0	49764.533	49764.550	-0.017
4	4	0	3	3	1	49766.447	49766.432	0.015
5	4	2	4	3	1	54025.070	54025.067	0.003
5	4	1	4	3	2	54038.345	54038.344	0.001
14	0	14	13	1	13	54315.997	54315.997	0.000
14	1	14	13	0	13	54406.676	54406.676	0.000
6	4	3	5	3	2	58261.154	58261.148	0.006
6	4	2	5	3	3	58314.533	58314.540	-0.007
7	4	4	6	3	3	62444.548	62444.551	-0.003
7	4	3	6	3	4	62604.996	62604.992	0.004
8	4	5	7	3	4	66531.090	66531.092	-0.002
8	4	4	7	3	5	66930.522	66930.523	-0.001
6	5	2	5	4	1	67637.590	67637.586	0.004
6	5	1	5	4	2	67638.264	67638.268	-0.004
9	4	6	8	3	5	70459.066	70459.063	0.003
9	4	5	8	3	6	71326.844	71326.843	0.001

S3: Rotational transitions of ^{13}CN isotopologue of succinonitrile

J	K_a	K_c	J'	K_a	K_c	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	4	1	3	3	0	50525.613	50525.619	-0.006
4	4	0	3	3	1	50527.268	50527.264	0.004
5	4	2	4	3	1	54761.887	54761.885	0.002
5	4	1	4	3	2	54773.489	54773.483	0.006
6	4	3	5	3	2	58976.341	58976.328	0.013
6	4	2	5	3	3	59022.958	59022.971	-0.013
7	4	4	6	3	3	63143.820	63143.816	0.004
7	4	3	6	3	4	63284.045	63284.052	-0.007
5	5	1	4	4	0	64350.319	64350.292	0.027
5	5	0	4	4	1	64350.319	64350.355	-0.036
8	4	5	7	3	4	67224.937	67224.947	-0.010
8	4	4	7	3	5	67574.512	67574.506	0.006
6	5	2	5	4	1	68594.197	68594.202	-0.005
6	5	1	5	4	2	68594.779	68594.767	0.012
9	4	6	8	3	5	71164.120	71164.107	0.013
9	4	5	8	3	6	71925.189	71925.189	0.000

S3: Rotational transitions of ^{15}N isotopologue of succinonitrile

J	K_a	K_c	J'	K_a	K_c	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	4	1	3	3	0	49870.226	49870.287	-0.061
4	4	0	3	3	1	49871.959	49871.941	0.018
5	4	2	4	3	1	54055.346	54055.366	-0.020
5	4	1	4	3	2	54067.042	54067.028	0.014
6	4	3	5	3	2	58218.577	58218.576	0.001
6	4	2	5	3	3	58265.472	58265.471	0.001
7	4	4	6	3	3	62334.723	62334.716	0.007
7	4	3	6	3	4	62475.676	62475.680	-0.004
5	5	1	4	4	0	63515.192	63515.160	0.032
5	5	0	4	4	1	63515.192	63515.223	-0.031
8	4	5	7	3	4	66364.286	66364.289	-0.003
8	4	4	7	3	5	66715.563	66715.562	0.001
6	5	2	5	4	1	67707.933	67707.939	-0.006
6	5	1	5	4	2	67708.523	67708.510	0.013
9	4	6	8	3	5	70251.643	70251.643	0.000

S4: Rotational transitions of ^{2}H (anti-H) isotopologue of succinonitrile

J	K_a	K_c	J'	K_a	K_c	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	4	1	3	3	0	48528.391	48528.365	0.026
4	4	0	3	3	1	48530.145	48530.139	0.006
5	4	2	4	3	1	52772.031	52772.021	0.010
5	4	1	4	3	2	52784.469	52784.528	-0.059
6	4	3	5	3	2	56992.609	56992.575	0.034
6	4	2	5	3	3	57042.895	57042.866	0.029
7	4	4	6	3	3	61163.328	61163.357	-0.029
7	4	3	6	3	4	61314.473	61314.480	-0.007
5	5	0	4	4	1	61782.129	61782.165	-0.036
5	5	1	4	4	0	61782.129	61782.094	0.035
8	4	5	7	3	4	65242.652	65242.635	0.017
8	4	4	7	3	5	65618.914	65618.914	0.000
6	5	2	5	4	1	66033.711	66033.710	0.001
6	5	1	5	4	2	66034.352	66034.347	0.005
9	4	6	8	3	5	69172.039	69172.040	-0.001
9	4	5	8	3	6	69989.727	69989.727	0.000
7	5	3	6	4	2	70279.609	70279.602	0.007
7	5	2	6	4	3	70282.781	70282.800	-0.019

S5: Rotational transitions of ^{2}H (anti-CN) isotopologue of succinonitrile

J	K_a	K_c	J'	K_a	K_c	$\nu_{obs.}$/MHz	$\nu_{calc.}$/MHz	Δν/MHz
4	4	1	3	3	0	48157.023	48157.028	-0.005
4	4	0	3	3	1	48159.289	48159.302	-0.013
5	4	2	4	3	1	52380.066	52380.065	0.001
5	4	1	4	3	2	52396.078	52396.102	-0.024
6	4	3	5	3	2	56574.523	56574.506	0.017
6	4	2	5	3	3	56639.035	56638.989	0.046
7	4	4	6	3	3	60707.109	60707.118	-0.009
7	4	3	6	3	4	60900.691	60900.712	-0.021
8	4	5	7	3	4	64726.125	64726.159	-0.034
8	4	4	7	3	5	65207.148	65207.163	-0.015
6	5	2	5	4	1	65540.891	65540.777	0.114
6	5	1	5	4	2	65541.562	65541.666	-0.104
9	4	6	8	3	5	68560.750	68560.742	0.008
9	4	5	8	3	6	69602.055	69602.045	0.010

S6:

M. J. Frisch. G. W. Trucks. H. B. Schlegel. G. E. Scuseria. M. A. Robb. J. R. Cheeseman. G. Scalmani. V. Barone. B. Mennucci. G. A. Petersson. H. Nakatsuji. M. Caricato. X. Li. H. P. Hratchian. A. F. Izmaylov. J. Bloino. G. Zheng. J. L. Sonnenberg. M. Hada. M. Ehara. K. Toyota. R. Fukuda. J. Hasegawa. M. Ishida. T. Nakajima. Y. Honda. O. Kitao. H. Nakai. T. Vreven. J. A. Montgomery. Jr.. J. E. Peralta. F. Ogliaro. M. Bearpark. J. J. Heyd. E. Brothers. K. N. Kudin. V. N. Staroverov. R. Kobayashi. J. Normand. K. Raghavachari. A. Rendell. J. C. Burant. S. S. Iyengar. J. Tomasi. M. Cossi. N. Rega. J. M. Millam. M. Klene. J. E. Knox. J. B. Cross. V. Bakken. C. Adamo. J. Jaramillo. R. Gomperts. R. E. Stratmann. O. Yazyev. A. J. Austin. R. Cammi. C. Pomelli. J. W. Ochterski. R. L. Martin. K. Morokuma. V. G. Zakrzewski. G. A. Voth. P. Salvador. J. J. Dannenberg. S. Dapprich. A. D. Daniels. Ö. Farkas. J. B. Foresman. J. V. Ortiz. J. Cioslowski. and D. J. Fox. Gaussian 09. Revision A.1. Gaussian. Inc.. Wallingford CT. 2009.