Electronic Supplementary Material (ESI)

Clonidine: molecule structure from gas-phase electron diffraction and quantum chemical calculations

Inna N. Kolesnikova *, Anatolii N. Rykov , Igor F. Shishkov, Victor A. Tafeenko, Leonid A. Aslanov

[a]Department of Chemistry, Lomonosov Moscow State University, Moscow 119991, Russia
*E-mail: kolesnikova@phys.chem.msu.ru.

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1 Information used for the GED model and results of the GED refinement

Table S1 Experimental intensities $I(s)$ and background lines $B(s)$ for clonidine.
1) Nozzle-to-Plate distance = 362.3 mm. Scale factor = 0.53(1) electrons' wavelength λ= 0.049988 Å, s in $Å^{-1}$

s	$I(s)$	$B(s)$	s	$I(s)$	$B(s)$
3.4	0.54730312	0.570601	11.0	0.52567541	0.52239242
3.6	0.54846914	0.58475209	11.2	0.52856442	0.52315327
3.8	0.54769755	0.59890317	11.4	0.5300357	0.52393669
4.0	0.54788661	0.61248457	11.6	0.52886426	0.52483926
4.2	0.56442034	0.62508736	11.8	0.52631748	0.5260438
4.4	0.59467537	0.63563348	12.0	0.52278873	0.52766829
4.6	0.6291482	0.6429818	12.2	0.5202981	0.52972297
4.8	0.65406861	0.64692225	12.4	0.52082432	0.53211993
5.0	0.67733225	0.64817669	12.6	0.52453115	0.53471968
5.2	0.68902711	0.64719805	12.8	0.52948715	0.53742547
5.4	0.69335453	0.64421686	13.0	0.53382516	0.54025662
5.6	0.69394545	0.63941965	13.2	0.53721985	0.54330471
5.8	0.68697468	0.63299379	13.4	0.54156688	0.54661308
6.0	0.66977066	0.62525168	13.6	0.54775475	0.55010715
6.2	0.64359303	0.61659328	13.8	0.55668414	0.5536795
6.4	0.61456521	0.60741479	14.0	0.56614603	0.55727578
6.6	0.5912247	0.59808432	14.2	0.57381137	0.56097917
6.8	0.57720399	0.58888526	14.4	0.57808351	0.56499504
7.0	0.5658096	0.58002125	14.6	0.58053404	0.56953932
7.2	0.55457021	0.57177393	14.8	0.5816826	0.57469046
7.4	0.5433938	0.56437109	15.0	0.58380968	0.58039482
7.6	0.53382693	0.55788334	15.2	0.58721797	0.58649277
7.8	0.53023379	0.55227457	15.4	0.59219154	0.59280621
8.0	0.53188583	0.54739219	15.6	0.59759865	0.59922051
8.2	0.53656742	0.54306882	15.8	0.60419018	0.60574829
8.4	0.54004752	0.53919843	16.0	0.61093058	0.61248118
8.6	0.54001631	0.53576737	16.2	0.61769314	0.6195769
8.8	0.53680761	0.53279072	16.4	0.62439813	0.62719816
9.0	0.53268169	0.53024341	16.6	0.63123236	0.63542161
9.2	0.53110734	0.52804532	16.8	0.63823386	0.64418063
9.4	0.53123715	0.52607946	17.0	0.64665926	0.65328236
9.6	0.53184809	0.52431116	17.2	0.65473316	0.66249116
9.8	0.53057416	0.52280441	17.4	0.66403168	0.67169997
10.0	0.52759149	0.52167931	10.8	0.52277844	0.5216808
10.2	0.52370299	0.5210249	11.0	0.52567541	0.52239242
10.4	0.52130825	0.52086396	11.2	0.52856442	0.52315327
10.6	0.52099621	0.52112485	17.4	0.66403168	0.67169997
10.8	0.52277844	0.5216808			

2) Nozzle-to-Plate distance = 193.9 mm. Scale factor = 0.64(2) electrons' wavelength λ= 0.050388 Å, s in $Å^{-1}$

s	*I*(*s*)	*B*(*s*)	*s*	*I*(*s*)	*B*(*s*)	*s*	*I*(*s*)	*B*(*s*)
6.8	0.619235	0.634517	15.6	0.473891	0.475779	24.4	0.417467	0.417091
7.0	0.610824	0.629312	15.8	0.47182	0.473736	24.6	0.415307	0.416434
7.2	0.603646	0.624107	16.0	0.470207	0.471789	24.8	0.414242	0.415786
7.4	0.590841	0.618937	16.2	0.468481	0.46992	25.0	0.413344	0.415141
7.6	0.582616	0.613858	16.4	0.466287	0.468097	25.2	0.412671	0.414505
7.8	0.579447	0.608859	16.6	0.463333	0.46629	25.4	0.412634	0.413892
8.0	0.584445	0.603869	16.8	0.459573	0.46449	25.6	0.412659	0.41331
8.2	0.590194	0.598788	17.0	0.4565	0.462714	25.8	0.411977	0.412766
8.4	0.594769	0.593595	17.2	0.454377	0.460979	26.0	0.411743	0.412276
8.6	0.595365	0.588318	17.4	0.452985	0.459298	26.2	0.411522	0.41184
8.8	0.588225	0.583029	17.6	0.452274	0.457677	26.4	0.411448	0.411451
9.0	0.580147	0.577884	17.8	0.452302	0.456117	26.6	0.411178	0.411107
9.2	0.575239	0.573026	18.0	0.452725	0.454604	26.8	0.411199	0.410813
9.4	0.575208	0.56849	18.2	0.453286	0.453126	27.0	0.411192	0.410571
9.6	0.573333	0.564215	18.4	0.454516	0.45169	27.2	0.410726	0.410382
9.8	0.570712	0.560148	18.6	0.455734	0.450313	27.4	0.410426	0.41025
10.0	0.563507	0.556241	18.8	0.456337	0.449007	27.6	0.410297	0.410177
10.2	0.556656	0.552464	19.0	0.456491	0.447766	27.8	0.410298	0.41016
10.4	0.549971	0.548773	19.2	0.454902	0.446555	28.0	0.410462	0.410195
10.6	0.544753	0.545145	19.4	0.45226	0.445334	28.2	0.410853	0.410281
10.8	0.542786	0.541592	19.6	0.448507	0.444074	28.4	0.411221	0.410417
11.0	0.541754	0.538111	19.8	0.444565	0.442759	28.6	0.411336	0.410606
11.2	0.540819	0.534691	20.0	0.440108	0.441385	28.8	0.41148	0.410859
11.4	0.538432	0.531318	20.2	0.436443	0.439967	29.0	0.411528	0.411193
11.6	0.532983	0.527988	20.4	0.433708	0.438527	29.2	0.411619	0.411627
11.8	0.525583	0.524709	20.6	0.432207	0.437091	29.4	0.41182	0.412176
12.0	0.516266	0.521484	20.8	0.431442	0.435685	29.6	0.41245	0.412846
12.2	0.507535	0.518322	21.0	0.431339	0.434326	29.8	0.41309	0.413626
12.4	0.502026	0.515243	21.2	0.430981	0.433012	30.0	0.414001	0.414496
12.6	0.499993	0.512264	21.4	0.429985	0.431735	30.2	0.414963	0.415425
12.8	0.500091	0.509391	21.6	0.428551	0.430498	30.4	0.415891	0.416383
13.0	0.49976	0.506615	21.8	0.427826	0.429309	30.6	0.417235	0.417339
13.2	0.4978	0.503922	22.0	0.427402	0.428161	30.8	0.417873	0.418272
13.4	0.495872	0.501305	22.2	0.427134	0.427044	31.0	0.418584	0.419195
13.6	0.496193	0.498761	22.4	0.426719	0.425947	31.2	0.419861	0.420134
13.8	0.498582	0.49629	22.6	0.426062	0.42487	31.4	0.420568	0.421114
14.0	0.502867	0.493892	22.8	0.424895	0.42382	31.6	0.421972	0.422168
14.2	0.50482	0.491547	23.0	0.424082	0.422811	31.8	0.423271	0.423313
14.4	0.503315	0.489235	23.2	0.423231	0.421849	32.0	0.424834	0.424556
14.6	0.498681	0.486943	23.4	0.423087	0.420934	32.2	0.426183	0.425892
14.8	0.492166	0.484656	23.6	0.422328	0.420062	32.4	0.42769	0.427313
15.0	0.485883	0.482379	23.8	0.421574	0.41924	32.6	0.429789	0.428793
15.2	0.480684	0.480124	24.0	0.420352	0.418474	32.8	0.431173	0.430272
15.4	0.476791	0.477915	24.2	0.418711	0.417763			

Table S2 Calculated and observed vibrational amplitudes in clonidine

Distance	GED	Calc[b]	GED[c]	Distance	GED	Calc[b]	GED[c]
	r_a	u	u		r_a	u	u
N3–H14	1.033	0.072	assumed	H14...Cl23	4.528	0.353	assumed
N1–H13	1.033	0.072	assumed	N1...C9	4.552	0.230	0.230(8)[7]
C9–H20	1.083	0.077	assumed	N6...H22	4.563	0.114	assumed
C11–H22	1.083	0.077	assumed	C10...H13	4.565	0.358	assumed
C10–H21	1.085	0.077	assumed	N3...C12	4.586	0.133	0.133(8)[7]
C5–H17	1.109	0.078	assumed	N6...H20	4.605	0.113	assumed
C4–H16	1.110	0.078	assumed	N3...Cl23	4.615	0.272	0.272(8)[7]
C5–H18	1.116	0.079	assumed	C2...C11	4.628	0.142	0.142(8)[7]
C4–H15	1.117	0.079	assumed	C4...C7	4.649	0.096	0.096(8)[7]
C2–N6	1.287	0.041	0.042(2)[1]	C7...H18	4.686	0.217	assumed
C2–N3	1.386	0.048	0.049(2)[1]	C5...C8	4.713	4.732	0.232(8)[7]
N6–C7	1.389	0.048	0.049(2)[1]	C12...H14	4.758	0.213	assumed
N1–C2	1.390	0.049	0.050(2)[1]	H21...Cl23	4.823	0.116	assumed
C11–C12	1.394	0.047	0.048(2)[1]	C8...H18	4.834	0.331	assumed
C8–C9	1.396	0.047	0.048(2)[1]	Cl19...H21	4.836	0.117	assumed
C9–C10	1.396	0.046	0.048(2)[1]	H14...Cl19	4.866	0.286	assumed
C10–C11	1.398	0.046	0.048(2)[1]	N1...C11	4.873	0.312	0.312(8)[7]
C7–C8	1.416	0.048	0.050(2)[1]	C8...H14	4.905	0.164	assumed
C7–C12	1.416	0.048	0.050(2)[1]	C7...H17	5.003	0.179	assumed
N3–C4	1.467	0.051	0.052(2)[1]	C7...H15	5.054	0.219	assumed
N1–C5	1.471	0.052	0.053(2)[1]	C2...C10	5.078	0.122	0.122(8)[7]
C4–C5	1.548	0.054	0.056(2)[1]	C4...Cl19	5.084	0.342	0.342(8)[7]
C12–Cl23	1.733	0.053	0.050(3)[2]	H17...Cl19	5.139	0.510	assumed
C8–Cl19	1.741	0.054	0.051(3)[2]	N1...C10	5.183	0.259	0.260(8)[7]
H15...H16	1.803	0.125	assumed	N1...H20	5.194	0.295	assumed
H17...H18	1.804	0.125	assumed	C2...H20	5.234	0.173	assumed
C2...H14	2.055	0.103	assumed	N3...Cl19	4.269	0.264	0.264(8)[7]
C2...H13	2.069	0.103	assumed	C5...C7	4.289	0.131	0.132(8)[7]
N1...H18	2.134	0.105	assumed	H20...H22	4.292	0.132	assumed
N1...H17	2.138	0.106	assumed	N1...Cl23	4.297	0.452	0.452(8)[7]
C12...H22	2.140	0.100	assumed	C5...Cl19	4.327	0.451	0.451(8)[7]
C8...H20	2.141	0.101	assumed	N6...H16	4.402	0.113	assumed
N3...H16	2.141	0.105	assumed	H13...H20	4.409	0.377	assumed
N3...H15	2.147	0.105	assumed	N6...H17	4.428	0.113	assumed
C9...H21	2.148	0.101	assumed	N3...C8	4.437	0.136	0.137(8)[7]
C11...H21	2.150	0.101	assumed	H13...Cl23	4.451	0.517	assumed
C10...H20	2.157	0.100	assumed	C11...H13	4.462	0.423	assumed
C10...H22	2.159	0.101	assumed	C2...C9	4.481	0.120	0.121(8)[7]
C4...H14	2.173	0.107	assumed	C9...Cl23	4.498	0.072	0.072(8)[7]
C5...H13	2.174	0.106	assumed	C11...Cl19	4.508	0.072	0.073(8)[7]
C4...H18	2.198	0.112	assumed	H14...Cl23	4.528	0.353	assumed
C5...H15	2.201	0.112	assumed	N1...C9	4.552	0.230	0.230(8)[7]
C4...H17	2.217	0.111	assumed	N6...H22	4.563	0.114	assumed
C5...H16	2.228	0.111	assumed	C10...H13	4.565	0.358	assumed
N1...N3	2.246	0.057	0.060(5)[3]	N3...C12	4.586	0.133	0.133(8)[7]
N3...C5	2.302	0.065	0.068(5)[3]	N6...H20	4.605	0.113	assumed
C2...C5	2.318	0.060	0.063(5)[3]	N3...Cl23	4.615	0.272	0.272(8)[7]

C2...C7	2.335	0.072	0.075(5)[3]	C2...C11	4.628	0.142	0.142(8)[7]
C2...C4	2.343	0.060	0.063(5)[3]	C4...C7	4.649	0.096	0.096(8)[7]
N3...N6	2.344	0.060	0.063(5)[3]	C7...H18	4.686	0.217	assumed
N1...C4	2.352	0.066	0.068(5)[3]	C5...C8	4.713	4.732	0.232(8)[7]
C8...C12	2.385	0.060	0.063(5)[3]	C12...H14	4.758	0.213	assumed
C10...C12	2.408	0.058	0.061(5)[3]	H21...Cl23	4.823	0.116	assumed
C8...C10	2.410	0.058	0.061(5)[3]	C8...H18	4.834	0.331	assumed
N1...N6	2.414	0.061	0.063(5)[3]	Cl19...H21	4.836	0.117	assumed
C9...C11	2.415	0.058	0.061(5)[3]	H14...Cl19	4.866	0.286	assumed
H15...H17	2.429	0.182	assumed	N1...C11	4.873	0.312	0.312(8)[7]
N6...C12	2.433	0.067	0.070(5)[3]	C8...H14	4.905	0.164	assumed
H16...H18	2.438	0.182	assumed	C7...H17	5.003	0.179	assumed
C7...C9	2.468	0.059	0.062(5)[3]	C7...H15	5.054	0.219	assumed
C7...C11	2.469	0.059	0.062(5)[3]	C2...C10	5.078	0.122	0.122(8)[7]
N6...C8	2.477	0.067	0.070(5)[3]	C4...Cl19	5.084	0.342	0.342(8)[7]
H20...H21	2.486	0.164	assumed	N1...C11	4.873	0.312	0.312(8)[7]
H21...H22	2.488	0.164	assumed	C8...H14	4.905	0.164	assumed
H13...H18	2.507	0.192	assumed	C7...H17	5.003	0.179	assumed
H14...H15	2.542	0.188	assumed	C7...H15	5.054	0.219	assumed
N6...H14	2.573	0.142	assumed	C2...C10	5.078	0.122	0.122(8)[7]
H14...H16	2.645	0.158	assumed	C4...Cl19	5.084	0.342	0.342(8)[7]
H13...H17	2.649	0.158	assumed	H17...Cl19	5.139	0.510	assumed
C11...Cl23	2.683	0.070	0.070(3)[4]	N1...C10	5.183	0.259	0.260(8)[7]
C9...Cl19	2.697	0.070	0.070(3)[4]	N1...H20	5.194	0.295	assumed
N6...H13	2.712	0.137	assumed	C2...H20	5.234	0.173	assumed
C7...Cl23	2.712	0.070	0.070(3)[4]	C5...C12	5.241	0.288	0.291(9)[8]
C7...Cl19	2.715	0.072	0.072(3)[4]	N6...H21	5.302	0.101	assumed
C7...H13	2.718	0.217	assumed	H13...H22	5.330	0.499	assumed
C9...C12	2.772	0.066	0.066(3)[4]	H15...Cl23	5.362	0.567	assumed
C8...C11	2.775	0.067	0.066(3)[4]	C4...C8	5.370	0.167	0.170(9)[8]
N3...H18	2.787	0.167	assumed	Cl19...Cl23	5.414	0.095	0.098(9)[8]
H22...Cl23	2.798	0.149	assumed	C8...H17	5.418	0.265	assumed
H16...H17	2.804	0.160	assumed	C2...H22	5.458	0.192	assumed
Cl19...H20	2.812	0.150	assumed	C4...Cl23	5.491	0.417	0.419(9)[8]
H13...Cl19	2.830	0.544	assumed	H13...H21	5.492	0.392	assumed
N1...H15	2.842	0.168	assumed	C4...C12	5.545	0.470	0.473(9)[8]
C7...C10	2.852	0.066	0.066(3)[4]	C5...Cl23	5.545	0.228	0.231(9)[8]
C8...H13	2.857	0.289	assumed	C7...H16	5.553	0.127	assumed
C2...H18	2.858	0.152	assumed	H20...Cl23	5.568	0.102	assumed
C2...H15	2.891	0.153	assumed	Cl19...H22	5.578	0.102	assumed
N1...C7	2.896	0.137	0.142(14)[5]	H16...Cl19	5.647	0.416	assumed
N6...Cl23	2.973	0.119	0.125(14)[5]	N1...H22	5.690	0.387	assumed
N6...Cl19	3.052	0.125	0.131(14)[5]	C12...H15	5.716	0.364	assumed
H15...H18	3.083	0.132	assumed	C12...H17	5.785	0.384	assumed
N3...H13	3.141	0.104	assumed	N3...C9	5.787	0.129	0.132(9)[8]
N1...H14	3.148	0.102	assumed	C12...H18	5.803	0.290	assumed
C2...C8	3.166	0.121	0.127(14)[5]	C5...C9	5.885	0.263	0.265(9)[8]
C2...H17	3.220	0.104	assumed	N3...C11	5.902	0.125	0.128(9)[8]
C2...H16	3.241	0.104	assumed	H15...Cl19	5.907	0.334	assumed
N3...H17	3.249	0.103	assumed	C8...H15	5.945	0.220	assumed
C5...H14	3.275	0.097	assumed	H17...Cl23	5.984	0.613	assumed
N1...H16	3.295	0.104	assumed	C9...H18	5.998	0.364	assumed

C2...Cl19	3.297	0.212	0.217(14)[5]	C11...H14	6.123	0.203	assumed
C4...H13	3.313	0.098	assumed	C2...H21	6.136	0.149	assumed
C2...C12	3.369	0.147	0.153(14)[5]	N1...H21	6.168	0.296	assumed
C12...H21	3.384	0.097	assumed	C8...H16	6.173	0.227	assumed
C8...H21	3.385	0.097	assumed	C9...H14	6.240	0.156	assumed
C11...H20	3.394	0.097	assumed	C5...C11	6.319	0.318	0.320(9)[8]
C9...H22	3.394	0.097	assumed	H18...Cl23	6.331	0.410	assumed
N1...C8	3.398	0.219	0.214(14)[5]	H18...H20	6.376	0.453	assumed
N1...Cl19	3.399	0.404	0.399(14)[5]	N3...C10	6.410	0.106	0.109(9)[8]
C7...H20	3.427	0.098	assumed	C5...H20	6.419	0.348	assumed
C7...H22	3.429	0.098	assumed	C9...H17	6.464	0.315	assumed
C4...N6	3.555	0.068	0.073(14)[5]	N3...H20	6.495	0.195	assumed
C5...N6	3.569	0.066	0.072(14)[5]	H16...Cl23	6.496	0.390	assumed
N3...C7	3.616	0.069	0.075(14)[5]	C12...H16	6.530	0.206	assumed
C12...H13	3.626	0.396	assumed	C5...C10	6.600	0.278	0.281(9)[8]
N6...C11	3.719	0.068	0.074(14)[5]	C4...C9	6.660	0.178	0.181(9)[8]
C2...Cl23	3.726	0.250	0.256(14)[5]	N3...H22	6.677	0.187	assumed
N6...C9	3.749	0.068	0.074(14)[5]	C10...H14	6.758	0.160	assumed
H14...H18	3.771	0.187	assumed	C11...H17	6.774	0.427	assumed
N1...C12	3.814	0.300	0.306(14)[5]	C4...C11	6.802	0.236	0.239(9)[8]
H13...H15	3.826	0.186	assumed	C11...H18	6.810	0.333	assumed
C12...H20	3.845	0.098	assumed	H14...H22	6.822	0.263	assumed
C8...H22	3.848	0.098	assumed	C10...H18	6.896	0.345	assumed
C9...H13	3.861	0.312	assumed	H17...H20	6.980	0.410	assumed
C7...H21	3.926	0.098	assumed	C11...H15	6.981	0.380	assumed
C7...H14	3.936	0.146	assumed	H14...H20	7.007	0.203	assumed
C10...Cl23	3.982	0.070	0.076(4)[6]	C10...H17	7.081	0.360	assumed
C8...Cl23	3.986	0.070	0.077(4)[6]	C5...H22	7.114	0.406	assumed
C12...Cl19	3.991	0.071	0.078(4)[6]	C9...H15	7.173	0.248	assumed
C10...Cl19	3.994	0.070	0.077(4)[6]	C4...C10	7.288	0.187	0.190(9)[8]
N6...H15	4.002	0.183	assumed	C4...H20	7.309	0.255	assumed
N6...H18	4.018	0.179	assumed	N3...H21	7.471	0.135	assumed
H13...H14	4.022	0.129	assumed	H17...H22	7.485	0.547	assumed
H18...Cl19	4.062	0.548	assumed	C9...H16	7.492	0.234	assumed
H14...H17	4.149	0.143	assumed	C4...H22	7.537	0.320	assumed
H13...H16	4.176	0.147	assumed	C5...H21	7.566	0.325	assumed
N6...C10	4.231	0.071	0.077(4)[6]	H15...H22	7.595	0.475	assumed
N3...Cl19	4.269	0.264	0.264(8)[7]	C10...H15	7.629	0.307	assumed
C5...C7	4.289	0.131	0.132(8)[7]	H18...H22	7.689	0.393	assumed
H20...H22	4.292	0.132	assumed	C11...H16	7.790	0.214	assumed
N1...Cl23	4.297	0.452	0.452(8)[7]	H14...H21	7.823	0.178	assumed
C5...Cl19	4.327	0.451	0.451(8)[7]	H18...H21	7.836	0.390	assumed
N6...H16	4.402	0.113	assumed	H15...H20	7.906	0.288	assumed
H13...H20	4.409	0.377	assumed	H17...H21	7.987	0.420	assumed
N6...H17	4.428	0.113	assumed	H16...H20	8.068	0.323	assumed
N3...C8	4.437	0.136	0.137(8)[7]	C10...H16	8.214	0.199	assumed
H13...Cl23	4.451	0.517	assumed	C4...H21	8.317	0.224	assumed
C11...H13	4.462	0.423	assumed	H16...H22	8.554	0.291	assumed
C2...C9	4.481	0.120	0.121(8)[7]	H15...H21	8.642	0.342	assumed
C9...Cl23	4.498	0.072	0.072(8)[7]	H16...H21	9.244	0.233	assumed
C11...Cl19	4.508	0.072	0.073(8)[7]				

[a]Values of distances (r_a), and amplitudes (u) are in Å**.**

[b] Calculated with B3LYP/6-31G(d,p) quadratic force constants.

[c]The same numeric superscripts indicate that these amplitudes were refined in one group; differences between their values were assumed from theoretical calculation. Amplitudes without superscript were constrained to the calculated values.

Table S3 Matrix of correlation for GED refinement. Parameters 10 and 20 are the scale factors for LD and SD, respectively. The definition of all other parameters can be found in Tab. 4 and S2.

	10	20	b	c	d	e	f	g
10	1.0000							
20	0.5036	1.0000						
b	-0.1958	-0.1676	1.0000					
c	0.3205	0.3627	-0.3938	1.0000				
d	-0.4115	-0.3600	0.3804	-0.4945	1.0000			
e	0.0397	0.0012	-0.0583	-0.0359	-0.0210	1.0000		
f	-0.3584	-0.1979	0.3160	-0.0823	0.4296	-0.5576	1.0000	
g	0.0721	0.0881	-0.0323	0.3002	-0.0904	0.0108	-0.0302	1.0000
h	0.1669	0.2227	-0.3445	0.1841	-0.2652	0.0694	-0.2023	-0.0002
j	0.0479	0.0937	-0.1006	-0.1784	-0.1775	0.0140	-0.0478	-0.1331
k	-0.0643	0.0087	0.2971	-0.0003	0.1269	0.0224	0.0861	0.6005
l	-0.1441	-0.0349	0.2301	-0.0729	0.2315	-0.1068	0.2050	0.0769
n	-0.1064	0.0070	0.0929	-0.1659	0.0664	-0.0208	0.1158	-0.0201
1	0.1477	0.3451	0.2747	-0.5926	0.3120	-0.0087	-0.0420	-0.1218
2	0.1818	0.4141	0.0034	-0.1164	0.0157	0.0195	-0.0582	-0.0557
3	0.4015	0.5379	-0.3673	0.6451	-0.4254	-0.0914	-0.0230	0.0699
4	0.1240	0.2930	-0.1506	0.0013	-0.1412	0.0058	-0.1184	0.1013
5	-0.0791	-0.1271	-0.0003	0.0628	0.0975	-0.0883	0.0863	-0.0011
6	0.1835	0.2804	-0.0688	0.0800	-0.1039	-0.0295	-0.0291	-0.0289
7	0.1652	0.1674	-0.0467	0.0839	-0.1236	-0.0333	-0.0485	-0.0342
8	0.1340	0.1197	-0.0504	0.0294	-0.0891	0.0312	-0.1151	-0.0025

	h	j	k	l	n	1	2	3
h	1							
j	0.5573	1.0000						
k	-0.0431	-0.0700	1.0000					
l	-0.2790	-0.3505	0.2774	1.0000				
n	0.2167	0.4505	0.1955	0.5436	1.0000			
1	-0.0280	0.1626	0.0653	0.0740	0.1378	1.0000		
2	0.0434	0.1123	-0.0136	0.0118	0.0655	0.4221	1.0000	
3	0.2891	0.3151	-0.2645	-0.2403	0.0339	-0.1887	0.1221	1.0000
4	0.0214	-0.0959	0.0775	0.4103	0.2268	0.1830	0.1757	-0.0244
5	-0.4071	-0.4779	-0.1695	-0.3273	-0.5764	-0.1294	-0.0865	-0.1305
6	0.1462	0.0903	-0.0402	0.0592	0.1378	0.1143	0.1182	0.1625
7	-0.1929	-0.0809	-0.1604	-0.1738	-0.3372	0.0324	0.0737	0.1478

8	0.0504	0.0568	-0.0115	-0.1386	-0.1137	0.0515	0.0434	0.0660

	4	5	6	7	8
4	1.0000				
5	-0.0565	1.0000			
6	0.1242	-0.1237	1.0000		
7	-0.0275	0.1509	-0.0169	1.0000	
8	-0.0106	0.0178	0.0202	0.0812	1.0000

Table S4 Cartesian coordinates of clonidine obtained from GED refinement

Atom	X	Y	Z
N	-1.879695122	0.061381849	1.046286814
C	-1.621525359	-0.354747009	-0.255075602
N	-2.824103123	-0.723237773	-0.836023741
C	-3.882436265	-0.818042142	0.176752308
C	-3.335955311	0.193049119	1.215110806
N	-0.493527753	-0.443144532	-0.867288801
C	0.698482964	-0.011279429	-0.301246257
C	1.050676824	1.349209024	-0.116305465
C	2.305338525	1.754715559	0.343552
C	3.273135751	0.795193792	0.643510373
C	2.980065167	-0.5615769	0.481778341
C	1.720528173	-0.941189517	0.019220849
H	-1.242813675	0.773862716	1.445451949
H	-2.766308792	-1.41919726	-1.600798203
H	-3.955401568	-1.841794321	0.6194092
H	-4.874326819	-0.535179136	-0.235412588
H	-3.644956147	-0.054532861	2.252877592
H	-3.675717398	1.229133812	0.973877846
Cl	-0.128489424	2.572976726	-0.496357716
H	2.514285096	2.813438122	0.457540652
H	4.252667327	1.101996622	0.998625505
H	3.717659478	-1.323849668	0.710777044
Cl	1.394457007	-2.634182214	-0.16004164

2 Results of quantum-chemical calculations

2.1 Geometries and thermochemical properties for clonidine conformers obtained by the B3LYP/6-31G(d,p) calculations

Table S5 Cartesian coordinates of **I** conformer found using B3LYP/6-31G(d,p) calculations

Atom	X	Y	Z
N	-1.834760	0.104895	1.0228940
C	-1.578059	-0.288618	-0.2824940
N	-2.789733	-0.595301	-0.8710440
C	-3.835911	-0.666455	0.1438730
C	-3.273808	0.298651	1.2035580
N	-0.458636	-0.411442	-0.9024850
C	0.746536	-0.041067	-0.3282130
C	1.157555	1.300537	-0.1495600
C	2.422200	1.650600	0.3180220
C	3.339482	0.651186	0.6316690
C	2.984920	-0.688035	0.4748990
C	1.717418	-1.015492	0.0049410
H	-1.193364	0.768044	1.4349150
H	-2.758955	-1.258796	-1.6319920
H	-3.946332	-1.678452	0.5603010
H	-4.803203	-0.339542	-0.2462790
H	-3.591481	0.039230	2.2167030
H	-3.579877	1.332048	0.9883980
Cl	0.033293	2.601616	-0.5498240
H	2.677543	2.698523	0.4275070
H	4.328041	0.913991	0.9933760
H	3.683195	-1.481720	0.7151070
Cl	1.301080	-2.712687	-0.1739270

Thermochemical data for **I** conformer of clonidine calculated with B3LYP/6-31G(d,p) at 420 K using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.693	64.247	134.34
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.451
Vibrational	117.189	58.286	56.998

Ee =-1433.0377755 Ha
ZPE = 0.167018 Ha

Table S6 Cartesian coordinates of **A1** conformer found using B3LYP/6-31G(d,p) calculations

Atom	X	Y	Z
N	2.717484	-1.031707	-0.705422
C	1.719774	-0.353013	-0.267563
N	1.900095	0.391994	0.899259
C	3.361222	0.444376	1.088512
C	3.819613	-0.764846	0.22795
N	0.478482	-0.403357	-0.902015
C	-0.747155	-0.039116	-0.318684
C	-1.132630	1.305098	-0.142978
C	-2.362776	1.660219	0.405748
C	-3.272194	0.666381	0.757701
C	-2.951330	-0.674679	0.561767
C	-1.705928	-1.010924	0.039484
H	-0.062537	2.599212	-0.667955
H	-2.606439	2.708996	0.528579
H	-4.236096	0.937640	1.175223
H	-3.650189	-1.461179	0.821503
H	-1.322751	-2.709367	-0.186574
H	0.436961	-1.216493	-1.504457
Cl	1.414041	1.278206	0.951055
H	3.776317	1.388275	0.707863
H	3.627201	0.351252	2.145115
H	4.752687	-0.563496	-0.308518
Cl	3.991394	-1.650066	0.856247

Thermochemical data for **A1** conformer of clonidine calculated with B3LYP/6-31G(d,p) using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.566	64.196	134.701
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.468
Vibrational	117.062	58.234	57.343

Ee = -1433.0251552 Ha
ZPE = 0.166791 Ha

Table S7 Cartesian coordinates of **A2** conformer found using B3LYP/6-31G(d,p) calculations

Atom	X	Y	Z
N	-2.775005	-0.836195	-0.817439
C	-1.728716	-0.295096	-0.305932
N	-1.883486	0.425299	0.877165
C	-3.212368	0.048088	1.38456
C	-3.879388	-0.491107	0.088066
N	-0.484689	-0.381520	-0.922886
C	0.741161	-0.032825	-0.333924
C	1.693146	-1.014431	0.015584
C	2.935574	-0.692397	0.553835
C	3.254751	0.645073	0.777123
C	2.350627	1.647361	0.43513
C	1.122379	1.312048	-0.133993
H	1.302720	-2.708333	-0.241525
H	3.631496	-1.484631	0.803788
H	4.215655	0.907217	1.207513
H	2.597878	2.692827	0.57794
H	0.071735	2.608809	-0.655606
H	-0.459998	-1.147181	-1.583716
Cl	-1.110844	0.413767	1.531224
H	-3.139001	-0.733771	2.154231
H	-3.733289	0.908198	1.814394
H	-4.518602	-1.358834	0.28056
Cl	-4.509750	0.280950	-0.375272

Thermochemical data for **A2** conformer of clonidine calculated with B3LYP/6-31G(d,p) using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.448	64.389	136.112
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.460
Vibrational	116.944	58.427	58.012

Ee = -1433.023614 Ha
ZPE = 0.166456 Ha

Table S8 Cartesian coordinates of **A3** conformer found using B3LYP/6-31G(d,p) calculations

Atom	X	Y	Z
N	-1.776220	0.088168	1.057201
C	-1.640778	-0.413308	-0.110393
N	-2.773691	-0.945156	-0.741931
C	-3.916229	-0.473755	0.064113
C	-3.208547	-0.004551	1.372157
N	-0.445274	-0.516830	-0.826291
C	0.763495	-0.027707	-0.298769
C	1.827273	-0.890941	0.021911
C	3.050509	-0.426740	0.496104
C	3.233426	0.941470	0.677109
C	2.210570	1.831449	0.357214
C	1.002797	1.351517	-0.142879
H	1.614279	-2.627499	-0.190331
H	3.837199	-1.134663	0.729053
H	4.177713	1.315886	1.05825
H	2.346401	2.900455	0.472103
H	-0.210122	2.514419	-0.632533
H	-0.352885	-1.413825	-1.288882
Cl	-2.827371	-0.756901	-1.736849
H	-4.435525	0.355498	-0.433729
H	-4.639267	-1.276735	0.233888
H	-3.593162	0.956262	1.730699
Cl	-3.352574	-0.731487	2.181889

Thermochemical data for **A3** conformer of clonidine calculated with B3LYP/6-31G(d,p) using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.558	64.177	134.756
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.459
Vibrational	117.055	58.215	57.407

Ee = -1433.0251604 Ha
ZPE = 0.166740 Ha

Table S9 Equilibrium distribution of clonidine conformers at 420 K by means of B3LYP/6-31G(d,p) calculations

Conformer	ΔE_e	ΔH	S_{420}	p_{420}
I	0.0	0.0	135.7	100
A1	8.1	7.8	136.1	0
A2	8.9	8.5	136.7	0
A3	7.9	7.7	136.1	0

ΔE_e (kcal /mol) is the relative electronic energy; $H = E_e$ + ZPE (kcal·mol^{-1}), where ZPE is the zero point energy correction calculated from scaled vibrational frequencies; S_{420} (cal/(K·mol)) is the entropy value at 420 K obtained using scaled frequencies including the entropy of mixing (Rln2), since all conformers present as an equimolar mixture of the two optical isomers; $\Delta G_T(i) = \Delta H(i) + T\ \Delta S_T(i)$ is the Gibbs free energy difference (kcal·mol^{-1}); $p_T\ (i) = [\exp(-\Delta G_T\ (i) /RT)]/\Sigma[\exp(-G_T(i) /RT)]$ is the mole fraction of conformers (%).

2.2 Geometries and thermochemical properties for clonidine conformers obtained by the B3LYP/cc-pVTZ calculations

Table S10 Cartesian coordinates of **I** conformer found using B3LYP/cc-pVTZ calculations

Atom	X	Y	Z
N	-1.837584	0.099649	1.019084
C	-1.574738	-0.290820	-0.280993
N	-2.780756	-0.594687	-0.87445
C	-3.834237	-0.662430	0.130695
C	-3.275758	0.286861	1.199668
N	-0.456123	-0.412155	-0.887614
C	0.747940	-0.040914	-0.323059
C	1.153143	1.296983	-0.148103
C	2.413520	1.649357	0.311271
C	3.332506	0.657697	0.619436
C	2.982183	-0.677169	0.466814
C	1.718884	-1.008789	0.006219
H	-1.199492	0.752658	1.442601
H	-2.751845	-1.248831	-1.638572
H	-3.954964	-1.673101	0.535458
H	-4.791094	-0.325922	-0.264353
H	-3.592305	0.015381	2.2051
H	-3.579869	1.318798	0.998034
Cl	0.027552	2.589641	-0.541703
H	2.665268	2.694194	0.418086
H	4.318330	0.923037	0.974215
H	3.681704	-1.465265	0.703337
Cl	1.310381	-2.701715	-0.167987

Thermochemical data for **I** conformer of clonidine calculated with B3LYP/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.708	64.114	134.197
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.436
Vibrational	117.204	58.152	56.870

Ee = -1433.2785142 Ha
ZPE = 0.167101 Ha

Table S11 Cartesian coordinates of **A1** conformer found using B3LYP/cc-pVTZ calculations

Atom	X	Y	Z
N	2.702478	-1.071461	-0.703435
C	1.711656	-0.401551	-0.253611
N	1.913664	0.342737	0.904596
C	3.376220	0.401693	1.066751
C	3.821267	-0.805957	0.206931
N	0.461704	-0.470267	-0.855977
C	-0.750214	-0.041521	-0.301932
C	-1.080953	1.313926	-0.144956
C	-2.297625	1.722032	0.381738
C	-3.249899	0.775460	0.726933
C	-2.984493	-0.573621	0.543435
C	-1.752522	-0.964936	0.04522
H	0.396796	-1.296828	-1.431156
H	1.421757	1.219457	0.975582
H	3.776513	1.341464	0.673392
H	3.660386	0.314602	2.114182
H	4.738663	-0.607213	-0.347407
H	4.002410	-1.686901	0.831058
Cl	0.037844	2.556928	-0.671212
H	-2.497768	2.777262	0.491498
H	-4.203520	1.089488	1.126904
H	-3.717762	-1.325003	0.795237
Cl	-1.442728	-2.673782	-0.16812

Thermochemical data for **A1** conformer of clonidine calculated with B3LYP/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.603	64.062	134.453
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.454
Vibrational	117.099	58.100	57.108

Ee = -1433.26655 Ha
ZPE = 0.166928 Ha

Table S12 Cartesian coordinates of **A2** conformer found using B3LYP/cc-pVTZ calculations

Atom	X	Y	Z
N	-2.766112	-0.835771	-0.830016
C	-1.721916	-0.325703	-0.29842
N	-1.882708	0.362402	0.897673
C	-3.227767	0.007335	1.374566
C	-3.880366	-0.508829	0.066494
N	-0.473589	-0.423956	-0.892249
C	0.743693	-0.033137	-0.321861
C	1.723250	-0.982023	0.019328
C	2.955041	-0.624089	0.543376
C	3.236762	0.716848	0.760375
C	2.305563	1.687199	0.422571
C	1.088008	1.317271	-0.133133
H	-0.433982	-1.189183	-1.547126
H	-1.124640	0.324904	1.561588
H	-3.181492	-0.777186	2.136452
H	-3.738347	0.871149	1.797688
H	-4.515353	-1.378723	0.235237
H	-4.504215	0.265296	-0.391321
Cl	1.383780	-2.680871	-0.234802
H	3.673355	-1.392303	0.787228
H	4.189630	1.006718	1.180308
H	2.523875	2.735962	0.557223
Cl	0.006480	2.580013	-0.656075

Thermochemical data for **A2** conformer of clonidine calculated with B3LYP/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.498	64.243	135.208
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.446
Vibrational	116.994	58.281	57.871

Ee = -1433.265027 Ha
ZPE = 0.166595 Ha

Table S13 Cartesian coordinates of **A3** conformer found using B3LYP/cc-pVTZ calculations

Atom	X	Y	Z
N	-1.779415	0.096718	1.046757
C	-1.637112	-0.410272	-0.110422
N	-2.767057	-0.943544	-0.737214
C	-3.911095	-0.475241	0.065868
C	-3.208925	0.008832	1.365589
N	-0.442735	-0.519677	-0.816568
C	0.764883	-0.028074	-0.296983
C	1.822352	-0.889216	0.024649
C	3.040023	-0.428076	0.498409
C	3.223384	0.934393	0.679018
C	2.206685	1.821483	0.356752
C	1.004150	1.345063	-0.142841
H	-0.351007	-1.410574	-1.282866
H	-2.822315	-0.771764	-1.730744
H	-4.433572	0.342375	-0.437295
H	-4.623639	-1.279623	0.243057
H	-3.589096	0.971605	1.70916
H	-3.350935	-0.704141	2.181802
Cl	1.608568	-2.618474	-0.190067
H	3.822890	-1.133698	0.732311
H	4.163707	1.306590	1.060468
H	2.343311	2.886413	0.470024
Cl	-0.200389	2.505827	-0.635638

Thermochemical data for **A3** conformer of clonidine calculated with B3LYP/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.631	64.003	134.483
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.443
Vibrational	117.127	58.041	57.149

Ee = -1433.2669916 Ha
ZPE = 0.166946 Ha

Table S14 Equilibrium distribution of clonidine conformers at 420 K by means of B3LYP/cc-pVTZ calculations

Conformer	ΔE_e	ΔH	S_{420}	p_{420}
I	0.0	0.0	135.6	100
A1	7.5	7.4	135.8	0
A2	8.5	8.1	136.6	0
A3	7.2	7.1	135.9	0

ΔE_e (kcal /mol) is the relative electronic energy; $H = E_e$ + ZPE (kcal·mol^{-1}), where ZPE is the zero point energy correction calculated from scaled vibrational frequencies; S_{420} (cal/(K·mol)) is the entropy value at 420 K obtained using scaled frequencies including the entropy of mixing (Rln2), since all conformers present as an equimolar mixture of the two optical isomers; $\Delta G_T(i) = \Delta H(i) + T\ \Delta S_T(i)$ is the Gibbs free energy difference (kcal·mol^{-1}); $p_T\ (i) = [\exp(-\Delta G_T\ (i) /RT)]/\Sigma[\exp(-G_T(i) /RT)]$ is the mole fraction of conformers (%).

2.3 Geometries and thermochemical properties for clonidine conformers obtained by the MP2/cc-pVTZ calculations

Table S15 Cartesian coordinates of I conformer found using MP2/cc-pVTZ calculations

Atom	X	Y	Z
N	-1.704501	0.033546	1.012663
C	-1.531031	-0.333559	-0.309834
N	-2.775533	-0.613675	-0.832894
C	-3.735403	-0.716932	0.257116
C	-3.124615	0.269875	1.24871
N	-0.444154	-0.447567	-0.985336
C	0.732290	-0.040802	-0.372932
C	1.066400	1.312414	-0.170734
C	2.291776	1.714500	0.352618
C	3.234857	0.751318	0.695077
C	2.948992	-0.599145	0.5186
C	1.717141	-0.976231	-0.004802
H	-3.415553	1.292491	0.995475
H	-0.093472	2.531244	-0.602937
H	2.493932	2.768109	0.478878
H	4.191392	1.052663	1.097785
H	3.665727	-1.362514	0.783666
H	1.366858	-2.658191	-0.203222
Cl	-1.032723	0.690252	1.380081
H	-2.785023	-1.285400	-1.583937
H	-3.765782	-1.720264	0.690506
H	-4.733448	-0.426960	-0.059435
Cl	-3.399204	0.054978	2.27773

Thermochemical data for **I** conformer of clonidine calculated with MP2/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	119.173	64.596	134.194
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.354
Vibrational	116.669	58.634	56.950

Ee = -1428.6038924 Ha
ZPE = 0.166112 Ha

Table S16 Cartesian coordinates of **A1** conformer found using MP2/cc-pVTZ calculations

Atom	X	Y	Z
N	2.716807	-1.003898	-0.710601
C	1.679541	-0.375440	-0.289469
N	1.778860	0.304168	0.924179
C	3.228998	0.442378	1.11966
C	3.738224	-0.766006	0.319394
N	0.469206	-0.408683	-0.968866
C	-0.732570	-0.038134	-0.35724
C	-1.077540	1.309336	-0.162806
C	-2.279375	1.684536	0.42932
C	-3.193071	0.705502	0.804285
C	-2.906469	-0.639251	0.594172
C	-1.686206	-0.994549	0.030938
H	0.412736	-1.235612	-1.547303
H	1.251326	1.163430	0.980417
H	3.594499	1.376855	0.68516
H	3.491419	0.406345	2.17355
H	4.712422	-0.590609	-0.130697
H	3.813288	-1.648879	0.959296
Cl	0.004619	2.551900	-0.700327
H	-2.495248	2.733741	0.566331
H	-4.133485	0.991637	1.253219
H	-3.606367	-1.412481	0.874252
Cl	-1.323671	-2.669298	-0.208894

Thermochemical data for **A1** conformer of clonidine calculated with MP2/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations.

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	118.988	64.657	135.713
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.380
Vibrational	116.484	58.696	58.443

Ee = -1428.5909445 Ha
ZPE = 0.165716 Ha

Table S17 Cartesian coordinates of **A2** conformer found using MP2/cc-pVTZ calculations

Atom	X	Y	Z
N	2.778703	0.742923	-0.781844
C	1.698947	0.204115	-0.342338
N	1.770890	-0.518963	0.845111
C	3.031772	-0.072566	1.450845
C	3.807534	0.355806	0.194732
N	0.499157	0.263099	-1.037095
C	-0.721785	0.030553	-0.389787
C	-1.568268	1.084569	-0.005863
C	-2.797895	0.863149	0.604339
C	-3.197511	-0.443255	0.866781
C	-2.389245	-1.513877	0.499468
C	-2.389245	-1.513877	0.499468
H	0.503451	1.041772	-1.681472
H	0.947383	-0.485739	1.430146
H	2.870080	0.779634	2.116541
H	3.512755	-0.875948	2.002476
H	4.492163	1.178447	0.386064
H	4.384703	-0.481943	-0.204904
Cl	-1.055760	2.710483	-0.308249
H	-3.416039	1.705677	0.876866
H	-4.145944	-0.627832	1.351017
H	-2.697683	-2.533267	0.678381
Cl	-0.233906	-2.622258	-0.666264

Thermochemical data for **A2** conformer of clonidine calculated with MP2/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations.

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	118.928	64.696	135.395
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.371
Vibrational	116.424	58.734	58.134

Ee = -1428.5900023 Ha
ZPE = 0.165589 Ha

Table S18 Cartesian coordinates of **A3** conformer found using MP2/cc-pVTZ calculations

Atom	X	Y	Z
N	2.778701	0.742939	-0.781838
C	1.698948	0.204122	-0.342339
N	1.770894	-0.518970	0.845104
C	3.031777	-0.072566	1.450842
C	3.807535	0.355813	0.19473
N	0.499154	0.263106	-1.037098
C	-0.721784	0.030552	-0.389789
C	-1.568273	1.084565	-0.005859
C	-2.797902	0.863138	0.604336
C	-3.197517	-0.443268	0.866773
C	-2.389244	-1.513884	0.499461
C	-1.174845	-1.276833	-0.14011
H	0.503444	1.041798	-1.681453
H	0.947389	-0.485748	1.430144
H	2.870078	0.779634	2.116537
H	3.512758	-0.875951	2.00247
H	4.492167	1.178452	0.386066
H	4.384700	-0.481934	-0.204915
Cl	-1.055771	2.710483	-0.308241
H	-3.416045	1.705666	0.876866
H	-4.145953	-0.627852	1.351001
H	-2.697672	-2.533278	0.678371
Cl	-0.233892	-2.622256	-0.666261

Thermochemical data for **A3** conformer of clonidine calculated with MP2/cc-pVTZ using ideal gas, rigid rotor, harmonic normal mode approximations.

	E (Thermal), kcal/mol	$c_{v,}$ cal/(mol·K)	S, cal/(mol·K)
Total	118.928	64.696	135.393
Electronic	0.000	0.000	0.000
Translational	1.252	2.981	43.890
Rotational	1.252	2.981	33.371
Vibrational	116.424	58.734	58.132

Ee = -1428.5900019 Ha
ZPE = 0.165590 Ha