A Molecular Orbital Study of Tambjamine E and Analogs

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HF/6-31G* and B3LYP/6-31G* energy (kcal/mol) for protonated molecules in vacuum phase.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)	Enamine (E)	Enamine (Z)	Methoxy	"Proto"
0	1.8 (1.9)	3.5	2.7	2.5	0.6	0.2
10	1.6 (1.8)	1.3	--	--	0.6 at 8°	--
20	1.5 (1.7 at 16°)	1.1	--	--	--	--
30	1.7 (2.1)	3.1	3.0	2.6	2.2	2.6
60	4.1 (5.2)	5.8	5.3	5.0	8.0	9.4
90	5.8 (7.8)	7.7	6.8	6.5	12.2	14.4
120	3.0 (3.8)	4.6	3.8	3.4	7.0	8.1
150	0.3 (0.6)	1.6	1.2	0.4	1.6	2.0
166	**0.0** (--)	1.2 at 165°	--	--	--	--
180	0.05 **(0.0)**	1.4	0.8	**0.0**	**0.0**	**0.0**

[a]The global energy minimum (GEM) conformer energies are in bold face type. The B3LYP/6-31G* energies are in parentheses. The tambjamine (Z) relative energies are given relative to that of the tambjamine (E) GEM conformation. The enamine (E) relative energies are given relative to that of the enamine (Z) GEM conformation.

AM1 energy (kcal/mol) for protonated molecules in vacuum phase.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)	Enamine (E)	Enamine (Z)	Methoxy	"Proto"
0	1.0	2.6	1.6	1.4	0.85	0.40
30	1.7	3.2	2.4	2.2	2.5	2.2
60	3.5	5.0	4.5	4.2	6.9	7.2
90	4.5	6.0	5.6	5.3	9.8	10.9
120	3.1	4.5	4.1	3.7	6.6	7.3
150	0.86	2.2	1.5	1.0	1.8	2.0
180	**0.0**	1.3	0.51	**0.0**	**0.0**	**0.0**

[a]The global energy minimum (GEM) conformer energies are in bold face type. The tambjamine (Z) relative energies are given relative to that of the tambjamine (E) GEM conformation. The enamine (E) relative energies are given relative to that of the enamine (Z) GEM conformation.

AM1/SM5.4 energy (kcal/mol) for protonated molecules in solvent.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)	Enamine (E)	Enamine (Z)	Methoxy	"Proto"
0	0.5	2.0	1.0	1.1	0.5	0.3
30	1.2	2.7	1.6	1.7	2.1	2.0
60	2.7	4.1	2.8	2.9	5.7	5.8
90	3.3	4.7	3.3	3.3	7.6	7.8
120	2.4	3.6	2.5	2.3	5.5	5.8
150	0.7	1.8	1.0	0.7	1.6	1.7
180	**0.0**	1.0	0.3	**0.0**	**0.0**	**0.0**

[a]The global energy minimum (GEM) conformer energies are in bold face type. The tambjamine (Z) relative energies are given relative to that of the tambjamine (E) GEM conformer. The enamine (E) relative energies are given relative to that of the enamine (Z) GEM conformer.

HF/6-31G* and B3LYP/6-31G* energy (kcal/mol) for neutral molecules in vacuum phase.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)
0	4.16 (3.58)	**0.00**
10	4.37 (3.87)	--
30	3.58 (3.91)	1.49
60	7.81 (8.89)	5.44
90	10.33 (11.70)	8.46
120	9.04 (10.05)	6.92
150	9.29 (8.98)	4.60
180	8.80 (8.00)	4.11

[a]The global energy minimum (GEM) conformer energies are in bold face type. The B3LYP/6-31G* energies are in parentheses. The tambjamine (E) relative energies are given relative to that of the tambjamine (Z) GEM conformer.

AM1 energy (kcal/mol) for neutral molecules in vacuum phase.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)	Enamine (E)	Enamine (Z)	Methoxy	"Proto"
0	0.6	**0.0**	2.1	**0.0**	**0.0**	**0.0**
30	1.3	0.8	2.9	0.8	0.9	0.9
60	3.4	2.7	5.0	2.8	3.2	3.1
90	4.8	4.1	6.5	4.2	4.8	4.7
120	4.6	3.8	6.2	3.9	4.5	4.5
150	3.4	2.6	5.0	2.6	3.2	3.2
180	3.0	2.2	4.6	2.2	2.7	2.8

[a]The global energy minimum (GEM) conformer energies are in bold face type. The tambjamine (E) relative energies are given relative to that of the tambjamine (Z) GEM conformer. The enamine (E) relative energies are given relative to that of the enamine (Z) GEM conformer.

AM1/SM5.4 energy (kcal/mol) for neutral molecules in solvent.[a]

NCCN (°)	Tambjamine (E)	Tambjamine (Z)	Enamine (E)	Enamine (Z)	Methoxy	"Proto"
0	0.8	**0.0**	1.6	**0.0**	**0.0**	**0.0**
30	1.4	0.7	2.3	0.7	0.8	0.8
60	3.0	2.2	3.8	2.2	2.5	2.6
90	4.0	3.2	4.9	3.1	3.6	3.6
120	3.8	2.9	4.6	2.7	3.2	3.1
150	2.7	1.8	3.4	1.6	1.8	1.6
180	2.3	1.3	2.9	1.0	1.2	1.0

[a]The global energy minimum (GEM) conformer energies are in bold face type. The enamine (E) results are given relative to that of the enamine (Z) GEM conformer. The enamine (E) relative energies are given relative to that of the enamine (Z) GEM conformer.