

Mechanisms and energetics of potassium channel block by local anesthetics and antifungal agents

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Supporting Information

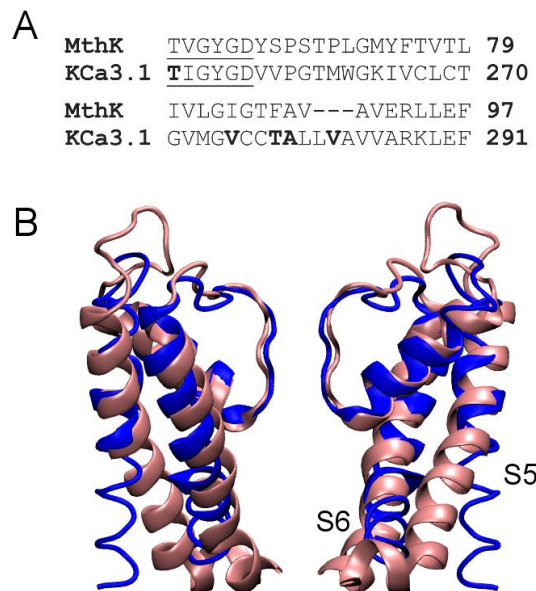


Figure S1. (A) Sequence alignment between MthK and KCa3.1 in the selectivity filter (underscored) and S6 helix region. (B) Structural alignment between MthK (blue, PDB ID 1LNQ) and Kv1.2 (pink, PDB ID 3LUT) in the pore domain. Positions of S5 and S6 helices are indicated.

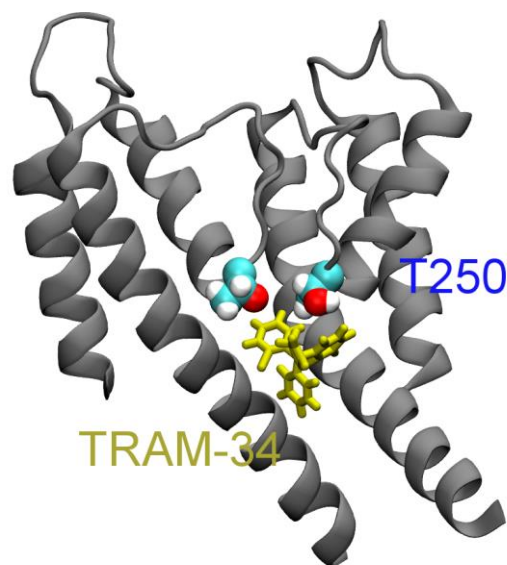


Figure S2. The position of TRAM-34 (yellow) relative to Thr250 of KCa3.1. Two adjacent subunits of the channel are shown as grey ribbons.

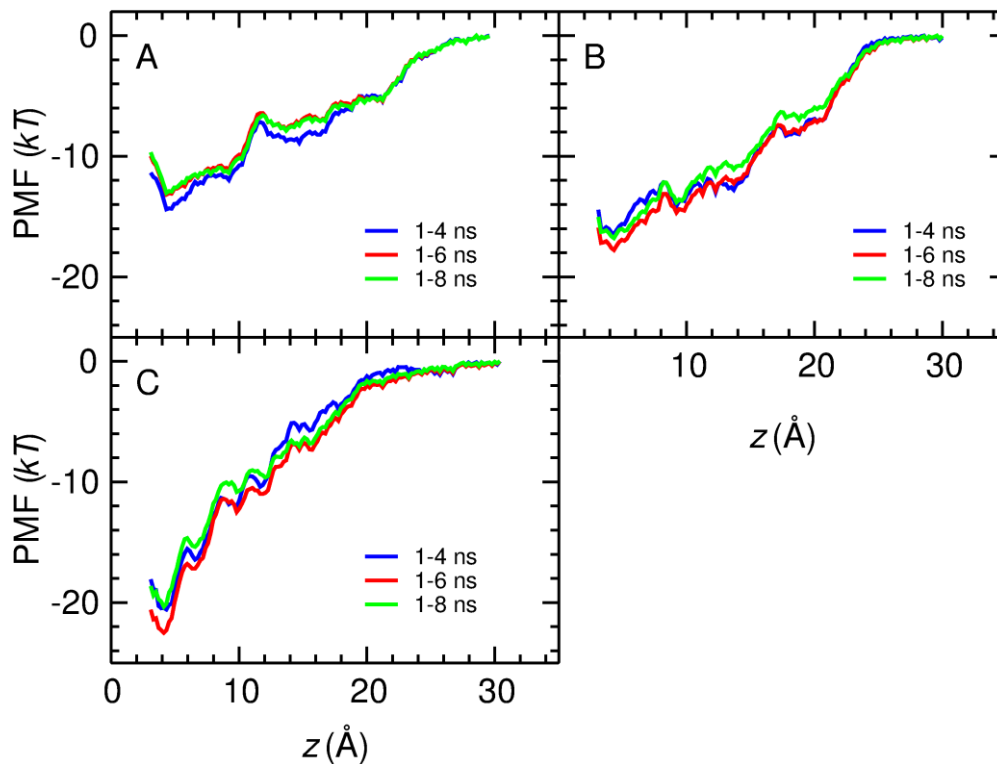


Figure S3. Block analysis of the PMF profiles of lidocaine-Kv1.2 (A), TRAM-34-Kv1.2 (B) and TRAM-34-K_{Ca}3.1 (C).

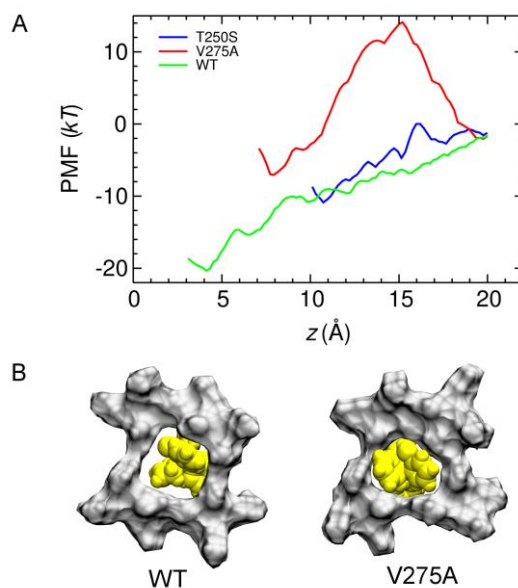


Figure S4. (A) PMF profiles for the binding of TRAM-34 to the wild type (WT) and two mutant (T250S and V275A) K_{Ca}3.1. In both mutant channels, the position of the minimum of the profiles is shifted toward the right, indicating that the drug binds to a more inward position. A large barrier of ~ 15 kT is observed at $z=15$ Å in the V275A mutant due to narrowing of channel wall after the mutation (see panel B). At this position, the drug is coordinated by a ring of four Val282 residues just below the Val275 ring. (B) The position of TRAM-34 (yellow) relative to the Val282 ring in the WT and V275A mutant K_{Ca}3.1 at the window $z=15$ Å.

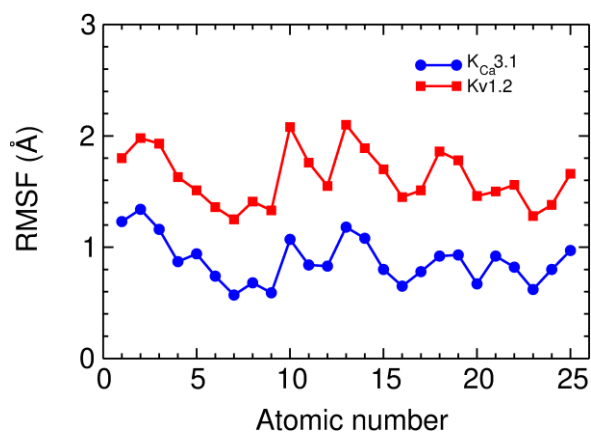


Figure S5. The root mean square fluctuation (RMSF) of the 25 heavy atoms of TRAM-34 bound to the inner cavity of Kv1.2 and K_{Ca}3.1 over the last 10 ns of the equilibrium simulation of 30 ns.

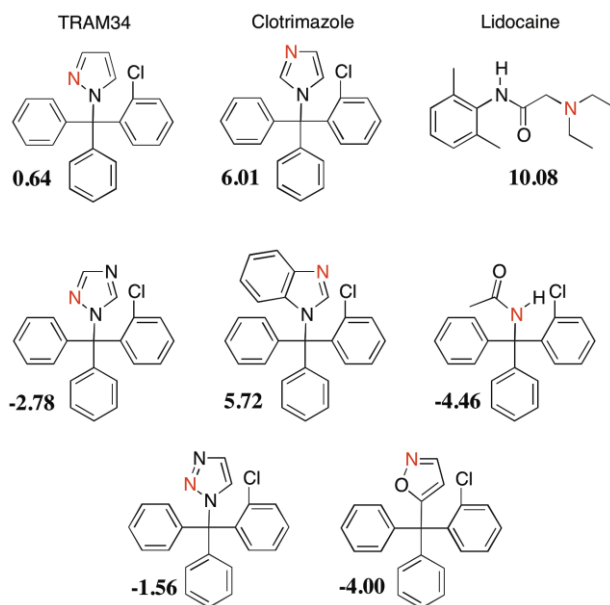


Figure S6. Analogues of TRAM-34 and the first principles calculated pKa values of their respective conjugate bases. Where protonation at multiple sites is possible, the most favored site (shown in red) is considered. Corresponding pKa values for TRAM-34, clotrimazole and lidocaine are shown for comparison.

Computational Procedures and Results

Methodology

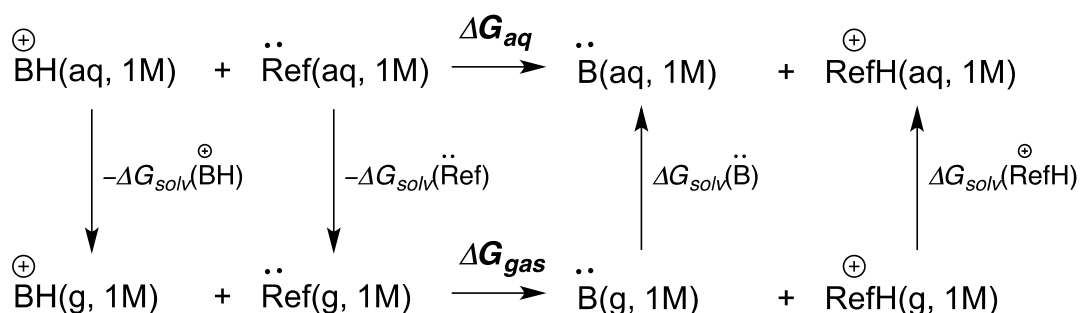
Standard *ab initio* and density functional theory calculations have been performed using Gaussian 09¹ and Molpro 2012.1² software packages. Geometries of all species were fully optimized using the M06-2X³/6-31+G(d) method, and the frequencies were calculated at the same levels and scaled by recommended scale factors.⁴ Full conformational searches at a resolution of 120° were performed for all other species in the present work. Accurate electronic energies were calculated using high-level composite *ab initio* G3(MP2,CC)(+) method.⁵ For large systems (over 15-20 heavy atoms), where high-level composite calculations were not feasible computationally, a double-layer ONIOM-type procedure was applied instead and the MP2/6-311+G(3df,2p) method was used for the full system.

Accurate gas-phase Gibbs free energies of all species at 25 °C include gas-phase entropies and thermal corrections, obtained using standard textbook formulas for the statistical thermodynamics of an ideal gas under the harmonic oscillator approximation⁶ in conjunction with the optimized geometries and scaled frequencies. Gibbs free energies of solvation in water were calculated for relaxed solution-phase geometries using UAKS-CPCM/B3LYP/6-31+G(d) method.⁷

In this work we define the pK_a of a basic *N*-containing functional group, B, as a negative logarithm of the equilibrium constant of the deprotonation of BH^+ in water. This value is calculated using the proton exchange method (Scheme 1) according to Equation 1:

$$pK_a = \frac{\Delta G_{aq}}{RT \ln(10)} + pK_a(Ref) \quad \text{Eq. 1}$$

In this scheme Ref is a reference base, structurally and electronically similar to the investigated species B and for which a reliable experimental pK_a is available. The described procedures were previously shown to reproduce experimental data within chemical accuracy.⁸⁻¹⁰



Scheme 1. pK_a calculation using the proton exchange scheme. Ref is a reference base.

Structures of the studied compounds are shown in Figure S7 below.

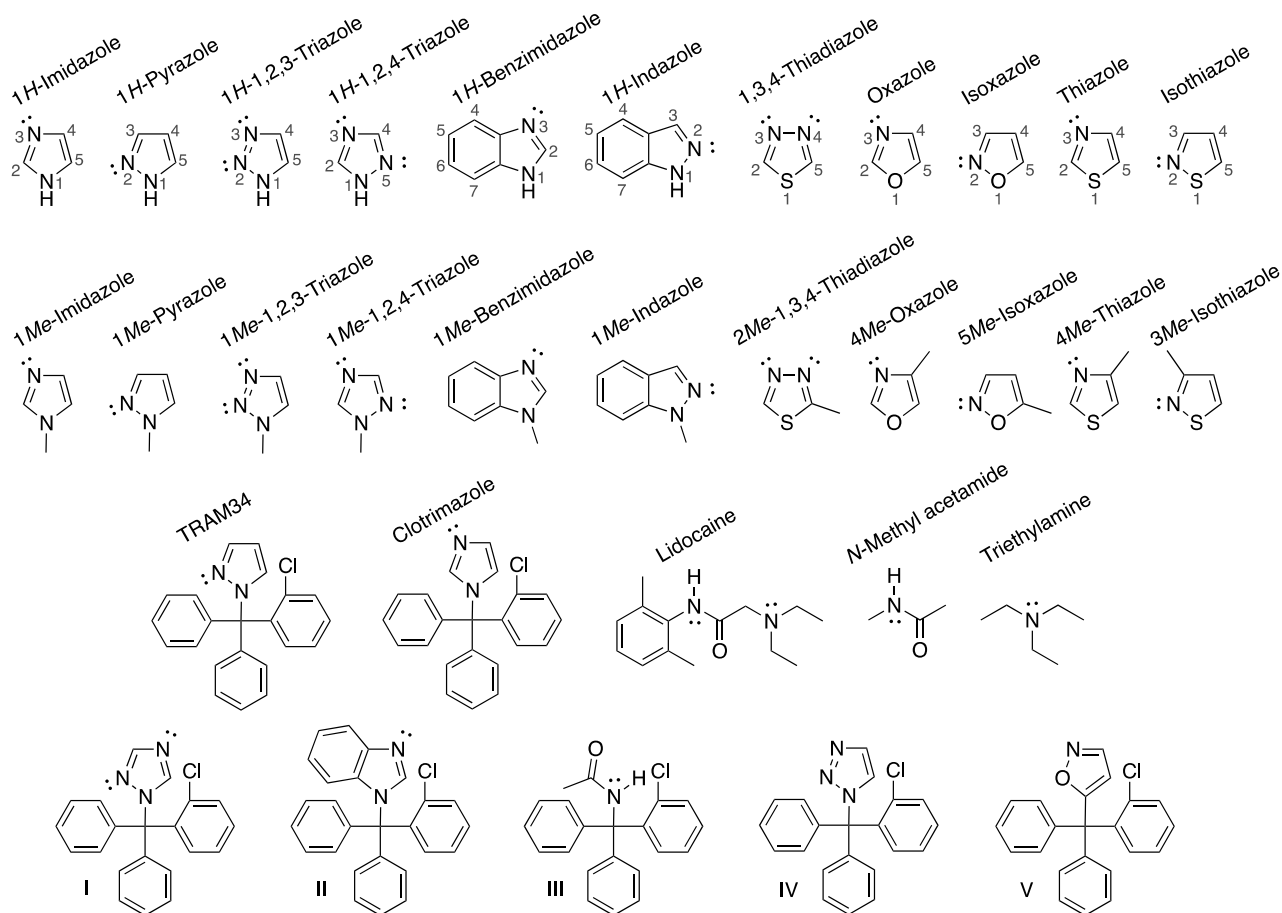


Figure S7. Structures and names of the investigated bases.

Experimental literature data

Table S1. pK_a values of the investigated bases, reported in the literature.

Compound ^a	pK_a	Reference	Comment
1 <i>H</i> -Imidazole (N3)	6.90	11	Original source not given
	6.99	12	Potentiometry
	6.99	13	Calorimetry
	6.99	14	Spectrophotometry
1 <i>H</i> -Pyrazole (N2)	2.48	15	Potentiometry
	2.49	14	Spectrophotometry
1 <i>H</i> -1,2,3-Triazole (N3)	1.15	16	Cited in Ref. 17
	1.17	16	Cited in Ref. 18
1 <i>H</i> -1,2,4-Triazole (N2)	2.20	11	Original source not given
	2.19	16	Cited in Ref. 18
1 <i>H</i> -1,2,4-Triazole (N4)	2.39	19	Cite Ref. 17
	2.45	16	Cited in Ref. 17
1 <i>H</i> -Benzimidazole (N3)	5.56 ^b		Not specified
1 <i>H</i> -Indazole (N2)	1.04 ^b		Not specified
1,3,4-Thiadiazole (N3=N4)	-4.90	11	Original source not given
Oxazole (N3)	0.80	11	Original source not given
	0.80	20	Not specified
Thiazole (N3)	2.50	11	Original source not given
	2.50	20	Not specified
	2.53	21	Spectroscopy
Isothiazole (N2)	-0.50	11	Original source not given
1 <i>Me</i> -Imidazole (N3)	7.12 ^b		Not specified
	7.11	14	Spectrophotometry
1 <i>Me</i> -Pyrazole (N2)	2.06	17	Cite Ref. 22, in French
1 <i>Me</i> -1,2,3-Triazole (N3)	1.23	16	Cited in Ref. 17
1 <i>Me</i> -1,2,4-Triazole (N4)	3.20	16	Cited in Ref. 17
1 <i>Me</i> -Benzimidazole (N3)	5.55 ^b		Not specified
1 <i>Me</i> -Indazole (N2)	0.30 ^b		Not specified
Clotrimazole (N3)	4.70	23	Original source not given
	6.10	24	Original source not given
	6.02	25	Potentiometry
Lidocaine	7.80	26	Original source not given
<i>N</i> -Methyl acetamide	-0.42	27	Conductivity
Triethylamine	10.74	28	Potentiometry, calorimetry

^a See Figure S7 for details.

^b Catalan, J., Claramunt, R. M., Elguero, J., Laynez, J. & Menendez, M. unpublished results, 1986.

Results

Table S2. pK_a values of the investigated bases, calculated using proton exchange method in aqueous solution at 25 °C.

B ^a	Ref and its pK_a ^b	pK_a (B)
1Me-Imidazole (N3)	1H-Imidazole (6.99)	7.10
Clotrimazole (N3)	1H-Imidazole	6.01
1Me-Pyrazole (N2)	1H-Pyrazole (2.49)	1.51
TRAM34 (N2)	1H-Pyrazole	0.64
1H-1,2,4-Triazole (N4)	1H-Imidazole	2.08
1Me-1,2,4-Triazole (N4)	1H-Imidazole	2.09
1H-1,2,4-Triazole (N2)	1H-Pyrazole	-1.91
1Me-1,2,4-Triazole (N2)	1H-Pyrazole	-2.78
1H-1,2,3-Triazole (N2)	1H-1,2,3-Triazole (N3) (1.17)	-0.83
1Me-1,2,3-Triazole (N2)	1H-1,2,3-Triazole (N3)	-1.56
1Me-1,2,3-Triazole (N3)	1H-1,2,3-Triazole (N3)	1.11
Lidocaine (N-amide)	N-Methyl acetamide (-0.42)	-1.73
Lidocaine (N-amine)	Triethylamine (10.74)	10.08
III (N-amide)	N-Methyl acetamide	-4.46
1Me-Benzimidazole (N3)	1H-Benzimidazole (5.56)	5.72
1H-Indazole (N2)	1H-Benzimidazole	1.64
1Me-Indazole (N2)	1H-Benzimidazole	0.96
4Me-Oxazole (N3)	Oxazole (0.80)	1.60
Isoxazole (N2)	Oxazole	-5.44
5Me-Isoxazole (N2)	Oxazole	-4.00
4Me-Thiazole (N3)	Thiazole (2.53)	3.29
Isothiazole (N2)	Thiazole	-2.45
3Me-Isothiazole (N2)	Thiazole	-0.36
1,3,4-Thiadiazole (N3=N4)	Thiazole	-0.71
2Me-1,3,4-Thiadiazole (N4)	Thiazole	0.02

^a See Figure S7 for details.

^b pK_a values in brackets are taken from refs. 29,30.

Comparing calculated pK_a values for clotrimazole and TRAM34 to those of their *N*-methyl analogues (Table S2) we conclude that triphenyl substituent lowers the pK_a by *ca.* 1 unit compared to methyl, hence small *N*-methyl models provide a reasonable estimate for the upper limit of pK_a of candidate blockers I-V in Figure S7.

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Appendix 1

Table S3. Contributions to the gas and solution-phase free energies of all the species in this study at 298.15 K.

Species ^a	E _e , Hartrees ^b		S ²⁹⁸ J mol ⁻¹ K ⁻¹	TC ²⁹⁸ Hartrees	ZPVE Hartrees	G ²⁹⁸ _{gas} Hartrees	ΔG ²⁹⁸ _{aq} kcal mol ⁻¹
	MP2/6- 311+G(3df,2p)	G3(MP2,cc)(+) or ONIOM					
1 <i>H</i> -Imidazole		-225.94101	273.8284	0.00478	0.06966	-225.89767	-12.42
1 <i>H</i> -Imidazole(H ⁺)		-226.31242	274.7362	0.00481	0.08316	-226.25565	-67.25
1 <i>Me</i> -Imidazole	-264.98913	-265.19844	312.2875	0.00644	0.09684	-265.13063	-8.68
1 <i>Me</i> -Imidazole(H ⁺)	-265.36377	-265.57754	312.1053	0.00650	0.11021	-265.49626	-58.85
Clotrimazole	-1415.75438	-1415.96369	621.5998	0.02125	0.32428	-1415.68876	-2.20
Clotrimazole(H ⁺)	-1416.14335	-1416.35711	622.2936	0.02141	0.33736	-1416.06901	-41.71
1 <i>H</i> -Pyrazole		-225.92349	273.5031	0.00476	0.06977	-225.88003	-11.35
1 <i>H</i> -Pyrazole(H ⁺)		-226.27458	277.7181	0.00503	0.08228	-226.21881	-73.03
1 <i>Me</i> -Pyrazole	-264.97508	-265.18353	314.3636	0.00645	0.09678	-265.11600	-6.27
1 <i>Me</i> -Pyrazole(H ⁺)	-265.32847	-265.54307	313.6665	0.00663	0.10958	-265.46248	-61.79
TRAM34	-1415.73970	-1415.94814	622.9761	0.02129	0.32389	-1415.67371	-0.03
TRAM34(H ⁺)	-1416.11326	-1416.32786	623.5834	0.02150	0.33678	-1416.04040	-41.67
1 <i>H</i> -1,2,4-Triazole		-241.96625	270.6537	0.00456	0.05879	-241.93364	-14.40
1 <i>H</i> -1,2,4-Triazole(H ⁺ @N4)		-242.31524	272.2528	0.00464	0.07163	-242.26989	-76.16
1 <i>H</i> -1,2,4-Triazole(H ⁺ @N2)		-242.29727	274.8456	0.00483	0.07083	-242.25281	-82.38
1 <i>Me</i> -1,2,4-Triazole		-281.22723	306.8266	0.00616	0.08600	-281.16992	-8.75
1 <i>Me</i> -1,2,4-Triazole(H ⁺ @N4)		-281.58567	307.9213	0.00628	0.09869	-281.51567	-64.56
1 <i>Me</i> -1,2,4-Triazole(H ⁺ @N2)		-281.56777	309.5244	0.00641	0.09825	-281.49827	-69.79
1 <i>H</i> -1,2,3-Triazole		-241.93862	271.1588	0.00459	0.05805	-241.90677	-16.51
1 <i>H</i> -1,2,3-Triazole(H ⁺ @N3)		-242.29066	271.7800	0.00460	0.07177	-242.24515	-75.42
1 <i>H</i> -1,2,3-Triazole(H ⁺ @N2)		-242.27002	274.1619	0.00478	0.07071	-242.22566	-84.92
1 <i>Me</i> -1,2,3-Triazole		-281.19960	310.2215	0.00627	0.08513	-281.14342	-10.81
1 <i>Me</i> -1,2,3-Triazole(H ⁺ @N3)		-281.56130	310.6891	0.00632	0.09864	-281.49162	-63.48
1 <i>Me</i> -1,2,3-Triazole(H ⁺ @N2)		-281.54140	312.5309	0.00647	0.09796	-281.47245	-71.87
Lidocaine		-730.58352	593.4203	0.01984	0.33318	-730.29788	-8.87

Lidocaine(H ⁺ @N-amide)		-730.92824	598.7366	0.02022	0.34532	-730.63069	-54.58
Lidocaine(H ⁺ @N-amine)		-730.97159	601.0358	0.02008	0.34755	-730.67221	-58.43
<i>N</i> -Methyl acetamide	-248.04401	-248.24105	342.9406	0.00782	0.09937	-248.17280	-11.49
<i>N</i> -Methyl acetamide(H ⁺)	-248.36767	-248.56860	343.0442	0.00777	0.11238	-248.48741	-70.41
Triethylamine		-292.05192	388.5266	0.01039	0.20112	-291.88454	-2.65
Triethylamine(H ⁺)		-292.43916	388.5602	0.01044	0.21625	-292.25660	-54.53
III	-1398.80733	-1399.00437	648.0970	0.02238	0.32682	-1398.72876	-4.43
III(H ⁺)	-1399.15167	-1399.35260	649.7155	0.02264	0.33925	-1399.06449	-44.58
1 <i>H</i> -Benzimidazole		-379.37808	331.3376	0.00725	0.11536	-379.29309	-11.93
1 <i>H</i> -Benzimidazole(H ⁺)		-379.75215	332.0282	0.00729	0.12893	-379.65363	-63.10
1 <i>Me</i> -Benzimidazole		-418.63726	366.4656	0.00893	0.14268	-418.52726	-7.95
1 <i>Me</i> -Benzimidazole(H ⁺)		-419.01781	366.7842	0.00904	0.15600	-418.89442	-55.19
1 <i>H</i> -Indazole		-379.35389	332.2956	0.00730	0.11538	-379.26895	-10.38
1 <i>H</i> -Indazole(H ⁺)		-379.70786	340.2256	0.00778	0.12761	-379.61111	-67.74
1 <i>Me</i> -Indazole		-418.61476	371.1322	0.00905	0.14239	-418.50546	-4.92
1 <i>Me</i> -Indazole(H ⁺)		-418.97483	380.1117	0.00941	0.15515	-418.85343	-57.71
Oxazole		-245.78260	270.8637	0.00456	0.05752	-245.75128	-5.15
Oxazole(H ⁺)		-246.12713	272.8939	0.00467	0.07043	-246.08302	-66.29
4 <i>Me</i> -Oxazole		-285.05274	306.2632	0.00621	0.08457	-284.99674	-4.41
4 <i>Me</i> -Oxazole(H ⁺)		-285.40407	309.0445	0.00636	0.09744	-285.33537	-62.32
Isoxazole		-245.74494	271.4037	0.00459	0.05694	-245.71423	-6.03
Isoxazole(H ⁺)		-246.07783	274.3797	0.00478	0.06974	-246.03447	-65.87
5 <i>Me</i> -Isoxazole		-285.01723	308.4470	0.00629	0.08396	-284.96201	-5.60
5 <i>Me</i> -Isoxazole(H ⁺)		-285.35975	314.5344	0.00658	0.09639	-285.29251	-60.97
Thiazole		-568.40342	282.9172	0.00493	0.05409	-568.37653	-5.21
Thiazole(H ⁺)		-568.75823	284.5042	0.00503	0.06709	-568.71842	-63.29
4 <i>Me</i> -Thiazole		-607.67330	318.0874	0.00663	0.08109	-607.62171	-4.34
4 <i>Me</i> -Thiazole(H ⁺)		-608.03407	321.0098	0.00677	0.09404	-607.96971	-59.62
Isothiazole		-568.40027	282.5970	0.00492	0.05392	-568.37351	-5.49
Isothiazole(H ⁺)		-568.74553	285.3875	0.00509	0.06660	-568.70625	-62.52
3 <i>Me</i> -Isothiazole		-607.67030	320.4073	0.00669	0.08079	-607.61920	-4.80
3 <i>Me</i> -Isothiazole(H ⁺)		-608.02369	326.9769	0.00694	0.09333	-607.96055	-59.28

1,3,4-Thiadiazole	-584.41244	275.2352	0.00479	0.04228	-584.39663	-8.04
1,3,4-Thiadiazole(H ⁺)	-584.75649	282.2065	0.00486	0.05555	-584.72813	-68.22
2 <i>Me</i> -1,3,4-Thiadiazole	-623.68382	318.2731	0.00655	0.06937	-623.64404	-7.53
2 <i>Me</i> -Thiadiazole(H ⁺)	-624.03602	320.7472	0.00666	0.08241	-623.98338	-63.79

^a (H⁺) denotes the protonated form (conjugate acid) of the base, @N denotes which nitrogen atom is protonated; ^b For those species, for which the MP2 energy is given, the total energy is calculated using two-layer ONIOM approximation, whereas high-level composite G3(MP2,CC)(+) energy is used for the rest of the compounds; ^c Calculated using UAKS-CPCM/B3LYP/6-31+G(d) method.

Appendix 2

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the M06-2X/6-31G(d) level.

```
1H-Imidazole 1\1\GINC-R2798\FOpt\RM062X\Gen\C3H4N2\ROOT\06-Nov-2013\0\#\M062X/gen
6 D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\im. freq\0,1\N,-1.6702801648,2.1727538781,0.\C,-
0.2968822737,2.1898912875 ,0.\C,0.20334168,0.9138418279,0.\N,-
0.9033321556,0.0974523527,0.\C,-2.
0010644241,0.9047723918,0.\H,0.2534930352,3.1192922349,0.\H,1.209111
63 27,0.5235672733,0.\H,-0.9031705296,-0.9120882187,0.\H,-
3.0081068002,0. 5120269724,0.\Version=EM64L-G09RevC.01\State=1-
A'\HF=-226.1296522\RMS D=4.160e-09\RMSF=1.173e-04\Dipole=0.4884685,-
1.4627399,0.\Quadrupole=1 .1245032,1.9757978,-
3.1003009,2.5740414,0.,0.\PG=CS [SG(C3H4N2)]\@

1H-Imidazole (H+) 1\1\GINC-R413\FOpt\RM062X\Gen\C3H5N2(1+)\ROOT\05-Nov-
2013\0\#\M062X/ge n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ im_p.freq\1,1\N,-
1.6549806975,2.1244348259,0.\C,-0.2777366742,2.21124
78604,0.\C,0.1880114635,0.9335696743,0.\N,-
0.9220275965,0.1137191844,0 .\C,-
2.0317779911,0.8481239335,0.\H,0.2421594073,3.1566945464,0.\H,1.1
943528735,0.5444848027,0.\H,-0.9047217263,-0.9017527767,0.\H,-
3.046794 4754,0.4781346864,0.\H,-
2.2952045834,2.9128332627,0.\Version=EM64L-G0 9RevC.01\State=1-
A'\HF=-226.4956762\RMSD=3.554e-09\RMSF=1.434e-04\Dipo le=-0.5476611,-
0.199652,0.\Quadrupole=2.8892396,5.0723876,-7.9616272,-
0.9175922,0.,0.\PG=CS [SG(C3H5N2)]\@

1Me-Imidazole 1\1\GINC-R442\FOpt\RM062X\Gen\C4H6N2\ROOT\05-Nov-2013\0\#\M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\mim. freq\0,1\N,-1.657146181,2.3081292567,-
0.2109673515\C,-0.3138862333,2.
3396070799,0.0643151285\C,0.1805336133,1.0659367744,0.1931239735\N,-
0. 8926986033,0.2315851872,-0.0095563846\C,-
1.9672086393,1.0335628064,-0.
2474966006\H,0.2212640724,3.2742252276,0.1542981687\H,1.1678437867,0
.6 818117967,0.4041713171\C,-0.8804523439,-
1.2171728762,0.0237437041\H,-2 .9505313075,0.6240094039,-
0.440791691\H,-0.2058085396,-1.6113992611,-0 .7404830579\H,-
1.8903343932,-1.5796103659,-0.1760119464\H,-0.564735231 4,-
1.5743150296,1.0072947403\Version=EM64L-G09RevC.01\State=1-A'\HF=-2
65.4203369\RMSD=3.200e-09\RMSF=7.249e-06\Dipole=0.4880541,-
1.6189327,0 .1347406\Quadrupole=1.5174051,0.3970862,-
1.9144913,3.0704702,0.6652325 ,0.5789299\PG=C01 [X(C4H6N2)]\@

1Me-Imidazole (H+) 1\1\GINC-R2858\FOpt\RM062X\Gen\C4H7N2(1+)\ROOT\06-Nov-
2013\0\#\M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ \mim_p.freq\1,1\N,-1.6364426668,2.2793884969,-
0.0636694085\C,-0.26688
74859,2.3525328411,0.0568690494\C,0.1804115658,1.0682979554,0.100702
62 98\N,-0.9254594761,0.2467486434,0.0059057817\C,-
2.0160350087,1.0003193 327,-
0.0928712153\H,0.2616388891,3.2921231644,0.1004803669\H,1.1796851
112,0.6692090076,0.1902238188\C,-0.8927982595,-
1.2215670105,0.01366628 5\H,-3.0303852495,0.6386413718,-
0.1810773553\H,-2.2690158108,3.0708670 892,-0.1224531967\H,-
0.4561162967,-1.5626005684,0.9527066953\H,-0.2983 457682,-
```

```

1.5685177741,-0.8319486698\H,-1.912218544,-1.5951635496,-0.075
2747813\\Version=EM64L-G09RevC.01\State=1-A\HF=-
265.7935663\RMSD=8.286 e-09\RMSF=5.436e-06\Dipole=-
0.5249874,0.2583179,-0.0473343\Quadrupole= 1.5786819,6.8543241,-
8.433006,-1.5198491,0.8961714,-0.1863358\PG=C01 [ X(C4H7N2) ]\@

```

Clotrimazole

```

1\1\GINC-R1304\FOpt\RM062X\Gen\C22H17Cl1N2\ROOT\08-Nov-
2013\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=161061273 6\\clot.freq\\0,1\N,-1.5920634748,2.647357166,-
0.0542970225\C,-1.37122 92764,2.3640507991,1.2701692203\C,-
1.2276966949,1.0153213898,1.4544355 001\N,-
1.3611228904,0.4468466386,0.2027773121\C,-1.5758228568,1.485472
0091,-0.6643796961\H,-1.3393143776,3.1442299992,2.0177201337\H,-
1.0523 645613,0.4156912047,2.3349305525\C,-1.1735030939,-
0.9980850452,-0.0856 548892\H,-1.7389732508,1.3365388961,-
1.7203881836\C,0.3391749595,-1.31 80612816,-0.1236443264\C,-
1.7571175665,-1.288861054,-1.4895605726\C,-1 .9064906588,-
1.7298625042,1.0565898605\C,1.2874079759,-0.3285269666,0.
160616884\C,2.6569430838,-0.5758049601,0.0954640993\C,3.1201261992,-
1. 8355131812,-0.2654430052\C,2.2032957428,-2.8365691165,-
0.5687584733\C, 0.8364491091,-2.5768445103,-
0.5040870067\H,0.950792106,0.6664712524,0.
4306200206\H,3.3545789771,0.2239282456,0.3233078318\H,4.1842493959,-
2. 0429438979,-0.3209312033\H,2.5347145666,-3.8265053619,-
0.8647288812\C1 , -0.2179189309,-3.9044833778,-0.9291011209\C,-
3.2329526251,-1.36584265 63,1.3315442199\C,-3.9362186559,-
1.954552586,2.3754519434\C,-3.3177698 606,-
2.9096465666,3.184364567\C,-1.992592548,-3.2521544453,2.942532766
7\C,-1.2897882044,-2.6622420779,1.88915322\H,-3.7088637106,-
0.59351021 04,0.731685847\H,-4.962892823,-
1.6567496357,2.5667258397\H,-3.86240842 35,-
3.3683583305,4.0042626014\H,-1.4906118959,-3.9771577054,3.57628600
19\H,-0.2504937716,-2.9333204726,1.739384572\C,-1.0231307745,-
0.879893 0518,-2.6108502334\C,-1.4948011365,-1.1070141256,-
3.8996801761\C,-2.70 8960758,-1.7642393253,-4.0937333434\C,-
3.4361134742,-2.1910212507,-2.9 872125564\C,-2.9641667918,-
1.9569983347,-1.6953404375\H,-0.0656099553, -0.3822210011,-
2.4756075933\H,-0.9074903443,-0.7774393045,-4.751622314 1\H,-
3.0771521178,-1.9506345649,-5.0981590918\H,-4.3740074348,-2.72170
13906,-3.1222749781\H,-3.533236177,-2.3368763074,-
0.8552598891\\Versio n=EM64L-G09RevC.01\State=1-A\HF=-
1417.8652727\RMSD=5.268e-09\RMSF=5.83 5e-06\Dipole=0.4717615,-
1.2570821,0.1844734\Quadrupole=9.9616954,-16.5
886121,6.6269167,3.976729,-0.5842841,-0.3956592\PG=C01
[X(C22H17Cl1N2) ]\@

```

Clotrimazole (H+)

```

1\1\GINC-R174\FOpt\RM062X\Gen\C22H18Cl1N2(1+)\ROOT\06-Nov-
2013\0\#M06 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=161061 2736\\clot_p.freq\\1,1\N,-
1.5504295739,2.6508681742,0.5598313484\C,-1.
2091450377,2.2159021989,1.8218581015\C,-
1.003912675,0.8771559845,1.715 3222476\N,-
1.2171314618,0.5266934007,0.394323374\C,-1.557547928,1.6174 93017,-
0.2840198984\H,-1.1448288333,2.8813786661,2.6681447676\H,-0.737
1611814,0.1411962689,2.4588616645\C,-1.1714158756,-0.8980941211,-
0.112 7007985\H,-1.8351329634,1.6544329711,-1.3263772063\C,-
1.9393776014,-1. 7206927256,0.9453424693\C,0.3054087427,-
1.3209755316,-0.2359060251\C,- 1.7941057835,-0.9590599565,-
1.519504249\C,-1.3381987366,-2.8272320258, 1.5568918587\C,-
1.996057611,-3.5872673913,2.5217749567\C,-3.2848104968 , -
3.2480877364,2.9136067281\C,-3.9048654799,-2.1418445951,2.3402481792
\C,-3.2404420085,-1.3910737975,1.3752258598\H,-0.3284360458,-
3.1043969 128,1.2796302483\H,-1.4909620813,-

```



```

4.4391174843,2.964898913\H,-3.809778 7721,-
3.8304983331,3.6638262227\H,-4.9078436379,-1.8511041396,2.634717
5534\C1,-4.129791833,-0.0166502843,0.7460518467\C,-1.1149177605,-
0.334 4284157,-2.5772624255\C,-1.6161619977,-0.3840573973,-
3.8731203229\C,-2 .7903469628,-1.0909714728,-4.1395268542\C,-
3.4454995955,-1.7486711228, -3.1042872139\C,-2.9508764943,-
1.6848298734,-1.8000701389\H,-0.1662520 9,0.1667554436,-
2.3911648494\H,-1.0772403285,0.1057198964,-4.678238718 5\H,-
3.1776928681,-1.1429109185,-5.1521479151\H,-4.3452436787,-2.32180
63275,-3.3043413286\H,-3.4718364153,-2.2211372431,-
1.0143161888\C,1.37 06378751,-
0.5826499361,0.2779431577\C,2.68555238,-1.0325412372,0.12354
74365\C,2.9474373238,-2.223551343,-0.5416185805\C,1.8861785333,-
2.9632 410709,-1.0679598561\C,0.5806217381,-2.511366952,-
0.924339131\H,1.2112 99692,0.3592202987,0.792367218\H,3.5013614446,-
0.4396071201,0.52508218 06\H,3.9685085909,-2.5717151138,-
0.6601106999\H,2.0766972055,-3.889528 5816,-1.600861725\H,-
0.2368507605,-3.0860927519,-1.353172498\H,-1.7892
719565,3.6019885924,0.3034202914\\Version=EM64L-G09RevC.01\State=1-
A\H F=-1418.2540226\RMSD=4.714e-09\RMSF=8.257e-
06\Dipole=0.3280541,2.34364 79,0.6693031\Quadrupole=-
9.4983391,12.365744,-2.8674049,0.3618735,-0.4 118668,1.2651347\PG=C01
[X(C22H18C11N2)]\\@

```

1H-Pyrazole

```

1\1\GINC-R331\FOpt\RM062X\Gen\C3H4N2\ROOT\05-Nov-2013\0\#\M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\py.f req\0,1\C,-
1.6580688506,2.6091631749,0.0003488121\C,-0.2540475823,2.7
727103905,0.0002241514\C,0.2392367485,1.4850776914,0.0001255321\N,-
0.8 406020976,0.6680543601,0.0002061198\N,-
2.0046670507,1.3281065524,0.000 3335359\H,-
2.4273791189,3.3687793021,0.0004484636\H,0.312346727,3.6915
981326,0.0002051512\H,1.2463528019,1.0946765216,0.0000128744\H,-
0.8538 215772,-0.3410161254,0.0001753596\\Version=EM64L-
G09RevC.01\State=1-A\ HF=-226.1116452\RMSD=8.090e-09\RMSF=5.124e-
05\Dipole=0.8937409,-0.3190 406,-0.0000931\Quadrupole=-
1.1769253,4.409592,-3.2326667,-2.2113978,-0 .0002858,0.0004707\PG=C01
[X(C3H4N2)]\\@

```

1H-Pyrazole (H⁺)

```

1\1\GINC-R332\FOpt\RM062X\Gen\C3H5N2(1+)\ROOT\05-Nov-
2013\0\#\M062X/ge n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\ py_p.freq\1,1\C,-
1.6550636145,2.6378214822,0.021495853\C,-0.271277785 1,2.767358475,-
0.0097557662\C,0.2308449532,1.471043108,-0.0102331811\N , -
0.8075139658,0.6254621491,0.0192689521\N,-1.9476707003,1.3308844652,
0.0384510344\H,-
2.4420878245,3.3792287134,0.0326790625\H,0.2962438112, 3.6851969812,-
0.0295651539\H,1.2454816829,1.0977167609,-0.0293609723\H , -
0.8129622135,-0.3900632985,0.0275998017\H,-2.853635617,0.8725406918,
0.0619320318\\Version=EM64L-G09RevC.01\State=1-A'\HF=-
226.4567876\RMSD =3.204e-09\RMSF=2.658e-05\Dipole=-0.5085417,-
0.8223324,0.0177497\Quadr upole=3.8441249,4.0826078,-
7.9267328,0.2319795,-0.2589418,-0.102228\PG =CS [SG(C3H5N2)]\\@

```

1Me-Pyrazole

```

1\1\GINC-R332\FOpt\RM062X\Gen\C4H6N2\ROOT\05-Nov-2013\0\#\M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\mpy. freq\0,1\C,-
1.6630804206,2.7138099373,0.0218957668\C,-0.2672342208,2.
9128413056,-0.0116336295\C,0.2540607395,1.6342016608,-
0.0111687442\N,- 0.7978556459,0.7825798671,0.0209091543\N,-
1.973222121,1.4213699682,0.0 411476838\H,-
2.4532948807,3.4518677634,0.0325003045\H,0.2772371109,3.8 446770005,-
0.0330849317\H,1.2710292997,1.2685130648,-0.0306260423\C,-0

```

```
.773780495,-0.6650157334,0.0362136522\H,0.2648052458,-
0.9977723207,0.0      083971885\H,-1.3066457811,-1.0509987087,-
0.8352467269\H,-1.2528888309,-
1.0321238047,0.9462763245\\Version=EM64L-G09RevC.01\State=1-A\HF=-
265      .4045882\RMSD=5.059e-09\RMSF=4.834e-05\Dipole=0.8667258,-
0.483746,-0.0      143769\Quadrupole=-1.2054308,4.1361682,-2.9307373,-
1.3888003,-0.026136 6,-0.0382517\PG=C01 [X(C4H6N2)]\\@
```

1Me-Pyrazole (H⁺)

```
1\1\GINC-R369\FOpt\RM062X\Gen\C4H7N2(1+)\ROOT\05-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\      mpy_p.freq\1,1\C,-
1.6691137448,2.7679053899,0.0213289116\C,-0.2916817
467,2.9189101516,-0.0111972654\C,0.2269527798,1.6253632056,-
0.01022540      67\N,-0.7879376338,0.754186055,0.0207467436\N,-
1.9350424727,1.45164219      44,0.0399820794\H,-
2.4699746103,3.4939712821,0.0321001334\H,0.26364198 8,3.8439128409,-
0.0328532312\H,1.2486199192,1.2712298898,-0.0297305676      \C,-
0.7797179367,-0.709119663,0.0366229613\H,-2.8325040689,0.977247639
7,0.0648463892\H,0.2611117529,-1.0281950704,0.0085111616\H,-
1.30099092      78,-1.0871982469,-0.8447391925\H,-1.2470532981,-
1.0677156688,0.9555872 832\\Version=EM64L-G09RevC.01\State=1-A\HF=-
265.7581905\RMSD=5.050e-09      \RMSF=5.226e-05\Dipole=-0.4831237,-
0.4546616,0.0156518\Quadrupole=3.02      97718,5.0843585,-8.1141303,-
0.5140518,-0.2454759,-0.1204016\PG=C01 [X(C4H7N2)]\\@
```

TRAM34

```
1\1\GINC-R2128\FOpt\RM062X\Gen\C22H17Cl1N2\ROOT\06-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=161061273 6\\tram.freq\0,1\C,-1.2917135783,2.6409051908,-
0.4108115049\C,-1.6434      742069,2.5911231899,0.9536102308\C,-
1.6485932976,1.2459572931,1.255338      515\N,-
1.3118095643,0.5845395752,0.1185621433\N,-1.0940740492,1.426652
7235,-0.9059154471\H,-1.8803864843,3.4085325253,1.6179913323\H,-
1.9053      492893,0.7286528128,2.1652930098\C,-1.1522049758,-
0.8670467215,-0.1342      179193\C,-1.7993456341,-1.1488448867,-
1.5091035874\C,-1.8077508693,-1.
6788722908,1.0042785828\C,0.3524547257,-1.2179431062,-
0.1282114882\C,-      1.0916593936,-1.8165834514,-2.5126452665\C,-
1.6483906639,-2.0896924609      ,-3.7603588412\C,-2.9461688038,-
1.6855032993,-4.0445780123\C,-3.673280      0953,-1.004706249,-
3.0733955985\C,-3.106443844,-0.7397625353,-1.830155      1058\H,-
0.0692636687,-2.120942301,-2.3257125526\H,-1.0559184951,-2.609
2044081,-4.5069549188\H,-3.3938989701,-1.8864405409,-
5.0130247343\H,-4      .6856473467,-0.6669302834,-3.2691735876\C1,-
4.1224730699,0.1272286638,      -0.7021725721\C,0.7354117604,-
2.5630783861,-0.0353753879\C,2.077756050      2,-2.925057102,-
0.0285764224\C,3.0673792754,-1.9430138502,-0.098432283
2\C,2.6956328254,-0.605478738,-0.1768792373\C,1.34628138,-
0.242171974,      -0.1949291991\H,-0.0283247872,-
3.3342422788,0.0356035843\H,2.350992592      3,-
3.9739639959,0.0408383656\H,4.1170149549,-2.2215998989,-0.085775399
3\H,3.454867025,0.1696998295,-
0.2252083016\H,1.0776201088,0.8056088152      ,-0.2677473444\C,-
1.2234270165,-1.6359270505,2.2787749458\C,-1.7471268      047,-
2.3734682685,3.3341288224\C,-2.8545812696,-3.1977988356,3.1287038
778\C,-3.419063661,-3.2767638541,1.8608184682\C,-2.8981630092,-
2.52469      30755,0.8055198752\H,-0.3336610948,-
1.030999344,2.4386961058\H,-1.2794      858189,-
2.3180240497,4.3127871544\H,-3.2617028534,-3.7825460852,3.9482
783551\H,-4.2695178288,-3.9275467857,1.6806289379\H,-3.3496124263,-
2.6      177900874,-0.176129746\H,-1.1785768277,3.5023615759,-
1.0550558489\\Ver      sion=EM64L-G09RevC.01\State=1-A\HF=-
1417.8480818\RMSD=4.448e-09\RMSF=6      .539e-06\Dipole=0.2225423,-
0.7947569,0.3082634\Quadrupole=-1.1142579,-
```

1.7153118,2.8295697,1.2746169,1.3469222,2.1714077\PG=C01
[X(C22H17C11N 2)]\@

TRAM34 (H⁺)

1\1\GINC-R156\FOpt\RM062X\Gen\C22H18C11N2(1+)\ROOT\08-Nov-
2013\0\#\M06 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=161061 2736\tram_p.freq\1,1\C,-
2.4367464189,1.881156198,1.6647731014\C,-1.1
795401104,2.4146877703,1.4284942486\C,-
0.4798396831,1.4321163863,0.728 725671\N,-
1.2801416957,0.3754350353,0.5527910518\N,-2.4635820794,0.657
8973529,1.1179157362\H,-
0.8095381502,3.380101337,1.7368021684\H,0.5396
277455,1.4124092557,0.3747783824\C,-1.0786819787,-0.9513379809,-
0.1474 873982\C,-1.8054699927,-
1.9917041862,0.7338500003\C,0.4314384867,-1.20 61600466,-
0.2944208096\C,-1.6910620352,-0.8338427921,-1.556274412\C,-2
.7633628418,-2.8480244755,0.1750472663\C,-3.4290270482,-
3.8072459823,0 .936025473\C,-3.1608371394,-
3.9247631006,2.2940911688\C,-2.2338738749,-
3.0716208918,2.8865794634\C,-1.5696099181,-
2.118593543,2.1195727221\H , -2.996379863,-2.7690711246,-
0.8799356627\H,-4.157301145,-4.4548217001 ,0.4593058167\H,-
3.6707028068,-4.6679056075,2.898662581\H,-2.015741889 8,-
3.1367365745,3.9474721965\Cl,-0.4510836295,-1.0869573294,2.98143934
38\C,-1.3916127714,-1.8404671984,-2.484313531\C,-1.9233152895,-
1.80051 30409,-3.7673440167\C,-2.7502808666,-0.7431413091,-
4.152590827\C,-3.03 3129046,0.2703391622,-3.2451738472\C,-
2.5070996582,0.2262603202,-1.950 7120491\H,-0.7325892539,-
2.6570666194,-2.1989429496\H,-1.6826281821,-2 .5905636562,-
4.4716802408\H,-3.158936211,-0.707390657,-5.157345369\H,-
3.6589924063,1.1074890333,-3.5379036047\H,-
2.7335473177,1.048717251,-1 .2785678327\C,1.0796708663,-
2.2627098934,0.344311715\C,2.4424896295,-2
.4819758495,0.1376279402\C,3.1692344193,-1.651317882,-
0.7083933603\C,2 .5224153891,-0.6089765395,-
1.374189778\C,1.161517234,-0.4008356187,-1.
1816181741\H,0.5343271413,-
2.9373177132,0.9951137793\H,2.9300720323,-3
.3109587347,0.6405600469\H,4.2291837649,-1.824060496,-
0.8657636163\H,3 .0718737276,0.026399094,-
2.0617118751\H,0.6556076716,0.3752463332,-1.7 529981327\H,-
3.300831743,2.2750439316,2.1806325659\H,-3.1937910617,-0.
0499089181,1.1309720477\Version=EM64L-G09RevC.01\State=1-A\HF=-
1418.2 226929\RMSD=3.388e-09\RMSF=5.312e-06\Dipole=-
1.1554521,1.3084976,0.465 1594\Quadrupole=-0.1646527,4.0498265,-
3.8851738,-1.0208716,-5.0440281, 1.6067794\PG=C01 [X(C22H18C11N2)]\@

**1H-1,2,4-
Triazole**

1\1\GINC-R1701\FOpt\RM062X\Gen\C2H3N3\ROOT\05-Nov-2013\0\#\M062X/gen
6 D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\124 tr.freq\0,1\N,-
1.4592692815,2.1373192606,0.\C,-0.0994188244,2.0871800
051,0.\N,0.4153170919,0.8718299659,0.\N,-
0.686062813,0.1005772109,0.\C , -
1.7955627037,0.8646269894,0.\H,0.5261416138,2.9679249613,0.\H,-0.597
2669396,-0.9056152318,0.\H,-
2.7980081435,0.4603968386,0.\Version=EM64 L-G09RevC.01\State=1-
A'\HF=-242.1624598\RMSD=6.236e-09\RMSF=1.620e-04\ Dipole=-0.3984017,-
1.1125483,0.\Quadrupole=-1.5263527,3.1525233,-1.626
1705,4.2239707,0.,0.\PG=CS [SG(C2H3N3)]\@

**1H-1,2,4-
Triazole(H⁺@N4)**

1\1\GINC-R1700\FOpt\RM062X\Gen\C2H4N3(1+)\ROOT\05-Nov-
2013\0\#\M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\124tr_p.freq\1,1\N,-

```

1.4572307032,2.0928022337,0.\C,-0.0833667106,2.1
093331805,0.\N,0.3838995103,0.8949650401,0.\N,-
0.7162453324,0.11537731
67,0.\C,-
1.8373379133,0.812529643,0.\H,0.5157381839,3.0087462883,0.\H,-
0.6105674403,-0.8968492784,0.\H,-2.8483277438,0.42806574,0.\H,-
2.0776
118507,2.8988198362,0.\Version=EM64L-G09RevC.01\State=1-
A'\HF=-242.50
51887\RMSD=7.348e-09\RMSF=6.449e-05\Dipole=-
1.4600721,0.2100657,0.\Qua
drupole=-0.1995733,6.5302528,-
6.3306795,1.028395,0.,0.\PG=CS [SG(C2H4N 3)]\@

1H-1,2,4-Triazole(H*@N2)
1\1\GINC-R1700\FOpt\RM062X\Gen\C2H4N3(1+)\ROOT\05-Nov-
2013\0\#\M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ 124tr_p1.freq\1,1\N,-1.4851121083,2.2647335697,-
0.0023872974\C,-0.15
73678273,2.2700311502,-
0.0016559697\N,0.3248378912,1.0226685033,0.0010
120907\N,-
0.7395732129,0.2001862821,0.0019993278\C,-1.8250987504,0.981
3165226,-0.000109078\H,0.4816305933,3.1439660624,-0.002979737\H,-
2.831
9351547,0.5834044831,0.0000938372\H,1.2820389086,0.6767259164,0.0022
11
936\H,-0.646250337,-0.8133124983,0.0040004704\Version=EM64L-
G09RevC.0 1\State=1-A'\HF=-242.4866957\RMSD=3.978e-09\RMSF=4.177e-
05\Dipole=1.14
10518,-
1.4764825,0.0034766\Quadrupole=3.7931593,2.3878976,-6.1810569,2
.6922309,0.0003931,-0.0149752\PG=CS [SG(C2H4N3)]\@

1Me-1,2,4-Triazole
1\1\GINC-R1701\FOpt\RM062X\Gen\C3H5N3\ROOT\05-Nov-2013\0\#\M062X/gen
6 D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\m12 4tr.freq\0,1\N,-1.4741091894,2.2803302764,-
0.2010338497\C,-0.16485698
67,2.2352753105,0.1557224173\N,0.3331019931,1.0190951875,0.299253679
2\
N,-0.7229907875,0.2356095466,0.016936438\C,-
1.7893380132,1.0019414249,-
0.2785476176\H,0.4384486922,3.1178484783,0.3133748368\C,-0.6062213,-
1
.2070338949,0.0574497959\H,-2.7552453893,0.5901513429,-
0.5387672776\H,
0.1492392945,-1.5337136463,-0.6594109491\H,-
1.5732422442,-1.6399440973
,-0.2028582196\H,-0.3188460695,-
1.5231099286,1.0618407463\Version=EM6 4L-G09RevC.01\State=1-A'\HF=-
281.4566154\RMSD=2.423e-09\RMSF=3.214e-05\
Dipole=-0.3224653,-
1.3394097,-0.0796063\Quadrupole=-1.1753064,2.112767
9,-
0.9374615,3.6173143,-0.0983881,0.9646769\PG=C01 [X(C3H5N3)]\@

1Me-1,2,4-Triazole(H*@N2)
1\1\GINC-R1700\FOpt\RM062X\Gen\C3H6N3(1+)\ROOT\05-Nov-
2013\0\#\M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ m124tr_p1.freq\1,1\N,-1.4481694669,2.2483820743,-
0.1082039558\C,-0.11
57192292,2.2449615171,0.2073362228\N,0.3252700967,1.0227993402,0.292
27
83133\N,-0.7472776992,0.2447151907,0.0253563246\C,-
1.8236942207,0.9666
972101,-
0.2179178383\H,0.477312657,3.1348562864,0.3626057367\C,-0.6048
702023,-1.2146395389,0.0367353675\H,-2.8111331995,0.5975124751,-
0.4582
07726\H,-2.0450137888,3.0604693885,-
0.2385510931\H,0.1389596234,-1.489
9769014,-0.7107016774\H,-
1.5710989699,-1.6581662498,-0.2001825976\H,-0
.2754356006,-
1.5171607924,1.0305929234\Version=EM64L-G09RevC.01\State =1-A'\HF=-
281.8084996\RMSD=2.762e-09\RMSF=3.602e-05\Dipole=-1.3544353,0
.5999216,-0.3122575\Quadrupole=-1.8100581,8.8055799,-6.9955218,-
0.8007 727,1.2944755,0.0608487\PG=C01 [X(C3H6N3)]\@

1Me-1,2,4-Triazole(H*@N2)
1\1\GINC-R1700\FOpt\RM062X\Gen\C3H6N3(1+)\ROOT\05-Nov-
2013\0\#\M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\
m124tr_p1.freq\1,1\N,-
1.4636447645,2.2751113863,-0.1937345378\C,-0.1
680758466,2.2812610927,0.0780417415\N,0.299140017,1.0297815213,0.188
12
04374\N,-0.7390767033,0.1964585472,-0.0218570764\C,-

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1.7912994524,0.985                                     3156497,-
0.2502405035\H,0.4602711244,3.153943184,0.2015530243\C,-0.609
5161627,-1.2627772913,0.018069386\H,-2.7774452536,0.5873814256,-
0.4536          493063\H,0.0911589418,-1.5861859322,-0.7534268564\H,-
1.5963266603,-1.6          773618725,-0.1851069063\H,-0.2786322419,-
1.5709256904,1.0111962743\H,1
.2349070022,0.6841379795,0.3873043229\\Version=EM64L-
G09RevC.01\State=      1-A\HF=-281.7903719\RMSD=7.760e-09\RMSF=1.540e-
05\Dipole=1.0780019,-1.
1516713,0.236388\Quadrupole=2.7652952,2.8576082,-
5.6229034,3.7026406,1 .8025635,0.695411\PG=C01 [X(C3H6N3)]\\@

1H-1,2,3-Triazole      1\1\GINC-R1897\FOpt\RM062X\Gen\C2H3N3\ROOT\05-Nov-2013\0\\#M062X/gen
6      D      SCF=Tight      INT(grid=ultrafine)      OPT      IOP(2/17=4)
maxdisk=268435456\\123      tr.freq\\0,1\N,-
2.2623143289,2.6932576834,0.\C,-0.9038231352,2.7881929      803,0.\C,-
0.3767039482,1.5195869725,0.\N,-1.4732970551,0.7282093597,0.      \N,-
2.601141717,1.4447088205,0.\H,-0.4035438267,3.7438949911,0.\H,0.62
97059872,1.1320915872,0.\H,-1.533451976,-
0.2806823946,0.\\Version=EM64      L-G09RevC.01\State=1-A'\HF=-
242.1333113\RMSD=2.171e-09\RMSF=1.282e-04\      Dipole=1.4978654,-
1.0423879,0.\Quadrupole=-1.749623,3.6552558,-1.90563
28,0.8629501,0.,0.\PG=CS [SG(C2H3N3)]\\@

1H-1,2,3-Triazole(H*@N3)      1\1\GINC-R1894\FOpt\RM062X\Gen\C2H4N3(1+)\ROOT\05-Nov-
2013\0\\#M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ \123tr_p.freq\\1,1\N,-2.2193001161,2.8130733721,-
0.0015112766\C,-0.869      9504655,2.9671403593,-0.0023911873\C,-
0.3807825843,1.6867526755,0.0008      40324\N,-
1.4891712946,0.9019232278,0.0033121938\N,-2.6057116244,1.5704
434317,0.0019252395\H,-0.3828790568,3.9308981977,-
0.0051218198\H,0.624      7655301,1.2931770196,0.0015354335\H,-
2.9387559958,3.5347725034,-0.0031      78002\H,-1.544224394,-
0.1156107978,0.0060350614\\Version=EM64L-G09RevC .01\State=1-A'\HF=-
242.4801349\RMSD=3.264e-09\RMSF=9.565e-05\Dipole=0.
5247424,0.2005149,-0.0007158\Quadrupole=0.0969709,6.3844113,-
6.4813822 ,-2.8128434,0.0051799,-0.0332048\PG=CS [SG(C2H4N3)]\\@

1H-1,2,3-Triazole(H*@N2)      1\1\GINC-R1896\FOpt\RM062X\Gen\C2H4N3(1+)\ROOT\05-Nov-
2013\0\\#M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ \123tr_p1.freq\\1,1\N,-2.2766854009,2.8482291508,-
0.0020468617\C,-0.94      25583692,2.9490036125,-0.0023730653\C,-
0.388751657,1.668882571,0.00095      78004\N,-
1.4355857589,0.83920183,0.0031819154\N,-2.5397030419,1.583374
5694,0.0012819118\H,-0.4511052841,3.9103428356,-
0.0049166052\H,0.63093      56414,1.3097477077,0.0018521229\H,-
1.4675809714,-0.1795358428,0.005854      6193\H,-
3.4848651563,1.202083664,0.0023255879\\Version=EM64L-G09RevC.0
1\State=1-A'\HF=-242.4584151\RMSD=5.816e-09\RMSF=4.168e-
05\Dipole=0.21      4545,-
1.553502,0.0040635\Quadrupole=3.3395697,3.0393673,-6.378937,3.18
15011,-0.0087936,-0.0248435\PG=CS [SG(C2H4N3)]\\@

1Me-1,2,3-Triazole      1\1\GINC-R94\FOpt\RM062X\Gen\C3H5N3\ROOT\06-Nov-2013\0\\#M062X/gen 6D
SCF=Tight      INT(grid=ultrafine)      OPT      IOP(2/17=4)
maxdisk=268435456\m123t      r.freq\\0,1\N,-2.219246721,2.8878866302,-
0.1941060324\C,-0.8758299471,      2.9379304162,0.0043992609\C,-
0.4062970184,1.6503545911,0.1159213045\N, -1.512945969,0.8865246922,-
0.0241546275\N,-2.5962323825,1.6485998894,-      0.2102081865\H,-
0.3439747019,3.8755405483,0.0536398594\H,0.5745733289,
1.2291927048,0.2753141371\C,-1.636887674,-
0.5582626379,0.0025665945\H,      -1.306374056,-
0.9471687357,0.9679985684\H,-1.0444075987,-1.0025287643,
0.8000575024\H,-2.6912592603,-0.7898403345,-

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0.1464323759\\Version=EM6                                4L-G09RevC.01\\State=1-A\\HF=-
281.4274209\\RMSD=6.564e-09\\RMSF=3.156e-05\\           Dipole=1.3679165,-
1.3173601,0.2455461\\Quadrupole=-1.1850409,2.4918859,-
1.306845,2.6175163,-0.0684494,0.2703421\\PG=C01 [X(C3H5N3)]\\@

1Me-1,2,3-
Triazole(H*@N3) 1\\1\\GINC-R92\\FOpt\\RM062X\\Gen\\C3H6N3(1+)\\ROOT\\06-Nov-
2013\\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\m 123tr_p.freq\\1,1\\N,-2.2150404321,2.8187182052,-
0.1045149911\\C,-0.8765 714793,2.9631181567,0.0504524989\\C,-
0.4048225855,1.6783408594,0.115369 8477\\N,-
1.5045556652,0.8866991786,-0.0068762386\\N,-2.6025492146,1.5723
519046,-0.1402139898\\H,-
0.3844205027,3.9228332057,0.1005653173\\H,0.591
7957636,1.2797089528,0.2346130646\\C,-1.5608371703,-0.5830116926,-
0.002 2281028\\H,-1.1719831501,-0.9438149596,0.9500995167\\H,-
0.9633594458,-0. 9574925054,-0.8335615723\\H,-2.6049126089,-
0.8668156685,-0.1221730482\\H , -2.9256965092,3.5421143631,-
0.1929623023\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-
281.7835968\\RMSD=4.946e-09\\RMSF=4.667e-06\\Dipole=0.4925802
,0.5412601,0.0532966\\Quadrupole=-1.5008677,8.8400449,-7.3391772,-
2.035 045,0.7064725,-0.3616355\\PG=C01 [X(C3H6N3)]\\@

1Me-1,2,3-
Triazole(H*@N2) 1\\1\\GINC-R1896\\FOpt\\RM062X\\Gen\\C3H6N3(1+)\\ROOT\\05-Nov-
2013\\0\\#M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\\ \\m123tr_p1.freq\\1,1\\N,-
2.2935971149,2.9876780939,-0.0051419987\\C,-0.9
640135098,3.0996710621,-0.0058682076\\C,-
0.4010647225,1.8210204483,0.00 05294212\\N,-
1.4304571308,0.9708384527,0.0051221085\\N,-2.5366525119,1.7
136670871,0.0011951652\\H,-0.4799663407,4.0646097192,-
0.0109120194\\H,0. 6230034792,1.475279971,0.0021530672\\C,-
1.4697893875,-0.4982114181,0.01 43879929\\H,-
3.4765619336,1.3211951396,0.0032375495\\H,-0.4392854547,-0.
8493354198,0.0062159562\\H,-1.9875918776,-0.8477793266,-
0.8801216237\\H, -1.9703734951,-
0.8371638094,0.9226925888\\Version=EM64L-G09RevC.01\\Sta te=1-A\\HF=-
281.7628226\\RMSD=7.355e-09\\RMSF=4.775e-05\\Dipole=0.2432354, -
1.2516704,0.0067883\\Quadrupole=2.6809285,3.5315585,-
6.212487,3.224779 2,-0.0175612,-0.0537254\\PG=C01 [X(C3H6N3)]\\@

Lidocaine 1\\1\\GINC-R142\\FOpt\\RM062X\\Gen\\C14H22N2O1\\ROOT\\07-Nov-
2013\\0\\#M062X/ge n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=1073741824\\ \\ld.freq\\0,1\\C,-1.9162248233,1.1232298596,-
0.4238768312\\C,-3.19403160 78,0.5794447794,-0.584954243\\C,-
3.399327575,-0.7955114319,-0.585751808 5\\C,-2.3169660724,-
1.6559566532,-0.4219718507\\C,-1.029018119,-1.153151 6787,-
0.2417931677\\C,-0.841486807,0.2385747265,-0.2423828497\\C,-1.7180
689892,2.6140956343,-0.4636399888\\H,-4.0356047559,1.2535094225,-
0.7243 284851\\H,-4.3996427932,-1.1971904194,-0.7184480899\\H,-
2.4705156598,-2. 7321909357,-0.4209442004\\C,0.1399076499,-
2.0790499891,-0.0296904336\\N, 0.4774618435,0.7462687418,-
0.0886345485\\H,-2.5607392951,3.0976141849,- 0.965070224\\H,-
0.8000106671,2.8754037139,-1.0015269217\\H,-1.6268887299
,3.0189072826,0.5490869077\\H,-0.1938528097,-
3.119069237,0.0099320949\\H ,0.6554820177,-
1.8446454803,0.9076639355\\H,0.8783528016,-1.9986726637, -
0.8374638514\\C,0.8703975527,1.5994861591,0.8952813967\\H,1.2326582272
, 0.4197252096,-
0.6873895126\\O,0.1531613736,2.0026989041,1.7964574549\\C,
2.3078207695,2.107792037,0.7587650892\\H,2.7394578578,2.1229223767,1.
76
87475076\\H,2.208083763,3.1576833615,0.454960055\\N,3.1362560403,1.379
14 21154,-

```

0.1950493691\C,4.1239863599,0.5187986565,0.4558849275\C,3.711105
 30242,2.2290991419,-1.2407107911\C,3.4717491934,-
 0.6502584268,1.181984
 3388\H,4.7474030586,1.0927589678,1.1643373843\H,4.7931201573,0.13634
 68 61,-0.3238835409\H,4.1281502217,1.5677555846,-
 2.0095136034\C,4.7839859 387,3.2156819815,-
 0.7725562307\H,2.8825133466,2.7717391652,-1.71092236
 7\H,2.7570730531,-0.3072916986,1.9388125164\H,4.2290606583,-
 1.25564935 02,1.6893590127\H,2.935934632,-
 1.2877237466,0.4726809855\H,5.668834056 3,2.6943996539,-
 0.3942008967\H,4.4084442593,3.8666880499,0.0246948867\
 H,5.1020278482,3.8529901401,-1.6035736879\\Version=EM64L-
 G09RevC.01\State=1-A\HF=-731.1738471\RMSD=8.951e-09\RMSF=3.626e-
 06\Dipole=1.3067914 , -0.3130069,-
 1.0024951\Quadrupole=5.8438732,2.0483259,-7.8921991,1.913
 7949,2.1675338,-3.4851617\PG=C01 [X(C14H22N2O1)]\@

**Lidocaine (H*⁺N-
amide)**

1\1\GINC-R93\FOpt\RM062X\Gen\C14H23N2O1(1+)\ROOT\07-Nov-
 2013\0\#\#M062X /gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
 maxdisk=10737418 24\ld_p.freq\1,1\C,-1.6729609823,0.7280288242,-
 0.2230676335\C,-2.922 689266,0.141412732,-0.4266217921\C,-
 3.0635799343,-1.2431367839,-0.4596 738238\C,-1.9564651259,-
 2.0712385442,-0.2950575197\C,-0.6860517722,-1. 5322864888,-
 0.0900692631\C,-0.591430308,-0.140158052,-0.063682695\C,-1
 .50159412,2.2260614787,-0.1916741275\H,-3.7907436344,0.7805181005,-
 0.5 571134852\H,-4.0441798217,-1.6807210968,-0.6166793371\H,-
 2.0737227304, -3.1503189462,-0.3259445106\C,0.5267821924,-
 2.4118613118,0.0771515431\
 N,0.7314060768,0.4550959785,0.1724803681\H,-
 2.4652307924,2.7205339504, -0.325889407\H,-
 0.8531304238,2.5854243664,-1.0028175018\H,-1.092597046
 9,2.5706878978,0.7645789129\H,0.2379335639,-
 3.4644032793,0.0719154082\ H,1.0420928333,-
 2.2238443076,1.0266499202\H,1.2491612738,-2.2730558481 , -
 0.7378564399\C,1.0472443709,0.8503715582,1.6464145924\H,1.5370963123
 , -0.155248206,-
 0.0773318002\O,0.1591305206,0.9152356999,2.4188991883\C
 ,2.5337906069,1.0950613595,1.8053879473\H,2.7455072027,1.1476654598,
 2.
 8819396703\H,2.7394470317,2.0876433315,1.3792385142\N,3.269871467,0.
 06 93193822,1.0798274739\C,3.5140964632,-
 1.0918209138,1.9602546589\C,4.48
 61583515,0.5903428949,0.4210608184\C,4.1441604151,-
 2.2663582316,1.2291 181166\H,2.5434217681,-
 1.390879154,2.3769559391\H,4.1361840815,-0.7976
 197876,2.8197341308\H,4.8521309432,-0.1913209758,-
 0.2498097451\C,5.595
 1349487,1.0465325443,1.365275439\H,4.1698366306,1.4217567804,-
 0.220003 5609\H,3.5892139823,-
 2.5070394908,0.3162540537\H,4.139072346,-3.147448
 3247,1.875823987\H,5.1842334557,-
 2.0677813282,0.9561627558\H,6.0114445
 444,0.2128215013,1.9380089453\H,5.24148386,1.8048980659,2.0730169301
 \H
 ,6.4118602835,1.4889671978,0.788750227\H,0.8397174322,1.3077099673,-
 0. 3949988981\\Version=EM64L-G09RevC.01\State=1-A\HF=-
 731.5115046\RMSD=8. 253e-09\RMSF=9.660e-
 06\Dipole=0.7501699,0.6339184,-0.659501\Quadrupole
 =13.8281514,0.3702635,-14.1984149,1.9451859,8.6068984,-
 1.3754543\PG=C0 1 [X(C14H23N2O1)]\@

Lidocaine (H⁺@N-amine)

1\1\GINC-R413\FOpt\RM062X\Gen\C14H23N2O1(1+)\ROOT\08-Nov-2013\0\#\M062 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741 824\ld_pl.freq\1,1\C,-1.8806263237,0.9820869843,-0.498897558\C,-3.06 7704755,0.2872533978,-0.2505155064\C,-3.0543870983,-1.0608382131,0.089 0815119\C,-1.8464483461,-1.7471422409,0.1870130266\C,-0.6373812785,-1. 0921740588,-0.0408885375\C,-0.6827719047,0.2681267323,-0.377355537\C,-1.9143876531,2.436953091,-0.8833562351\H,-4.0129241111,0.8158198569,-0.3369814098\H,-3.9888603371,-1.5817865785,0.2725729709\H,-1.8378838005,-2.8010468198,0.4500681787\C,0.6775772826,-1.8204395542,0.0722992356\N,0.5703549923,0.9276746291,-0.6322142464\H,-2.8930143431,2.6998582411,-1.2908718806\H,-1.1609577595,2.6707028331,-1.6437264303\H,-1.7236542167,3.0732129376,-0.0127831781\H,0.5239257595,-2.8336304902,0.44912201 58\H,1.3613042806,-1.3065980723,0.7574807116\H,1.1816263824,-1.9103541 567,-0.8986047476\C,1.0315791869,1.9632296984,0.0795586035\H,1.1739113196,0.5261533706,-1.3426393674\O,0.4703819506,2.4970874004,1.0286573374\C,2.3795926079,2.5518074075,-0.3824613843\H,2.2229038751,3.170901130 5,-1.2707581734\H,3.1308224935,1.7902006089,-0.6047431284\N,2.8537087933,3.4173026214,0.7350428004\C,3.6267980633,2.6097568598,1.7508919131\C,3.5416424169,4.6764825474,0.2773375593\C,3.9730669552,3.4181740298,2.987393748\H,4.5148916303,2.225382828,1.2438373451\H,2.9760666818,1.76 8435435,2.0044531804\H,2.8421030504,5.166310753,-0.4048002213\C,4.8797 438512,4.4096424057,-0.3873512284\H,3.6470621134,5.3120189902,1.1584266788\H,4.7212252078,4.1891228187,2.7870506828\H,4.3904065529,2.7428456401,3.7380703435\H,3.0832391617,3.8837672982,3.4234998471\H,4.78853916 29,3.7270447082,-1.2379148829\H,5.6158205682,4.006815601,0.3131977076\H,5.2740820574,5.3551069746,-0.7671668956\H,1.96431053,3.6748923537,1.2102771503\Version=EM64L-G09RevC.01\State=1-A\HF=-731.5552765\RMSD=6. 769e-09\RMSF=5.522e-06\Dipole=3.584633,1.8466717,-0.2090441\Quadrupole=11.5910226,3.2393425,-14.8303651,18.8000323,5.2858817,1.1404347\PG=C0 1 [X(C14H23N2O1)]\@

N-Methyl acetamide

1\1\GINC-R215\FOpt\RM062X\Gen\C3H7N1O1\ROOT\06-Nov-2013\0\#\M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268435456\ma a.freq\0,1\C,-2.4186212069,0.1310100764,0.0377463528\C,-1.1230722835,0.8810148008,0.2728812563\O,-1.085829966,1.931284446,0.8961194173\N,0. 0018890284,0.3217654456,-0.2491331787\C,1.2902277856,0.9662080573,-0.0 767947234\H,-3.1107178821,0.7904893142,-0.4915166814\H,-2.8627662791,-0.1075738883,1.0071943055\H,-2.2916320887,-0.7908610955,-0.5356799579\H,-0.0597540888,-0.5456046606,-0.7595036096\H,1.2796270459,1.966392216 2,-0.519022196\H,2.0553749835,0.3610266648,-0.5647459011\H,1.5279349517,1.0669186234,0.9859149162\Version=EM64L-G09RevC.01\State=1-A\HF=-24 8.4146252\RMSD=7.573e-09\RMSF=1.930e-05\Dipole=0.3530365,-1.2910436,-0.8329052\Quadrupole=2.7748393,-1.6466849,-1.1281544,1.0258882,0.043722 6,-0.7546058\PG=C01 [X(C3H7N1O1)]\@

N-Methyl acetamide (H⁺)

1\1\GINC-R1867\FOpt\RM062X\Gen\C3H8N1O1(1+)\ROOT\06-Nov-2013\0\#\M062X /gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26843545 6\maa_p.freq\1,1\C,-2.4416132343,0.1893185877,-


```

0.0439983576\C,-1.203      8206484,0.8896124191,0.4035792331\O,-
1.0400458621,1.7847694567,1.15045 12265\N,0.1034239642,0.3138856567,-
0.2662788839\C,1.3324887489,1.11352      42446,0.0541431132\H,-
2.6318487192,0.4070878517,-1.1013276509\H,-3.278
1422605,0.5544451194,0.5525155599\H,-2.3469685961,-
0.8949328687,0.0728      456603\H,0.2225525321,-
0.6588138035,0.0466823803\H,1.1847574063,2.1292      177171,-
0.3091475815\H,2.1839323602,0.6433296047,-0.4366675868\H,1.461
463924,1.1238895017,1.1348761893\H,-0.0388706153,0.2620925128,-
1.28325      23019\\Version=EM64L-G09RevC.01\State=1-A\HF=-
248.7348907\RMSD=5.002e-      09\RMSF=6.970e-06\Dipole=0.6224527,-
1.3441711,-1.2094942\Quadrupole=4.      9970481,-2.3379544,-
2.6590936,0.9287263,-0.2928979,-0.2617358\PG=C01 [ X(C3H8N1O1) ]\\@

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Triethylamine

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1\1\GINC-R415\FOpt\RM062X\Gen\C6H15N1\ROOT\06-Nov-2013\0\\#M062X/gen
6      D      SCF=Tight      INT(grid=ultrafine)      OPT      IOP(2/17=4)
maxdisk=268435456\\net      3.freq\0,1\N,-0.9681923529,0.8928754502,-
0.0240578631\C,0.4924735532,      0.8770201488,-0.0915721259\C,-
1.5487943471,2.2300045859,-0.1037325381\      C,-
1.513934692,0.1855363678,1.1305839761\C,1.2314934557,1.5804531478,1
.0526922624\H,0.7853875748,1.3233972351,-
1.0470525046\H,0.8108299667,-      0.1687621495,-0.1461840274\H,-
2.6369386756,2.0975252423,-0.1354258805\      C,-
1.1113659248,3.0134925175,-1.3356677668\H,-1.3364824841,2.823730168
3,0.8070670333\H,-1.300617762,0.7203162297,2.0769711275\C,-
1.038531769      1,-1.2581250867,1.2432562315\H,-
2.6044475382,0.1919671549,1.0150257603
\H,0.9742263524,2.6438325966,1.1082054947\H,2.3132937206,1.507372895
3,      0.9010930286\H,1.0000688148,1.1282096587,2.0232397345\H,-
1.2255594589,      2.4013528512,-2.2361967804\H,-
0.0694101022,3.3421432619,-1.2701682768\      H,-
1.7305114854,3.9090238835,-1.4447227272\H,0.0102039394,-1.327104818
7,1.5488190589\H,-1.1543872133,-1.7727961323,0.2838820242\H,-
1.6333920      918,-1.7868877029,1.9940970463\\Version=EM64L-
G09RevC.01\State=1-A'\HF      =-292.2633053\RMSD=5.937e-09\RMSF=7.276e-
06\Dipole=0.0960145,0.1219615
,0.1993001\Quadrupole=0.786505,0.2084878,-0.9949929,-0.3713744,-
0.6113 973,-1.1657368\PG=CS [SG(C2H1N1),X(C4H14) ]\\@

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Triethylamine (H⁺)

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1\1\GINC-R424\FOpt\RM062X\Gen\C6H16N1(1+)\ROOT\06-Nov-
2013\0\\#M062X/g en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\      \net3_p.freq\1,1\N,-0.9972034881,0.8694387218,-
0.0559629188\C,0.51488      76507,0.8319804989,-0.0527545235\C,-
1.5713463235,2.2601655647,-0.21848      49707\C,-
1.5382863066,0.1242521349,1.1439294453\C,1.1336031845,1.51004 45414,-
1.2620177514\H,0.7808797072,-0.2274457297,-0.0163574073\H,0.835
1827852,1.2913470101,0.8848485745\H,-1.1927893117,2.6368602851,-
1.1701      198171\C,-1.2227927483,3.1895761444,0.929161997\H,-
2.6505100988,2.1343      496869,-0.3204344653\H,-1.1071431465,-
0.8782455767,1.0841412396\C,-3.0
549544548,0.0661975931,1.1791992756\H,-
1.1250200408,0.6157367637,2.027 3094842\H,0.7153049201,1.1319996599,-
2.2010791195\H,2.2033354218,1.287      5088861,-
1.270016697\H,1.0259249114,2.5967045654,-1.2347602482\H,-0.14
54697673,3.3478449496,1.0264121479\H,-
1.6200378107,2.8397779764,1.8857      005638\H,-
1.6767029536,4.1625783141,0.7255298827\H,-3.4714344498,-0.31
13139838,0.2391157868\H,-3.5068691386,1.0342151934,1.4069801129\H,-
3.3      53311957,-0.6278731235,1.9686052095\H,-
1.3001465847,0.3451599237,-0.88      57858007\\Version=EM64L-
G09RevC.01\State=1-A\HF=-292.6451274\RMSD=4.20      2e-09\RMSF=9.659e-
06\Dipole=-0.008359,-0.4257271,-0.2661198\Quadrupole

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=1.2705021,0.3386542,-1.6091563,0.5958649,-2.462488,-
0.4990635\PG=C01 [X(C6H16N1)]\@

III

1\1\GINC-R453\FOpt\RM062X\Gen\C21H18Cl1N1O1\ROOT\07-Nov-
2013\0\#M062X /gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=16106127 36\63.freq\0,1\C,-2.499405518,3.1403071499,-
1.126895438\C,-1.4107062 384,2.9987413691,-0.0819840894\O,-
0.9083815574,3.9560531964,0.47997130 73\N,-
1.0371875625,1.7032512003,0.1797906581\H,-2.0388140061,3.1141652
683,-2.1207130982\H,-2.9909619157,4.104181278,-0.9939460918\H,-
3.23759 5078,2.3353074635,-
1.0686664387\C,0.2310076529,1.3527587708,0.84287511 26\H,-
1.3737617761,1.009243779,-0.4764230514\C,1.3679250104,2.18993547
13,0.2159980616\C,0.4439895035,-
0.1605866285,0.6359707637\C,0.12875736
6,1.5485585343,2.369666339\C,1.6508507599,2.1512934889,-
1.1582611089\C ,2.6657599277,2.9154692532,-
1.7286628031\C,3.426099153,3.763576034,-0.
931280482\C,3.1504260969,3.8467440163,0.4288920937\C,2.1343581896,3.
07 32824053,0.9823954568\C1,0.7424174974,1.1450497078,-
2.2758486242\H,2.8 455160238,2.840735249,-
2.796136335\H,4.2149189792,4.3610357828,-1.3778
928364\H,3.7132011514,4.5234498961,1.0641745028\H,1.9113141791,3.177
87 9281,2.0375391001\C,-0.629642244,-1.0259221208,0.8735900636\C,-
0.47371 86204,-2.4039366905,0.7532434347\C,0.766605787,-
2.940607537,0.41042907 13\C,1.8451667642,-
2.0866322924,0.1961034837\C,1.6855088043,-0.7058412
959,0.3084364033\H,-1.589655013,-0.6177345849,1.1818311898\H,-
1.319740 8276,-3.0589975005,0.9399332916\H,0.8917017945,-
4.0152964235,0.3177804 589\H,2.8180256074,-2.4918611429,-
0.0665870492\H,2.5359159548,-0.05369
87341,0.1286081232\C,1.1566263813,1.0605602081,3.1873880382\C,1.0940
53 414,1.1903262069,4.5702029624\C,-
0.0111319126,1.7996174192,5.166069490 2\C,-
1.0424938487,2.273579805,4.3626480405\C,-0.973486283,2.1498263682
,2.9732171297\H,2.0166512346,0.571305185,2.7358866145\H,1.9046187941
,0 .8068653307,5.1831337744\H,-
0.0662241314,1.8984666019,6.2462024296\H,-
1.9095598435,2.7489879486,4.8119881103\H,-
1.7831486502,2.5347912823,2. 3661089407\Version=EM64L-
G09RevC.01\State=1-A\HF=-1400.8616665\RMSD=7 .151e-09\RMSF=2.446e-
06\Dipole=0.0891404,-0.7750061,-0.1693294\Quadrup ole=6.4351999,-
5.8761751,-0.5590248,3.6076701,0.8545781,-0.8680211\PG=
C01
[X(C21H18Cl1N1O1)]\@

III (H⁺)

1\1\GINC-R342\FOpt\RM062X\Gen\C21H19Cl1N1O1(1+)\ROOT\07-Nov-
2013\0\#M 062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=1610 612736\63_p.freq\1,1\C,-3.5826197561,1.3002109506,-
0.5004643139\C,-2 .4210772653,2.1524019389,-0.9069152265\O,-
2.4011201061,3.1011851809,-1 .6120604072\N,-
1.1120296661,1.7251227939,-0.2015663087\H,-3.3938332187
,0.2475405159,-0.72786207\H,-4.464010823,1.6425590362,-
1.0426642025\H, -
3.7591052324,1.3983929088,0.577050931\C,0.3205003542,2.0689348182,-
0. 7809790682\H,-1.1485497524,0.7062194304,-
0.0687799532\C,0.2365473481,2 .3030516651,-
2.2898652295\C,1.1790289031,0.8451991721,-0.4298621678\C,
0.7827310684,3.3106721178,-0.0078774567\C,-
0.3406638307,1.3817810181,- 3.1758806295\C,-
0.3444653861,1.5771614056,-4.5506185166\C,0.2606579209
,2.7135909072,-5.0819278493\C,0.8576110491,3.6366688227,-
4.2314039736\ C,0.8406948259,3.4307866984,-2.8537942494\C1,-
1.1102775352,-0.08710219 63,-2.5926080731\H,-

```

0.8139224187,0.8401168932,-5.1935712857\H,0.262845
4524,2.8675788715,-6.156049723\H,1.3374270571,4.5230245023,-
4.63274848                                02\H,1.3133012444,4.1603169684,-
2.2057602296\C,1.1316142575,0.31685592
43,0.8679102277\C,1.9282117214,-
0.7667650241,1.225120049\C,2.802293282                                9,-
1.3243192004,0.2924909904\C,2.8763979257,-0.7858500657,-0.988890195
\C,2.0694645652,0.2928048767,-
1.3511569487\H,0.5055933833,0.7723694884
,1.634663865\H,1.8775038471,-
1.1628206103,2.2343973459\H,3.4282998065,                                -
2.1667840601,0.5684931898\H,3.5624730336,-1.2054743659,-
1.7177363916\                                H,2.1438849028,0.698928736,-
2.3549893935\C,2.0709857932,3.3763951356,0
.5298690762\C,2.4942543399,4.521923602,1.2039719888\C,1.636731723,5.
60 79583179,1.3552399158\C,0.3535835778,5.5536565861,0.8122852414\C,-
0.06
76697636,4.4175597595,0.1266146259\H,2.7535571799,2.5397434005,0.423
36
39414\H,3.4984841586,4.5577777297,1.6141523411\H,1.9669342236,6.4951
59 1095,1.8861436327\H,-0.3175871249,6.4014467878,0.9074003803\H,-
1.04667                                10741,4.4218088179,-0.3446325777\H,-
1.1406749924,2.1497006348,0.737035                                178\\Version=EM64L-
G09RevC.01\State=1-A\HF=-1401.2037685\RMSD=5.923e-0 9\RMSF=6.789e-
06\Dipole=-1.105738,-0.3018415,1.1531812\Quadrupole=1.95 05501,-
3.5373542,1.5868041,2.2281785,-2.9101859,-0.181643\PG=C01 [X(C2
1H19C11N1O1)]\@

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1H-Benzimidazole

```

1\1\GINC-R809\FOpt\RM062X\Gen\C7H6N2\ROOT\05-Nov-2013\0\#M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=536870912\bi.f req\0,1\C,-
1.563084317,3.1026604627,0.0641225944\C,-2.711189017,2.328 5492869,-
0.0026698707\C,-2.6471728776,0.9196643486,-0.0223809463\C,-1.
4347768464,0.2462772808,0.0240902595\C,-
0.2834447561,1.034539324,0.091                                2637491\C,-
0.3286577814,2.4436806987,0.1118682421\N,0.9533359132,2.968
5254453,0.1809698522\C,1.7353794682,1.92735909,0.201152108\N,1.06264
37                                761,0.7322482619,0.1500471334\H,-
1.6026515653,4.1872258441,0.079755612                                5\H,-
3.6826837927,2.8117421879,-0.0408174748\H,-3.568891723,0.34815996
05,-0.0751967014\H,-1.3889678358,-
0.8385303344,0.0087485311\H,2.816194
6034,1.9613164695,0.2528164691\H,1.4782580904,-
0.1873078696,0.15486213 05\\Version=EM64L-G09RevC.01\State=1-A'\HF=-
379.7210591\RMSD=7.902e-09 \RMSF=3.402e-05\Dipole=0.3559715,-
1.3709517,-0.0052911\Quadrupole=4.95 57429,0.5469042,-5.5026471,-
5.6544805,0.4041356,-0.1695233\PG=CS [SG(C 7H6N2)]\@

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1H-Benzimidazole (H⁺)

```

1\1\GINC-R828\FOpt\RM062X\Gen\C7H7N2(1+)\ROOT\05-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=536870912\bi_p.freq\1,1\C,-
1.5828602236,3.1254725956,0.0723642242\C,-2.71454381
42,2.330861986,0.0003563228\C,-2.6378234181,0.9211198044,-
0.0249818035 \C,-1.4264758032,0.2519056632,0.0207157833\C,-
0.2855361351,1.053093578                                4,0.0933254827\C,-
0.3615962348,2.4507066341,0.118435758\N,0.9549963044
,2.9040978974,0.1922502881\C,1.7833827109,1.864657804,0.2119113817\N
,1                                .0725980437,0.7428542629,0.1537317131\H,-
1.6435587908,4.2081918727,0.0                                916560673\H,-
3.6895741984,2.8046241935,-0.0378294246\H,-3.5557771947,0
.3460492908,-0.0819713706\H,-1.3693213392,-
0.8310021684,0.00117926\H,2
.8615761171,1.9223580113,0.2661702211\H,1.4734273673,-

```

0.189334315,0.15
 41192037\H,1.2523266085,3.8736528891,0.2268468925\\Version=EM64L-
 G09Re vC.01\State=1-A\HF=-380.08969\RMSD=6.398e-09\RMSF=9.507e-
 05\Dipole=1.9
 954403,0.1067914,0.1002711\Quadrupole=11.2392543,3.2497423,-
 14.4889965 ,0.4127171,1.2769724,0.3873551\PG=C01 [X(C7H7N2)]\@

**1Me-
Benzimidazole**

1\1\GINC-R869\FOpt\RM062X\Gen\C8H8N2\ROOT\05-Nov-2013\0\#M062X/gen
 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
 maxdisk=536870912\\mbi. freq\0,1\C,-
 1.6241233275,3.1846015503,0.0710413239\C,-2.7623956357,2.
 3946584036,0.0001199454\C,-2.682002405,0.9868426146,-0.02280046\C,-
 1.4 60476817,0.3283866935,0.0245292337\C,-
 0.3206396724,1.1330143632,0.0957 219818\C,-
 0.3815696646,2.542215614,0.1197307303\N,0.8953940464,3.07487
 40798,0.1925739987\C,1.6801426137,2.0336510535,0.211262166\N,1.02359
 12 199,0.830814887,0.1557659662\H,-
 1.6794996359,4.2685552991,0.0890412992 \H,-
 3.7398459181,2.8658283206,-0.0388176824\H,-3.5970779024,0.40495824
 62,-0.0787414563\H,-1.4001642299,-
 0.7561544242,0.0069022028\H,2.762304
 0994,2.0686644217,0.2650226519\C,1.604347278,-
 0.4928527897,0.159687989 1\H,2.6907994273,-
 0.4007240843,0.2098762816\H,1.335932492,-1.030456925 7,-
 0.7547114119\H,1.2559540317,-1.0607873231,1.02762524\\Version=EM64L -
 G09RevC.01\State=1-A\HF=-419.0131032\RMSD=7.885e-09\RMSF=3.536e-
 05\Di pole=0.4526206,-1.4992358,-0.0062291\Quadrupole=5.2089863,-
 0.3938087,- 4.8151777,-5.3077246,0.3912882,-0.1754773\PG=C01
 [X(C8H8N2)]\@

**1Me-
Benzimidazole (H⁺
)**

1\1\GINC-R885\FOpt\RM062X\Gen\C8H9N2(1+)\ROOT\05-Nov-
 2013\0\#M062X/ge n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
 maxdisk=536870912\\ mbi_p.freq\1,1\C,-
 1.6573158284,3.2048266311,0.0699146555\C,-2.7738019
 583,2.3879204086,-0.0005085392\C,-2.6704361623,0.9800739992,-
 0.0223558 074\C,-1.4449662098,0.3360068481,0.0254380362\C,-
 0.3196955027,1.159860 6014,0.0963549067\C,-
 0.4229487246,2.554974552,0.1180518848\N,0.8840534
 401,3.0282005606,0.1912861107\C,1.724067153,1.9925176658,0.212672141
 2\ N,1.0407557167,0.8562756457,0.1572024057\H,-
 1.7393887217,4.2862157379, 0.0865917135\H,-
 3.7578267854,2.8426927392,-0.040095609\H,-3.5773243825 ,0.387589114,-
 0.0781490789\H,-1.3671465618,-0.7460048348,0.0086650538\
 H,2.8018183052,2.0651468696,0.2669353547\C,1.6005390192,-
 0.4954202314,
 0.1593458166\H,1.1697531345,4.0006526429,0.2238230154\H,2.6869816325
 ,- 0.4287386271,0.2094414377\H,1.3058574733,-1.0053216587,-
 0.7594183526\H ,1.2249349628,-
 1.0363286642,1.0295948547\\Version=EM64L-G09RevC.01\Sta te=1-A\HF=-
 419.3877869\RMSD=7.640e-09\RMSF=2.227e-05\Dipole=1.7175146,
 0.2581025,0.089402\Quadrupole=9.5225442,5.0063729,-14.5289171,-
 0.46664 36,1.1747548,0.3510882\PG=C01 [X(C8H9N2)]\@

1H-Indazole

1\1\GINC-R1038\FOpt\RM062X\Gen\C7H6N2\ROOT\05-Nov-2013\0\#M062X/gen
 6 D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
 maxdisk=268435456\\in. freq\0,1\C,-1.8081075907,2.3119141476,0.\C,-
 3.0209049966,1.6517748612 ,0.\C,-3.0836612841,0.2367709404,0.\C,-
 1.9432118531,-0.5421915395,0.\C , -0.7125461988,0.1363708345,0.\C,-
 0.6280566523,1.5449916343,0.\C,0.777
 4670569,1.8111698877,0.\N,1.4742271893,0.6963059618,0.\N,0.576411514
 9, -0.309394173,0.\H,-1.7635044078,3.3970928352,0.\H,-
 3.9456528074,2.2201 961393,0.\H,-4.0558829468,-0.2471647899,0.\H,-
 1.9971298329,-1.62654224

```

95,0.\H,1.2882089209,2.7644117639,0.\H,0.9121938884,-
1.2602462539,0.\
Version=EM64L-G09RevC.01\State=1-A'\HF=-
379.6961276\RMSD=3.869e-09\RMSF=5.360e-05\Dipole=-0.585886,-
0.4195592,0.\Quadrupole=-2.748814,7.3095
937,-4.5607797,-
0.9193613,0.,0.\PG=CS [SG(C7H6N2)]\@

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1H-Indazole (H⁺)

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1\1\GINC-R1038\FOpt\RM062X\Gen\C7H7N2 (1+)\ROOT\05-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\
\in_p.freq\1,1\C,-
1.8048855436,2.3302324106,0.\C,-3.001919645,1.66210
0696,0.\C,-
3.0583592899,0.2376425909,0.\C,-1.9308011894,-0.5511944086,
0.\C,-
0.702625391,0.1338156303,0.\C,-0.6211026957,1.5503962119,0.\C,0.
7499256233,1.8549676019,0.\N,1.4203540381,0.7072151125,0.\N,0.571727
73
34,-0.340885331,0.\H,-1.7555998342,3.4137570807,0.\H,-
3.9313579094,2.2
207968796,0.\H,-4.031758964,-0.2427227879,0.\H,-
1.9867279354,-1.633946
9869,0.\H,1.275643024,2.8002116488,0.\H,0.9160203927,-
1.2936745588,0.\
H,2.425317586,0.5623682099,0.\Version=EM64L-
G09RevC.01\State=1-A'\HF=
-380.0438061\RMSD=5.176e-09\RMSF=8.199e-
05\Dipole=2.0330428,-0.4850244
0.\Quadrupole=13.3279328,1.6297685,-
14.9577013,-1.9445469,0.,0.\PG=CS [SG(C7H7N2)]\@

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1Me-Indazole

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1\1\GINC-R331\FOpt\RM062X\Gen\C8H8N2\ROOT\05-Nov-2013\0\#M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\min.
freq\0,1\C,-1.8548262374,2.3735526682,-
0.002828756\C,-3.0576561475,1.
6939447242,-0.001724006\C,-
3.0999490452,0.2781096674,0.0023102556\C,-1
.9472315258,-
0.4836197125,0.0052284188\C,-0.7272011994,0.2150912687,0.
0039391364\C,-
0.6633287606,1.6253235134,0.00011711\C,0.7377332643,1.90
38234468,0.0003361718\N,1.4423646916,0.7918423822,0.0041984009\N,0.5
60
5879866,-0.2293245387,0.0058800079\H,-1.8281848621,3.4594099561,-
0.005
8877472\H,-3.9908986236,2.2484601375,-0.0039272838\H,-
4.065290269,-0.2
195648072,0.003169938\H,-1.9840319596,-
1.5690184498,0.0084873049\H,1.2
426651884,2.8601357665,-
0.002071142\C,1.0152954266,-1.5999249727,0.011
5257586\H,2.1046333828,-1.5798265506,0.0047318254\H,0.6538326135,-
2.12
82404233,-0.8763476385\H,0.6647660763,-
2.1180040764,0.9098122451\Vers
ion=EM64L-G09RevC.01\State=1-A'\HF=-
418.9897012\RMSD=4.876e-09\RMSF=5.3
33e-05\Dipole=-0.4459201,-
0.5527649,0.0013517\Quadrupole=-2.0038027,6.
6386932,-4.6348905,-
1.8303721,0.0058958,-0.0333654\PG=C01 [X(C8H8N2)]\@

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1Me-Indazole (H⁺)

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1\1\GINC-R92\FOpt\RM062X\Gen\C8H9N2 (1+)\ROOT\06-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=536870912\m
in_p.freq\1,1\C,-1.8550608368,2.3918392531,-
0.0189629769\C,-3.0429190
528,1.7088389095,-0.0069987708\C,-
3.080540526,0.2833150126,0.020806302
8\C,-1.943080505,-
0.4892227735,0.0412473672\C,-0.7195364932,0.20965062
22,0.0358365125\C,-0.660400955,1.6281165905,-
0.001170159\C,0.704255062
8,1.9483567384,-
0.0119975107\N,1.3825682355,0.8026348668,0.0157680153\
N,0.5545094913,-0.2619325146,0.0631712108\H,-
1.820104651,3.4757157933,
-0.0425289422\H,-
3.9799966482,2.2545678713,-0.021026927\H,-4.047848311
9,-
0.2091549395,0.0242049104\H,-1.9909643268,-1.5723271664,0.056310943
5\H,1.2216386906,2.8978436209,-0.0283279732\C,1.0536993457,-
1.62830335
59,-
0.0185564632\H,2.3889962527,0.6679709245,0.0313114986\H,1.23714919
48,-1.9106527951,-1.057988089\H,1.9677203411,-
1.7140579347,0.572052635
1\H,0.3006576923,-
2.2826957235,0.4197594157\Version=EM64L-G09RevC.01\
State=1-A'\HF=-
419.3431389\RMSD=6.467e-09\RMSF=3.107e-06\Dipole=1.79195
34,-

```

0.3377147,-0.0191111\Quadrupole=11.5527263,3.2552173,-14.8079436,-
2.275199,0.0253785,-0.2019117\PG=C01 [X(C8H9N2)]\@

Oxazole

1\1\GINC-R397\FOpt\RM062X\Gen\C3H3N1O1\ROOT\05-Nov-
2013\0\#\M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\oz .freq\0,1\N,-
1.2510381163,1.8208755766,0.\C,0.1375307537,1.7878253568
,0.\C,0.5478041171,0.4978368574,0.\O,-0.5632060951,-
0.2897798954,0.\C,-
1.5949276542,0.5777265437,0.\H,0.728345113,2.6912342831,0.\H,1.50152
5 4728,-0.0040848485,0.\H,-
2.588843591,0.1552661263,0.\Version=EM64L-G0 9RevC.01\State=1-
A'\HF=-245.9802679\RMSD=7.103e-09\RMSF=2.287e-05\Dipo le=0.462231,-
0.4384956,0.\Quadrupole=3.3164576,-1.7607595,-1.5556981,2
.4450317,0.,0.\PG=CS [SG(C3H3N1O1)]\@

Oxazole (H⁺)

1\1\GINC-R215\FOpt\RM062X\Gen\C3H4N1O1(1+)\ROOT\05-Nov-
2013\0\#\M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \oz_p.freq\1,1\N,-
1.2458676325,1.757787347,0.0226119412\C,0.14501868
45,1.8041568271,0.0114051196\C,0.5380507367,0.5142478592,-
0.0050893957 \O,-0.5801549384,-0.2745340352,-0.0037663253\C,-
1.6274669072,0.4998820
472,0.0129503734\H,0.7008381684,2.7293910748,0.0162008374\H,1.492721
49 09,0.0118783137,-0.0182454628\H,-
2.6301631236,0.0934750186,0.017214442 1\H,-
1.8722062989,2.5602353286,0.0360798933\Version=EM64L-G09RevC.01\
State=1-A'\HF=-246.3188742\RMSD=6.309e-09\RMSF=1.112e-04\Dipole=-
0.599 5588,0.8917957,0.0141569\Quadrupole=5.1724783,1.0735541,-
6.2460324,-0. 8270973,-0.1043706,0.0818314\PG=CS [SG(C3H4N1O1)]\@

4Me-Oxazole

1\1\GINC-R94\FOpt\RM062X\Gen\C4H5N1O1\ROOT\05-Nov-2013\0\#\M062X/gen
6 D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\moz .freq\0,1\N,-
1.299360461,1.6673897474,0.3187649088\C,0.0627572873,1.6
618215253,0.0237073132\C,0.4258469392,0.3910982229,-0.2766593647\O,-
0. 679790275,-0.4038137123,-0.1770002377\C,-
1.6652279178,0.4383874532,0.1
832628259\C,0.8770723683,2.9106919222,0.0659726343\H,1.3481601149,-
0.0 901217246,-0.5600643627\H,-
2.6480297153,0.0116263557,0.3208926514\H,0. 4798603908,3.6493227921,-
0.6364540208\H,1.9187100184,2.7069711484,-0.1
946974122\H,0.8475012501,3.3521962697,1.0664250645\Version=EM64L-
G09R evC.01\State=1-A'\HF=-285.2810184\RMSD=2.593e-09\RMSF=2.537e-
05\Dipole= 0.4832029,-0.2437259,-0.1469292\Quadrupole=2.4287764,-
0.9419153,-1.486 861,2.4248485,-0.4266165,-0.4255989\PG=C01
[X(C4H5N1O1)]\@

4Me-Oxazole (H⁺)

1\1\GINC-R302\FOpt\RM062X\Gen\C4H6N1O1(1+)\ROOT\05-Nov-
2013\0\#\M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \moz_p.freq\1,1\N,-
1.2967814677,1.6348787364,0.2054203409\C,0.085847 1672,1.6839681295,-
0.0154666581\C,0.4228845778,0.3954677032,-0.2501141 062\O,-
0.7037236152,-0.3827761045,-0.1728472915\C,-1.7116630607,0.3917
539866,0.1005697111\C,0.8752523796,2.9452978727,0.0306791168\H,1.349
25 24735,-0.1103746555,-0.472512866\H,-2.7129291865,-
0.0023378068,0.21166 90521\H,-
1.8930632853,2.433048424,0.4136225635\H,0.5219675149,3.654010 4857,-
0.7235642599\H,1.9244606911,2.7253024126,-0.1715336812\H,0.80742
58111,3.4119308162,1.0175280785\Version=EM64L-G09RevC.01\State=1-
A'\HF =-285.6264378\RMSD=3.308e-09\RMSF=4.129e-05\Dipole=-
0.8398421,0.509326 4,0.2090338\Quadrupole=5.6334992,0.6688078,-
6.302307,0.9386293,-1.9026 479,0.8737616\PG=C01 [X(C4H6N1O1)]\@

Isoxazole 1\1\GINC-R534\FOpt\RM062X\Gen\C3H3N1O1\ROOT\05-Nov-2013\0\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268435456\io z.freq\0,1\C,-1.329601938,2.4267696824,0.0696293106\C,0.082430563,2.6195083049,0.0905428358\C,0.5482076374,1.3709108965,0.3460557977\O,-0.4 707765419,0.5126340162,0.467226441\N,-1.6565591326,1.1821185249,0.2921 5192\H,-2.1150617474,3.1509791745,-0.099531592\H,0.6444023426,3.527894 4904,-0.0587098303\H,1.5351187234,0.9486153458,0.4662074162\Version=EM64L-G09RevC.01\State=1-A'\HF=-245.9403974\RMSD=9.305e-09\RMSF=1.518e-04\Dipole=0.857253,0.8673496,-0.1294677\Quadrupole=1.1824649,0.4686395,-1.6511044,-2.348067,0.5650744,-0.5201516\PG=CS [SG(C3H3N1O1)]\@

Isoxazole (H⁺) 1\1\GINC-R573\FOpt\RM062X\Gen\C3H4N1O1(1+)\ROOT\05-Nov-2013\0\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268435456 \ioz_p.freq\1,1\C,-1.3238017371,2.4752562309,0.0555573183\C,0.073173853,2.6184413658,0.0934328166\C,0.5359187638,1.3561595291,0.3481746546 \O,-0.476535914,0.4926231816,0.4626367594\N,-1.5978193381,1.2066648683,0.2793889774\H,-2.1146503012,3.1961100248,-0.1144238074\H,0.6456369941,3.5229464211,-0.0479858801\H,1.5198812568,0.9234776139,0.4732449291\H,-2.4631035772,0.6732807644,0.3392642322\Version=EM64L-G09RevC.01\State=1-A'\HF=-246.2679145\RMSD=8.817e-09\RMSF=7.411e-05\Dipole=-0.557799,0.3824934,-0.0963911\Quadrupole=6.0060476,0.0592409,-6.0652885,0.4398 337,0.478362,-1.1613972\PG=C01 [X(C3H4N1O1)]\@

5Me-Isoxazole 1\1\GINC-R511\FOpt\RM062X\Gen\C4H5N1O1\ROOT\05-Nov-2013\0\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268435456\mi oz.freq\0,1\C,-1.4531714842,2.5007889979,0.0458842065\C,-0.0410747672,2.6819192421,0.0750210449\C,0.4294066723,1.4317142436,0.3337574664\O,-0.6053840597,0.5830103221,0.4484696052\N,-1.7912311777,1.2593124855,0.2664841009\H,-2.2320174148,3.2314230588,-0.1280377339\H,0.527124306,3.587463798,-0.0714991458\C,1.7888883616,0.8514919811,0.5056632024\H,2.5442676256,1.6302671272,0.3874965573\H,1.9693232961,0.0690423163,-0.2371783469\H,1.8936586421,0.4061064272,1.4992990428\Version=EM64L-G09RevC.01\State=1-A'\HF=-285.2435917\RMSD=7.543e-09\RMSF=4.866e-05\Dipole=1.0997892,0.7340304,-0.0897038\Quadrupole=0.1571574,1.1130639,-1.270221 3,-3.1532001,0.6704649,-0.6234395\PG=C01 [X(C4H5N1O1)]\@

5Me-Isoxazole (H⁺) 1\1\GINC-R511\FOpt\RM062X\Gen\C4H6N1O1(1+)\ROOT\05-Nov-2013\0\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268435456 \mioz_p.freq\1,1\C,-1.4524082099,2.53496195,0.0395918582\C,-0.0611624849,2.6773959785,0.0754856479\C,0.4252130276,1.4150882599,0.3364673168 \O,-0.6019179382,0.5546781311,0.4529281058\N,-1.7281358849,1.26603364 49,0.267394767\H,-2.2438101895,3.2543357076,-0.1323964596\H,0.50883365 68,3.5825574901,-0.0701708511\C,1.7817516628,0.8472121351,0.505871088\H,-2.5918486001,0.7329902024,0.329135321\H,2.5258815578,1.6345460068,0.3844209179\H,1.9586167147,0.0651788697,-0.2386147833\H,1.8832866878,0.405261624,1.5016770715\Version=EM64L-G09RevC.01\State=1-A'\HF=-285.58 11139\RMSD=5.721e-09\RMSF=7.138e-05\Dipole=-0.8855832,0.4269383,-0.120 5328\Quadrupole=8.3703412,-1.0843552,-7.285986,-1.247181,0.9601127,-1.2858373\PG=C01 [X(C4H6N1O1)]\@

Thiazole 1\1\GINC-R133\FOpt\RM062X\Gen\C3H3N1S1\ROOT\05-Nov-
2013\0\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\sz .freq\0,1\N,-1.6331131094,2.3136079487,0.\C,-
0.2586331626,2.351961602 2,0.\C,0.3679396609,1.1413736052,0.\S,-
0.8040204338,-0.1195056887,0.\C , -
2.0488939313,1.0853428586,0.\H,0.2427726879,3.3119309472,0.\H,1.4280
909751,0.9316231603,0.\H,-
3.0946226867,0.8017755665,0.\Version=EM64L- G09RevC.01\State=1-
A'\HF=-568.9453058\RMSD=6.435e-09\RMSF=1.636e-04\Di pole=0.4314001,-
0.5107517,0.\Quadrupole=3.3977075,-1.3260903,-2.071617
2,2.8551844,0.,0.\PG=CS [SG(C3H3N1S1)]\@

Thiazole(H⁺) 1\1\GINC-R744\FOpt\RM062X\Gen\C3H4N1S1(1+)\ROOT\05-Nov-
2013\0\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \sz_p.freq\1,1\N,-
1.6693789936,2.2576483776,0.\C,-0.2970724916,2.393
0328521,0.\C,0.3146686999,1.1826565307,0.\S,-0.8372041395,-
0.096772481 ,0.\C,-
2.1072417494,1.0071606859,0.\H,0.1538063392,3.3761135383,0.\H,1
.3773376685,0.9795754706,0.\H,-3.1582976005,0.745817539,0.\H,-
2.302667 733,3.0558874867,0.\Version=EM64L-G09RevC.01\State=1-
A'\HF=-569.29354 84\RMSD=8.857e-09\RMSF=1.479e-04\Dipole=-
0.5703404,0.9063555,0.\Quadru pole=4.2723795,3.2962181,-7.5685977,-
1.3542272,0.,0.\PG=CS [SG(C3H4N1S 1)]\@

4Me-Thiazole 1\1\GINC-R644\FOpt\RM062X\Gen\C4H5N1S1\ROOT\05-Nov-
2013\0\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\ms z.freq\0,1\N,-
1.7307059194,2.1619080124,0.2486021758\C,-0.3738170178,
2.2394129675,0.0020749286\C,0.2252787949,1.0415899013,-
0.2621658685\S, -0.9286481774,-0.2361332586,-0.205519315\C,-
2.1446849382,0.9364980956,
0.1721359251\C,0.2975587468,3.5773167149,0.044133524\H,1.2665931624,
0. 8519962463,-0.4826944386\H,-
3.1742677666,0.6368808682,0.3288083395\H,-
0.1516762665,4.2508870035,-
0.6919284521\H,1.3654972365,3.4879942291,-0
.1682410632\H,0.1726821453,4.0339692198,1.0306242443\Version=EM64L-
G0 9RevC.01\State=1-A'\HF=-608.245725\RMSD=4.747e-09\RMSF=7.717e-
06\Dipole =0.43786,-0.2928279,-0.1196488\Quadrupole=2.4009268,-
0.2840791,-2.1168 477,2.8259753,-0.5076349,-0.295094\PG=C01
[X(C4H5N1S1)]\@

4Me-Thiazole(H⁺) 1\1\GINC-R133\FOpt\RM062X\Gen\C4H6N1S1(1+)\ROOT\05-Nov-
2013\0\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \msz_p.freq\1,1\N,-
1.7136944959,2.1184720344,0.1598006136\C,-0.34680 99485,2.262233034,-
0.0307995472\C,0.217374407,1.0423255885,-0.24197573 59\S,-
0.9459288221,-0.2259547403,-0.1990572195\C,-2.1764469226,0.87818
36494,0.1002251241\C,0.2921019813,3.6115231175,0.0134776691\H,1.2625
56 1438,0.8282363831,-0.4210773855\H,-
3.2215059603,0.6262917526,0.2309493 058\H,-
2.3246048083,2.9151793479,0.3342223377\H,-0.1201014196,4.264149
0255,-0.7619829472\H,1.3649930194,3.5161168629,-
0.1566998836\H,0.14135
68258,4.0828939445,0.9893076686\Version=EM64L-G09RevC.01\State=1-
A'\HF =-608.5998734\RMSD=7.793e-09\RMSF=2.395e-05\Dipole=-
0.7166142,0.544567 9,0.1640817\Quadrupole=4.1648869,3.4823247,-
7.6472116,0.4543502,-1.783 9417,1.1271771\PG=C01 [X(C4H6N1S1)]\@

Isothiazole 1\1\GINC-R397\FOpt\RM062X\Gen\C3H3N1S1\ROOT\05-Nov-
2013\0\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\is z.freq\0,1\C,-
1.0669665726,2.2018785146,0.\C,0.3583084927,2.270328688


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2,0.\C,0.88113186,1.007226559,0.\S,-0.3930065049,-
0.1340456571,0.\N,-1.6018806108,1.0036623062,0.\H,-
1.7314301292,3.0604564142,0.\H,0.936408
2326,3.1856658827,0.\H,1.9217752321,0.709987292,0.\Version=EM64L-
G09R evC.01\State=1-A'\HF=-568.9377253\RMSD=2.492e-09\RMSF=1.429e-
04\Dipole =0.9409804,0.405636,0.\Quadrupole=-0.298514,2.6288961,-
2.3303821,-1.18 18802,0.,0.\PG=CS [SG(C3H3N1S1)]\@

Isothiazole (H+) 1\1\GINC-R497\FOpt\RM062X\Gen\C3H4N1S1(1+)\ROOT\05-Nov-
2013\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \isz_p.freq\1,1\C,-
1.0783922991,2.2359504034,0.010008655\C,0.3219690 432,2.2695113351,-
0.0036103426\C,0.8360937089,0.9917596106,0.002203092 2\S,-
0.3678262761,-0.1973216588,0.023636736\N,-1.551677608,0.992799551
6,0.0249366115\H,-
1.7680283926,3.0727111701,0.009563286\H,0.9155845249 ,3.1739337572,-
0.0168451362\H,1.8794038235,0.694551265,-0.0052426558\H ,
-2.540636573,0.7471845232,0.0364146738\Version=EM64L-G09RevC.01\Stat
e=1-A'\HF=-569.2791567\RMSD=3.193e-09\RMSF=8.200e-05\Dipole=-
0.5026633 ,0.3841118,0.0015679\Quadrupole=5.4966803,1.9908659,-
7.4875462,-0.6703 077,-0.1180657,-0.0730789\PG=CS [SG(C3H4N1S1)]\@

3Me-Isothiazole 1\1\GINC-R513\FOpt\RM062X\Gen\C4H5N1S1\ROOT\06-Nov-
2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\mi sz.freq\0,1\C,-
1.0054111607,2.0799618321,0.0511009979\C,0.4200657005, 2.1199756624,-
0.1023542929\C,0.9431074915,0.8625751752,-0.0275648646\S ,
-0.3235744812,-0.2629768808,0.2211294897\N,-1.5253416854,0.8866368572
,0.2285189667\C,-
1.8966657169,3.2870036506,0.0200680633\H,0.9945027755 ,3.0259342624,-
0.2559146138\H,1.9788544876,0.5578396066,-0.1046569275\ H,-
1.8074185081,3.810317329,-0.9374083848\H,-1.6232232545,3.9912857885
,0.8124020267\H,-
2.9349096484,2.9826097169,0.1608395392\Version=EM64L -
G09RevC.01\State=1-A'\HF=-608.2386943\RMSD=5.974e-09\RMSF=6.591e-
06\Di pole=0.8011594,0.5665648,-
0.1423174\Quadrupole=0.5911394,1.826926,-2.4 180654,-2.0041161,-
0.1124803,-0.2313563\PG=C01 [X(C4H5N1S1)]\@

3Me- 1\1\GINC-R251\FOpt\RM062X\Gen\C4H6N1S1(1+)\ROOT\06-Nov-
Isothiazole (H+) 2013\0\#M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \misz_p.freq\1,1\C,-
1.0072375864,2.1137191271,0.0154856167\C,0.40123 10766,2.1184670607,-
0.0936932599\C,0.9146379782,0.8489151225,-0.036487 8388\S,-
0.2871858803,-0.3360198474,0.1467749478\N,-1.4643884141,0.8681
537411,0.1458417383\C,-1.9230056498,3.2895092427,-
0.003408243\H,0.9940 593642,3.0170511197,-
0.2080623008\H,1.9550646805,0.5482632517,-0.09392 96664\H,-
2.4492606511,0.62612796,0.2403975774\H,-1.799631257,3.8351469 74,-
0.9437393462\H,-1.6648885677,3.968322449,0.8149854113\H,-2.9692420
931,2.9965427989,0.0989383635\Version=EM64L-G09RevC.01\State=1-
A'\HF=- 608.58862\RMSD=4.854e-09\RMSF=1.412e-06\Dipole=-
0.3058569,0.2029816,0. 0082096\Quadrupole=4.7314678,3.2245909,-
7.9560587,-1.9849415,-0.838198 6,-0.7084601\PG=C01 [X(C4H6N1S1)]\@

1,3,4- 1\1\GINC-R215\FOpt\RM062X\Gen\C2H2N2S1\ROOT\05-Nov-
Thiadiazole 2013\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\td z.freq\0,1\N,-1.5966803955,2.6531955736,0.\N,-
0.2330875347,2.69841405 57,0.\C,0.3014796101,1.517734868,0.\S,-
0.8332743681,0.2148141132,0.\C, -
2.0518534906,1.4396953346,0.\H,1.3716423945,1.3563763828,0.\H,-
3.1089 752561,1.2077933749,0.\Version=EM64L-G09RevC.01\State=1-
A1\HF=-584.96 14886\RMSD=2.949e-09\RMSF=6.497e-05\Dipole=0.0460251,-

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1.3879162,0.\Qua drupole=4.8025722,-4.3547573,-
0.4478149,0.3040031,0.,0.\PG=C02V [C2(S1 ),SGV(C2H2N2)]\ \@

1,3,4- 1\1\GINC-R246\FOpt\RM062X\Gen\C2H3N2S1(1+)\ROOT\05-Nov-
Thiadiazole(H+) 2013\0\#\M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \tdz_p.freq\1,1\N,-
1.6088626392,2.6020825663,0.\N,-0.269990728,2.742
3407686,0.\C,0.2693900092,1.5655769977,0.\S,-
0.8529932032,0.243396586, 0.\C,-
2.0990691945,1.3812731725,0.\H,1.3431970659,1.4183618247,0.\H,-3
.1617227604,1.1650410423,0.\H,-
2.1654785499,3.4577370418,0.\Version=E M64L-G09RevC.01\State=1-
A'\HF=-585.2993897\RMSD=3.671e-09\RMSF=9.962e-05\Dipole=-0.9442116,-
0.0144078,0.\Quadrupole=5.4164075,0.2957435,-5.7 12151,-
3.8683528,0.,0.\PG=CS [SG(C2H3N2S1)]\ \@

2Me-1,3,4- 1\1\GINC-R172\FOpt\RM062X\Gen\C3H4N2S1\ROOT\05-Nov-
Thiadiazole 2013\0\#\M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456\mt dz.freq\0,1\N,-1.7969229383,2.7027959295,-
0.0016354526\N,-0.432558826 2,2.7325912366,-
0.0000940307\C,0.1094567485,1.5530230699,0.0019869627\ S,-
1.0570354034,0.2598683534,0.0021598842\C,-2.2654935656,1.4965508361
,-0.0006679712\C,1.5863525094,1.323662193,0.0049223439\H,-
3.3252200284 ,1.2757299642,-
0.0017141001\H,2.0813573806,2.2963205167,-0.0038989452\
H,1.8989655668,0.7554214542,-
0.8756373418\H,1.8975585566,0.7726764464,
0.8969486509\Version=EM64L-G09RevC.01\State=1-A\HF=-
624.2639486\RMSD= 9.858e-09\RMSF=4.058e-05\Dipole=0.338795,-
1.3524762,0.0026101\Quadrupo le=5.4402048,-4.9297557,-
0.5104491,1.4975508,0.0070215,0.0075289\PG=C0 1 [X(C3H4N2S1)]\ \@

2Me- 1\1\GINC-R172\FOpt\RM062X\Gen\C3H5N2S1(1+)\ROOT\05-Nov-
Thiadiazole(H+) 2013\0\#\M062X/ gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=268435456 \mtdz_p.freq\1,1\N,-1.776546341,2.6412149592,-
0.0007811111\N,-0.4343
700373,2.7571897004,0.0006277563\C,0.1076108096,1.5764683935,0.00221
31 4\S,-1.0666357286,0.2730096583,0.0018302412\C,-
2.2917947197,1.43337608 35,-
0.000522359\C,1.5785679374,1.3398473967,0.0050925798\H,-3.35868009
22,1.2406077294,-0.0017520603\H,-2.3162730692,3.5068377032,-
0.00216892 95\H,2.0834974358,2.3070091893,-
0.0042202971\H,1.8795017446,0.76797207 98,-
0.8769570112\H,1.8781620607,0.7862071068,0.8992580509\Version=EM6
4L-G09RevC.01\State=1-A\HF=-624.6100748\RMSD=6.279e-09\RMSF=5.299e-
05\ Dipole=-1.1673727,0.0389981,-0.0008298\Quadrupole=8.6617226,-
1.5497169 , -7.1120057,-4.1204057,0.0268948,-0.0097023\PG=C01
[X(C3H5N2S1)]\ \@

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