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Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: https://www.math.utah.edu/~beebe/

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[?]. ^{19} [?]. $^1A_1$ [?]. $^1A\prime$ [?]. $^1\Delta_g$ [?, ?]. $^1\Phi_g$ [?]. $^1\Pi_u$ [?]. $^1\Sigma$ [?, ?, ?]. $^1\Sigma^+$ [?, ?, ?]. $^1\Sigma_g^+$ [?]. $^1\Sigma_g^+$ [?, ?]. ^{2} [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $^{2+}$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $^{2+/3+}$ [?]. ^{2,6} [?]. $^{2-}$ [?]. $^{2-}_4$ [?]. $^{2-}_{II}$ [?]. ^{207} [?]. ^{29} [?]. $^2\Lambda$ [?]. $^{2n-}$ [?]. $^2\Pi_g$ [?]. $^2\Sigma^+$ [?, ?, ?, ?]. ^{3} [?, ?, ?, ?, ?, ?]. $^{3+}$ [?, ?, ?, ?]. $^{3-}$ [?, ?]. ^{35} [?]. ^{377} [?]. $^3\Pi_g$ [?]. $^3\Sigma^-$ [?]. ^{4} [?, ?, ?]. $^{4+}$ [?, ?]. $^{4-}$ [?]. ^{5} [?]. $^{5+}$ [?, ?, ?]. ^{6} [?, ?]. $^{6+}$ [?, ?]. $^{6-}$ [?, ?]. $^{7+}$ [?]. ^{9} [?]. ^{e} [?]. $^\infty$ [?]. ^{M} [?]. ^{N} [?]. $^{n+}$ [?]. ^{o} [?]. $^\prime$ [?, ?, ?, ?, ?]. $_0$ [?]. $_{0.4}$ [?]. $_{0.6}$ [?]. $_{0.8}$ [?]. $_1$ [?, ?, ?, ?, ?, ?, ?, ?]. $_{1-x}$ [?, ?]. $_{1.2}$ [?]. $_{10}$ [?, ?, ?]. $_{105}$ [?]. $_{111}$ [?]. $_{12}$ [?, ?, ?, ?]. $_{123}$ [?]. $_{13}$ [?]. $_{14}$ [?]. $^2_1$ [?]. $_{1A}$ [?]. $_2$ [?, ?]. $_2$ [?, ?]. $_{20}$ [?]. $_{24}$ [?]. $_{240}$ [?]. $_{26}$ [?]. $_{28}$ [?, ?]. $^+_2$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $^-_2$ [?, ?, ?]. $_{2h}$ [?]. $_{2n}$ [?]. $_2 \longrightarrow$ [?]. $_3$ [?, ?]. $_{3-\delta}$ [?]. $_{3-x}$ [?, ?]. $_{3-y}$ [?]. $_{32}$ [?]. $^+_3$ [?, ?, ?, ?]. $^-_3$ [?]. $^2_3$ [?]. $_3 \longrightarrow$ [?]. $_4$ [?, ?]. $_{40}$ [?, ?]. $^{+1}_4$ [?]. $^{2-}_4$ [?]. $_4 \longrightarrow$ [?]. $_5$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $_{5+\delta}$ [?]. $^{2+}_5$ [?]. $_6$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $_{60}$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $^{2-}_{60}$ [?]. $^{3-}_{60}$ [?]. $_7$ [?, ?, ?, ?, ?, ?]. $_{7+\delta}$ [?]. $_{70}$ [?, ?, ?]. $_{78}$ [?, ?]. $_8$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $_{80}$ [?, ?]. $_{81}$ [?]. $_{86}$ [?]. $_{87}$ [?]. $_{88}$ [?]. $_9$ [?, ?, ?]. $_{93}$ [?]. $_a$ [?]. $_B$ [?]. $_C$ [?, ?, ?, ?, ?, ?, ?, ?, ?]. $_{\text{cam}}$ [?]. $_g$ [?, ?, ?]. $_I$ [?]. $_{II} \longrightarrow$ [?]. $_\infty$ [?]. $_J$ [?]. $_k$ [?]. $_m$ [?]. $_n$ [?, ?]. $_s[\rho]$ [?]. $_u$ [?]. $_x$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $_x[\rho]$ [?]. $_y$ [?, ?, ?]. $_z$ [?]. A [?]. $\mathrm{A_2B_2} \leftarrow \mathrm{X^2A_1}$ [?]. α [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $\alpha 2$ [?]. α^2 [?]. α_N [?, ?]. as [?]. B [?, ?, ?, ?]. β [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. β_1 [?, ?, ?]. β_2 [?]. $\mathcal{L}_N$ [?]. $\mathcal{S}_N$ [?]. $\cdot$ [?, ?, ?, ?, ?]. $\cdots$ [?]. $\chi^{(2)}$ [?]. D [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. D_{2h} [?]. δ [?, ?, ?, ?, ?, ?]. $\Delta^{-1/2}$ [?]. $\delta E/\delta\rho$ [?]. e [?, ?, ?]. ϵ [?]. η [?]. η^5 [?, ?]. f [?]. $f(r)$ [?, ?]. f^6 [?]. G [?, ?, ?]. γ [?, ?, ?, ?]. $h-b-1$ [?, ?]. I [?]. I_h [?]. j [?, ?]. $J=0$ [?]. K_a [?]. $\kappa-\pi$ [?]. L^2 [?, ?]. λ [?]. $\lambda, \mu, \nu \geq -2$ [?]. $\langle 1/r \rangle$ [?, ?]. $\langle r^n \rangle$ [?]. $\leftarrow$ [?]. $\leftrightarrow$ [?, ?]. $\longleftrightarrow$ [?]. m [?]. $m=0,1$ [?]. μ [?, ?, ?]. μ_3 [?]. N [?, ?]. $n=1,2$ [?]. $n=1,5$ [?]. $n=1,7$ [?]. $n=45$ [?]. N^6 [?]. $\nabla^2 n/n$ [?]. $\nabla n/n$ [?]. nl^N [?]. $n \leq 7$ [?]. $\mathrm{NO_2}$ [?]. $N\prime$ [?]. ν [?]. ν_{17} [?]. O [?]. O_4 [?]. O_h [?]. $O \supset C_4$ [?]. p [?, ?, ?]. P^o [?]. π [?, ?]. $\pi* \leftarrow n$ [?]. π^*

[?]. π^2 [?]. $\pi^2 + \pi^2$ [?]. π^4 [?]. $\pi \to \pi$ [?]. $\pi \to \pi*$ [?]. $\prime$ [?, ?, ?, ?, ?]. R [?]. r_{12}^{-2} [?]. r_{12}^{-1} [?]. $r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu}$ [?]. r_{ij} [?]. $\rho(r)$ [?, ?]. $\to$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $\rightleftharpoons$ [?]. S [?, ?, ?, ?, ?, ?, ?]. $S = 0, 1/2$ [?]. S_1 [?]. Σ [?, ?, ?, ?, ?, ?]. $\Sigma^+ \not\leftrightarrow \Sigma^-$ [?]. sp [?]. t [?]. T_1 [?]. T_c [?]. $T_c[\rho]$ [?]. $U(2n)$ [?, ?, ?]. v [?, ?]. $v\prime$ [?]. $Y'' = F(X, Y)$ [?]. Z [?, ?]. $Z = 1--24$ [?].

***** [?, ?].

-2 [?]. **-acetylpropanamide** [?]. **-adrenergic** [?]. **-adrenoceptor** [?, ?, ?]. **-Al** [?]. **-alanine** [?]. **-Alkane** [?]. **-Alkanes** [?]. **-allyl** [?]. **-aminobutyric** [?]. **-aminohexanoic** [?]. **-aminoimidazole** [?]. **-aminopentane** [?]. **-aminophenyl** [?]. **-androstane** [?]. **-Argon** [?, ?]. **-Atom** [?]. **-Atomic** [?]. **-Azido-3prime-deoxythymidine** [?]. **-bend** [?]. **-Benzohydroquinone** [?]. **-Bi** [?]. **-bipyridyl-3** [?]. **-bis** [?]. **-bithiophene** [?]. **-Butane** [?]. **-Butyl** [?]. **-Butylbenzene** [?]. **-butyrolactone** [?]. **-C** [?, ?]. **-Chemisorbed** [?]. **-conjugated** [?, ?]. **-Conjugation** [?, ?]. **-cristobalite** [?]. **-cyclodextrin** [?, ?]. **-cyclopropan** [?]. **-D** [?, ?, ?]. **-DCNQI** [?]. **-deoxyadenosine-5** [?]. **-dianthryl** [?]. **-difluorobenzene** [?]. **-DIIS** [?]. **-Dimensional** [?, ?, ?, ?, ?]. **-diol** [?]. **-doped** [?, ?, ?]. **-Electron** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **-electronic** [?]. **-Electrons** [?, ?]. **-elements** [?]. **-Ethyl-Indole-3-Acetic** [?]. **-fluoropropane** [?]. **-fluorotoluene** [?]. **-Fold** [?, ?, ?, ?]. **-Framework** [?]. **-function** [?]. **-glycylcarbonyl** [?, ?]. **-Halogenobenzoic** [?]. **-HD** [?]. **-helical** [?]. **-helices** [?, ?]. **-heptane-HZSM-** [?]. **-His** [?]. **-hydrido-bridged** [?]. **-hydroxyketones** [?]. **-hydroxypentanoic** [?]. **-Hydroxypropionic** [?]. **-Hydroxytetronic** [?]. **-Hydroxyurea** [?]. **-Indacene** [?]. **-indole** [?]. **-ionone** [?]. **-K** [?]. **-ketoenolyl** [?]. **-Ketoesters** [?]. **-krypton** [?]. **-layer** [?]. **-manifold** [?]. **-Membered** [?]. **-Methyl** [?]. **-methyl-** [?]. **-methyl-derivatives** [?]. **-Methylacetamide** [?]. **-Methylformamide** [?]. **-Methylpyridones** [?]. **-methylthio-** [?]. **-MSH** [?]. [?]NaSaha:1999:LES. **-Neon** [?]. **-Ni** [?]. **-one** [?]. **-opioid** [?]. **-Pairing** [?]. **-phosphate** [?]. **-pleated** [?]. **-poly** [?]. **-polyazamacrocyclic** [?]. **-propiolactone** [?]. **-protonation** [?]. **-Pyridylacetic** [?]. **-quinonenediimine** [?]. **-reduced** [?]. **-related** [?]. **-Representability** [?, ?, ?]. **-representable** [?, ?, ?]. **-residue** [?]. **-S** [?]. **-separation** [?]. **-Sextet** [?]. **-SiO** [?]. **-Spiral** [?, ?]. **-state** [?]. **-subunit** [?]. **-tensor** [?]. **-Tensors** [?]. **-Tetrasilane** [?]. **-tetrazine** [?]. **-Type** [?, ?, ?, ?, ?]. **-wave** [?].

/1 [?]. **/6** [?, ?]. **/6-31** [?, ?]. **/blood** [?]. [?]CSaha:1999:LES. **/Cu** [?]. **/INDO** [?]. **/M** [?]. **/MC** [?]. **/MCLR** [?]. **/Molecular** [?]. [?]NSaha:1999:LES. **/Q** [?].

7-cyclooctatetraene [?].

8-tetrachlorodibenzo-p-dioxin [?].

9 [?, ?]. **9-dimethylguanine** [?]. **9-j** [?].

= [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?].

A/T [?]. **AA** [?]. **Ab-initio** [?, ?, ?, ?]. **Abacus** [?, ?]. **able** [?]. **above** [?]. **above-threshold** [?]. **abrupt** [?]. **Absolute** [?, ?]. **Absorbed** [?]. **Absorption** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Abstraction** [?, ?, ?, ?, ?]. **AC** [?]. **Academic** [?, ?, ?, ?, ?]. **Acceleration** [?, ?]. **accelerator** [?]. **Accelerators** [?]. **Acceptor** [?, ?, ?, ?, ?, ?, ?]. **acceptors** [?]. **Account** [?, ?]. **Accounts** [?]. **ACCs** [?]. **Accuracy** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Accurate** [?, ?]. **ACE** [?]. **ACES** [?]. **Acetaldehyde** [?]. **Acetaldehyde/Vinyl** [?]. **Acetaldimine** [?]. **Acetaldimine/Vinylamine** [?]. **acetate** [?, ?]. **Acetic** [?, ?, ?, ?, ?, ?]. **Acetone** [?, ?, ?]. **Acetonitrile** [?]. **Acetyl** [?]. **Acetylene** [?, ?, ?, ?, ?]. **Acetyloxyl** [?]. **acetylpropanamide** [?]. **ACh** [?]. **AChE** [?, ?]. **AChE-catalyzed** [?, ?]. **Achieving** [?]. **Acid** [?, ?]. **Acid-Base** [?]. **Acidic** [?]. **Acidities** [?, ?, ?, ?]. **Acidity** [?]. **Acids** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **ACPQ** [?, ?]. **acrylonitrile** [?, ?]. **action** [?, ?, ?]. **Activated** [?]. **Activating** [?]. **Activation** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Activation/Cyclization** [?]. **Active** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Active-site** [?, ?, ?]. **Active-Space** [?]. **Activity** [?, ?]. **actual** [?]. **Actually** [?]. **Acylation** [?, ?, ?]. **acylhydrazones** [?]. **ad** [?]. **Adams** [?]. **Adaptation** [?]. **Adapted** [?, ?]. **Adatom** [?]. **adatoms** [?]. **Addendum** [?, ?, ?]. **Addition** [?, ?, ?, ?, ?, ?]. **additions** [?]. **Additive** [?]. **additivity** [?]. **Adducts** [?, ?]. **Adenine** [?, ?, ?, ?, ?, ?]. **Adiabatic** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Adiabaticity** [?]. **Adjoint** [?]. **Adler** [?]. **admissibility** [?]. **adrenergic** [?, ?]. **adrenoceptor** [?, ?, ?]. **Adsorbate** [?, ?]. **Adsorbates** [?, ?, ?, ?, ?]. **Adsorbed** [?, ?, ?, ?, ?, ?, ?]. **Adsorption** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Advanced** [?, ?, ?]. **Advances** [?, ?, ?, ?]. **Advantages** [?]. **Affinities** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Affinity** [?, ?, ?, ?, ?, ?]. **aflatoxin** [?]. **AG** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **AgCl** [?]. **agent** [?]. **agents** [?, ?, ?, ?]. **AgF** [?]. **Aggregate** [?, ?, ?]. **Aggregates** [?]. **Aggregation** [?, ?, ?, ?]. **Agonist** [?, ?, ?]. **Agostic** [?]. **AGP** [?]. **Agreement** [?]. **AH** [?, ?]. **Aib** [?]. **Aid** [?, ?, ?]. **aims** [?]. **Al**