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$(0.0 \leq x \leq 0.3)$ [?]. (110) [?]. $(4s)$ [?]. $(5s)$ [?]. (C_{2v}) [?]. $(d+s)^3$ [?]. (Γ) [?]. $(J = 0)$ [?, ?]. $(n = 0, 1, 2)$ [?]. $(n = 1, 2, , 6)$ [?]. $(n = 1, 2, 4)$ [?]. $(n = 1--3)$ [?]. $(n = 1--4)$ [?, ?]. $(n = 1--6)$ [?]. $(n = 2--12)$ [?]. $(n = 2- - 14)$ [?]. $(n = 2--4)$ [?, ?]. $(n = 4, 5, 6)$ [?]. $(x = 2--16)$ [?]. + [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $0s$ [?]. $1, 4$ [?]. $1\,^1$ [?]. $1\,^1B_u^+$ [?]. $1\,^2$ [?]. $1 - x$ [?]. $1/2$ [?]. $1/r_{ij}$ [?]. $1/Z$ [?]. $10D_q$ [?]. **$187.00** [?]. $1s$ [?]. 2 [?, ?, ?, ?, ?]. $2\,^1A_g^-$ [?]. $2\,^3$ [?]. 20 [?]. **$208** [?]. 3 [?, ?, ?, ?]. $3n$ [?, ?]. 4 [?, ?]. $4n + 2$ [?]. 5 [?]. 540 [?]. 6 [?]. **$60.00** [?]. 7 [?]. **$79.00** [?]. = [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $[2 + 2]$ [?]. * [?, ?, ?]. $^+$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?]. ^{19} [?]. $^{1}A_1$ [?]. $^{1}A\prime$ [?]. $^{1}\Delta_g$ [?, ?]. $^{1}\Phi_g$ [?]. $^{1}\Pi_u$ [?]. $^{1}\Sigma$ [?, ?, ?]. $^{1}\Sigma^+$ [?, ?, ?]. $^{1}\Sigma_g^+$ [?]. $^{1}\Sigma_g^+$ [?, ?]. ^{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} [?]. $^{\prime}$ [?, ?, ?, ?, ?]. $_{0}$ [?]. $_{0.4}$ [?]. $_{0.6}$ [?]. $_{0.8}$ [?]. $_{1}$ [?, ?, ?, ?, ?, ?, ?, ?]. $_{1-x}$ [?, ?]. $_{1.2}$ [?]. $_{10}$ [?, ?, ?]. $_{105}$ [?]. $_{111}$ [?]. $_{12}$ [?, ?, ?, ?]. $_{123}$ [?]. $_{13}$ [?]. $_{14}$ [?]. $_{1}^{2}$ [?]. $_{1A}$ [?]. $_{2}$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?]. π^2 [?]. $\pi^2 + \pi^2$ [?]. π^4 [?]. $\pi \rightarrow \pi$ [?]. $\pi \rightarrow \pi*$ [?]. $\prime$ [?, ?, ?, ?, ?]. R [?]. r_{12}^{-2} [?]. r_{12}^{-1} [?]. $r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu}$ [?]. r_{ij} [?]. $\rho(r)$ [?, ?]. $\rightarrow$ [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. $\rightleftharpoons$ [?]. S [?, ?, ?, ?, ?, ?, ?]. $S = 0, 1/2$ [?]. S_1 [?]. Σ [?, ?, ?, ?, ?, ?]. $\Sigma^+ \leftrightarrow \Sigma^-$ [?]. 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** [?].

0 [?, ?, ?, ?, ?, ?, ?, ?]. **0-19-506643-X** [?]. **0-19-508091-2** [?]. **0-19-508523-X** [?]. **0-19-509775-0** [?]. **0-19-855573-3** [?]. **0-387-57874-9** [?]. **0-387-94376-5** [?]. **0-387-94380-3** [?]. **0-444-82171-6** [?]. **0-7923-3264-4** [?]. **0-7923-3664-X** [?].

1 [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **1-Bisnitroxyphenylethylene** [?]. **1-D** [?, ?]. **1-dimethyl** [?]. **1000-Tesla** [?]. **11-14** [?]. **11-diene** [?]. **13-atom** [?]. **13-Molecule** [?]. **13C** [?, ?]. **155.00** [?]. **158** [?]. **18-crown-6** [?]. **1980** [?]. **1984** [?]. **1986** [?]. **1987** [?, ?, ?, ?]. **1988** [?, ?, ?]. **1989** [?, ?, ?, ?]. **1990** [?, ?, ?]. **1991** [?, ?, ?, ?, ?, ?, ?]. **1992** [?, ?, ?, ?, ?, ?, ?]. **1993** [?, ?, ?]. **1994** [?, ?]. **1995** [?, ?]. **1996** [?, ?]. **1b** [?]. **1b-adrenergic** [?]. **1D** [?, ?]. **1S** [?].

2 [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **2-** [?, ?]. **2-alkenylfurans** [?]. **2-Aminoethanethiol** [?]. **2-Aminoethanol** [?]. **2-D** [?, ?]. **2-diazacyclobutadienes** [?]. **2-Dihydro-1** [?]. **2-dimethylcyclopropanone** [?]. **2-Dithietes** [?]. **2-electron** [?]. **2-Hydroxypropanal** [?]. **2-Hydroxypyridine** [?]. **2-isomer** [?]. **2-Nitrophenylcyanate** [?]. **2-Nitrophenylthiocyanate** [?]. **2-Pyridone** [?, ?]. **2-substituted-1** [?]. **2-Trifluoromethylvinyl** [?]. **2/6** [?]. **2/6-31** [?]. **20-component** [?]. **202nd** [?]. **21G** [?]. **21st** [?]. **23S** [?]. **273K** [?]. **28H4** [?]. **29-July** [?]. **2D** [?]. **2e** [?]. **2N** [?]. **2nd** [?, ?, ?]. **2NH** [?].

3 [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **3-21G** [?]. **3-540-57801-3** [?]. **3-540-57962-1** [?]. **3-540-58703-9** [?]. **3-Aminopropionamide** [?]. **3-calculated** [?]. **3-center** [?]. **3-di-** [?]. **3-dialkylnitroxybenzenes** [?]. **3-Didehydroproline** [?]. **3-dienes** [?]. **3-Diketopiperazine** [?]. **3-Dimensional** [?]. **3-dimethylimidazol-2-ylidene** [?]. **3-Dimethyluracil** [?]. **3-Dipolar** [?]. **3-Isothiazolones** [?]. **3-j** [?]. **3-methyl** [?]. **3-pyridinecarboxylic** [?]. **3-Pyridyl-** [?]. **3-substituted** [?]. **3-Triazole** [?]. **31G** [?, ?]. **330** [?]. **3d** [?, ?, ?]. **3p** [?]. **3prime** [?]. **3S** [?].

4 [?, ?, ?]. **4-** [?]. **4-31G** [?]. **4-aminobutanol** [?]. **4-chloro-indole-3-acetic** [?]. **4-Currents** [?]. **4-dihydropyridines** [?]. **4-Diphenylpentane** [?]. **4-Nitro-1** [?]. **4-phenylene** [?]. **4-trioxane** [?]. **4.2** [?]. **45.00** [?]. **48** [?]. **4CuCl** [?]. **4d** [?]. **4th** [?, ?].

5 [?, ?, ?, ?]. **5-** [?]. **5-C** [?, ?]. **5-Contracted** [?]. **5-Fluorouracil** [?]. **5-hexatriene** [?]. **5-HT** [?]. **5-lipoxygenase** [?]. **5-Me** [?]. **5-tetranitroimidazole** [?]. **5-trinitroimidazole** [?]. **55A** [?].

6 [?, ?]. **6-31** [?, ?]. **6-31G** [?]. **6-benzyl** [?]. **6-dihydronicotinic** [?]. **6-Dimethoxy-1** [?]. **6-furfuryl** [?]. **6-j** [?]. **6-thioguanine** [?]. **60th** [?].

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** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Al-doped** [?]. **alanine** [?]. **Alberte** [?]. **Alcohol** [?, ?, ?, ?, ?]. **Alcohols** [?, ?]. **alcoholysis** [?]. **Aldehyde** [?]. **Aldehydic** [?]. **Alder** [?, ?, ?]. **Algebra** [?, ?, ?, ?, ?, ?]. **Algebraic** [?, ?]. **Algebrants** [?, ?, ?]. **Algorithm** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Algorithmic** [?]. **Algorithms** [?, ?, ?, ?, ?, ?, ?, ?]. **AlH** [?, ?]. **alignment** [?]. **aliphatic** [?, ?]. **Alkali** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Alkali-Doped** [?, ?]. **alkali-earth** [?]. **Alkaline** [?, ?, ?, ?, ?, ?, ?, ?]. **Alkaline-Earth** [?]. **Alkaline-Earth-Intercalated** [?]. **alkaloids** [?]. **Alkane** [?, ?]. **Alkanes** [?, ?, ?, ?]. **Alkenes** [?]. **alkenylfurans** [?]. **Alkoxo** [?]. **Alkoxo-Bridged** [?]. **Alkyl** [?]. **alkylating** [?, ?]. **Alkylation** [?]. **Alkylidenes** [?]. **Alkylperoxyl** [?]. **Alkynes** [?]. **All-** [?]. **All-Electron** [?, ?, ?, ?, ?]. **All-trans** [?, ?, ?]. **All-Valence** [?, ?]. **Allene** [?]. **Allinger** [?]. **allotropic** [?]. **Allowed** [?]. **alloy** [?, ?, ?]. **Alloys** [?, ?, ?]. **Allyl** [?, ?, ?]. **allyl-nickel** [?]. **Allylic** [?, ?]. **almost** [?]. **AlO** [?]. **Along** [?, ?, ?, ?, ?, ?, ?]. **alpha** [?, ?, ?, ?]. **alpha-Aminoisobutyric** [?]. **alpha-function** [?]. **alpha-particles** [?]. **Alternant** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Alternating** [?]. **Alternation** [?, ?, ?, ?, ?]. **Alternative** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Altmann** [?]. **Alumina** [?, ?]. **Aluminum** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **AM** [?, ?, ?]. **AM1** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **AM1-based** [?]. **am7** [?]. **America** [?]. **American** [?]. **Amides** [?, ?, ?]. **Amine** [?]. **Amino** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Amino-Nitro** [?]. **Aminoalkylation** [?]. **aminobutanol** [?]. **aminobutyric** [?]. **Aminoethanethiol** [?]. **Aminoethanol** [?]. **aminohexanoic** [?]. **aminoimidazole** [?]. **Aminoisobutyric** [?]. **aminopentane** [?]. **aminophenyl** [?]. **Aminopropionamide** [?]. **Ammonia** [?, ?, ?, ?, ?]. **AMO** [?]. **Among** [?, ?, ?, ?]. **Amorphous** [?, ?, ?]. **Amphipathic** [?]. **Amplitude** [?, ?]. **Amplitudes** [?, ?, ?]. **Amsterdam** [?, ?]. **Analgesic** [?, ?]. **analog** [?]. **analogous** [?]. **Analogs** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **analogues** [?, ?]. **Analyses** [?, ?, ?]. **Analysis** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Anomalous [?, ?]. **anomeric** [?]. **Ansatz** [?, ?]. **ansätze** [?]. **Antagonist** [?, ?]. **Antagonists** [?, ?, ?, ?]. **Antalya** [?]. **Antarafacial** [?]. **anthracene** [?]. **anthraquinone** [?]. **anti** [?, ?]. **anti-malarial** [?]. **Antiaromaticity** [?, ?, ?]. **antibiotic** [?]. **antibiotics** [?]. **Antibound** [?]. **anticancer** [?, ?]. **Anticonvulsant** [?, ?]. **Anticonvulsivant** [?]. **antidepressant** [?]. **Antiferromagnetic** [?, ?]. **antihydrogen** [?]. **antileishmanial** [?]. **antimalarial** [?, ?]. **antioxidant** [?]. **antiparallel** [?, ?]. **Antiparallel-spin** [?]. **antisite** [?]. **Antisymmetry** [?, ?]. **Antitumor** [?, ?, ?]. **Antiviral** [?]. **Any** [?, ?]. **Aperiodic** [?, ?, ?]. **Apoenzyme** [?]. **Apomorphines** [?]. **appearing** [?]. **Applicability** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Application** [?, ?, ?, ?, ?, ?, ?, ?, ?,

Atkins [?]. **Atom**
[?, ?, ?,

[?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **behind** [?]. **being** [?]. **Beings** [?]. **BEM** [?]. **Benchmark** [?, ?, ?]. **bend** [?]. **Bending** [?, ?]. **Benoxaprofen** [?]. **Bent** [?, ?]. **Bent-bond** [?]. **benz** [?]. **Benzaldehydes** [?]. **Benzene** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Benzene-Tetracyanoethylene** [?]. **BenzeneAr** [?]. **Benzenes** [?, ?]. **Benzenoid** [?, ?, ?, ?, ?, ?]. **benzenoids** [?]. **benzo** [?, ?]. **Benzocyclobutadiene** [?]. **Benzocyclobutadienes** [?]. **Benzocyclobutenes** [?]. **benzodiazepine** [?, ?]. **benzofuran** [?]. **Benzohydroquinone** [?]. **benzoic** [?, ?]. **Benzoyloxyl** [?]. **benzyl** [?]. **benzylidene** [?]. **Benzylimidazole** [?]. **Bergman** [?]. **Berlin** [?, ?, ?, ?]. **Bernard** [?, ?]. **Berry** [?]. **Beryllium** [?, ?, ?, ?, ?, ?, ?, ?]. **Bessel** [?, ?]. **Bethe** [?, ?, ?, ?, ?]. **Between** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

borazine [?]. **borealis** [?]. **Born** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Born-von** [?]. **Boron** [?, ?, ?, ?, ?, ?, ?, ?]. **boron-like** [?]. **Boron-Nitrogen** [?]. **Boronlike** [?]. **borrowing** [?]. **Bose** [?]. **Boson** [?]. **Bosonic** [?]. **Boston** [?, ?]. **Both** [?, ?, ?, ?]. **bottlenecks** [?]. **Bound** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Boundaries** [?, ?]. **Boundary** [?, ?, ?, ?, ?, ?, ?]. **Bounded** [?]. **Bounds** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Box** [?, ?, ?, ?, ?]. **Boxes** [?, ?, ?]. **Boys** [?]. **BPh** [?]. **Br** [?]. **Bragg** [?]. **brain** [?]. **Branch** [?]. **branched** [?]. **branching** [?]. **Brandt** [?]. **Breach** [?]. **Breaking** [?, ?, ?, ?, ?, ?, ?]. **breaks** [?]. **breakthrough** [?]. **Breathing** [?]. **Breit** [?, ?, ?, ?, ?]. **Brewer** [?]. **bridge** [?]. **Bridged** [?, ?, ?, ?, ?]. **Bridges** [?]. **Brillouin** [?, ?, ?, ?, ?]. **Britain** [?]. **Broken** [?, ?, ?, ?, ?, ?, ?]. **Broken-symmetry** [?]. **bromide** [?]. **bromine** [?]. **Brownian** [?]. **Brueckner** [?, ?, ?, ?, ?, ?, ?]. **Brueckner-Coupled-Cluster** [?]. **BSSE** [?, ?, ?, ?, ?, ?, ?]. **BSSE-Free** [?, ?, ?, ?, ?]. **buckminsterfullerene** [?, ?, ?]. **Building** [?, ?, ?, ?]. **Built** [?, ?, ?]. **Bulk** [?, ?, ?, ?]. **bupivacaine** [?]. **Butadiene** [?, ?, ?]. **Butane** [?]. **Butenolide** [?]. **Butyl** [?]. **Butylbenzene** [?]. **butylcyclopropanone** [?]. **butyrolactone** [?].

C [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?, ?]. **cancérogène** [?]. **Cannabinoid** [?, ?]. **cannabinoids** [?]. **Canonical** [?, ?, ?]. **capacities** [?]. **capacity** [?, ?]. **Capping** [?]. **Capture** [?, ?, ?, ?, ?]. **Car** [?]. **Carbanions** [?]. **Carbene** [?, ?, ?]. **Carbenes** [?, ?, ?]. **carbide** [?]. **Carbides** [?]. **Carbó** [?]. **carboanion** [?]. **carbocation** [?]. **Carbon** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **carbon-** [?]. **Carbon-Carbon** [?]. **Carbonic** [?, ?]. **Carbonyl** [?, ?, ?, ?]. **Carbonyls** [?, ?, ?, ?, ?, ?]. **Carborane** [?]. **Carborane-hydrocarbon** [?]. **Carboxyl** [?]. **Carboxylic** [?, ?]. **carbyne** [?, ?]. **carcinogen** [?]. **Carcinogens** [?]. **Cardiac** [?]. **cardiotonics** [?]. **Career** [?]. **Carlo** [?, ?]. **Carotenoids** [?]. **carriers** [?]. **Cartesian** [?, ?, ?, ?, ?, ?]. **CAS** [?, ?, ?]. **CAS-SCF** [?]. **case** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **cases** [?, ?]. **Casimir** [?, ?]. **CASMP2** [?]. **CASPT2** [?]. **CASSCF** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **CASVB** [?, ?]. **Catacondensed** [?]. **Catalysis** [?, ?, ?, ?, ?, ?]. **Catalysts** [?, ?]. **Catalytic** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **catalyzed** [?, ?, ?, ?, ?, ?]. **catastrophe** [?]. **catecholamine** [?]. **cathodic** [?]. **Cation** [?, ?, ?, ?, ?, ?, ?, ?]. **Cationic** [?, ?, ?]. **Cations** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Cauchy** [?]. **Caused** [?, ?]. **causing** [?]. **Cavities** [?, ?, ?]. **Cavity** [?]. **CBC** [?]. **CC** [?]. **CCCH** [?]. **CCD** [?, ?]. **CCSD** [?, ?, ?, ?]. **CCSDT** [?]. **CD** [?, ?, ?, ?]. **CdS** [?]. **CECAM** [?, ?]. **CECAM-NSF** [?]. **Cell** [?, ?, ?, ?, ?, ?, ?]. **Cell-Shedding** [?]. **Cells** [?, ?, ?]. **Cellular** [?, ?]. **Cellulose** [?, ?]. **Center** [?, ?]. **Centered** [?, ?, ?, ?]. **Centers** [?, ?, ?, ?]. **central** [?, ?, ?, ?]. **centricity** [?]. **Century** [?]. **CEQ** [?]. **cerium** [?]. **Certain** [?, ?, ?, ?, ?, ?, ?]. **CF** [?, ?]. **CFHH** [?, ?]. **CFPHGLF** [?]. **CG** [?]. **CGA** [?]. **CGCGTTAACGCG** [?]. **CH** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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Conjecture [?]. **conjectured** [?]. **Conjoint** [?]. **Conjugacy** [?]. **conjugate** [?]. **Conjugated** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Conjugation** [?, ?, ?, ?, ?, ?]. **Connect** [?]. **Connected** [?, ?, ?]. **Connecting** [?]. **Connection** [?, ?, ?, ?, ?, ?, ?, ?]. **Connections** [?, ?]. **Connectivity** [?]. **Conquer** [?, ?]. **Conrotatory** [?]. **conscious** [?, ?]. **Consequences** [?, ?]. **Conservation** [?]. **Consideration** [?]. **Considerations** [?, ?, ?]. **Considered** [?]. **Considering** [?]. **Consistency** [?, ?, ?]. **Consistent** [?, ?]. **Constant** [?, ?, ?, ?, ?, ?]. **Constants** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Constrained** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Constraints** [?, ?, ?, ?, ?]. **constructed** [?]. **Construction** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Contact** [?, ?]. **Containing** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Contemporary** [?]. **Content** [?, ?, ?]. **Contents** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **context** [?, ?]. **continued** [?]. **Continuous** [?, ?, ?, ?, ?, ?]. **Continuum** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Contour** [?]. **Contracted** [?, ?, ?, ?, ?, ?, ?]. **Contracting** [?]. **contraction** [?, ?]. **Contribution** [?, ?, ?, ?]. **Contributions** [?, ?]. **Control** [?, ?, ?, ?]. **Controlling** [?]. **Conventional** [?, ?]. **converged** [?]. **Convergence** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Convergent** [?]. **Conversion** [?, ?]. **Converters** [?]. **convolution** [?]. **Cooper** [?, ?]. **Cooperative** [?]. **Cooperativity** [?, ?]. **Coordinate** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **coordinated** [?]. **Coordinates** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Coordination** [?, ?, ?]. **copacking** [?]. **Copenhagen** [?]. **coplanar** [?]. **copolymers** [?]. **Copper** [?, ?, ?, ?, ?, ?, ?]. **Core** [?, ?]. **Core-Level** [?, ?]. **core-optimized** [?]. **Core-Valency** [?]. **Coriolis** [?, ?]. **Coronene** [?]. **Coronene-Coronene** [?]. **Correct** [?, ?]. **Corrected** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Correction** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Corrections** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Correctly** [?]. **corrector** [?]. **Correlated** [?, ?]. **Correlation** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Coulomb-Hole [?]. **Coulomb-Hole-Hartree** [?]. **Coulombic** [?, ?]. **Count** [?, ?]. **counterexample** [?]. **Counterion** [?, ?]. **counterions** [?]. **Counterpoise** [?, ?]. **Coupled** [?, ?, ?,

dC [?]. **DCl** [?]. **DCNQI** [?]. **DCS** [?, ?, ?, ?]. **deactivation** [?]. **deacylation** [?]. **deaminations** [?]. **deaminoarginine** [?]. **Debye** [?]. **decane** [?]. **Decarboxylation** [?, ?]. **Decay** [?, ?, ?, ?, ?]. **Decomplexation** [?]. **Decomposition** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Decompositions** [?, ?]. **decoupled** [?, ?]. **Decoupling** [?]. **decsilane** [?]. **Dedication** [?]. **Deduced** [?, ?, ?]. **Deep** [?]. **Defect** [?, ?, ?, ?]. **Defects** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Deficiency** [?]. **Define** [?]. **Defined** [?]. **defining** [?]. **Definite** [?, ?]. **Definition** [?, ?, ?, ?, ?]. **Deformation** [?]. **Deformations** [?]. **deformed** [?]. **Defranceschi** [?, ?]. **Degeneracy** [?]. **Degenerate** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **degenerated** [?]. **degree** [?]. **Degrees** [?]. **Dehydration** [?]. **dehydroalanine** [?]. **Dehydrogenase** [?, ?, ?, ?]. **del** [?]. **del-operator** [?]. **Delayed** [?]. **Delhalle** [?]. **Delocalization** [?, ?]. **Delocalized** [?]. **delta** [?]. **delta-doped** [?]. **Deltafunction** [?]. **Denmark** [?]. **Dennis** [?]. **denominator** [?]. **dense** [?, ?, ?]. **Densities** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Descriptions [?, ?, ?, ?, ?]. **descriptor** [?]. **Descriptors** [?, ?, ?, ?, ?]. **Design** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **designing** [?, ?]. **desorption** [?]. **Destabilization** [?]. **Detachment** [?, ?]. **Detailed** [?]. **Determinantal** [?, ?, ?]. **Determinants** [?, ?, ?, ?, ?, ?]. **Determination** [?, ?]. **Determine** [?, ?, ?]. **Determined** [?, ?]. **Determining** [?, ?, ?, ?, ?]. **Detour** [?]. **developed** [?]. **Development** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Developments** [?, ?, ?, ?]. **Deviation** [?]. **devices** [?]. **Devoted** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **DEWAR** [?, ?, ?]. **DEWAR-PI** [?]. **Dexanabinol** [?]. **DF** [?]. **DFT** [?, ?]. **DFT-evaluated** [?]. **DFT-LDA** [?]. **dG** [?]. **Di-** [?]. **Diabatic** [?]. **Diacetylene** [?]. **Diagnosing** [?]. **Diagonal** [?, ?, ?]. **Diagonalization** [?, ?]. **Diagram** [?]. **Diagrammatic** [?, ?, ?, ?]. **diagrams** [?, ?]. **dialane** [?]. **dialkylnitroxybenzenes** [?]. **Diamagnetic** [?]. **Diamond** [?]. **Diamondlike** [?]. **dianthryl** [?]. **Diatomic** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Dipole-Moment [?]. **Dipole-Octupole** [?]. **Dipositronium** [?]. **Diprotonated** [?]. **dipyridyl** [?]. **Dirac** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Direct** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **directional** [?]. **Directly** [?, ?]. **Dirichlet** [?, ?]. **discovery** [?]. **Discrete** [?, ?, ?, ?, ?, ?, ?]. **discretized** [?]. **Discrimination** [?]. **disk** [?]. **Diskette** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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?, ?]. **Electronic-phase** [?, ?]. **electronically** [?]. **electronics** [?, ?, ?, ?]. **Electrons** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Electrons-in-a-Box** [?]. **Electrophilic** [?, ?, ?, ?, ?, ?]. **electropolymerization** [?]. **Electrostatic** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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[?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **failure** [?]. **famous** [?]. **Faraday** [?]. **Fast** [?, ?, ?, ?]. **fate** [?]. **fatty** [?]. **Favorable** [?]. **FCP** [?, ?]. **Fe** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Fe-Al** [?]. **Fe-His** [?]. **feasibility** [?]. **features** [?]. **FeCO** [?]. **feedback** [?]. **Feenberg** [?]. **Fellows** [?]. **Femtosecond** [?, ?]. **FeN** [?]. **Ferguson** [?]. **Fermi** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Fermi-Edge** [?]. **fermion** [?, ?, ?]. **Ferredoxin** [?]. **ferrocene** [?]. **ferromagnets** [?]. **Feshbach** [?, ?]. **Few** [?, ?, ?, ?, ?, ?]. **Few-Body** [?, ?]. **few-electron** [?]. **Feynman** [?, ?, ?, ?]. **FF** [?, ?]. **FFT** [?]. **FH** [?]. **fibered** [?]. **Fibonacci** [?]. **Field** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?]. **Forming** [?, ?]. **Formosinho** [?]. **Forms** [?, ?, ?, ?]. **Formula** [?, ?, ?, ?, ?, ?, ?, ?]. **formulae** [?]. **Formulas** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Formulation** [?, ?]. **formulations** [?, ?]. **Formyloxyl** [?]. **Förner** [?]. **Forward** [?]. **Foundation** [?, ?]. **Foundations** [?, ?, ?, ?]. **Four** [?, ?, ?, ?, ?, ?, ?, ?]. **Four-Body** [?, ?]. **four-center** [?, ?]. **Four-Membered** [?]. **Fourier** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Fourth** [?, ?, ?]. **Fourth-Order** [?]. **FPLMTO** [?]. **Fr** [?]. **Fractal** [?, ?, ?]. **Fractals** [?]. **fraction** [?]. **Fractional** [?, ?, ?, ?]. **Fractionally** [?, ?]. **Fragment** [?, ?, ?, ?, ?, ?, ?, ?]. **Fragment-Based** [?, ?]. **Fragmentation** [?, ?, ?, ?, ?]. **Fragments** [?, ?, ?, ?]. **Frames** [?]. **Framework** [?, ?, ?, ?, ?, ?, ?]. **Frameworks** [?]. **France** [?]. **Franck** [?, ?, ?, ?, ?, ?, ?, ?]. **Frank** [?, ?]. **Free** [?, ?]. **free-base** [?]. **Free-Energy** [?]. **Free-Radical** [?]. **Freedom** [?]. **Freeman** [?]. **Freeon** [?, ?, ?, ?]. **Frequencies** [?, ?]. **Frequency** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Frequency-Dependent** [?, ?, ?, ?, ?, ?, ?]. **Frictional** [?]. **Friedel** [?]. **Friedrichs** [?]. **Friend** [?]. **Frohlich** [?, ?]. **frontier** [?, ?, ?]. **Frontiers** [?, ?, ?]. **Frost** [?]. **Frozen** [?, ?, ?, ?]. **Frozen-Core** [?, ?]. **FSGO** [?]. **Fukui** [?, ?, ?]. **Fukutome** [?]. **Full** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Full-CI** [?]. **Full-Electron** [?]. **Full-Potential** [?, ?]. **Fullerene** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **fullerene-related** [?]. **Fullerenes** [?, ?, ?, ?, ?, ?]. **fullerides** [?, ?]. **Fullerites** [?]. **Fully** [?, ?, ?, ?, ?]. **Function** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

functions [?, ?, ?,

GROMOS [?]. **GROMOS-MD** [?]. **groove** [?]. **groove-binding** [?]. **Ground** [?, ?, ?,

heteroanalogs [?]. **heteroaromatic** [?]. **heteroatom** [?]. **Heterocumulenes** [?]. **Heterocycle** [?]. **Heterocycles** [?]. **heterocyclic** [?]. **heterofullerene** [?]. **Heterogeneous** [?, ?, ?, ?]. **Heteronuclear** [?, ?]. **Heterosiliranes** [?]. **Heterosubstituted** [?]. **heuristic** [?]. **Hexagonal** [?, ?, ?]. **Hexamers** [?]. **hexanuclear** [?]. **Hexatriene** [?, ?]. **hexyl** [?]. **HF** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Hg** [?]. **HgC** [?]. **HgO** [?]. **HH** [?]. **HH-GLF** [?]. **HI** [?, ?]. **Hierarchical** [?, ?]. **Hierarchies** [?]. **Hierarchy** [?]. **High** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?, ?, ?, ?, ?]. **Hypermodified** [?, ?, ?]. **Hyperpolarizabilities** [?, ?]. **Hyperpolarizability** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **hyperradius** [?]. **Hyperspherical** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Hypersurface** [?, ?, ?]. **hypersurfaces** [?]. **hypervalence** [?]. **Hypervalent** [?, ?]. **hypervelocity** [?]. **Hypervirial** [?]. **hypothesis** [?]. **HZSM** [?].

Iachello [?]. **IBM** [?]. **Ice** [?, ?]. **Icons** [?, ?]. **Icosahedral** [?, ?]. **Idazoxan** [?]. **Idea** [?]. **Ideal** [?, ?, ?]. **idempotency** [?]. **Identical** [?]. **identify** [?, ?]. **Identifying** [?]. **Ih** [?]. **II** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?, ?, ?,

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L [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **L-KALA** [?]. **L-Proline** [?]. **Labarthe** [?]. **Labeled** [?]. **Lability** [?]. **LaC** [?]. **Lack** [?]. **LACO** [?]. **Ladder** [?, ?, ?, ?]. **LADH** [?]. **Ladik** [?]. **lag** [?]. **Lagrange** [?, ?, ?]. **Lagrangian** [?]. **Lagrangians** [?]. **Laguerre** [?, ?, ?, ?]. **Lamb** [?]. **lamella** [?]. **Lanczos** [?, ?]. **Landau** [?]. **Landscapes** [?, ?]. **Langevin** [?]. **Langhoff** [?]. **Language** [?, ?]. **Lanthanide** [?, ?, ?, ?, ?, ?]. **LaO** [?]. **LAP** [?]. **Laplace** [?]. **Laplacian** [?]. **LAPW** [?]. **Large** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

local-density [?, ?, ?]. **Local-Exchange** [?]. **Local-Scaling** [?, ?, ?, ?, ?, ?, ?, ?]. **local-spin-density** [?]. **Locality** [?, ?]. **Localization** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Localization-Consistent** [?]. **Localized** [?, ?]. **locally** [?, ?, ?]. **Locate** [?]. **Located** [?]. **locations** [?]. **logarithm** [?]. **logarithmic** [?]. **Logic** [?]. **Logical** [?]. **London** [?, ?, ?, ?]. **Lone** [?, ?]. **Long** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Long-** [?]. **Long-Range** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Longitudinal** [?, ?]. **Look** [?, ?]. **Looking** [?]. **loop** [?]. **loop-to-edge** [?]. **LORG** [?]. **Louis** [?, ?]. **Low** [?, ?]. **Low-Dimensional** [?, ?]. **Low-energy** [?, ?, ?]. **Low-Gap** [?]. **Low-Lying** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **low-molecular-weight** [?]. **Low-Order** [?, ?]. **low-Rydberg** [?]. **Low-Spin** [?, ?]. **Low-Temperature** [?]. **Low-Wave-Number** [?]. **Löwdin** [?, ?]. **Lower** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Lower-Bound** [?, ?]. **Lower-Lying** [?]. **Lowest** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Lr** [?]. **LSD** [?, ?, ?, ?, ?, ?, ?]. **LSD-CGA** [?]. **Ltd** [?, ?]. **LTP** [?]. **Lu** [?]. **Lucas** [?]. **Ludeña** [?]. **Lund** [?]. **Lyapunov** [?]. **Lying** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Masthead [?, ?, ?,

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N [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Nonconventional [?]. **noncorrosive** [?]. **noncovalent** [?]. **nondegenerate** [?]. **nondisjoint** [?]. **Nonempirical** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Nonequilibrium** [?, ?, ?, ?]. **Noninteger** [?]. **Nonintegrable** [?]. **Noninteracting** [?, ?]. **Noniterative** [?]. **Nonlinear** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

ONOO [?]. **ONOOH** [?]. **Onset** [?]. **Open**
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[?, ?].
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Oxohydride [?]. **Oxygen** [?, ?]. **Ozone** [?, ?, ?, ?].

P [?, ?]. **p-phenylenevinylene** [?, ?]. **P450** [?, ?, ?]. **P450cam** [?]. **Package** [?]. **packet** [?, ?, ?]. **packets** [?]. **Packing** [?]. **Padé** [?, ?, ?, ?, ?]. **Padé-Type** [?]. **PAF** [?, ?]. **page** [?]. **pages** [?, ?, ?, ?]. **PAH** [?]. **Pair** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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Present-Day [?]. **Press** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Press/Gordon** [?]. **Pressure** [?, ?]. **Pressure-Induced** [?]. **Price** [?]. **Primary** [?, ?]. **Principal** [?]. **Principle** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Principles** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **prism** [?]. **Pro** [?]. **Probabilities** [?, ?, ?, ?]. **Probability** [?]. **Probed** [?]. **Probes** [?, ?, ?, ?]. **Problem** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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[?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **requirement** [?]. **requirements** [?, ?, ?, ?]. **Requisites** [?]. **Research** [?, ?, ?, ?, ?, ?]. **Resemblance** [?, ?]. **Reservoir** [?]. **Residue** [?, ?, ?]. **Residues** [?, ?]. **Resistance** [?, ?, ?]. **Resolution** [?, ?, ?, ?, ?, ?, ?, ?]. **Resolutions** [?]. **Resolved** [?, ?, ?, ?, ?, ?]. **Resonance** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Resonance-Stabilized** [?]. **Resonances** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Resonant** [?]. **respect** [?]. **Response** [?, ?]. **restraining** [?]. **Restricted** [?, ?, ?, ?, ?, ?, ?, ?]. **Restrictions** [?, ?]. **Results** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **retards** [?, ?]. **Retrospective** [?]. **Returning** [?]. **revealed** [?, ?]. **Reversal** [?, ?]. **Reverse** [?, ?]. **reversed** [?]. **Reversible** [?, ?, ?]. **Review** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Scaling-Nesting [?]. **scanning** [?, ?, ?, ?]. **scattered** [?]. **Scattering** [?, ?, ?,

[?, ?]. **Serine** [?, ?, ?, ?]. **session** [?]. **Set** [?, ?]. **Sets** [?, ?]. **settings** [?]. **seven** [?]. **seven-component** [?]. **Several** [?, ?, ?, ?]. **Sextet** [?]. **SGA** [?]. **SH** [?, ?, ?, ?]. **Shake** [?, ?, ?, ?]. **Shake-Up** [?, ?, ?]. **Shakeup** [?, ?]. **Shallow** [?, ?]. **Sham** [?, ?]. **Shannon** [?, ?]. **Shape** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Shaped** [?, ?, ?]. **Shapes** [?, ?, ?]. **Sharing** [?]. **Shedding** [?]. **sheets** [?]. **Shell** [?, ?]. **shell-structure** [?]. **Shells** [?, ?]. **Shepard** [?]. **Shepard-Type** [?]. **Shevelko** [?, ?]. **Shielding** [?, ?, ?, ?, ?, ?, ?, ?]. **Shift** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Shifting** [?, ?]. **Shifts** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Shiotani** [?]. **Shock** [?, ?]. **shocked** [?]. **Shopping** [?]. **Short** [?, ?, ?]. **Short-Range** [?, ?]. **SI** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Si-** [?]. **SIC** [?, ?]. **Side** [?, ?, ?, ?, ?, ?]. **Side-Chain** [?]. **Side-Group** [?]. **Siegert** [?]. **Siegmund** [?]. **SiGeH** [?]. **Sighted** [?]. **Sign** [?, ?]. **signal** [?]. **Signed** [?]. **significance** [?]. **Significant** [?]. **Signs** [?]. **SIH** [?, ?, ?]. **silacarbonyl** [?]. **silagermylyne** [?]. **Silatranes** [?]. **Silica** [?]. **Silicon** [?, ?]. **silicon-based** [?]. **Silole** [?]. **Silver** [?]. **Silverman** [?]. **Similar** [?]. **Similarity** [?, ?]. **Simon** [?]. **Simple** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

size-extensive [?]. **Sketch** [?, ?]. **Slater** [?, ?, ?,

[?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Spin-averaged** [?]. **Spin-Catalysis** [?]. **Spin-Coupled** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Spin-Dependent** [?]. **spin-extended** [?]. **Spin-Free** [?, ?, ?]. **Spin-Independent** [?]. **Spin-Mediated** [?]. **Spin-multiplet** [?]. **Spin-Orbit** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Spin-Paired** [?]. **Spin-Polarized** [?, ?, ?, ?]. **Spin-Projected** [?]. **Spin-Spin** [?, ?]. **Spin-Unrestricted** [?, ?]. **spinel** [?]. **spinless** [?]. **Spiral** [?, ?]. **spiro** [?]. **spirochromics** [?]. **spironaphthoxazines** [?]. **Spline** [?, ?, ?]. **split** [?]. **Splitting** [?, ?, ?, ?, ?, ?, ?, ?]. **Splittings** [?]. **sponsored** [?]. **Spontaneous** [?]. **spontaneously** [?]. **spore** [?]. **Springer** [?, ?, ?, ?, ?, ?, ?]. **Springer-Verlag** [?, ?, ?, ?, ?, ?]. **Square** [?, ?, ?]. **Square-Cell** [?, ?]. **Square-Pyramidal** [?]. **Squared** [?]. **Squares** [?, ?]. **Squeezed** [?, ?, ?]. **Squeezing** [?]. **SSCH** [?]. **SSH** [?]. **ST** [?]. **Stabilities** [?, ?]. **Stability** [?, ?]. **Stabilization** [?, ?, ?, ?, ?]. **Stabilized** [?, ?, ?, ?]. **Stabilizing** [?]. **Stable** [?, ?, ?, ?, ?, ?, ?, ?]. **stack** [?, ?]. **stacked** [?]. **Stacking** [?]. **Stages** [?, ?]. **staggered** [?]. **Standard** [?, ?, ?, ?, ?, ?, ?]. **Stands** [?]. **Stark** [?, ?]. **starting** [?]. **State** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

Structural [?, ?]. **Structure** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

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target [?]. **Targeted** [?]. **Targets** [?]. **Tautomeric** [?, ?]. **Tautomerism** [?, ?, ?, ?, ?, ?]. **Tautomerization** [?, ?, ?]. **Tautomers** [?, ?, ?, ?]. **Taylor** [?]. **TB** [?]. **TB-LMTO** [?]. **TCNQ** [?]. **td** [?]. **TDHF** [?]. **Te** [?]. **Teacher** [?]. **Technique** [?, ?, ?, ?, ?, ?, ?, ?]. **Techniques** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Technology** [?]. **TeCl** [?]. **Teller** [?, ?, ?, ?, ?, ?, ?, ?, ?]. **Temperature** [?, ?, ?, ?, ?, ?]. **Temperature-induced** [?]. **Temperatures** [?]. **template** [?]. **Temporal** [?, ?]. **tendencies** [?]. **Tennyson** [?]. **Tensor** [?, ?, ?, ?, ?]. **Tensorial** [?, ?, ?, ?]. **Tensors** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **tentative** [?, ?]. **teratogenicity** [?]. **term** [?, ?]. **Terminal** [?]. **Terms** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **tert}** [?]. **tert}-butylcyclopropanone** [?]. **Tesla** [?]. **Test** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Testimony** [?]. **Testing** [?, ?]. **Testosterone** [?]. **tests** [?, ?]. **tetracaine** [?]. **tetrachlorodibenzo** [?]. **Tetrachloromethane** [?]. **Tetracyanoethylene** [?]. **Tetrafluoride** [?]. **Tetrafluorobenzene** [?]. **tetrahedral** [?]. **tetrahedrane** [?]. **Tetrahydrocannabinols** [?]. **Tetrahydrofuran** [?]. **Tetrakis** [?]. **tetrameter** [?]. **tetramethylene** [?]. **tetranitroimidazole** [?]. **tetrapeptide** [?]. **Tetrasilane** [?]. **Tetratomic** [?]. **tetrazine** [?]. **tetrazole** [?]. **TG** [?]. **théaories** [?, ?]. **Theinyl** [?]. **Theinyl-Imino** [?]. **Their** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

theory [?, ?, ?,

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Understanding [?, ?, ?, ?, ?, ?]. **Unexpected** [?]. **unfolded** [?]. **unfolding** [?]. **Uniaxial** [?]. **Unification** [?]. **Unified** [?, ?, ?]. **uniformly** [?, ?]. **Unimolecular** [?, ?, ?, ?]. **Union** [?]. **Unique** [?]. **Uniqueness** [?, ?, ?, ?, ?, ?]. **Unit** [?, ?]. **Unitary** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Unitary-group-based** [?]. **Units** [?, ?, ?, ?]. **Universal** [?, ?, ?, ?, ?, ?, ?, ?]. **University** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **unknown** [?]. **unlike** [?]. **unrelaxed** [?]. **Unrestricted** [?, ?, ?, ?]. **Unsaturated** [?, ?, ?, ?]. **unstable** [?]. **until** [?]. **unusual** [?, ?]. **upon** [?, ?, ?, ?]. **Upper** [?, ?, ?, ?, ?, ?, ?, ?]. **Upper-** [?]. **UPt** [?]. **Uracil** [?, ?, ?]. **uranium** [?, ?]. **Urea** [?, ?]. **Urea-Nitrate** [?]. **urocanic** [?]. **Use** [?, ?]. **Used** [?, ?, ?, ?]. **Usefulness** [?]. **Using** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?, ?, ?, ?, ?, ?, ?, ?, ?]. **Vision** [?]. **Visualization** [?, ?]. **Vitae** [?, ?, ?]. **vitro** [?]. **VO** [?]. **void** [?]. **Vol** [?, ?, ?, ?, ?, ?, ?, ?]. **voltage** [?]. **Volume** [?, ?]. **Volume-Dependent** [?]. **volumes** [?]. **Voronoi** [?]. **VPA** [?]. **VPGG** [?]. **vs** [?, ?, ?, ?, ?, ?, ?]. **VSCC** [?].

W [?, ?, ?, ?]. **Waals** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?]. **Wagging** [?]. **walk** [?]. **walking** [?]. **Walks** [?, ?]. **wall** [?]. **Walls** [?]. **Wannier** [?, ?]. **Water** [?, ?]. **Water-Assisted** [?]. **Water-Carbon** [?]. **Watson** [?, ?]. **Waugh** [?]. **Waugh-type** [?]. **Wave** [?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,

[?]. **Zinc** [?, ?]. **Zinn** [?]. **Zinn-Justin** [?]. **zippers** [?]. **Zn** [?]. **ZnO** [?, ?, ?, ?, ?]. **ZnS** [?, ?, ?]. **ZnSe** [?, ?, ?, ?]. **Zr** [?, ?, ?]. **ZrO** [?]. **ZrSiO** [?]. **Zwitterionic** [?].