

ChemEssen, Inc. 1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 | Fax: +82.2.3143.5920

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# **Chemical Big Data**

Provided By

**C**hemical **C**ompounds **D**EEP **P**ROFILING **S**ERVICES

Over 3 Trillion Data Points for More Than 1 Billion Chemical Compounds



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# **Refined Experimental Properties**

The experimental data was collected to validate the reliability of our predicted properties. Due to frequent measuring errors in the raw experimental data, we implemented a systematic refinement process involving basic analysis, statistical filtering, and similarity analysis. For more details, see <u>our refinement example</u> using the normal boiling point as a case study.

Property Name	Number of Compounds	Number of Data Points
Constant Properties		
Absolute Entropy of Ideal Gas at 298.15 K and 1 bar	1,864	1,864
Acentric Factor	1,857	1,857
Critical Compressibility Factor	1,355	1,355
Critical Pressure	3,157	3,157
Critical Temperature	2,668	2,668
Critical Volume	2,468	2,468
Dipole Moment	9,707	9,707
Electron Affinity	200	200
Enthalpy (Heat) of Formation for Ideal Gas at 298.15 K	1,960	1,960
Enthalpy (Heat) of Fusion at Melting Point	3,930	3,930
Flash Point	3,728	3,728
Gibbs Energy of Formation for Ideal Gas at 298.15 K and 1 bar	1,823	1,823
Heat (Enthalpy) of Vaporization at 298.15 K	2,875	2,875
Heat (Enthalpy) of Vaporization at Normal Boiling Point	1,210	1,210
Ionization Potential	6,079	6,079
Liquid Density at Normal Boiling Point	1,813	1,813
Liquid Molar Volume at 298.15 K	8,140	8,140



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Lower Flammability Limit Temperature	1,067	1,067
Lower Flammability Limit Volume Percent	391	391
Magnetic Susceptibility	1,205	1,205
Net Standard State Enthalpy (Heat) of Combustion at 298.15 K	2,163	2,163
Normal Boiling Point	35,489	35,489
Parachor	965	965
Polarizability	380	380
Radius of Gyration	1,367	1,367
Refractive Index	60,974	60,974
Solubility Parameter at 298.15 K	1,494	1,494
Standard State Absolute Entropy at 298.15 K and 1 bar	1,105	1,105
Standard State Enthalpy (Heat) of Formation at 298.15 K and 1 bar	3,506	3,506
Standard State Gibbs Energy of Formation at 298.15 K and 1 bar	1,170	1,170
Upper Flammability Limit Temperature	1,421	1,421
Upper Flammability Limit Volume Percent	972	972
Melting Point	3,583	3,583
LogP (Octanol-Water Partition Coefficient)	29,199	29,199
LogS (Water Solubility)	7,443	7,443
Temperature Dependent Properties		
Heat Capacity of Ideal Gas	1,105	19,353
Heat Capacity of Liquid	919	17,093
Heat of Vaporization	1,371	35,941
Liquid Density	2,770	19,686
Second Virial Coefficient	485	14,829
Surface Tension	1,195	11,984
Thermal Conductivity of Gas	889	8,936
Thermal Conductivity of Liquid	1,480	18,084





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Vapor Pressure of Liquid	2,939	41,257
Viscosity of Gas	1,256	12,557
Viscosity of Liquid	1,841	30,367

# **Reliability-Proven Predicted Properties**

The property data listed below is produced using our proprietary technology, backed by 41 patents, and has been validated to demonstrate proven reliability. The compounds, composed of C, H, N, O, S, F, Cl, Br, I, Si, P, and/or As, span a wide range of structures and compositions.

View Our Technology | View Reliability

Property Name	Number of Compounds	Average Accuracy(%)*
Absolute Entropy of Ideal Gas at 298.15 K and 1 bar	1+ Billion	98.67%
Acentric Factor	1+ Billion	94.45%
Critical Compressibility Factor	1+ Billion	91.70%
Critical Pressure	1+ Billion	93.00%
Critical Temperature	1+ Billion	97.14%
Critical Volume	1+ Billion	97.15%
Enthalpy (Heat) of Formation for Ideal Gas at 298.15 K	1+ Billion	90.15%
Flash Point	1+ Billion	99.94%
Heat (Enthalpy) of Vaporization at 298.15 K	1+ Billion	78.44%
Heat (Enthalpy) of Vaporization at Normal Boiling Point	1+ Billion	97.31%
Liquid Density at Normal Boiling Point	1+ Billion	98.92%



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Liquid Molar Volume at 298.15 K	1+ Billion	94.82%
LogS (Water Solubility)	1+ Billion	86.61%
Lower Flammability Limit Temperature	1+ Billion	98.92%
Lower Flammability Limit Volume Percent	1+ Billion	66.33%
Magnetic Susceptibility	1+ Billion	85.64%
Net Standard State Enthalpy (Heat) of Combustion at 298.15 K	1+ Billion	86.94%
Normal Boiling Point	1+ Billion	99.69%
Melting Point	1+ Billion	83.08%
Parachor	1+ Billion	94.41%
Polarizability	1+ Billion	84.13%
Refractive Index	1+ Billion	84.11%
Solubility Parameter at 298.15 K	1+ Billion	98.94%
Standard State Absolute Entropy at 298.15 K and 1 bar	1+ Billion	94.52%
Standard State Enthalpy (Heat) of Formation at 298.15 K and 1 bar	1+ Billion	79.53%
Upper Flammability Limit Temperature	1+ Billion	96.66%
Upper Flammability Limit Volume Percent	1+ Billion	92.96%

## **Molecular Structure and Identifier**

We offer molecular structures and identifiers as listed below. The optimized 3D structures are produced using a quantum chemical process. We perform conformer analysis to select the lowest energy structure, followed by geometry optimization with the DFT-B3LYP functional and 6-31G basis set. All optimized structures are verified to ensure the absence of imaginary frequencies.



C h e m E s s e n , l n c .

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Structure & Identifier	Number of Compounds
3D Structure Data (Mol) File	1+ Billion
2D Structure Data (Mol) File	1+ Billion
SMILES String	1+ Billion
InChl	1+ Billion
InChlKey	1+ Billion

# **Molecular Descriptors**

We offer over 3,000 2-dimensional molecular descriptors for more than 1 billion compounds, organized into 20 distinct categories, providing detailed insights into molecular behavior for AI-driven research.

#### ► Constitutional Descriptors (43)

	<b>Constitutional Descriptors</b>	Number of Compounds
1.	Molecular Weight	1+ Billion
2.	Average Molecular Weight	1+ Billion
3.	Sum of Atomic van der Waals Volumes (Scaled on Carbon Atom)	1+ Billion
4.	Sum of Atomic Sanderson Electronegativities (Scaled on Carbon Atom)	1+ Billion
5.	Sum of Atomic Polarizabilities (Scaled on Carbon Atom)	1+ Billion



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6.	Sum of First Ionization Potentials (Scaled on Carbon Atom)	1+ Billion
7.	Mean Atomic van der Waals Volume (Scaled on Carbon Atom)	1+ Billion
8.	Mean Atomic Sanderson Electronegativity (Scaled on Carbon Atom)	1+ Billion
9.	Mean Atomic Polarizability (Scaled on Carbon Atom)	1+ Billion
10.	Mean First Ionization Potential (Scaled on Carbon Atom)	1+ Billion
11.	Number of Atoms	1+ Billion
12.	Number of Non-H Atoms	1+ Billion
13.	Number of Bonds	1+ Billion
14.	Number of Non-H Bonds	1+ Billion
15.	Number of Multiple Bonds	1+ Billion
16.	Sum of Conventional Bond Orders (H-Depleted)	1+ Billion
17.	Number of Rotatable Bonds	1+ Billion
18.	Rotatable Bond Fraction	1+ Billion
19.	Number of Double Bonds	1+ Billion
20.	Number of Triple Bonds	1+ Billion
21.	Number of Aromatic Bonds	1+ Billion
22.	Number of Hydrogen Atoms	1+ Billion
23.	Number of Carbon Atoms	1+ Billion
24.	Number of Nitrogen Atoms	1+ Billion
25.	Number of Oxygen Atoms	1+ Billion
26.	Number of Phosphorous Atoms	1+ Billion
27.	Number of Sulfur Atoms	1+ Billion
28.	Number of Fluorine Atoms	1+ Billion
29.	Number of Chlorine Atoms	1+ Billion
30.	Number of Bromine Atoms	1+ Billion
31.	Number of lodine Atoms	1+ Billion



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32.	Number of Boron Atoms	1+ Billion
33.	Number of Heavy Atoms	1+ Billion
34.	Number of Heteroatoms	1+ Billion
35.	Number of Halogen Atoms	1+ Billion
36.	Percentage of H Atoms	1+ Billion
37.	Percentage of C Atoms	1+ Billion
38.	Percentage of N Atoms	1+ Billion
39.	Percentage of O Atoms	1+ Billion
40.	Percentage of Halogen Atoms	1+ Billion
41.	Number of sp3 Hybridized Carbon Atoms	1+ Billion
42.	Number of sp2 Hybridized Carbon Atoms	1+ Billion
43.	Number of sp Hybridized Carbon Atoms	1+ Billion

## ▶ Ring Descriptors (32)

	<b>Ring Descriptors</b>	Number of Compounds
1.	Number of Rings (Cyclomatic Number)	1+ Billion
2.	Number of Circuits	1+ Billion
3.	Total Ring Size	1+ Billion
4.	Ring Perimeter	1+ Billion
5.	Ring Bridge Count	1+ Billion
6.	Molecular Cyclized Degree	1+ Billion
7.	Ring Fusion Density	1+ Billion
8.	Ring Complexity Index	1+ Billion
9.	Number of Ring Systems	1+ Billion



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10.	Normalized Number of Ring Systems	1+ Billion
11.	Number of 3-Membered Rings	1+ Billion
12.	Number of 4-Membered Rings	1+ Billion
13.	Number of 5-Membered Rings	1+ Billion
14.	Number of 6-Membered Rings	1+ Billion
15.	Number of 7-Membered Rings	1+ Billion
16.	Number of 8-Membered Rings	1+ Billion
17.	Number of 9-Membered Rings	1+ Billion
18.	Number of 10-Membered Rings	1+ Billion
19.	Number of 11-Membered Rings	1+ Billion
20.	Number of 12-Membered Rings	1+ Billion
21.	Number of Benzene-Like Rings	1+ Billion
22.	Aromatic Ratio	1+ Billion
23.	Distance/Detour Ring Index of Order 3	1+ Billion
24.	Distance/Detour Ring Index of Order 4	1+ Billion
25.	Distance/Detour Ring Index of Order 5	1+ Billion
26.	Distance/Detour Ring Index of Order 6	1+ Billion
27.	Distance/Detour Ring Index of Order 7	1+ Billion
28.	Distance/Detour Ring Index of Order 8	1+ Billion
29.	Distance/Detour Ring Index of Order 9	1+ Billion
30.	Distance/Detour Ring Index of Order 10	1+ Billion
31.	Distance/Detour Ring Index of Order 11	1+ Billion
32.	Distance/Detour Ring Index of Order 12	1+ Billion

## ► Topological Descriptors (75)



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	Topological Descriptors	Number of Compounds
1.	First Zagreb Index	1+ Billion
2.	First Zagreb Index by Valence Vertex Degrees	1+ Billion
3.	First Zagreb Index by Kupchik Vertex Degrees	1+ Billion
4.	First Zagreb Index by Madan Vertex Degrees	1+ Billion
5.	First Zagreb Index by Perturbation Vertex Degrees	1+ Billion
6.	First Zagreb Index by Multiplicative Perturbation Vertex Degrees	1+ Billion
7.	Second Zagreb Index	1+ Billion
8.	Second Zagreb Index by Valence Vertex Degrees	1+ Billion
9.	Second Zagreb Index by Kupchik Vertex Degrees	1+ Billion
10.	Second Zagreb Index by Madan Vertex Degrees	1+ Billion
11.	Second Zagreb Index by Perturbation Vertex Degrees	1+ Billion
12.	Second Zagreb Index by Multiplicative Perturbation Vertex Degrees	1+ Billion
13.	Overall Modified Zagreb Index of Order 0	1+ Billion
14.	Overall Modified Zagreb Index of Order 0 by Valence Vertex Degrees	1+ Billion
15.	Overall Modified Zagreb Index of Order 1	1+ Billion
16.	Overall Modified Zagreb Index of Order 1 by Valence Vertex Degrees	1+ Billion
17.	Quadratic Index	1+ Billion
18.	Bertz Branching Index	1+ Billion
19.	Dragon Branching Index	1+ Billion
20.	Narumi Simple Topological Index (Log Function)	1+ Billion
21.	Narumi Harmonic Topological Index	1+ Billion
22.	Narumi Geometric Topological Index	1+ Billion
23.	Total Structure Connectivity Index	1+ Billion
24.	Pogliani Index	1+ Billion



Ramification Index	1+ Billion
Kier Benzene-Likeliness Index	1+ Billion
Polarity Number	1+ Billion
-	1+ Billion
Mean Square Distance Index (Balaban)	1+ Billion
Superpendentic Index	1+ Billion
2D Petitjean Shape Index	1+ Billion
Eccentricity	1+ Billion
Average Eccentricity	1+ Billion
Eccentric	1+ Billion
Mean Distance Degree Deviation	1+ Billion
Unipolarity	1+ Billion
Centralization	1+ Billion
Variation	1+ Billion
Radial Centric Information Index	1+ Billion
Schultz Molecular Topological Index (MTI)	1+ Billion
Schultz Molecular Topological Index by Valence Vertex Degrees	1+ Billion
Gutman Molecular Topological Index	1+ Billion
Gutman Molecular Topological Index by Valence Vertex Degrees	1+ Billion
Xu Index	1+ Billion
Eccentric Connectivity Index	1+ Billion
All-Path Wiener Index	1+ Billion
1-Path Kier Alpha-Modified Shape Index	1+ Billion
2-Path Kier Alpha-Modified Shape Index	1+ Billion
3-Path Kier Alpha-Modified Shape Index	1+ Billion
Kier Flexibility Index	1+ Billion
	Kier Benzene-Likeliness IndexPolarity NumberLog of Product of Row Sums (PRS)Mean Square Distance Index (Balaban)Superpendentic Index2D Petitjean Shape IndexEccentricityAverage EccentricityEccentricMean Distance Degree DeviationUnipolarityCentralizationVariationSchultz Molecular Topological Index (MTI)Schultz Molecular Topological Index by Valence Vertex DegreesGutman Molecular Topological Index by Valence Vertex DegreesXu IndexEccentric Connectivity IndexAll-Path Kier Alpha-Modified Shape Index3-Path Kier Alpha-Modified Shape Index3-Path Kier Alpha-Modified Shape Index



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51.	Path/Walk 2 - Randic Shape Index	1+ Billion
52.	Path/Walk 3 - Randic Shape Index	1+ Billion
53.	Path/Walk 4 - Randic Shape Index	1+ Billion
54.	Path/Walk 5 - Randic Shape Index	1+ Billion
55.	Maximal Electrotopological Negative Variation	1+ Billion
56.	Maximal Electrotopological Positive Variation	1+ Billion
57.	Molecular Electrotopological Variation	1+ Billion
58.	E-State Topological Parameter	1+ Billion
59.	Intrinsic State Pseudoconnectivity Index - Type S	1+ Billion
60.	Intrinsic State Pseudoconnectivity Index - Type S Average	1+ Billion
61.	Intrinsic State Pseudoconnectivity Index - Type 0	1+ Billion
62.	Intrinsic State Pseudoconnectivity Index - Type 1	1+ Billion
63.	Intrinsic State Pseudoconnectivity Index - Type T	1+ Billion
64.	Intrinsic State Pseudoconnectivity Index - Type 0d	1+ Billion
65.	Intrinsic State Pseudoconnectivity Index - Type 1d	1+ Billion
66.	Intrinsic State Pseudoconnectivity Index - Type 1s	1+ Billion
67.	Electrotopological State Pseudoconnectivity Index - Type S Average	1+ Billion
68.	Electrotopological State Pseudoconnectivity Index - Type 0	1+ Billion
69.	Electrotopological State Pseudoconnectivity Index - Type 1	1+ Billion
70.	Electrotopological State Pseudoconnectivity Index - Type T	1+ Billion
71.	Electrotopological State Pseudoconnectivity Index - Type 0d	1+ Billion
72.	Electrotopological State Pseudoconnectivity Index - Type 1d	1+ Billion
73.	Electrotopological State Pseudoconnectivity Index - Type 1s	1+ Billion
74.	Balaban Centric Index	1+ Billion
75.	Lopping Centric Index	1+ Billion





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#### Walk And Path Counts (46)

	Walk And Path Counts	Number of Compounds
1.	Molecular Walk Count of Order 1	1+ Billion
2.	Molecular Walk Count of Order 2	1+ Billion
3.	Molecular Walk Count of Order 3	1+ Billion
4.	Molecular Walk Count of Order 4	1+ Billion
5.	Molecular Walk Count of Order 5	1+ Billion
6.	Molecular Walk Count of Order 6	1+ Billion
7.	Molecular Walk Count of Order 7	1+ Billion
8.	Molecular Walk Count of Order 8	1+ Billion
9.	Molecular Walk Count of Order 9	1+ Billion
10.	Molecular Walk Count of Order 10	1+ Billion
11.	Self-Returning Walk Count of Order 2	1+ Billion
12.	Self-Returning Walk Count of Order 3	1+ Billion
13.	Self-Returning Walk Count of Order 4	1+ Billion
14.	Self-Returning Walk Count of Order 5	1+ Billion
15.	Self-Returning Walk Count of Order 6	1+ Billion
16.	Self-Returning Walk Count of Order 7	1+ Billion
17.	Self-Returning Walk Count of Order 8	1+ Billion
18.	Self-Returning Walk Count of Order 9	1+ Billion
19.	Self-Returning Walk Count of Order 10	1+ Billion
20.	Molecular Path Count of Order 1 (No. of Non-H Bonds)	1+ Billion
21.	Molecular Path Count of Order 2 (Gordon-Scantlebury Index)	1+ Billion
22.	Molecular Path Count of Order 3	1+ Billion



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23.	Molecular Path Count of Order 4	1+ Billion
24.	Molecular Path Count of Order 5	1+ Billion
25.	Molecular Path Count of Order 6	1+ Billion
26.	Molecular Path Count of Order 7	1+ Billion
27.	Molecular Path Count of Order 8	1+ Billion
28.	Molecular Path Count of Order 9	1+ Billion
29.	Molecular Path Count of Order 10	1+ Billion
30.	Molecular Multiple Path Count of Order 1	1+ Billion
31.	Molecular Multiple Path Count of Order 2	1+ Billion
32.	Molecular Multiple Path Count of Order 3	1+ Billion
33.	Molecular Multiple Path Count of Order 4	1+ Billion
34.	Molecular Multiple Path Count of Order 5	1+ Billion
35.	Molecular Multiple Path Count of Order 6	1+ Billion
36.	Molecular Multiple Path Count of Order 7	1+ Billion
37.	Molecular Multiple Path Count of Order 8	1+ Billion
38.	Molecular Multiple Path Count of Order 9	1+ Billion
39.	Molecular Multiple Path Count of Order 10	1+ Billion
40.	Total Walk Count	1+ Billion
41.	Total Path Count	1+ Billion
42.	Conventional Bond Order ID Number	1+ Billion
43.	Ratio of Multiple Path Count Over Path Count	1+ Billion
44.	Difference Between Multiple Path Count And Path Count	1+ Billion
45.	Randic ID Number	1+ Billion
46.	Balaban ID Number	1+ Billion





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#### Connectivity Indices (37)

	Connectivity Indices	Number of Compounds
1.	Connectivity Index of Order 0	1+ Billion
2.	Connectivity Index of Order 1 (Randic Connectivity Index)	1+ Billion
3.	Connectivity Index of Order 2	1+ Billion
4.	Connectivity Index of Order 3	1+ Billion
5.	Connectivity Index of Order 4	1+ Billion
6.	Connectivity Index of Order 5	1+ Billion
7.	Average Connectivity Index of Order 0	1+ Billion
8.	Average Connectivity Index of Order 1	1+ Billion
9.	Average Connectivity Index of Order 2	1+ Billion
10.	Average Connectivity Index of Order 3	1+ Billion
11.	Average Connectivity Index of Order 4	1+ Billion
12.	Average Connectivity Index of Order 5	1+ Billion
13.	Valence Connectivity Index of Order 0	1+ Billion
14.	Valence Connectivity Index of Order 1	1+ Billion
15.	Valence Connectivity Index of Order 2	1+ Billion
16.	Valence Connectivity Index of Order 3	1+ Billion
17.	Valence Connectivity Index of Order 4	1+ Billion
18.	Valence Connectivity Index of Order 5	1+ Billion
19.	Average Valence Connectivity Index of Order 0	1+ Billion
20.	Average Valence Connectivity Index of Order 1	1+ Billion
21.	Average Valence Connectivity Index of Order 2	1+ Billion
22.	Average Valence Connectivity Index of Order 3	1+ Billion

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23.	Average Valence Connectivity Index of Order 4	1+ Billion
24.	Average Valence Connectivity Index of Order 5	1+ Billion
25.	Solvation Connectivity Index of Order 0	1+ Billion
26.	Solvation Connectivity Index of Order 1	1+ Billion
27.	Solvation Connectivity Index of Order 2	1+ Billion
28.	Solvation Connectivity Index of Order 3	1+ Billion
29.	Solvation Connectivity Index of Order 4	1+ Billion
30.	Solvation Connectivity Index of Order 5	1+ Billion
31.	Modified Randic Index	1+ Billion
32.	Reciprocal Distance Sum Randic-Like Index	1+ Billion
33.	Reciprocal Distance Sum Inverse Randic-Like Index	1+ Billion
34.	Kupchik Connectivity Index	1+ Billion
35.	Connectivity Topochemical Index	1+ Billion
36.	Perturbation Connectivity Index	1+ Billion
37.	Multiplicative Perturbation Connectivity Index	1+ Billion

### ► Information Indices (48)

	Information Indices	Number of Compounds
1.	Information Index on Molecular Size	1+ Billion
2.	Total Information Index on Atomic Composition	1+ Billion
3.	Mean Information Index on Atomic Composition	1+ Billion
4.	Mean Information Content on The Distance Equality	1+ Billion
5.	Mean Information Content on The Distance Magnitude	1+ Billion



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6.	Mean Information Content on The Distance Degree Equality
7.	Mean Information Content on The Distance Degree Magnitude
8.	Total Information Content on The Distance Equality
9.	Total Information Content on The Distance Magnitude
10.	Mean Information Content on The Vertex Degree Equality
11.	Mean Information Content on The Vertex Degree Magnitude
12.	Kier Symmetry Index
13.	Graph Vertex Complexity Index
14.	Graph Distance Complexity Index (Log Function)
15.	Balaban U Index
16.	Balaban V Index
17.	Balaban X Index
18.	Balaban Y Index
19.	Information Content Index (Neighborhood Symmetry of 0-Order)
20.	Information Content Index (Neighborhood Symmetry of 1-Order)
21.	Information Content Index (Neighborhood Symmetry of 2-Order)
22.	Information Content Index (Neighborhood Symmetry of 3-Order)
23.	Information Content Index (Neighborhood Symmetry of 4-Order)
24.	Information Content Index (Neighborhood Symmetry of 5-Order)
25.	Total Information Content Index (Neighborhood Symmetry of 0-Order)
26.	Total Information Content Index (Neighborhood Symmetry of 1-Order)
27.	Total Information Content Index (Neighborhood Symmetry of 2-Order)
28.	Total Information Content Index (Neighborhood Symmetry of 3-Order)
29.	Total Information Content Index (Neighborhood Symmetry of 4-Order)
30.	Total Information Content Index (Neighborhood Symmetry of 5-Order)
31.	Structural Information Content Index (Neighborhood Symmetry of 0-Order)



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32.	Structural Information Content Index (Neighborhood Symmetry of 1-Order)	1+ Billion
33.	Structural Information Content Index (Neighborhood Symmetry of 2-Order)	1+ Billion
34.	Structural Information Content Index (Neighborhood Symmetry of 3-Order)	1+ Billion
35.	Structural Information Content Index (Neighborhood Symmetry of 4-Order)	1+ Billion
36.	Structural Information Content Index (Neighborhood Symmetry of 5-Order)	1+ Billion
37.	Complementary Information Content Index (Neighborhood Symmetry of 0-Order)	1+ Billion
38.	Complementary Information Content Index (Neighborhood Symmetry of 1-Order)	1+ Billion
39.	Complementary Information Content Index (Neighborhood Symmetry of 2-Order)	1+ Billion
40.	Complementary Information Content Index (Neighborhood Symmetry of 3-Order)	1+ Billion
41.	Complementary Information Content Index (Neighborhood Symmetry of 4-Order)	1+ Billion
42.	Complementary Information Content Index (Neighborhood Symmetry of 5-Order)	1+ Billion
43.	Bond Information Content Index (Neighborhood Symmetry of 0-Order)	1+ Billion
44.	Bond Information Content Index (Neighborhood Symmetry of 1-Order)	1+ Billion
45.	Bond Information Content Index (Neighborhood Symmetry of 2-Order)	1+ Billion
46.	Bond Information Content Index (Neighborhood Symmetry of 3-Order)	1+ Billion
47.	Bond Information Content Index (Neighborhood Symmetry of 4-Order)	1+ Billion
48.	Bond Information Content Index (Neighborhood Symmetry of 5-Order)	1+ Billion

# > 2D Matrix-Based Descriptors (550)

	2D Matrix-Based Descriptors	Number of Compounds
1.	Balaban-Like Index from Adjacency Matrix	1+ Billion
2.	Spectral Positive Sum from Adjacency Matrix	1+ Billion
3.	Normalized Spectral Positive Sum from Adjacency Matrix	1+ Billion



4.	Logarithmic Spectral Positive Sum from Adjacency Matrix	1+ Billion
5.	Leading Eigenvalue from Adjacency Matrix (Lovasz-Pelikan Index)	1+ Billion
6.	Normalized Leading Eigenvalue from Adjacency Matrix	1+ Billion
7.	Spectral Diameter from Adjacency Matrix	1+ Billion
8.	Spectral Absolute Deviation from Adjacency Matrix	1+ Billion
9.	Spectral Mean Absolute Deviation from Adjacency Matrix	1+ Billion
10.	Hosoya-Like Index (Log Function) from Adjacency Matrix	1+ Billion
11.	Estrada-Like Index (Log Function) from Adjacency Matrix	1+ Billion
12.	Coefficient Sum of The Last Eigenvector from Adjacency Matrix	1+ Billion
13.	Average Coefficient of The Last Eigenvector from Adjacency Matrix	1+ Billion
14.	Logarithmic Coefficient Sum of The Last Eigenvector from Adjacency Matrix	1+ Billion
15.	Randic-Like Eigenvector-Based Index from Adjacency Matrix	1+ Billion
16.	Normalized Randic-Like Eigenvector-Based Index from Adjacency Matrix	1+ Billion
17.	Logarithmic Randic-Like Eigenvector-Based Index from Adjacency Matrix	1+ Billion
18.	Wiener-Like Index from Topological Distance Matrix (Wiener Index)	1+ Billion
19.	Average Wiener-Like Index from Topological Distance Matrix	1+ Billion
20.	Average Vertex Sum from Topological Distance Matrix	1+ Billion
21.	Harary-Like Index from Topological Distance Matrix (Harary Index)	1+ Billion
22.	Randic-Like Index from Topological Distance Matrix	1+ Billion
23.	Average Randic-Like Index from Topological Distance Matrix	1+ Billion
24.	Balaban-Like Index from Topological Distance Matrix (Balaban Distance Connectivity Index)	1+ Billion
25.	Hyper-Wiener-Like Index (Log Function) from Topological Distance Matrix	1+ Billion
26.	Spectral Positive Sum from Topological Distance Matrix	1+ Billion
27.	Normalized Spectral Positive Sum from Topological Distance Matrix	1+ Billion
28.	Logarithmic Spectral Positive Sum from Topological Distance Matrix	1+ Billion
29.	Leading Eigenvalue from Topological Distance Matrix	1+ Billion



3	0.	Normalized Leading Eigenvalue from Topological Distance Matrix	1+ Billion
3	1.	Spectral Diameter from Topological Distance Matrix	1+ Billion
3	2.	Spectral Absolute Deviation from Topological Distance Matrix	1+ Billion
3	3.	Spectral Mean Absolute Deviation from Topological Distance Matrix	1+ Billion
3	4.	Hosoya-Like Index (Log Function) from Topological Distance Matrix	1+ Billion
3	5.	Estrada-Like Index (Log Function) from Topological Distance Matrix	1+ Billion
3	6.	Spectral Moment of Order 2 from Topological Distance Matrix	1+ Billion
3	7.	Spectral Moment of Order 3 from Topological Distance Matrix	1+ Billion
3	8.	Spectral Moment of Order 4 from Topological Distance Matrix	1+ Billion
3	9.	Spectral Moment of Order 5 from Topological Distance Matrix	1+ Billion
4	0.	Spectral Moment of Order 6 from Topological Distance Matrix	1+ Billion
4	1.	Coefficient Sum of The Last Eigenvector from Topological Distance Matrix	1+ Billion
4	2.	Average Coefficient of The Last Eigenvector from Topological Distance Matrix	1+ Billion
4	3.	Logarithmic Coefficient Sum of The Last Eigenvector from Topological Distance Matrix	1+ Billion
4	4.	Randic-Like Eigenvector-Based Index from Topological Distance Matrix	1+ Billion
4	5.	Normalized Randic-Like Eigenvector-Based Index from Topological Distance Matrix	1+ Billion
4	6.	Logarithmic Randic-Like Eigenvector-Based Index from Topological Distance Matrix	1+ Billion
4	7.	Quasi-Wiener Index (Kirchhoff Number) from Laplace Matrix	1+ Billion
4	8.	First Mohar Index from Laplace Matrix	1+ Billion
4	9.	Second Mohar Index from Laplace Matrix	1+ Billion
5	0.	Spanning Tree Number (Log Function) from Laplace Matrix	1+ Billion
5	1.	Spectral Positive Sum from Laplace Matrix	1+ Billion
5	2.	Normalized Spectral Positive Sum from Laplace Matrix	1+ Billion
5	3.	Logarithmic Spectral Positive Sum from Laplace Matrix	1+ Billion
5	4.	Leading Eigenvalue from Laplace Matrix	1+ Billion
5	5.	Normalized Leading Eigenvalue from Laplace Matrix	1+ Billion



56.	Spectral Diameter from Laplace Matrix	1+ Billion
57.	Spectral Absolute Deviation from Laplace Matrix	1+ Billion
58.	Spectral Mean Absolute Deviation from Laplace Matrix	1+ Billion
59.	Hosoya-Like Index (Log Function) from Laplace Matrix	1+ Billion
60.	Estrada-Like Index (Log Function) from Laplace Matrix	1+ Billion
61.	Spectral Moment of Order 2 from Laplace Matrix	1+ Billion
62.	Spectral Moment of Order 3 from Laplace Matrix	1+ Billion
63.	Spectral Moment of Order 4 from Laplace Matrix	1+ Billion
64.	Spectral Moment of Order 5 from Laplace Matrix	1+ Billion
65.	Spectral Moment of Order 6 from Laplace Matrix	1+ Billion
66.	Coefficient Sum of The Last Eigenvector from Laplace Matrix	1+ Billion
67.	Average Coefficient of The Last Eigenvector from Laplace Matrix	1+ Billion
68.	Logarithmic Coefficient Sum of The Last Eigenvector from Laplace Matrix	1+ Billion
69.	Randic-Like Eigenvector-Based Index from Laplace Matrix	1+ Billion
70.	Normalized Randic-Like Eigenvector-Based Index from Laplace Matrix	1+ Billion
71.	Logarithmic Randic-Like Eigenvector-Based Index from Laplace Matrix	1+ Billion
72.	Average Vertex Sum from Chi Matrix	1+ Billion
73.	Harary-Like Index from Chi Matrix	1+ Billion
74.	Randic-Like Index from Chi Matrix	1+ Billion
75.	Average Randic-Like Index from Chi Matrix	1+ Billion
76.	Balaban-Like Index from Chi Matrix	1+ Billion
77.	Hyper-Wiener-Like Index (Log Function) from Chi Matrix	1+ Billion
78.	Spectral Positive Sum from Chi Matrix	1+ Billion
79.	Normalized Spectral Positive Sum from Chi Matrix	1+ Billion
80.	Logarithmic Spectral Positive Sum from Chi Matrix	1+ Billion
81.	Leading Eigenvalue from Chi Matrix	1+ Billion



82.	Normalized Leading Eigenvalue from Chi Matrix	1+ Billion
83.	Spectral Diameter from Chi Matrix	1+ Billion
84.	Spectral Absolute Deviation from Chi Matrix	1+ Billion
85.	Spectral Mean Absolute Deviation from Chi Matrix	1+ Billion
86.	Hosoya-Like Index (Log Function) from Chi Matrix	1+ Billion
87.	Estrada-Like Index (Log Function) from Chi Matrix	1+ Billion
88.	Spectral Moment of Order 2 from Chi Matrix	1+ Billion
89.	Spectral Moment of Order 3 from Chi Matrix	1+ Billion
90.	Spectral Moment of Order 4 from Chi Matrix	1+ Billion
91.	Spectral Moment of Order 5 from Chi Matrix	1+ Billion
92.	Spectral Moment of Order 6 from Chi Matrix	1+ Billion
93.	Coefficient Sum of The Last Eigenvector from Chi Matrix	1+ Billion
94.	Average Coefficient of The Last Eigenvector from Chi Matrix	1+ Billion
95.	Logarithmic Coefficient Sum of The Last Eigenvector from Chi Matrix	1+ Billion
96.	Randic-Like Eigenvector-Based Index from Chi Matrix	1+ Billion
97.	Normalized Randic-Like Eigenvector-Based Index from Chi Matrix	1+ Billion
98.	Logarithmic Randic-Like Eigenvector-Based Index from Chi Matrix	1+ Billion
99.	Wiener-Like Index from Reciprocal Squared Distance Matrix	1+ Billion
100.	Average Wiener-Like Index from Reciprocal Squared Distance Matrix	1+ Billion
101.	Average Vertex Sum from Reciprocal Squared Distance Matrix	1+ Billion
102.	Randic-Like Index from Reciprocal Squared Distance Matrix	1+ Billion
103.	Average Randic-Like Index from Reciprocal Squared Distance Matrix	1+ Billion
104.	Balaban-Like Index from Reciprocal Squared Distance Matrix	1+ Billion
105.	Hyper-Wiener-Like Index (Log Function) from Reciprocal Squared Distance Matrix	1+ Billion
106.	Spectral Positive Sum from Reciprocal Squared Distance Matrix	1+ Billion
107.	Normalized Spectral Positive Sum from Reciprocal Squared Distance Matrix	1+ Billion



108. Logarithmic Spectral Positive Sum from Reciprocal Squared Distance Matrix	1+ Billion
109. Leading Eigenvalue from Reciprocal Squared Distance Matrix	1+ Billion
110. Normalized Leading Eigenvalue from Reciprocal Squared Distance Matrix	1+ Billion
111. Spectral Diameter from Reciprocal Squared Distance Matrix	1+ Billion
112. Spectral Absolute Deviation from Reciprocal Squared Distance Matrix	1+ Billion
113. Spectral Mean Absolute Deviation from Reciprocal Squared Distance Matrix	1+ Billion
114. Hosoya-Like Index (Log Function) from Reciprocal Squared Distance Matrix	1+ Billion
115. Estrada-Like Index (Log Function) from Reciprocal Squared Distance Matrix	1+ Billion
116. Spectral Moment of Order 2 from Reciprocal Squared Distance Matrix	1+ Billion
117. Spectral Moment of Order 3 from Reciprocal Squared Distance Matrix	1+ Billion
118. Spectral Moment of Order 4 from Reciprocal Squared Distance Matrix	1+ Billion
119. Spectral Moment of Order 5 from Reciprocal Squared Distance Matrix	1+ Billion
120. Spectral Moment of Order 6 from Reciprocal Squared Distance Matrix	1+ Billion
121. Coefficient Sum of The Last Eigenvector from Reciprocal Squared Distance Matrix	1+ Billion
122. Average Coefficient of The Last Eigenvector from Reciprocal Squared Distance Matrix	1+ Billion
123. Logarithmic Coefficient Sum of The Last Eigenvector from Reciprocal Squared Distance Matrix	1+ Billion
124. Randic-Like Eigenvector-Based Index from Reciprocal Squared Distance Matrix	1+ Billion
125. Normalized Randic-Like Eigenvector-Based Index from Reciprocal Squared Distance Matrix	1+ Billion
126. Logarithmic Randic-Like Eigenvector-Based Index from Reciprocal Squared Distance Matrix	1+ Billion
127. Wiener-Like Index from Detour Matrix (Detour Index)	1+ Billion
128. Average Wiener-Like Index from Detour Matrix	1+ Billion
129. Average Vertex Sum from Detour Matrix	1+ Billion
130. Harary-Like Index from Detour Matrix	1+ Billion
131. Randic-Like Index from Detour Matrix	1+ Billion
132. Average Randic-Like Index from Detour Matrix	1+ Billion
133. Balaban-Like Index from Detour Matrix	1+ Billion



134. Hyper-Wiener-Like Index (Log Function) from Detour Matrix	1+ Billion
135. Spectral Positive Sum from Detour Matrix	1+ Billion
136. Normalized Spectral Positive Sum from Detour Matrix	1+ Billion
137. Logarithmic Spectral Positive Sum from Detour Matrix	1+ Billion
138. Leading Eigenvalue from Detour Matrix	1+ Billion
139. Normalized Leading Eigenvalue from Detour Matrix	1+ Billion
140. Spectral Diameter from Detour Matrix	1+ Billion
141. Spectral Absolute Deviation from Detour Matrix	1+ Billion
142. Spectral Mean Absolute Deviation from Detour Matrix	1+ Billion
143. Hosoya-Like Index (Log Function) from Detour Matrix	1+ Billion
144. Estrada-Like Index (Log Function) from Detour Matrix	1+ Billion
145. Spectral Moment of Order 2 from Detour Matrix	1+ Billion
146. Spectral Moment of Order 3 from Detour Matrix	1+ Billion
147. Spectral Moment of Order 4 from Detour Matrix	1+ Billion
148. Spectral Moment of Order 5 from Detour Matrix	1+ Billion
149. Spectral Moment of Order 6 from Detour Matrix	1+ Billion
150. Coefficient Sum of The Last Eigenvector from Detour Matrix	1+ Billion
151. Average Coefficient of The Last Eigenvector from Detour Matrix	1+ Billion
152. Logarithmic Coefficient Sum of The Last Eigenvector from Detour Matrix	1+ Billion
153. Randic-Like Eigenvector-Based Index from Detour Matrix	1+ Billion
154. Normalized Randic-Like Eigenvector-Based Index from Detour Matrix	1+ Billion
155. Logarithmic Randic-Like Eigenvector-Based Index from Detour Matrix	1+ Billion
156. Wiener-Like Index from Distance/Detour Matrix	1+ Billion
157. Average Wiener-Like Index from Distance/Detour Matrix	1+ Billion
158. Average Vertex Sum from Distance/Detour Matrix	1+ Billion
159. Harary-Like Index from Distance/Detour Matrix	1+ Billion



160. Randic-Like Index from Distance/Detour Matrix	1+ Billion
161. Average Randic-Like Index from Distance/Detour Matrix	1+ Billion
162. Balaban-Like Index from Distance/Detour Matrix	1+ Billion
163. Hyper-Wiener-Like Index (Log Function) from Distance/Detour Matrix	1+ Billion
164. Spectral Positive Sum from Distance/Detour Matrix	1+ Billion
165. Normalized Spectral Positive Sum from Distance/Detour Matrix	1+ Billion
166. Logarithmic Spectral Positive Sum from Distance/Detour Matrix	1+ Billion
167. Leading Eigenvalue from Distance/Detour Matrix	1+ Billion
168. Normalized Leading Eigenvalue from Distance/Detour Matrix	1+ Billion
169. Spectral Diameter from Distance/Detour Matrix	1+ Billion
170. Spectral Absolute Deviation from Distance/Detour Matrix	1+ Billion
171. Spectral Mean Absolute Deviation from Distance/Detour Matrix	1+ Billion
172. Hosoya-Like Index (Log Function) from Distance/Detour Matrix	1+ Billion
173. Estrada-Like Index (Log Function) from Distance/Detour Matrix	1+ Billion
174. Spectral Moment of Order 2 from Distance/Detour Matrix	1+ Billion
175. Spectral Moment of Order 3 from Distance/Detour Matrix	1+ Billion
176. Spectral Moment of Order 4 from Distance/Detour Matrix	1+ Billion
177. Spectral Moment of Order 5 from Distance/Detour Matrix	1+ Billion
178. Spectral Moment of Order 6 from Distance/Detour Matrix	1+ Billion
179. Coefficient Sum of The Last Eigenvector from Distance/Detour Matrix	1+ Billion
180. Average Coefficient of The Last Eigenvector from Distance/Detour Matrix	1+ Billion
181. Logarithmic Coefficient Sum of The Last Eigenvector from Distance/Detour Matrix	1+ Billion
182. Randic-Like Eigenvector-Based Index from Distance/Detour Matrix	1+ Billion
183. Normalized Randic-Like Eigenvector-Based Index from Distance/Detour Matrix	1+ Billion
184. Logarithmic Randic-Like Eigenvector-Based Index from Distance/Detour Matrix	1+ Billion
185. Wiener-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion



186. Average Wiener-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
187. Average Vertex Sum from Barysz Matrix Weighted by Atomic Number	1+ Billion
188. Harary-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
189. Randic-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
190. Average Randic-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
191. Balaban-Like Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
192. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by Atomic Number	1+ Billion
193. Graph Energy from Barysz Matrix Weighted by Atomic Number	1+ Billion
194. Spectral Positive Sum from Barysz Matrix Weighted by Atomic Number	1+ Billion
195. Normalized Spectral Positive Sum from Barysz Matrix Weighted by Atomic Number	1+ Billion
196. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by Atomic Number	1+ Billion
197. Leading Eigenvalue from Barysz Matrix Weighted by Atomic Number	1+ Billion
198. Normalized Leading Eigenvalue from Barysz Matrix Weighted by Atomic Number	1+ Billion
199. Spectral Diameter from Barysz Matrix Weighted by Atomic Number	1+ Billion
200. Spectral Absolute Deviation from Barysz Matrix Weighted by Atomic Number	1+ Billion
201. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by Atomic Number	1+ Billion
202. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by Atomic Number	1+ Billion
203. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by Atomic Number	1+ Billion
204. Spectral Moment of Order 1 from Barysz Matrix Weighted by Atomic Number	1+ Billion
205. Spectral Moment of Order 2 from Barysz Matrix Weighted by Atomic Number	1+ Billion
206. Spectral Moment of Order 3 from Barysz Matrix Weighted by Atomic Number	1+ Billion
207. Spectral Moment of Order 4 from Barysz Matrix Weighted by Atomic Number	1+ Billion
208. Spectral Moment of Order 5 from Barysz Matrix Weighted by Atomic Number	1+ Billion
209. Spectral Moment of Order 6 from Barysz Matrix Weighted by Atomic Number	1+ Billion
210. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Atomic Number	1+ Billion
211. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by Atomic Number	1+ Billion





212. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Atomic Number	1+ Billion
213. Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
214. Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
215. Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Atomic Number	1+ Billion
216. Wiener-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
217. Average Wiener-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
218. Average Vertex Sum from Barysz Matrix Weighted by Mass	1+ Billion
219. Harary-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
220. Randic-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
221. Average Randic-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
222. Balaban-Like Index from Barysz Matrix Weighted by Mass	1+ Billion
223. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by Mass	1+ Billion
224. Graph Energy from Barysz Matrix Weighted by Mass	1+ Billion
225. Spectral Positive Sum from Barysz Matrix Weighted by Mass	1+ Billion
226. Normalized Spectral Positive Sum from Barysz Matrix Weighted by Mass	1+ Billion
227. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by Mass	1+ Billion
228. Leading Eigenvalue from Barysz Matrix Weighted by Mass	1+ Billion
229. Normalized Leading Eigenvalue from Barysz Matrix Weighted by Mass	1+ Billion
230. Spectral Diameter from Barysz Matrix Weighted by Mass	1+ Billion
231. Spectral Absolute Deviation from Barysz Matrix Weighted by Mass	1+ Billion
232. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by Mass	1+ Billion
233. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by Mass	1+ Billion
234. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by Mass	1+ Billion
235. Spectral Moment of Order 1 from Barysz Matrix Weighted by Mass	1+ Billion
236. Spectral Moment of Order 2 from Barysz Matrix Weighted by Mass	1+ Billion
237. Spectral Moment of Order 3 from Barysz Matrix Weighted by Mass	1+ Billion



238. Spectral Moment of Order 4 from Barysz Matrix Weighted by Mass	1+ Billion
239. Spectral Moment of Order 5 from Barysz Matrix Weighted by Mass	1+ Billion
240. Spectral Moment of Order 6 from Barysz Matrix Weighted by Mass	1+ Billion
241. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Mass	1+ Billion
242. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by Mass	1+ Billion
243. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Mass	1+ Billion
244. Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Mass	1+ Billion
245. Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Mass	1+ Billion
246. Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Mass	1+ Billion
247. Wiener-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
248. Average Wiener-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
249. Average Vertex Sum from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
250. Harary-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
251. Randic-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
252. Average Randic-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
253. Balaban-Like Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
254. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
255. Graph Energy from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
256. Spectral Positive Sum from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
257. Normalized Spectral Positive Sum from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
258. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
259. Leading Eigenvalue from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
260. Normalized Leading Eigenvalue from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
261. Spectral Diameter from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
262. Spectral Absolute Deviation from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
263. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by van der Waals Volume	1+ Billion



264. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
265. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
266. Spectral Moment of Order 1 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
267. Spectral Moment of Order 2 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
268. Spectral Moment of Order 3 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
269. Spectral Moment of Order 4 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
270. Spectral Moment of Order 5 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
271. Spectral Moment of Order 6 from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
272. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
273. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
274. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by van der Waals V	/olume 1+ Billion
275. Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by van der Waals Volume	1+ Billion
276. Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by van der Waals Volu	ume 1+ Billion
277. Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by van der Waals Volu	ume 1+ Billion
278. Wiener-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
279. Average Wiener-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
280. Average Vertex Sum from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
281. Harary-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
282. Randic-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
283. Average Randic-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
284. Balaban-Like Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
285. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
286. Graph Energy from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
287. Spectral Positive Sum from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
288. Normalized Spectral Positive Sum from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
289. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion



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290. Leading Eigenvalue from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
291. Normalized Leading Eigenvalue from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
292. Spectral Diameter from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
293. Spectral Absolute Deviation from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
294. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
295. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
296. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
297. Spectral Moment of Order 1 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
298. Spectral Moment of Order 2 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
299. Spectral Moment of Order 3 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
300. Spectral Moment of Order 4 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
301. Spectral Moment of Order 5 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
302. Spectral Moment of Order 6 from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
303. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
304. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
305. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
306. Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
307. Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
308. Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Sanderson Electronegativity	1+ Billion
309. Wiener-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion
310. Average Wiener-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion
311. Average Vertex Sum from Barysz Matrix Weighted by Polarizability	1+ Billion
312. Harary-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion
313. Randic-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion
314. Average Randic-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion
315. Balaban-Like Index from Barysz Matrix Weighted by Polarizability	1+ Billion



316. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by Polarizability	1+ Billion
317. Graph Energy from Barysz Matrix Weighted by Polarizability	1+ Billion
318. Spectral Positive Sum from Barysz Matrix Weighted by Polarizability	1+ Billion
319. Normalized Spectral Positive Sum from Barysz Matrix Weighted by Polarizability	1+ Billion
320. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by Polarizability	1+ Billion
321. Leading Eigenvalue from Barysz Matrix Weighted by Polarizability	1+ Billion
322. Normalized Leading Eigenvalue from Barysz Matrix Weighted by Polarizability	1+ Billion
323. Spectral Diameter from Barysz Matrix Weighted by Polarizability	1+ Billion
324. Spectral Absolute Deviation from Barysz Matrix Weighted by Polarizability	1+ Billion
325. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by Polarizability	1+ Billion
326. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by Polarizability	1+ Billion
327. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by Polarizability	1+ Billion
328. Spectral Moment of Order 1 from Barysz Matrix Weighted by Polarizability	1+ Billion
329. Spectral Moment of Order 2 from Barysz Matrix Weighted by Polarizability	1+ Billion
330. Spectral Moment of Order 3 from Barysz Matrix Weighted by Polarizability	1+ Billion
331. Spectral Moment of Order 4 from Barysz Matrix Weighted by Polarizability	1+ Billion
332. Spectral Moment of Order 5 from Barysz Matrix Weighted by Polarizability	1+ Billion
333. Spectral Moment of Order 6 from Barysz Matrix Weighted by Polarizability	1+ Billion
334. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Polarizability	1+ Billion
335. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by Polarizability	1+ Billion
336. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Polarizability	1+ Billion
337. Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Polarizability	1+ Billion
338. Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Polarizability	1+ Billion
339. Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Polarizability	1+ Billion
340. Wiener-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
341. Average Wiener-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion



342. Average Vertex Sum from Barysz Matrix Weighted by Ionization Potential	1+ Billion
343. Harary-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
344. Randic-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
345. Average Randic-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
346. Balaban-Like Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
347. Hyper-Wiener-Like Index (Log Function) from Barysz Matrix Weighted by Ionization Potential	1+ Billion
348. Graph Energy from Barysz Matrix Weighted by Ionization Potential	1+ Billion
349. Spectral Positive Sum from Barysz Matrix Weighted by Ionization Potential	1+ Billion
350. Normalized Spectral Positive Sum from Barysz Matrix Weighted by Ionization Potential	1+ Billion
351. Logarithmic Spectral Positive Sum from Barysz Matrix Weighted by Ionization Potential	1+ Billion
352. Leading Eigenvalue from Barysz Matrix Weighted by Ionization Potential	1+ Billion
353. Normalized Leading Eigenvalue from Barysz Matrix Weighted by Ionization Potential	1+ Billion
354. Spectral Diameter from Barysz Matrix Weighted by Ionization Potential	1+ Billion
355. Spectral Absolute Deviation from Barysz Matrix Weighted by Ionization Potential	1+ Billion
356. Spectral Mean Absolute Deviation from Barysz Matrix Weighted by Ionization Potential	1+ Billion
357. Hosoya-Like Index (Log Function) from Barysz Matrix Weighted by Ionization Potential	1+ Billion
358. Estrada-Like Index (Log Function) from Barysz Matrix Weighted by Ionization Potential	1+ Billion
359. Spectral Moment of Order 1 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
360. Spectral Moment of Order 2 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
361. Spectral Moment of Order 3 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
362. Spectral Moment of Order 4 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
363. Spectral Moment of Order 5 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
364. Spectral Moment of Order 6 from Barysz Matrix Weighted by Ionization Potential	1+ Billion
365. Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Ionization Potential	1+ Billion
366. Average Coefficient of The Last Eigenvector from Barysz Matrix Weighted by Ionization Potential	1+ Billion
367. Logarithmic Coefficient Sum of The Last Eigenvector from Barysz Matrix Weighted by Ionization Potential	1+ Billion



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368.	Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
369.	Normalized Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
370.	Logarithmic Randic-Like Eigenvector-Based Index from Barysz Matrix Weighted by Ionization Potential	1+ Billion
371.	Wiener-Like Index from Burden Matrix Weighted by Mass	1+ Billion
372.	Average Wiener-Like Index from Burden Matrix Weighted by Mass	1+ Billion
373.	Average Vertex Sum from Burden Matrix Weighted by Mass	1+ Billion
374.	Randic-Like Index from Burden Matrix Weighted by Mass	1+ Billion
375.	Average Randic-Like Index from Burden Matrix Weighted by Mass	1+ Billion
376.	Balaban-Like Index from Burden Matrix Weighted by Mass	1+ Billion
377.	Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by Mass	1+ Billion
378.	Graph Energy from Burden Matrix Weighted by Mass	1+ Billion
379.	Spectral Positive Sum from Burden Matrix Weighted by Mass	1+ Billion
380.	Normalized Spectral Positive Sum from Burden Matrix Weighted by Mass	1+ Billion
381.	Logarithmic Spectral Positive Sum from Burden Matrix Weighted by Mass	1+ Billion
382.	Leading Eigenvalue from Burden Matrix Weighted by Mass	1+ Billion
383.	Normalized Leading Eigenvalue from Burden Matrix Weighted by Mass	1+ Billion
384.	Spectral Diameter from Burden Matrix Weighted by Mass	1+ Billion
385.	Spectral Absolute Deviation from Burden Matrix Weighted by Mass	1+ Billion
386.	Spectral Mean Absolute Deviation from Burden Matrix Weighted by Mass	1+ Billion
387.	Hosoya-Like Index (Log Function) from Burden Matrix Weighted by Mass	1+ Billion
388.	Estrada-Like Index (Log Function) from Burden Matrix Weighted by Mass	1+ Billion
389.	Spectral Moment of Order 1 from Burden Matrix Weighted by Mass	1+ Billion
390.	Spectral Moment of Order 2 from Burden Matrix Weighted by Mass	1+ Billion
391.	Spectral Moment of Order 3 from Burden Matrix Weighted by Mass	1+ Billion
392.	Spectral Moment of Order 4 from Burden Matrix Weighted by Mass	1+ Billion
393.	Spectral Moment of Order 5 from Burden Matrix Weighted by Mass	1+ Billion





1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

394.	Spectral Moment of Order 6 from Burden Matrix Weighted by Mass	1+ Billion
395.	Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Mass	1+ Billion
396.	Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by Mass	1+ Billion
397.	Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Mass	1+ Billion
398.	Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Mass	1+ Billion
399.	Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Mass	1+ Billion
400.	Logarithmic Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Mass	1+ Billion
401.	Wiener-Like Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
402.	Average Wiener-Like Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
403.	Average Vertex Sum from Burden Matrix Weighted by van der Waals Volume	1+ Billion
404.	Randic-Like Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
405.	Average Randic-Like Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
406.	Balaban-Like Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
407.	Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by van der Waals Volume	1+ Billion
408.	Graph Energy from Burden Matrix Weighted by van der Waals Volume	1+ Billion
409.	Spectral Positive Sum from Burden Matrix Weighted by van der Waals Volume	1+ Billion
410.	Normalized Spectral Positive Sum from Burden Matrix Weighted by van der Waals Volume	1+ Billion
411.	Logarithmic Spectral Positive Sum from Burden Matrix Weighted by van der Waals Volume	1+ Billion
412.	Leading Eigenvalue from Burden Matrix Weighted by van der Waals Volume	1+ Billion
413.	Normalized Leading Eigenvalue from Burden Matrix Weighted by van der Waals Volume	1+ Billion
414.	Spectral Diameter from Burden Matrix Weighted by van der Waals Volume	1+ Billion
415.	Spectral Absolute Deviation from Burden Matrix Weighted by van der Waals Volume	1+ Billion
416.	Spectral Mean Absolute Deviation from Burden Matrix Weighted by van der Waals Volume	1+ Billion
417.	Hosoya-Like Index (Log Function) from Burden Matrix Weighted by van der Waals Volume	1+ Billion
418.	Estrada-Like Index (Log Function) from Burden Matrix Weighted by van der Waals Volume	1+ Billion
419.	Spectral Moment of Order 1 from Burden Matrix Weighted by van der Waals Volume	1+ Billion

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420. Spectral Moment of Order 2 from Burden Matrix Weighted by van der Waals Volume	1+ Billion
421. Spectral Moment of Order 3 from Burden Matrix Weighted by van der Waals Volume	1+ Billion
422. Spectral Moment of Order 4 from Burden Matrix Weighted by van der Waals Volume	1+ Billion
423. Spectral Moment of Order 5 from Burden Matrix Weighted by van der Waals Volume	1+ Billion
424. Spectral Moment of Order 6 from Burden Matrix Weighted by van der Waals Volume	1+ Billion
425. Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by van der Waals Volume	1+ Billion
426. Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by van der Waals Volume	1+ Billion
427. Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by van der Waals Volume	1+ Billion
428. Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
429. Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
430. Logarithmic Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by van der Waals Volume	1+ Billion
431. Wiener-Like Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
432. Average Wiener-Like Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
433. Average Vertex Sum from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
434. Randic-Like Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
435. Average Randic-Like Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
436. Balaban-Like Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
437. Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
438. Graph Energy from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
439. Spectral Positive Sum from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
440. Normalized Spectral Positive Sum from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
441. Logarithmic Spectral Positive Sum from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
442. Leading Eigenvalue from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
443. Normalized Leading Eigenvalue from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
444. Spectral Diameter from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
445. Spectral Absolute Deviation from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion





446. Spectral Mean Absolute Deviation from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
447. Hosoya-Like Index (Log Function) from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
448. Estrada-Like Index (Log Function) from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
449. Spectral Moment of Order 1 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
450. Spectral Moment of Order 2 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
451. Spectral Moment of Order 3 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
452. Spectral Moment of Order 4 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
453. Spectral Moment of Order 5 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
454. Spectral Moment of Order 6 from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
455. Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
456. Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
457. Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
458. Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
459. Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
460. Logarithmic Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
461. Wiener-Like Index from Burden Matrix Weighted by Polarizability	1+ Billion
462. Average Wiener-Like Index from Burden Matrix Weighted by Polarizability	1+ Billion
463. Average Vertex Sum from Burden Matrix Weighted by Polarizability	1+ Billion
464. Randic-Like Index from Burden Matrix Weighted by Polarizability	1+ Billion
465. Average Randic-Like Index from Burden Matrix Weighted by Polarizability	1+ Billion
466. Balaban-Like Index from Burden Matrix Weighted by Polarizability	1+ Billion
467. Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by Polarizability	1+ Billion
468. Graph Energy from Burden Matrix Weighted by Polarizability	1+ Billion
469. Spectral Positive Sum from Burden Matrix Weighted by Polarizability	1+ Billion
470. Normalized Spectral Positive Sum from Burden Matrix Weighted by Polarizability	1+ Billion
471. Logarithmic Spectral Positive Sum from Burden Matrix Weighted by Polarizability	1+ Billion



472. Leading Eigenvalue from Burden Matrix Weighted by Polarizability	1+ Billion
473. Normalized Leading Eigenvalue from Burden Matrix Weighted by Polarizability	1+ Billion
474. Spectral Diameter from Burden Matrix Weighted by Polarizability	1+ Billion
475. Spectral Absolute Deviation from Burden Matrix Weighted by Polarizability	1+ Billion
476. Spectral Mean Absolute Deviation from Burden Matrix Weighted by Polarizability	1+ Billion
477. Hosoya-Like Index (Log Function) from Burden Matrix Weighted by Polarizability	1+ Billion
478. Estrada-Like Index (Log Function) from Burden Matrix Weighted by Polarizability	1+ Billion
479. Spectral Moment of Order 1 from Burden Matrix Weighted by Polarizability	1+ Billion
480. Spectral Moment of Order 2 from Burden Matrix Weighted by Polarizability	1+ Billion
481. Spectral Moment of Order 3 from Burden Matrix Weighted by Polarizability	1+ Billion
482. Spectral Moment of Order 4 from Burden Matrix Weighted by Polarizability	1+ Billion
483. Spectral Moment of Order 5 from Burden Matrix Weighted by Polarizability	1+ Billion
484. Spectral Moment of Order 6 from Burden Matrix Weighted by Polarizability	1+ Billion
485. Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Polarizability	1+ Billion
486. Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by Polarizability	1+ Billion
487. Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Polarizability	1+ Billion
488. Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Polarizability	1+ Billion
489. Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Polarizability	1+ Billion
490. Logarithmic Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Polarizability	1+ Billion
491. Wiener-Like Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
492. Average Wiener-Like Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
493. Average Vertex Sum from Burden Matrix Weighted by Ionization Potential	1+ Billion
494. Randic-Like Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
495. Average Randic-Like Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
496. Balaban-Like Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
497. Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by Ionization Potential	1+ Billion





498.	Graph Energy from Burden Matrix Weighted by Ionization Potential	1+ Billion
499.	Spectral Positive Sum from Burden Matrix Weighted by Ionization Potential	1+ Billion
500.	Normalized Spectral Positive Sum from Burden Matrix Weighted by Ionization Potential	1+ Billion
501.	Logarithmic Spectral Positive Sum from Burden Matrix Weighted by Ionization Potential	1+ Billion
502.	Leading Eigenvalue from Burden Matrix Weighted by Ionization Potential	1+ Billion
503.	Normalized Leading Eigenvalue from Burden Matrix Weighted by Ionization Potential	1+ Billion
504.	Spectral Diameter from Burden Matrix Weighted by Ionization Potential	1+ Billion
505.	Spectral Absolute Deviation from Burden Matrix Weighted by Ionization Potential	1+ Billion
506.	Spectral Mean Absolute Deviation from Burden Matrix Weighted by Ionization Potential	1+ Billion
507.	Hosoya-Like Index (Log Function) from Burden Matrix Weighted by Ionization Potential	1+ Billion
508.	Estrada-Like Index (Log Function) from Burden Matrix Weighted by Ionization Potential	1+ Billion
509.	Spectral Moment of Order 1 from Burden Matrix Weighted by Ionization Potential	1+ Billion
510.	Spectral Moment of Order 2 from Burden Matrix Weighted by Ionization Potential	1+ Billion
511.	Spectral Moment of Order 3 from Burden Matrix Weighted by Ionization Potential	1+ Billion
512.	Spectral Moment of Order 4 from Burden Matrix Weighted by Ionization Potential	1+ Billion
513.	Spectral Moment of Order 5 from Burden Matrix Weighted by Ionization Potential	1+ Billion
514.	Spectral Moment of Order 6 from Burden Matrix Weighted by Ionization Potential	1+ Billion
515.	Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Ionization Potential	1+ Billion
516.	Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by Ionization Potential	1+ Billion
517.	Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by Ionization Potential	1+ Billion
518.	Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
519.	Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
520.	Logarithmic Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by Ionization Potential	1+ Billion
521.	Wiener-Like Index from Burden Matrix Weighted by I-State	1+ Billion
522.	Average Wiener-Like Index from Burden Matrix Weighted by I-State	1+ Billion
523.	Average Vertex Sum from Burden Matrix Weighted by I-State	1+ Billion



524. Randic-Like Index from Burden Matrix Weighted by I-State	1+ Billion
525. Average Randic-Like Index from Burden Matrix Weighted by I-State	1+ Billion
526. Balaban-Like Index from Burden Matrix Weighted by I-State	1+ Billion
527. Hyper-Wiener-Like Index (Log Function) from Burden Matrix Weighted by I-State	1+ Billion
528. Graph Energy from Burden Matrix Weighted by I-State	1+ Billion
529. Spectral Positive Sum from Burden Matrix Weighted by I-State	1+ Billion
530. Normalized Spectral Positive Sum from Burden Matrix Weighted by I-State	1+ Billion
531. Logarithmic Spectral Positive Sum from Burden Matrix Weighted by I-State	1+ Billion
532. Leading Eigenvalue from Burden Matrix Weighted by I-State	1+ Billion
533. Normalized Leading Eigenvalue from Burden Matrix Weighted by I-State	1+ Billion
534. Spectral Diameter from Burden Matrix Weighted by I-State	1+ Billion
535. Spectral Absolute Deviation from Burden Matrix Weighted by I-State	1+ Billion
536. Spectral Mean Absolute Deviation from Burden Matrix Weighted by I-State	1+ Billion
537. Hosoya-Like Index (Log Function) from Burden Matrix Weighted by I-State	1+ Billion
538. Estrada-Like Index (Log Function) from Burden Matrix Weighted by I-State	1+ Billion
539. Spectral Moment of Order 1 from Burden Matrix Weighted by I-State	1+ Billion
540. Spectral Moment of Order 2 from Burden Matrix Weighted by I-State	1+ Billion
541. Spectral Moment of Order 3 from Burden Matrix Weighted by I-State	1+ Billion
542. Spectral Moment of Order 4 from Burden Matrix Weighted by I-State	1+ Billion
543. Spectral Moment of Order 5 from Burden Matrix Weighted by I-State	1+ Billion
544. Spectral Moment of Order 6 from Burden Matrix Weighted by I-State	1+ Billion
545. Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by I-State	1+ Billion
546. Average Coefficient of The Last Eigenvector from Burden Matrix Weighted by I-State	1+ Billion
547. Logarithmic Coefficient Sum of The Last Eigenvector from Burden Matrix Weighted by I-State	1+ Billion
548. Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by I-State	1+ Billion
549. Normalized Randic-Like Eigenvector-Based Index from Burden Matrix Weighted by I-State	1+ Billion



1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

# ► 2D Autocorrelation Indices (213)

	2D Autocorrelation Indices	Number of Compounds
1.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by Mass	1+ Billion
2.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by Mass	1+ Billion
3.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by Mass	1+ Billion
4.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by Mass	1+ Billion
5.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by Mass	1+ Billion
6.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by Mass	1+ Billion
7.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by Mass	1+ Billion
8.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by Mass	1+ Billion
9.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by van der Waals Volume	1+ Billion
10.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by van der Waals Volume	1+ Billion
11.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by van der Waals Volume	1+ Billion
12.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by van der Waals Volume	1+ Billion
13.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by van der Waals Volume	1+ Billion
14.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by van der Waals Volume	1+ Billion
15.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by van der Waals Volume	1+ Billion
16.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by van der Waals Volume	1+ Billion
17.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
18.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
19.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion



20.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
21.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
22.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
23.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
24.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by Sanderson Electronegativity	1+ Billion
25.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by Polarizability	1+ Billion
26.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by Polarizability	1+ Billion
27.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by Polarizability	1+ Billion
28.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by Polarizability	1+ Billion
29.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by Polarizability	1+ Billion
30.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by Polarizability	1+ Billion
31.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by Polarizability	1+ Billion
32.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by Polarizability	1+ Billion
33.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by Ionization Potential	1+ Billion
34.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by Ionization Potential	1+ Billion
35.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by Ionization Potential	1+ Billion
36.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by Ionization Potential	1+ Billion
37.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by Ionization Potential	1+ Billion
38.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by Ionization Potential	1+ Billion
39.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by Ionization Potential	1+ Billion
40.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by Ionization Potential	1+ Billion
41.	Broto-Moreau Autocorrelation of Lag 1 (Log Function) Weighted by I-State	1+ Billion
42.	Broto-Moreau Autocorrelation of Lag 2 (Log Function) Weighted by I-State	1+ Billion
43.	Broto-Moreau Autocorrelation of Lag 3 (Log Function) Weighted by I-State	1+ Billion
44.	Broto-Moreau Autocorrelation of Lag 4 (Log Function) Weighted by I-State	1+ Billion
45.	Broto-Moreau Autocorrelation of Lag 5 (Log Function) Weighted by I-State	1+ Billion



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46.	Broto-Moreau Autocorrelation of Lag 6 (Log Function) Weighted by I-State	1+ Billion
47.	Broto-Moreau Autocorrelation of Lag 7 (Log Function) Weighted by I-State	1+ Billion
48.	Broto-Moreau Autocorrelation of Lag 8 (Log Function) Weighted by I-State	1+ Billion
49.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by Mass	1+ Billion
50.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by Mass	1+ Billion
51.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by Mass	1+ Billion
52.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by Mass	1+ Billion
53.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by Mass	1+ Billion
54.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by Mass	1+ Billion
55.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by Mass	1+ Billion
56.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by Mass	1+ Billion
57.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by van der Waals Volume	1+ Billion
58.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by van der Waals Volume	1+ Billion
59.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by van der Waals Volume	1+ Billion
60.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by van der Waals Volume	1+ Billion
61.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by van der Waals Volume	1+ Billion
62.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by van der Waals Volume	1+ Billion
63.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by van der Waals Volume	1+ Billion
64.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by van der Waals Volume	1+ Billion
65.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by Sanderson Electronegativity	1+ Billion
66.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by Sanderson Electronegativity	1+ Billion
67.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by Sanderson Electronegativity	1+ Billion
68.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by Sanderson Electronegativity	1+ Billion
69.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by Sanderson Electronegativity	1+ Billion
70.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by Sanderson Electronegativity	1+ Billion
71.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by Sanderson Electronegativity	1+ Billion



ChemEssen, Inc.	С	h	е	m	Е	s	s	е	n	,	I	n	С	
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72.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by Sanderson Electronegativity	1+ Billion
73.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by Polarizability	1+ Billion
74.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by Polarizability	1+ Billion
75.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by Polarizability	1+ Billion
76.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by Polarizability	1+ Billion
77.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by Polarizability	1+ Billion
78.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by Polarizability	1+ Billion
79.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by Polarizability	1+ Billion
80.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by Polarizability	1+ Billion
81.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by Ionization Potential	1+ Billion
82.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by Ionization Potential	1+ Billion
83.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by Ionization Potential	1+ Billion
84.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by Ionization Potential	1+ Billion
85.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by Ionization Potential	1+ Billion
86.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by Ionization Potential	1+ Billion
87.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by Ionization Potential	1+ Billion
88.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by Ionization Potential	1+ Billion
89.	Centred Broto-Moreau Autocorrelation of Lag 1 Weighted by I-State	1+ Billion
90.	Centred Broto-Moreau Autocorrelation of Lag 2 Weighted by I-State	1+ Billion
91.	Centred Broto-Moreau Autocorrelation of Lag 3 Weighted by I-State	1+ Billion
92.	Centred Broto-Moreau Autocorrelation of Lag 4 Weighted by I-State	1+ Billion
93.	Centred Broto-Moreau Autocorrelation of Lag 5 Weighted by I-State	1+ Billion
94.	Centred Broto-Moreau Autocorrelation of Lag 6 Weighted by I-State	1+ Billion
95.	Centred Broto-Moreau Autocorrelation of Lag 7 Weighted by I-State	1+ Billion
96.	Centred Broto-Moreau Autocorrelation of Lag 8 Weighted by I-State	1+ Billion
97.	Moran Autocorrelation of Lag 1 Weighted by Mass	1+ Billion



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98.	Moran Autocorrelation of Lag 2 Weighted by Mass	1+ Billion
99.	Moran Autocorrelation of Lag 3 Weighted by Mass	1+ Billion
100.	Moran Autocorrelation of Lag 4 Weighted by Mass	1+ Billion
101.	Moran Autocorrelation of Lag 5 Weighted by Mass	1+ Billion
102.	Moran Autocorrelation of Lag 6 Weighted by Mass	1+ Billion
103.	Moran Autocorrelation of Lag 7 Weighted by Mass	1+ Billion
104.	Moran Autocorrelation of Lag 8 Weighted by Mass	1+ Billion
105.	Moran Autocorrelation of Lag 1 Weighted by van der Waals Volume	1+ Billion
106.	Moran Autocorrelation of Lag 2 Weighted by van der Waals Volume	1+ Billion
107.	Moran Autocorrelation of Lag 3 Weighted by van der Waals Volume	1+ Billion
108.	Moran Autocorrelation of Lag 4 Weighted by van der Waals Volume	1+ Billion
109.	Moran Autocorrelation of Lag 5 Weighted by van der Waals Volume	1+ Billion
110.	Moran Autocorrelation of Lag 6 Weighted by van der Waals Volume	1+ Billion
111.	Moran Autocorrelation of Lag 7 Weighted by van der Waals Volume	1+ Billion
112.	Moran Autocorrelation of Lag 8 Weighted by van der Waals Volume	1+ Billion
113.	Moran Autocorrelation of Lag 1 Weighted by Sanderson Electronegativity	1+ Billion
114.	Moran Autocorrelation of Lag 2 Weighted by Sanderson Electronegativity	1+ Billion
115.	Moran Autocorrelation of Lag 3 Weighted by Sanderson Electronegativity	1+ Billion
116.	Moran Autocorrelation of Lag 4 Weighted by Sanderson Electronegativity	1+ Billion
117.	Moran Autocorrelation of Lag 5 Weighted by Sanderson Electronegativity	1+ Billion
118.	Moran Autocorrelation of Lag 6 Weighted by Sanderson Electronegativity	1+ Billion
119.	Moran Autocorrelation of Lag 7 Weighted by Sanderson Electronegativity	1+ Billion
120.	Moran Autocorrelation of Lag 8 Weighted by Sanderson Electronegativity	1+ Billion
121.	Moran Autocorrelation of Lag 1 Weighted by Polarizability	1+ Billion
122.	Moran Autocorrelation of Lag 2 Weighted by Polarizability	1+ Billion
123.	Moran Autocorrelation of Lag 3 Weighted by Polarizability	1+ Billion



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124. Moran Autocorrelation of Lag 4 Weighted by Polarizability	1+ Billion
125. Moran Autocorrelation of Lag 5 Weighted by Polarizability	1+ Billion
126. Moran Autocorrelation of Lag 6 Weighted by Polarizability	1+ Billion
127. Moran Autocorrelation of Lag 7 Weighted by Polarizability	1+ Billion
128. Moran Autocorrelation of Lag 8 Weighted by Polarizability	1+ Billion
129. Moran Autocorrelation of Lag 1 Weighted by Ionization Potential	1+ Billion
130. Moran Autocorrelation of Lag 2 Weighted by Ionization Potential	1+ Billion
131. Moran Autocorrelation of Lag 3 Weighted by Ionization Potential	1+ Billion
132. Moran Autocorrelation of Lag 4 Weighted by Ionization Potential	1+ Billion
133. Moran Autocorrelation of Lag 5 Weighted by Ionization Potential	1+ Billion
134. Moran Autocorrelation of Lag 6 Weighted by Ionization Potential	1+ Billion
135. Moran Autocorrelation of Lag 7 Weighted by Ionization Potential	1+ Billion
136. Moran Autocorrelation of Lag 8 Weighted by Ionization Potential	1+ Billion
137. Moran Autocorrelation of Lag 1 Weighted by I-State	1+ Billion
138. Moran Autocorrelation of Lag 2 Weighted by I-State	1+ Billion
139. Moran Autocorrelation of Lag 3 Weighted by I-State	1+ Billion
140. Moran Autocorrelation of Lag 4 Weighted by I-State	1+ Billion
141. Moran Autocorrelation of Lag 5 Weighted by I-State	1+ Billion
142. Moran Autocorrelation of Lag 6 Weighted by I-State	1+ Billion
143. Moran Autocorrelation of Lag 7 Weighted by I-State	1+ Billion
144. Moran Autocorrelation of Lag 8 Weighted by I-State	1+ Billion
145. Geary Autocorrelation of Lag 1 Weighted by Mass	1+ Billion
146. Geary Autocorrelation of Lag 2 Weighted by Mass	1+ Billion
147. Geary Autocorrelation of Lag 3 Weighted by Mass	1+ Billion
148. Geary Autocorrelation of Lag 4 Weighted by Mass	1+ Billion
149. Geary Autocorrelation of Lag 5 Weighted by Mass	1+ Billion



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150.	Geary Autocorrelation of Lag 6 Weighted by Mass	1+ Billion
151.	Geary Autocorrelation of Lag 7 Weighted by Mass	1+ Billion
152.	Geary Autocorrelation of Lag 8 Weighted by Mass	1+ Billion
153.	Geary Autocorrelation of Lag 1 Weighted by van der Waals Volume	1+ Billion
154.	Geary Autocorrelation of Lag 2 Weighted by van der Waals Volume	1+ Billion
155.	Geary Autocorrelation of Lag 3 Weighted by van der Waals Volume	1+ Billion
156.	Geary Autocorrelation of Lag 4 Weighted by van der Waals Volume	1+ Billion
157.	Geary Autocorrelation of Lag 5 Weighted by van der Waals Volume	1+ Billion
158.	Geary Autocorrelation of Lag 6 Weighted by van der Waals Volume	1+ Billion
159.	Geary Autocorrelation of Lag 7 Weighted by van der Waals Volume	1+ Billion
160.	Geary Autocorrelation of Lag 8 Weighted by van der Waals Volume	1+ Billion
161.	Geary Autocorrelation of Lag 1 Weighted by Sanderson Electronegativity	1+ Billion
162.	Geary Autocorrelation of Lag 2 Weighted by Sanderson Electronegativity	1+ Billion
163.	Geary Autocorrelation of Lag 3 Weighted by Sanderson Electronegativity	1+ Billion
164.	Geary Autocorrelation of Lag 4 Weighted by Sanderson Electronegativity	1+ Billion
165.	Geary Autocorrelation of Lag 5 Weighted by Sanderson Electronegativity	1+ Billion
166.	Geary Autocorrelation of Lag 6 Weighted by Sanderson Electronegativity	1+ Billion
167.	Geary Autocorrelation of Lag 7 Weighted by Sanderson Electronegativity	1+ Billion
168.	Geary Autocorrelation of Lag 8 Weighted by Sanderson Electronegativity	1+ Billion
169.	Geary Autocorrelation of Lag 1 Weighted by Polarizability	1+ Billion
170.	Geary Autocorrelation of Lag 2 Weighted by Polarizability	1+ Billion
171.	Geary Autocorrelation of Lag 3 Weighted by Polarizability	1+ Billion
172.	Geary Autocorrelation of Lag 4 Weighted by Polarizability	1+ Billion
173.	Geary Autocorrelation of Lag 5 Weighted by Polarizability	1+ Billion
174.	Geary Autocorrelation of Lag 6 Weighted by Polarizability	1+ Billion
175.	Geary Autocorrelation of Lag 7 Weighted by Polarizability	1+ Billion



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176.	Geary Autocorrelation of Lag 8 Weighted by Polarizability	1+ Billion
177.	Geary Autocorrelation of Lag 1 Weighted by Ionization Potential	1+ Billion
178.	Geary Autocorrelation of Lag 2 Weighted by Ionization Potential	1+ Billion
179.	Geary Autocorrelation of Lag 3 Weighted by Ionization Potential	1+ Billion
180.	Geary Autocorrelation of Lag 4 Weighted by Ionization Potential	1+ Billion
181.	Geary Autocorrelation of Lag 5 Weighted by Ionization Potential	1+ Billion
182.	Geary Autocorrelation of Lag 6 Weighted by Ionization Potential	1+ Billion
183.	Geary Autocorrelation of Lag 7 Weighted by Ionization Potential	1+ Billion
184.	Geary Autocorrelation of Lag 8 Weighted by Ionization Potential	1+ Billion
185.	Geary Autocorrelation of Lag 1 Weighted by I-State	1+ Billion
186.	Geary Autocorrelation of Lag 2 Weighted by I-State	1+ Billion
187.	Geary Autocorrelation of Lag 3 Weighted by I-State	1+ Billion
188.	Geary Autocorrelation of Lag 4 Weighted by I-State	1+ Billion
189.	Geary Autocorrelation of Lag 5 Weighted by I-State	1+ Billion
190.	Geary Autocorrelation of Lag 6 Weighted by I-State	1+ Billion
191.	Geary Autocorrelation of Lag 7 Weighted by I-State	1+ Billion
192.	Geary Autocorrelation of Lag 8 Weighted by I-State	1+ Billion
193.	Topological Charge Index of Order 1	1+ Billion
194.	Topological Charge Index of Order 2	1+ Billion
195.	Topological Charge Index of Order 3	1+ Billion
196.	Topological Charge Index of Order 4	1+ Billion
197.	Topological Charge Index of Order 5	1+ Billion
198.	Topological Charge Index of Order 6	1+ Billion
199.	Topological Charge Index of Order 7	1+ Billion
200.	Topological Charge Index of Order 8	1+ Billion
201.	Topological Charge Index of Order 9	1+ Billion



1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

202. Topological Charge Index of Order 101+ Billion203. Mean Topological Charge Index of Order 11+ Billion204. Mean Topological Charge Index of Order 21+ Billion205. Mean Topological Charge Index of Order 31+ Billion206. Mean Topological Charge Index of Order 41+ Billion207. Mean Topological Charge Index of Order 51+ Billion208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion213. Global Topological Charge Index1+ Billion		
204. Mean Topological Charge Index of Order 21+ Billion205. Mean Topological Charge Index of Order 31+ Billion206. Mean Topological Charge Index of Order 41+ Billion207. Mean Topological Charge Index of Order 51+ Billion208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	202. Topological Charge Index of Order 10	1+ Billion
205. Mean Topological Charge Index of Order 31+ Billion206. Mean Topological Charge Index of Order 41+ Billion207. Mean Topological Charge Index of Order 51+ Billion208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	203. Mean Topological Charge Index of Order 1	1+ Billion
206. Mean Topological Charge Index of Order 41+ Billion207. Mean Topological Charge Index of Order 51+ Billion208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	204. Mean Topological Charge Index of Order 2	1+ Billion
207. Mean Topological Charge Index of Order 51+ Billion208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	205. Mean Topological Charge Index of Order 3	1+ Billion
208. Mean Topological Charge Index of Order 61+ Billion209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	206. Mean Topological Charge Index of Order 4	1+ Billion
209. Mean Topological Charge Index of Order 71+ Billion210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	207. Mean Topological Charge Index of Order 5	1+ Billion
210. Mean Topological Charge Index of Order 81+ Billion211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	208. Mean Topological Charge Index of Order 6	1+ Billion
211. Mean Topological Charge Index of Order 91+ Billion212. Mean Topological Charge Index of Order 101+ Billion	209. Mean Topological Charge Index of Order 7	1+ Billion
212. Mean Topological Charge Index of Order 101+ Billion	210. Mean Topological Charge Index of Order 8	1+ Billion
	211. Mean Topological Charge Index of Order 9	1+ Billion
213. Global Topological Charge Index1+ Billion	212. Mean Topological Charge Index of Order 10	1+ Billion
	213. Global Topological Charge Index	1+ Billion

# **Burden Eigenvalue Descriptors (96)**

	Burden Eigenvalue Descriptors	Number of Compounds
1.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by Mass	1+ Billion
2.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by Mass	1+ Billion
3.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by Mass	1+ Billion
4.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by Mass	1+ Billion
5.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by Mass	1+ Billion
6.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by Mass	1+ Billion
7.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by Mass	1+ Billion
8.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by Mass	1+ Billion



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9.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
10.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
11.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
12.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
13.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
14.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
15.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
16.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
17.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
18.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
19.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
20.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
21.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
22.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
23.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
24.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
25.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by Polarizability	1+ Billion
26.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by Polarizability	1+ Billion
27.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by Polarizability	1+ Billion
28.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by Polarizability	1+ Billion
29.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by Polarizability	1+ Billion
30.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by Polarizability	1+ Billion
31.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by Polarizability	1+ Billion
32.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by Polarizability	1+ Billion
33.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by Ionization Potential	1+ Billion
34.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by Ionization Potential	1+ Billion

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35.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by Ionization Potential	1+ Billion
36.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by Ionization Potential	1+ Billion
37.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by Ionization Potential	1+ Billion
38.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by Ionization Potential	1+ Billion
39.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by Ionization Potential	1+ Billion
40.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by Ionization Potential	1+ Billion
41.	Largest Eigenvalue n. 1 of Burden Matrix Weighted by I-State	1+ Billion
42.	Largest Eigenvalue n. 2 of Burden Matrix Weighted by I-State	1+ Billion
43.	Largest Eigenvalue n. 3 of Burden Matrix Weighted by I-State	1+ Billion
44.	Largest Eigenvalue n. 4 of Burden Matrix Weighted by I-State	1+ Billion
45.	Largest Eigenvalue n. 5 of Burden Matrix Weighted by I-State	1+ Billion
46.	Largest Eigenvalue n. 6 of Burden Matrix Weighted by I-State	1+ Billion
47.	Largest Eigenvalue n. 7 of Burden Matrix Weighted by I-State	1+ Billion
48.	Largest Eigenvalue n. 8 of Burden Matrix Weighted by I-State	1+ Billion
49.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by Mass	1+ Billion
50.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by Mass	1+ Billion
51.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by Mass	1+ Billion
52.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by Mass	1+ Billion
53.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by Mass	1+ Billion
54.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by Mass	1+ Billion
55.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by Mass	1+ Billion
56.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by Mass	1+ Billion
57.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
58.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
59.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
60.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by van der Waals Volume	1+ Billion



61.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
62.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
63.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
64.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by van der Waals Volume	1+ Billion
65.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
66.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
67.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
68.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
69.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
70.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
71.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
72.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by Sanderson Electronegativity	1+ Billion
73.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by Polarizability	1+ Billion
74.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by Polarizability	1+ Billion
75.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by Polarizability	1+ Billion
76.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by Polarizability	1+ Billion
77.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by Polarizability	1+ Billion
78.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by Polarizability	1+ Billion
79.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by Polarizability	1+ Billion
80.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by Polarizability	1+ Billion
81.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by Ionization Potential	1+ Billion
82.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by Ionization Potential	1+ Billion
83.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by Ionization Potential	1+ Billion
84.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by Ionization Potential	1+ Billion
85.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by Ionization Potential	1+ Billion
86.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by Ionization Potential	1+ Billion



1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chernessen.com

87.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by Ionization Potential	1+ Billion
88.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by Ionization Potential	1+ Billion
89.	Smallest Eigenvalue n. 1 of Burden Matrix Weighted by I-State	1+ Billion
90.	Smallest Eigenvalue n. 2 of Burden Matrix Weighted by I-State	1+ Billion
91.	Smallest Eigenvalue n. 3 of Burden Matrix Weighted by I-State	1+ Billion
92.	Smallest Eigenvalue n. 4 of Burden Matrix Weighted by I-State	1+ Billion
93.	Smallest Eigenvalue n. 5 of Burden Matrix Weighted by I-State	1+ Billion
94.	Smallest Eigenvalue n. 6 of Burden Matrix Weighted by I-State	1+ Billion
95.	Smallest Eigenvalue n. 7 of Burden Matrix Weighted by I-State	1+ Billion
96.	Smallest Eigenvalue n. 8 of Burden Matrix Weighted by I-State	1+ Billion

# ▶ P\_VSA-Like Descriptors (45)

	P_VSA-Like Descriptors	Number of Compounds
1.	P_VSA-Like on LogP, Bin 1	1+ Billion
2.	P_VSA-Like on LogP, Bin 2	1+ Billion
3.	P_VSA-Like on LogP, Bin 3	1+ Billion
4.	P_VSA-Like on LogP, Bin 4	1+ Billion
5.	P_VSA-Like on LogP, Bin 5	1+ Billion
6.	P_VSA-Like on LogP, Bin 6	1+ Billion
7.	P_VSA-Like on LogP, Bin 7	1+ Billion
8.	P_VSA-Like on LogP, Bin 8	1+ Billion
9.	P_VSA-Like on Molar Refractivity, Bin 1	1+ Billion
10.	P_VSA-Like on Molar Refractivity, Bin 2	1+ Billion



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11.	P_VSA-Like on Molar Refractivity, Bin 3	1+ Billion
12.	P_VSA-Like on Molar Refractivity, Bin 4	1+ Billion
13.	P_VSA-Like on Molar Refractivity, Bin 5	1+ Billion
14.	P_VSA-Like on Molar Refractivity, Bin 6	1+ Billion
15.	P_VSA-Like on Molar Refractivity, Bin 7	1+ Billion
16.	P_VSA-Like on Molar Refractivity, Bin 8	1+ Billion
17.	P_VSA-Like on Mass, Bin 1	1+ Billion
18.	P_VSA-Like on Mass, Bin 2	1+ Billion
19.	P_VSA-Like on Mass, Bin 3	1+ Billion
20.	P_VSA-Like on Mass, Bin 4	1+ Billion
21.	P_VSA-Like on Mass, Bin 5	1+ Billion
22.	P_VSA-Like on van der Waals Volume, Bin 1	1+ Billion
23.	P_VSA-Like on van der Waals Volume, Bin 2	1+ Billion
24.	P_VSA-Like on van der Waals Volume, Bin 3	1+ Billion
25.	P_VSA-Like on van der Waals Volume, Bin 4	1+ Billion
26.	P_VSA-Like on Sanderson Electronegativity, Bin 1	1+ Billion
27.	P_VSA-Like on Sanderson Electronegativity, Bin 2	1+ Billion
28.	P_VSA-Like on Sanderson Electronegativity, Bin 3	1+ Billion
29.	P_VSA-Like on Sanderson Electronegativity, Bin 4	1+ Billion
30.	P_VSA-Like on Sanderson Electronegativity, Bin 5	1+ Billion
31.	P_VSA-Like on Sanderson Electronegativity, Bin 6	1+ Billion
32.	P_VSA-Like on Polarizability, Bin 1	1+ Billion
33.	P_VSA-Like on Polarizability, Bin 2	1+ Billion
34.	P_VSA-Like on Polarizability, Bin 3	1+ Billion
35.	P_VSA-Like on Polarizability, Bin 4	1+ Billion
36.	P_VSA-Like on Ionization Potential, Bin 1	1+ Billion





1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

37.	P_VSA-Like on Ionization Potential, Bin 2	1+ Billion
38.	P_VSA-Like on Ionization Potential, Bin 3	1+ Billion
39.	P_VSA-Like on Ionization Potential, Bin 4	1+ Billion
40.	P_VSA-Like on I-State, Bin 1	1+ Billion
41.	P_VSA-Like on I-State, Bin 2	1+ Billion
42.	P_VSA-Like on I-State, Bin 3	1+ Billion
43.	P_VSA-Like on I-State, Bin 4	1+ Billion
44.	P_VSA-Like on I-State, Bin 5	1+ Billion
45.	P_VSA-Like on I-State, Bin 6	1+ Billion

# **ETA Indices (23)**

	ETA Indices	Number of Compounds
1.	ETA Core Count	1+ Billion
2.	ETA Average Core Count	1+ Billion
3.	ETA Electronegativity Measure	1+ Billion
4.	ETA Average Electronegativity Measure	1+ Billion
5.	ETA Sigma VEM Count	1+ Billion
6.	ETA Sigma Average VEM Count	1+ Billion
7.	ETA Pi And Lone Pair VEM Count	1+ Billion
8.	ETA Pi And Lone Pair Average VEM Count	1+ Billion
9.	ETA VEM Count	1+ Billion
10.	ETA Average VEM Count	1+ Billion



11.	ETA Composite Index	1+ Billion
12.	ETA Average Composite Index	1+ Billion
13.	ETA Local Composite Index	1+ Billion
14.	ETA Average Local Composite Index	1+ Billion
15.	ETA Functionality Index	1+ Billion
16.	ETA Average Functionality Index	1+ Billion
17.	ETA Local Functionality Index	1+ Billion
18.	ETA Average Local Functionality Index	1+ Billion
19.	ETA Branching Index	1+ Billion
20.	ETA Average Branching Index	1+ Billion
21.	ETA P Shape Index	1+ Billion
22.	ETA Y Shape Index	1+ Billion
23.	ETA X Shape Index	1+ Billion

# ► Edge Adjacency Indices (324)

	Edge Adjacency Indices	Number of Compounds
1.	Leading Eigenvalue from Edge Adjacency Mat.	1+ Billion
2.	Normalized Leading Eigenvalue from Edge Adjacency Mat.	1+ Billion
3.	Spectral Diameter from Edge Adjacency Mat.	1+ Billion
4.	Spectral Absolute Deviation from Edge Adjacency Mat.	1+ Billion
5.	Spectral Mean Absolute Deviation from Edge Adjacency Mat.	1+ Billion
6.	Leading Eigenvalue from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
7.	Normalized Leading Eigenvalue from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion

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8.	Spectral Diameter from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
9.	Spectral Absolute Deviation from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
10.	Spectral Mean Absolute Deviation from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
11.	Leading Eigenvalue from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
12.	Normalized Leading Eigenvalue from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
13.	Spectral Diameter from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
14.	Spectral Absolute Deviation from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
15.	Spectral Mean Absolute Deviation from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
16.	Leading Eigenvalue from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
17.	Normalized Leading Eigenvalue from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
18.	Spectral Diameter from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
19.	Spectral Absolute Deviation from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
20.	Spectral Mean Absolute Deviation from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
21.	Leading Eigenvalue from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
22.	Normalized Leading Eigenvalue from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
23.	Spectral Diameter from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
24.	Spectral Absolute Deviation from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
25.	Spectral Mean Absolute Deviation from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
26.	Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
27.	Normalized Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
28.	Spectral Diameter from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
29.	Spectral Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
30.	Spectral Mean Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
31.	Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
32.	Normalized Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
33.	Spectral Diameter from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion



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34.	Spectral Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
35.	Spectral Mean Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
36.	Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
37.	Normalized Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
38.	Spectral Diameter from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
39.	Spectral Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
40.	Spectral Mean Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
41.	Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
42.	Normalized Leading Eigenvalue from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
43.	Spectral Diameter from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
44.	Spectral Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
45.	Spectral Mean Absolute Deviation from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
46.	Connectivity-Like Index of Order 0 from Edge Adjacency Mat.	1+ Billion
47.	Connectivity-Like Index of Order 1 from Edge Adjacency Mat.	1+ Billion
48.	Connectivity-Like Index of Order 0 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
49.	Connectivity-Like Index of Order 1 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
50.	Connectivity-Like Index of Order 0 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
51.	Connectivity-Like Index of Order 1 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
52.	Connectivity-Like Index of Order 0 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
53.	Connectivity-Like Index of Order 1 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
54.	Connectivity-Like Index of Order 0 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
55.	Connectivity-Like Index of Order 1 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
56.	Connectivity-Like Index of Order 0 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
57.	Connectivity-Like Index of Order 1 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
58.	Connectivity-Like Index of Order 0 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
59.	Connectivity-Like Index of Order 1 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion



ChemEssen, Inc.

1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

60.	Connectivity-Like Index of Order 0 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
61.	Connectivity-Like Index of Order 1 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
62.	Connectivity-Like Index of Order 0 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
63.	Connectivity-Like Index of Order 1 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
64.	Spectral Moment of Order 2 from Edge Adjacency Mat.	1+ Billion
65.	Spectral Moment of Order 3 from Edge Adjacency Mat.	1+ Billion
66.	Spectral Moment of Order 4 from Edge Adjacency Mat.	1+ Billion
67.	Spectral Moment of Order 5 from Edge Adjacency Mat.	1+ Billion
68.	Spectral Moment of Order 6 from Edge Adjacency Mat.	1+ Billion
69.	Spectral Moment of Order 7 from Edge Adjacency Mat.	1+ Billion
70.	Spectral Moment of Order 8 from Edge Adjacency Mat.	1+ Billion
71.	Spectral Moment of Order 9 from Edge Adjacency Mat.	1+ Billion
72.	Spectral Moment of Order 10 from Edge Adjacency Mat.	1+ Billion
73.	Spectral Moment of Order 11 from Edge Adjacency Mat.	1+ Billion
74.	Spectral Moment of Order 12 from Edge Adjacency Mat.	1+ Billion
75.	Spectral Moment of Order 13 from Edge Adjacency Mat.	1+ Billion
76.	Spectral Moment of Order 14 from Edge Adjacency Mat.	1+ Billion
77.	Spectral Moment of Order 15 from Edge Adjacency Mat.	1+ Billion
78.	Spectral Moment of Order 2 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
79.	Spectral Moment of Order 3 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
80.	Spectral Moment of Order 4 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
81.	Spectral Moment of Order 5 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
82.	Spectral Moment of Order 6 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
83.	Spectral Moment of Order 7 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
84.	Spectral Moment of Order 8 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
85.	Spectral Moment of Order 9 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion

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86.	Spectral Moment of Order 10 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
87.	Spectral Moment of Order 11 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
88.	Spectral Moment of Order 12 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
89.	Spectral Moment of Order 13 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
90.	Spectral Moment of Order 14 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
91.	Spectral Moment of Order 15 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
92.	Spectral Moment of Order 2 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
93.	Spectral Moment of Order 3 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
94.	Spectral Moment of Order 4 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
95.	Spectral Moment of Order 5 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
96.	Spectral Moment of Order 6 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
97.	Spectral Moment of Order 7 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
98.	Spectral Moment of Order 8 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
99.	Spectral Moment of Order 9 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
100.	Spectral Moment of Order 10 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
101.	Spectral Moment of Order 11 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
102.	Spectral Moment of Order 12 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
103.	Spectral Moment of Order 13 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
104.	Spectral Moment of Order 14 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
105.	Spectral Moment of Order 15 from Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
106.	Spectral Moment of Order 2 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
107.	Spectral Moment of Order 3 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
108.	Spectral Moment of Order 4 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
109.	Spectral Moment of Order 5 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
110.	Spectral Moment of Order 6 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
111.	Spectral Moment of Order 7 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion



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112. Spectral Moment of Order 8 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
113. Spectral Moment of Order 9 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
114. Spectral Moment of Order 10 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
115. Spectral Moment of Order 11 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
116. Spectral Moment of Order 12 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
117. Spectral Moment of Order 13 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
118. Spectral Moment of Order 14 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
119. Spectral Moment of Order 15 from Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
120. Spectral Moment of Order 2 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
121. Spectral Moment of Order 3 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
122. Spectral Moment of Order 4 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
123. Spectral Moment of Order 5 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
124. Spectral Moment of Order 6 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
125. Spectral Moment of Order 7 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
126. Spectral Moment of Order 8 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
127. Spectral Moment of Order 9 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
128. Spectral Moment of Order 10 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
129. Spectral Moment of Order 11 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
130. Spectral Moment of Order 12 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
131. Spectral Moment of Order 13 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
132. Spectral Moment of Order 14 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
133. Spectral Moment of Order 15 from Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
134. Spectral Moment of Order 2 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
135. Spectral Moment of Order 3 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
136. Spectral Moment of Order 4 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
137. Spectral Moment of Order 5 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion



138. Spectral Moment of Order 6 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
139. Spectral Moment of Order 7 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
140. Spectral Moment of Order 8 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
141. Spectral Moment of Order 9 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
142. Spectral Moment of Order 10 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
143. Spectral Moment of Order 11 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
144. Spectral Moment of Order 12 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
145. Spectral Moment of Order 13 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
146. Spectral Moment of Order 14 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
147. Spectral Moment of Order 15 from Augmented Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
148. Spectral Moment of Order 2 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
149. Spectral Moment of Order 3 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
150. Spectral Moment of Order 4 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
151. Spectral Moment of Order 5 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
152. Spectral Moment of Order 6 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
153. Spectral Moment of Order 7 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
154. Spectral Moment of Order 8 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
155. Spectral Moment of Order 9 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
156. Spectral Moment of Order 10 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
157. Spectral Moment of Order 11 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
158. Spectral Moment of Order 12 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
159. Spectral Moment of Order 13 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
160. Spectral Moment of Order 14 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
161. Spectral Moment of Order 15 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
162. Spectral Moment of Order 2 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
163. Spectral Moment of Order 3 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion



164. Spectral Moment of Order 4 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
165. Spectral Moment of Order 5 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
166. Spectral Moment of Order 6 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
167. Spectral Moment of Order 7 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
168. Spectral Moment of Order 8 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
169. Spectral Moment of Order 9 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
170. Spectral Moment of Order 10 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
171. Spectral Moment of Order 11 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
172. Spectral Moment of Order 12 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
173. Spectral Moment of Order 13 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
174. Spectral Moment of Order 14 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
175. Spectral Moment of Order 15 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
176. Spectral Moment of Order 2 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
177. Spectral Moment of Order 3 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
178. Spectral Moment of Order 4 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
179. Spectral Moment of Order 5 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
180. Spectral Moment of Order 6 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
181. Spectral Moment of Order 7 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
182. Spectral Moment of Order 8 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
183. Spectral Moment of Order 9 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
184. Spectral Moment of Order 10 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
185. Spectral Moment of Order 11 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
186. Spectral Moment of Order 12 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
187. Spectral Moment of Order 13 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
188. Spectral Moment of Order 14 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
189. Spectral Moment of Order 15 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion



190. Eigenvalue n. 1 from Edge Adjacency Mat.	1+ Billion
191. Eigenvalue n. 2 from Edge Adjacency Mat.	1+ Billion
192. Eigenvalue n. 3 from Edge Adjacency Mat.	1+ Billion
193. Eigenvalue n. 4 from Edge Adjacency Mat.	1+ Billion
194. Eigenvalue n. 5 from Edge Adjacency Mat.	1+ Billion
195. Eigenvalue n. 6 from Edge Adjacency Mat.	1+ Billion
196. Eigenvalue n. 7 from Edge Adjacency Mat.	1+ Billion
197. Eigenvalue n. 8 from Edge Adjacency Mat.	1+ Billion
198. Eigenvalue n. 9 from Edge Adjacency Mat.	1+ Billion
199. Eigenvalue n. 10 from Edge Adjacency Mat.	1+ Billion
200. Eigenvalue n. 11 from Edge Adjacency Mat.	1+ Billion
201. Eigenvalue n. 12 from Edge Adjacency Mat.	1+ Billion
202. Eigenvalue n. 13 from Edge Adjacency Mat.	1+ Billion
203. Eigenvalue n. 14 from Edge Adjacency Mat.	1+ Billion
204. Eigenvalue n. 15 from Edge Adjacency Mat.	1+ Billion
205. Eigenvalue n. 1 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
206. Eigenvalue n. 2 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
207. Eigenvalue n. 3 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
208. Eigenvalue n. 4 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
209. Eigenvalue n. 5 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
210. Eigenvalue n. 6 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
211. Eigenvalue n. 7 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
212. Eigenvalue n. 8 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
213. Eigenvalue n. 9 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
214. Eigenvalue n. 10 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion
215. Eigenvalue n. 11 from Edge Adjacency Mat. Weighted by Edge Degree	1+ Billion



ChemEssen, Inc.

1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

216. Eigenvalue n. 12 from Edge Adjacency Mat. Weighted by Edge Degree 217. Eigenvalue n. 13 from Edge Adjacency Mat. Weighted by Edge Degree 218. Eigenvalue n. 14 from Edge Adjacency Mat. Weighted by Edge Degree 219. Eigenvalue n. 15 from Edge Adjacency Mat. Weighted by Edge Degree 220. Eigenvalue n. 1 from Edge Adjacency Mat. Weighted by Bond Order 221. Eigenvalue n. 2 from Edge Adjacency Mat. Weighted by Bond Order 222. Eigenvalue n. 3 from Edge Adjacency Mat. Weighted by Bond Order 223. Eigenvalue n. 4 from Edge Adjacency Mat. Weighted by Bond Order 224. Eigenvalue n. 5 from Edge Adjacency Mat. Weighted by Bond Order 225. Eigenvalue n. 6 from Edge Adjacency Mat. Weighted by Bond Order 226. Eigenvalue n. 7 from Edge Adjacency Mat. Weighted by Bond Order 227. Eigenvalue n. 8 from Edge Adjacency Mat. Weighted by Bond Order 228. Eigenvalue n. 9 from Edge Adjacency Mat. Weighted by Bond Order 229. Eigenvalue n. 10 from Edge Adjacency Mat. Weighted by Bond Order 230. Eigenvalue n. 11 from Edge Adjacency Mat. Weighted by Bond Order 231. Eigenvalue n. 12 from Edge Adjacency Mat. Weighted by Bond Order 232. Eigenvalue n. 13 from Edge Adjacency Mat. Weighted by Bond Order 233. Eigenvalue n. 14 from Edge Adjacency Mat. Weighted by Bond Order 234. Eigenvalue n. 15 from Edge Adjacency Mat. Weighted by Bond Order 235. Eigenvalue n. 1 from Edge Adjacency Mat. Weighted by Dipole Moment 236. Eigenvalue n. 2 from Edge Adjacency Mat. Weighted by Dipole Moment 237. Eigenvalue n. 3 from Edge Adjacency Mat. Weighted by Dipole Moment 238. Eigenvalue n. 4 from Edge Adjacency Mat. Weighted by Dipole Moment 239. Eigenvalue n. 5 from Edge Adjacency Mat. Weighted by Dipole Moment 240. Eigenvalue n. 6 from Edge Adjacency Mat. Weighted by Dipole Moment 241. Eigenvalue n. 7 from Edge Adjacency Mat. Weighted by Dipole Moment

1+ Billion
1+ Billion



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242. Eigenvalue n. 8 from Edge Adjacency Mat. Weighted by Dipole Moment
243. Eigenvalue n. 9 from Edge Adjacency Mat. Weighted by Dipole Moment
244. Eigenvalue n. 10 from Edge Adjacency Mat. Weighted by Dipole Moment
245. Eigenvalue n. 11 from Edge Adjacency Mat. Weighted by Dipole Moment
246. Eigenvalue n. 12 from Edge Adjacency Mat. Weighted by Dipole Moment
247. Eigenvalue n. 13 from Edge Adjacency Mat. Weighted by Dipole Moment
248. Eigenvalue n. 14 from Edge Adjacency Mat. Weighted by Dipole Moment
249. Eigenvalue n. 15 from Edge Adjacency Mat. Weighted by Dipole Moment
250. Eigenvalue n. 1 from Edge Adjacency Mat. Weighted by Resonance Integral
251. Eigenvalue n. 2 from Edge Adjacency Mat. Weighted by Resonance Integral
252. Eigenvalue n. 3 from Edge Adjacency Mat. Weighted by Resonance Integral
253. Eigenvalue n. 4 from Edge Adjacency Mat. Weighted by Resonance Integral
254. Eigenvalue n. 5 from Edge Adjacency Mat. Weighted by Resonance Integral
255. Eigenvalue n. 6 from Edge Adjacency Mat. Weighted by Resonance Integral
256. Eigenvalue n. 7 from Edge Adjacency Mat. Weighted by Resonance Integral
257. Eigenvalue n. 8 from Edge Adjacency Mat. Weighted by Resonance Integral
258. Eigenvalue n. 9 from Edge Adjacency Mat. Weighted by Resonance Integral
259. Eigenvalue n. 10 from Edge Adjacency Mat. Weighted by Resonance Integral
260. Eigenvalue n. 11 from Edge Adjacency Mat. Weighted by Resonance Integral
261. Eigenvalue n. 12 from Edge Adjacency Mat. Weighted by Resonance Integral
262. Eigenvalue n. 13 from Edge Adjacency Mat. Weighted by Resonance Integral
263. Eigenvalue n. 14 from Edge Adjacency Mat. Weighted by Resonance Integral
264. Eigenvalue n. 15 from Edge Adjacency Mat. Weighted by Resonance Integral
265. Eigenvalue n. 1 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
266. Eigenvalue n. 2 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
267. Eigenvalue n. 3 from Augmented Edge Adjacency Mat. Weighted by Edge Degree

1+ Billion
1+ Billion



ChemEssen, Inc.

1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

1+ Billion 1+ Billion

268. Eigenvalue n. 4 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
269. Eigenvalue n. 5 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
270. Eigenvalue n. 6 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
271. Eigenvalue n. 7 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
272. Eigenvalue n. 8 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
273. Eigenvalue n. 9 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
274. Eigenvalue n. 10 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
275. Eigenvalue n. 11 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
276. Eigenvalue n. 12 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
277. Eigenvalue n. 13 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
278. Eigenvalue n. 14 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
279. Eigenvalue n. 15 from Augmented Edge Adjacency Mat. Weighted by Edge Degree
280. Eigenvalue n. 1 from Augmented Edge Adjacency Mat. Weighted by Bond Order
281. Eigenvalue n. 2 from Augmented Edge Adjacency Mat. Weighted by Bond Order
282. Eigenvalue n. 3 from Augmented Edge Adjacency Mat. Weighted by Bond Order
283. Eigenvalue n. 4 from Augmented Edge Adjacency Mat. Weighted by Bond Order
284. Eigenvalue n. 5 from Augmented Edge Adjacency Mat. Weighted by Bond Order
285. Eigenvalue n. 6 from Augmented Edge Adjacency Mat. Weighted by Bond Order
286. Eigenvalue n. 7 from Augmented Edge Adjacency Mat. Weighted by Bond Order
287. Eigenvalue n. 8 from Augmented Edge Adjacency Mat. Weighted by Bond Order
288. Eigenvalue n. 9 from Augmented Edge Adjacency Mat. Weighted by Bond Order
289. Eigenvalue n. 10 from Augmented Edge Adjacency Mat. Weighted by Bond Order
290. Eigenvalue n. 11 from Augmented Edge Adjacency Mat. Weighted by Bond Order
291. Eigenvalue n. 12 from Augmented Edge Adjacency Mat. Weighted by Bond Order
292. Eigenvalue n. 13 from Augmented Edge Adjacency Mat. Weighted by Bond Order
293. Eigenvalue n. 14 from Augmented Edge Adjacency Mat. Weighted by Bond Order



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294. Eigenvalue n. 15 from Augmented Edge Adjacency Mat. Weighted by Bond Order	1+ Billion
295. Eigenvalue n. 1 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
296. Eigenvalue n. 2 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
297. Eigenvalue n. 3 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
298. Eigenvalue n. 4 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
299. Eigenvalue n. 5 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
300. Eigenvalue n. 6 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
301. Eigenvalue n. 7 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
302. Eigenvalue n. 8 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
303. Eigenvalue n. 9 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
304. Eigenvalue n. 10 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
305. Eigenvalue n. 11 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
306. Eigenvalue n. 12 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
307. Eigenvalue n. 13 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
308. Eigenvalue n. 14 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
309. Eigenvalue n. 15 from Augmented Edge Adjacency Mat. Weighted by Dipole Moment	1+ Billion
310. Eigenvalue n. 1 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
311. Eigenvalue n. 2 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
312. Eigenvalue n. 3 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
313. Eigenvalue n. 4 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
314. Eigenvalue n. 5 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
315. Eigenvalue n. 6 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
316. Eigenvalue n. 7 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
317. Eigenvalue n. 8 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
318. Eigenvalue n. 9 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
319. Eigenvalue n. 10 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion



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320. Eigenvalue n. 11 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
321. Eigenvalue n. 12 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
322. Eigenvalue n. 13 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
323. Eigenvalue n. 14 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion
324. Eigenvalue n. 15 from Augmented Edge Adjacency Mat. Weighted by Resonance Integral	1+ Billion

# Functional Group Counts (155)

	Functional Group Counts	Number of Compounds
1.	Number of Terminal Primary C(sp3)	1+ Billion
2.	Number of Total Secondary C(sp3)	1+ Billion
3.	Number of Total Tertiary C(sp3)	1+ Billion
4.	Number of Total Quaternary C(sp3)	1+ Billion
5.	Number of Ring Secondary C(sp3)	1+ Billion
6.	Number of Ring Tertiary C(sp3)	1+ Billion
7.	Number of Ring Quaternary C(sp3)	1+ Billion
8.	Number of Aromatic C(sp2)	1+ Billion
9.	Number of Unsubstituted Benzene C(sp2)	1+ Billion
10.	Number of Substituted Benzene C(sp2)	1+ Billion
11.	Number of Non-Aromatic Conjugated C(sp2)	1+ Billion
12.	Number of Terminal Primary C(sp2)	1+ Billion
13.	Number of Aliphatic Secondary C(sp2)	1+ Billion
14.	Number of Aliphatic Tertiary C(sp2)	1+ Billion
15.	Number of Allenes Groups	1+ Billion



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16.	Number of Terminal C(sp)	1+ Billion
17.	Number of Non-Terminal C(sp)	1+ Billion
18.	Number of Cyanates (Aliphatic)	1+ Billion
19.	Number of Cyanates (Aromatic)	1+ Billion
20.	Number of Isocyanates (Aliphatic)	1+ Billion
21.	Number of Isocyanates (Aromatic)	1+ Billion
22.	Number of Thiocyanates (Aliphatic)	1+ Billion
23.	Number of Thiocyanates (Aromatic)	1+ Billion
24.	Number of Isothiocyanates (Aliphatic)	1+ Billion
25.	Number of Isothiocyanates (Aromatic)	1+ Billion
26.	Number of Carboxylic Acids (Aliphatic)	1+ Billion
27.	Number of Carboxylic Acids (Aromatic)	1+ Billion
28.	Number of Esters (Aliphatic)	1+ Billion
29.	Number of Esters (Aromatic)	1+ Billion
30.	Number of Primary Amides (Aliphatic)	1+ Billion
31.	Number of Primary Amides (Aromatic)	1+ Billion
32.	Number of Secondary Amides (Aliphatic)	1+ Billion
33.	Number of Secondary Amides (Aromatic)	1+ Billion
34.	Number of Tertiary Amides (Aliphatic)	1+ Billion
35.	Number of Tertiary Amides (Aromatic)	1+ Billion
36.	Number of (Thio-) Carbamates (Aliphatic)	1+ Billion
37.	Number of (Thio-) Carbamates (Aromatic)	1+ Billion
38.	Number of Acyl Halogenides (Aliphatic)	1+ Billion
39.	Number of Acyl Halogenides (Aromatic)	1+ Billion
40.	Number of Thioacids (Aliphatic)	1+ Billion
41.	Number of Thioacids (Aromatic)	1+ Billion



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42.	Number of Dithioacids (Aliphatic)	1+ Billion
43.	Number of Dithioacids (Aromatic)	1+ Billion
44.	Number of Thioesters (Aliphatic)	1+ Billion
45.	Number of Thioesters (Aromatic)	1+ Billion
46.	Number of Dithioesters (Aliphatic)	1+ Billion
47.	Number of Dithioesters (Aromatic)	1+ Billion
48.	Number of Aldehydes (Aliphatic)	1+ Billion
49.	Number of Aldehydes (Aromatic)	1+ Billion
50.	Number of Ketones (Aliphatic)	1+ Billion
51.	Number of Ketones (Aromatic)	1+ Billion
52.	Number of Urea (-Thio) Derivatives	1+ Billion
53.	Number of Carbonate (-Thio) Derivatives	1+ Billion
54.	Number of Amidine Derivatives	1+ Billion
55.	Number of Guanidine Derivatives	1+ Billion
56.	Number of Imines (Aliphatic)	1+ Billion
57.	Number of Imines (Aromatic)	1+ Billion
58.	Number of Oximes (Aliphatic)	1+ Billion
59.	Number of Oximes (Aromatic)	1+ Billion
60.	Number of Primary Amines (Aliphatic)	1+ Billion
61.	Number of Primary Amines (Aromatic)	1+ Billion
62.	Number of Secondary Amines (Aliphatic)	1+ Billion
63.	Number of Secondary Amines (Aromatic)	1+ Billion
64.	Number of Tertiary Amines (Aliphatic)	1+ Billion
65.	Number of Tertiary Amines (Aromatic)	1+ Billion
66.	Number of N Hydrazines	1+ Billion
67.	Number of N Azo-Derivatives	1+ Billion



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68.	Number of Nitriles (Aliphatic)	1+ Billion
69.	Number of Nitriles (Aromatic)	1+ Billion
70.	Number of Positively Charged N	1+ Billion
71.	Number of Quaternary N	1+ Billion
72.	Number of Hydroxylamines (Aliphatic)	1+ Billion
73.	Number of Hydroxylamines (Aromatic)	1+ Billion
74.	Number of N-Nitroso Groups (Aliphatic)	1+ Billion
75.	Number of N-Nitroso Groups (Aromatic)	1+ Billion
76.	Number of Nitroso Groups (Aliphatic)	1+ Billion
77.	Number of Nitroso Groups (Aromatic)	1+ Billion
78.	Number of Nitro Groups (Aliphatic)	1+ Billion
79.	Number of Nitro Groups (Aromatic)	1+ Billion
80.	Number of Imides (-Thio)	1+ Billion
81.	Number of Hydrazones	1+ Billion
82.	Number of Hydroxyl Groups	1+ Billion
83.	Number of Aromatic Hydroxyls	1+ Billion
84.	Number of Primary Alcohols	1+ Billion
85.	Number of Secondary Alcohols	1+ Billion
86.	Number of Tertiary Alcohols	1+ Billion
87.	Number of Ethers (Aliphatic)	1+ Billion
88.	Number of Ethers (Aromatic)	1+ Billion
89.	Number of Hypohalogenides (Aliphatic)	1+ Billion
90.	Number of Hypohalogenides (Aromatic)	1+ Billion
91.	Number of Anhydrides (-Thio)	1+ Billion
92.	Number of Water Molecules	1+ Billion
93.	Number of Thiols	1+ Billion



94.	Number of Thioketones	1+ Billion
95.	Number of Sulfides	1+ Billion
96.	Number of Disulfides	1+ Billion
97.	Number of Sulfoxides	1+ Billion
98.	Number of Sulfones	1+ Billion
99.	Number of Sulfenic (Thio-) Acids	1+ Billion
100.	Number of Sulfinic (Thio-/Dithio-) Acids	1+ Billion
101.	Number of Sulfonic (Thio-/Dithio-) Acids	1+ Billion
102.	Number of Sulfuric (Thio-/Dithio-) Acids	1+ Billion
103.	Number of Sulfites (Thio-/Dithio-)	1+ Billion
104.	Number of Sulfonates (Thio-/Dithio-)	1+ Billion
105.	Number of Sulfates (Thio-/Dithio-)	1+ Billion
106.	Number of Sulfonamides (Thio-/Dithio-)	1+ Billion
107.	Number of Phosphites/Thiophosphites	1+ Billion
108.	Number of Phosphates/Thiophosphates	1+ Billion
109.	Number of Phosphanes	1+ Billion
110.	Number of Phosphonates (Thio-)	1+ Billion
111.	. Number of Phosphoranes (Thio-)	1+ Billion
112.	Number of CH2RX	1+ Billion
113.	Number of CHR2X	1+ Billion
114.	Number of CR3X	1+ Billion
115.	Number of R=CHX	1+ Billion
116.	Number of R=CRX	1+ Billion
117.	Number of R#CX	1+ Billion
118.	Number of CHRX2	1+ Billion
119.	Number of CR2X2	1+ Billion



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120. Number of R=CX2	1+ Billion
121. Number of CRX3	1+ Billion
122. Number of X on Aromatic Ring	1+ Billion
123. Number of X on Ring C(sp3)	1+ Billion
124. Number of X on Ring C(sp2)	1+ Billion
125. Number of X on Exo-Conjugated C	1+ Billion
126. Number of Aziridines	1+ Billion
127. Number of Oxiranes	1+ Billion
128. Number of Thiranes	1+ Billion
129. Number of Azetidines	1+ Billion
130. Number of Oxetanes	1+ Billion
131. Number of Thioethanes	1+ Billion
132. Number of Beta-Lactams	1+ Billion
133. Number of Pyrrolidines	1+ Billion
134. Number of Oxolanes	1+ Billion
135. Number of Tetrahydro-Thiophenes	1+ Billion
136. Number of Pyrroles	1+ Billion
137. Number of Pyrazoles	1+ Billion
138. Number of Imidazoles	1+ Billion
139. Number of Furanes	1+ Billion
140. Number of Thiophenes	1+ Billion
141. Number of Oxazoles	1+ Billion
142. Number of Isoxazoles	1+ Billion
143. Number of Thiazoles	1+ Billion
144. Number of Isothiazoles	1+ Billion
145. Number of Triazoles	1+ Billion



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146. Number of Pyridines	1+ Billion
147. Number of Pyridazines	1+ Billion
148. Number of Pyrimidines	1+ Billion
149. Number of Pyrazines	1+ Billion
150. Number of 1-3-5-Triazines	1+ Billion
151. Number of 1-2-4-Triazines	1+ Billion
152. Number of Donor Atoms for H-Bonds (N And O)	1+ Billion
153. Number of Acceptor Atoms for H-Bonds (N,O,F)	1+ Billion
154. Number of Intramolecular H-Bonds (With N,O,F)	1+ Billion
155. Number of Sulfenic (Thio-) Acids	1+ Billion

# ► Atom-Centred Fragments (115)

	Atom-Centred Fragments	Number of Compounds
1.	CH3R/CH4	1+ Billion
2.	CH2R2	1+ Billion
3.	CHR3	1+ Billion
4.	CR4	1+ Billion
5.	СНЗХ	1+ Billion
6.	CH2RX	1+ Billion
7.	CH2X2	1+ Billion
8.	CHR2X	1+ Billion
9.	CHRX2	1+ Billion
10.	CHX3	1+ Billion





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11.	CR3X	1+ Billion
12.	CR2X2	1+ Billion
13.	CRX3	1+ Billion
14.	CX4	1+ Billion
15.	=CH2	1+ Billion
16.	=CHR	1+ Billion
17.	=CR2	1+ Billion
18.	=CHX	1+ Billion
19.	=CRX	1+ Billion
20.	=CX2	1+ Billion
21.	#CH	1+ Billion
22.	#CR/R=C=R	1+ Billion
23.	#CX	1+ Billion
24.	RCHR	1+ Billion
25.	RCRR	1+ Billion
26.	RCXR	1+ Billion
27.	RCHX	1+ Billion
28.	RCRX	1+ Billion
29.	RCXX	1+ Billion
30.	XCHX	1+ Billion
31.	XCRX	1+ Billion
32.	XCXX	1+ Billion
33.	RCHX	1+ Billion
34.	RCRX	1+ Billion
35.	RCXX	1+ Billion
36.	Al-CH=X	1+ Billion

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37.	Ar-CH=X	1+ Billion
38.	Al-C(=X)-Al	1+ Billion
39.	Ar-C(=X)-R	1+ Billion
40.	R-C(=X)-X / R-C#X / X=C=X	1+ Billion
41.	X-C(=X)-X	1+ Billion
42.	XCHX	1+ Billion
43.	XCRX	1+ Billion
44.	XCXX	1+ Billion
45.	H Attached to C0(sp3) No X Attached to Next C	1+ Billion
46.	H Attached to C1(sp3)/C0(sp2)	1+ Billion
47.	H Attached to C2(sp3)/C1(sp2)/C0(sp)	1+ Billion
48.	H Attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)	1+ Billion
49.	H Attached to Heteroatom	1+ Billion
50.	H Attached to Alpha-C	1+ Billion
51.	H Attached to C0(sp3) With 1X Attached to Next C	1+ Billion
52.	H Attached to C0(sp3) With 2X Attached to Next C	1+ Billion
53.	H Attached to C0(sp3) With 3X Attached to Next C	1+ Billion
54.	H Attached to C0(sp3) With 4X Attached to Next C	1+ Billion
55.	Alcohol	1+ Billion
56.	Phenol / Enol / Carboxyl OH	1+ Billion
57.	=0	1+ Billion
58.	Al-O-Al	1+ Billion
59.	Al-O-Ar / Ar-O-Ar / ROR / R-O-C=X	1+ Billion
60.	0	1+ Billion
61.	O- (Negatively Charged)	1+ Billion
62.	R-O-O-R	1+ Billion



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63.	Any-Se-Any	1+ Billion
64.	=Se	1+ Billion
65.	Al-NH2	1+ Billion
66.	Al2-NH	1+ Billion
67.	Al3-N	1+ Billion
68.	Ar-NH2 / X-NH2	1+ Billion
69.	Ar-NH-Al	1+ Billion
70.	Ar-NAI2	1+ Billion
71.	RCO-NN-X=X	1+ Billion
72.	Ar2NH / Ar3N / Ar2N-Al / RNR	1+ Billion
73.	R#N / R=N-	1+ Billion
74.	RNR / RNX	1+ Billion
75.	Ar-NO2 / RN(R)O / RO-NO	1+ Billion
76.	Al-NO2	1+ Billion
77.	Ar-N=X / X-N=X	1+ Billion
78.	N+ (Positively Charged)	1+ Billion
79.	F Attached to C1(sp3)	1+ Billion
80.	F Attached to C2(sp3)	1+ Billion
81.	F Attached to C3(sp3)	1+ Billion
82.	F Attached to C1(sp2)	1+ Billion
83.	F Attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	1+ Billion
84.	Cl Attached to C1(sp3)	1+ Billion
85.	Cl Attached to C2(sp3)	1+ Billion
86.	Cl Attached to C3(sp3)	1+ Billion
87.	Cl Attached to C1(sp2)	1+ Billion
88.	Cl Attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	1+ Billion



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89.	Br Attached to C1(sp3)	1+ Billion
90.	Br Attached to C2(sp3)	1+ Billion
91.	Br Attached to C3(sp3)	1+ Billion
92.	Br Attached to C1(sp2)	1+ Billion
93.	Br Attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	1+ Billion
94.	I Attached to C1(sp3)	1+ Billion
95.	I Attached to C2(sp3)	1+ Billion
96.	I Attached to C3(sp3)	1+ Billion
97.	I Attached to C1(sp2)	1+ Billion
98.	I Attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	1+ Billion
99.	Fluoride Ion	1+ Billion
100.	. Chloride Ion	1+ Billion
101.	. Bromide Ion	1+ Billion
102.	. lodide lon	1+ Billion
103.	. R-SH	1+ Billion
104.	. R2S/RS-SR	1+ Billion
105.	. R=S	1+ Billion
106.	. R-SO-R	1+ Billion
107.	. R-SO2-R	1+ Billion
108.	. >Si<	1+ Billion
109.	. >B- as in Boranes	1+ Billion
110.	. Pylids	1+ Billion
111.	. R3-P=X	1+ Billion
112.	. X3-P=X (Phosphate)	1+ Billion
113.	. PX3 (Phosphite)	1+ Billion
114.	. PR3 (Phosphine)	1+ Billion





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115. C-P(X)2=X (Phosphonate)
```

1+ Billion

# Atom-Type E-State Indices (169)

	Atom-Type E-State Indices	Number of Compounds
1.	Sum of sCH3 E-States	1+ Billion
2.	Sum of dCH2 E-States	1+ Billion
3.	Sum of ssCH2 E-States	1+ Billion
4.	Sum of tCH E-States	1+ Billion
5.	Sum of dsCH E-States	1+ Billion
6.	Sum of aaCH E-States	1+ Billion
7.	Sum of sssCH E-States	1+ Billion
8.	Sum of ddC E-States	1+ Billion
9.	Sum of tsC E-States	1+ Billion
10.	Sum of dssC E-States	1+ Billion
11.	Sum of aasC E-States	1+ Billion
12.	Sum of aaaC E-States	1+ Billion
13.	Sum of ssssC E-States	1+ Billion
14.	Sum of sNH2 E-States	1+ Billion
15.	Sum of ssNH E-States	1+ Billion
16.	Sum of dNH E-States	1+ Billion
17.	Sum of sssN E-States	1+ Billion
18.	Sum of dsN E-States	1+ Billion
19.	Sum of aaN E-States	1+ Billion

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20.	Sum of tN E-States	1+ Billion
21.	Sum of sNH3+ E-States	1+ Billion
22.	Sum of ssNH2+ E-States	1+ Billion
23.	Sum of dNH2+ E-States	1+ Billion
24.	Sum of sssNH+ E-States	1+ Billion
25.	Sum of ssssN+ E-States	1+ Billion
26.	Sum of ddsN E-States	1+ Billion
27.	Sum of aasN E-States	1+ Billion
28.	Sum of aaNH E-States	1+ Billion
29.	Sum of sOH E-States	1+ Billion
30.	Sum of dO E-States	1+ Billion
31.	Sum of ssO E-States	1+ Billion
32.	Sum of aaO E-States	1+ Billion
33.	Sum of sPH2 E-States	1+ Billion
34.	Sum of ssPH E-States	1+ Billion
35.	Sum of sssP E-States	1+ Billion
36.	Sum of dsssP E-States	1+ Billion
37.	Sum of ddsP E-States	1+ Billion
38.	Sum of sssssP E-States	1+ Billion
39.	Sum of sSH E-States	1+ Billion
40.	Sum of dS E-States	1+ Billion
41.	Sum of ssS E-States	1+ Billion
42.	Sum of aaS E-States	1+ Billion
43.	Sum of dssS E-States	1+ Billion
44.	Sum of ddssS E-States	1+ Billion
45.	Sum of ssssssS E-States	1+ Billion



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46.	Sum of sF E-States	1+ Billion
47.	Sum of sCl E-States	1+ Billion
48.	Sum of sBr E-States	1+ Billion
49.	Sum of sl E-States	1+ Billion
50.	Sum of sLi E-States	1+ Billion
51.	Sum of ssBe E-States	1+ Billion
52.	Sum of ssssBe- E-States	1+ Billion
53.	Sum of sBH2 E-States	1+ Billion
54.	Sum of ssBH E-States	1+ Billion
55.	Sum of sssB E-States	1+ Billion
56.	Sum of ssssB- E-States	1+ Billion
57.	Sum of sGeH3 E-States	1+ Billion
58.	Sum of ssGeH2 E-States	1+ Billion
59.	Sum of sssGeH E-States	1+ Billion
60.	Sum of ssssGe E-States	1+ Billion
61.	Sum of sAsH2 E-States	1+ Billion
62.	Sum of ssAsH E-States	1+ Billion
63.	Sum of sssAs E-States	1+ Billion
64.	Sum of sssssAs E-States	1+ Billion
65.	Sum of dsssAs E-States	1+ Billion
66.	Sum of ddsAs E-States	1+ Billion
67.	Sum of sSeH E-States	1+ Billion
68.	Sum of dSe E-States	1+ Billion
69.	Sum of ssSe E-States	1+ Billion
70.	Sum of aaSe E-States	1+ Billion
71.	Sum of dssSe E-States	1+ Billion



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72.	Sum of ssssssSe E-States	1+ Billion
73.	Sum of ddssSe E-States	1+ Billion
74.	Sum of sSnH3 E-States	1+ Billion
75.	Sum of ssSnH2 E-States	1+ Billion
76.	Sum of sssSnH E-States	1+ Billion
77.	Sum of ssssSn E-States	1+ Billion
78.	Sum of sPbH3 E-States	1+ Billion
79.	Sum of ssPbH2 E-States	1+ Billion
80.	Sum of sssPbH E-States	1+ Billion
81.	Sum of ssssPb E-States	1+ Billion
82.	Sum of sSiH3 E-States	1+ Billion
83.	Sum of ssSiH2 E-States	1+ Billion
84.	Sum of sssSiH E-States	1+ Billion
85.	Sum of ssssSi E-States	1+ Billion
86.	Number of Atoms of Type sCH3	1+ Billion
87.	Number of Atoms of Type dCH2	1+ Billion
88.	Number of Atoms of Type ssCH2	1+ Billion
89.	Number of Atoms of Type tCH	1+ Billion
90.	Number of Atoms of Type dsCH	1+ Billion
91.	Number of Atoms of Type aaCH	1+ Billion
92.	Number of Atoms of Type sssCH	1+ Billion
93.	Number of Atoms of Type ddC	1+ Billion
94.	Number of Atoms of Type tsC	1+ Billion
95.	Number of Atoms of Type dssC	1+ Billion
96.	Number of Atoms of Type aasC	1+ Billion
97.	Number of Atoms of Type aaaC	1+ Billion





98. Number of Atoms of Type ssssC	1+ Billion
99. Number of Atoms of Type sNH2	1+ Billion
100. Number of Atoms of Type ssNH	1+ Billion
101. Number of Atoms of Type dNH	1+ Billion
102. Number of Atoms of Type sssN	1+ Billion
103. Number of Atoms of Type dsN	1+ Billion
104. Number of Atoms of Type aaN	1+ Billion
105. Number of Atoms of Type tN	1+ Billion
106. Number of Atoms of Type sNH3+	1+ Billion
107. Number of Atoms of Type ssNH2+	1+ Billion
108. Number of Atoms of Type dNH2+	1+ Billion
109. Number of Atoms of Type sssNH+	1+ Billion
110. Number of Atoms of Type ssssN+	1+ Billion
111. Number of Atoms of Type ddsN	1+ Billion
112. Number of Atoms of Type aasN	1+ Billion
113. Number of Atoms of Type aaNH	1+ Billion
114. Number of Atoms of Type dO	1+ Billion
115. Number of Atoms of Type ssO	1+ Billion
116. Number of Atoms of Type aaO	1+ Billion
117. Number of Atoms of Type sPH2	1+ Billion
118. Number of Atoms of Type ssPH	1+ Billion
119. Number of Atoms of Type sssP	1+ Billion
120. Number of Atoms of Type dsssP	1+ Billion
121. Number of Atoms of Type ddsP	1+ Billion
122. Number of Atoms of Type sssssP	1+ Billion
123. Number of Atoms of Type sSH	1+ Billion



C h e m E s s e n , l n c .

124. Number of Atoms of Type dS	1+ Billion
125. Number of Atoms of Type ssS	1+ Billion
126. Number of Atoms of Type aaS	1+ Billion
127. Number of Atoms of Type dssS	1+ Billion
128. Number of Atoms of Type ddssS	1+ Billion
129. Number of Atoms of Type ssssssS	1+ Billion
130. Number of Atoms of Type sF	1+ Billion
131. Number of Atoms of Type sCl	1+ Billion
132. Number of Atoms of Type sBr	1+ Billion
133. Number of Atoms of Type sl	1+ Billion
134. Number of Atoms of Type sLi	1+ Billion
135. Number of Atoms of Type ssBe	1+ Billion
136. Number of Atoms of Type ssssBe-	1+ Billion
137. Number of Atoms of Type sBH2	1+ Billion
138. Number of Atoms of Type ssBH	1+ Billion
139. Number of Atoms of Type sssB	1+ Billion
140. Number of Atoms of Type ssssB-	1+ Billion
141. Number of Atoms of Type sGeH3	1+ Billion
142. Number of Atoms of Type ssGeH2	1+ Billion
143. Number of Atoms of Type sssGeH	1+ Billion
144. Number of Atoms of Type ssssGe	1+ Billion
145. Number of Atoms of Type sAsH2	1+ Billion
146. Number of Atoms of Type ssAsH	1+ Billion
147. Number of Atoms of Type sssAs	1+ Billion
148. Number of Atoms of Type sssssAs	1+ Billion
149. Number of Atoms of Type dsssAs	1+ Billion





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150. Number of Atoms of Type ddsAs	1+ Billion
151. Number of Atoms of Type sSeH	1+ Billion
152. Number of Atoms of Type dSe	1+ Billion
153. Number of Atoms of Type ssSe	1+ Billion
154. Number of Atoms of Type aaSe	1+ Billion
155. Number of Atoms of Type dssSe	1+ Billion
156. Number of Atoms of Type ssssssSe	1+ Billion
157. Number of Atoms of Type ddssSe	1+ Billion
158. Number of Atoms of Type sSnH3	1+ Billion
159. Number of Atoms of Type ssSnH2	1+ Billion
160. Number of Atoms of Type sssSnH	1+ Billion
161. Number of Atoms of Type ssssSn	1+ Billion
162. Number of Atoms of Type sPbH3	1+ Billion
163. Number of Atoms of Type ssPbH2	1+ Billion
164. Number of Atoms of Type sssPbH	1+ Billion
165. Number of Atoms of Type ssssPb	1+ Billion
166. Number of Atoms of Type sSiH3	1+ Billion
167. Number of Atoms of Type ssSiH2	1+ Billion
168. Number of Atoms of Type sssSiH	1+ Billion
169. Number of Atoms of Type ssssSi	1+ Billion

# ► CATS 2D Descriptors (150)

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C h e m E s s e n , l n c .

1.	CATS2D Donor-Donor at Lag 00	1+ Billion
2.	CATS2D Donor-Donor at Lag 01	1+ Billion
3.	CATS2D Donor-Donor at Lag 02	1+ Billion
4.	CATS2D Donor-Donor at Lag 03	1+ Billion
5.	CATS2D Donor-Donor at Lag 04	1+ Billion
6.	CATS2D Donor-Donor at Lag 05	1+ Billion
7.	CATS2D Donor-Donor at Lag 06	1+ Billion
8.	CATS2D Donor-Donor at Lag 07	1+ Billion
9.	CATS2D Donor-Donor at Lag 08	1+ Billion
10.	CATS2D Donor-Donor at Lag 09	1+ Billion
11.	CATS2D Donor-Acceptor at Lag 00	1+ Billion
12.	CATS2D Donor-Acceptor at Lag 01	1+ Billion
13.	CATS2D Donor-Acceptor at Lag 02	1+ Billion
14.	CATS2D Donor-Acceptor at Lag 03	1+ Billion
15.	CATS2D Donor-Acceptor at Lag 04	1+ Billion
16.	CATS2D Donor-Acceptor at Lag 05	1+ Billion
17.	CATS2D Donor-Acceptor at Lag 06	1+ Billion
18.	CATS2D Donor-Acceptor at Lag 07	1+ Billion
19.	CATS2D Donor-Acceptor at Lag 08	1+ Billion
20.	CATS2D Donor-Acceptor at Lag 09	1+ Billion
21.	CATS2D Donor-Positive at Lag 00	1+ Billion
22.	CATS2D Donor-Positive at Lag 01	1+ Billion
23.	CATS2D Donor-Positive at Lag 02	1+ Billion
24.	CATS2D Donor-Positive at Lag 03	1+ Billion
25.	CATS2D Donor-Positive at Lag 04	1+ Billion
26.	CATS2D Donor-Positive at Lag 05	1+ Billion



C h e m E s s e n , l n c .

27.	CATS2D Donor-Positive at Lag 06	1+ Billion
28.	CATS2D Donor-Positive at Lag 07	1+ Billion
29.	CATS2D Donor-Positive at Lag 08	1+ Billion
30.	CATS2D Donor-Positive at Lag 09	1+ Billion
31.	CATS2D Donor-Negative at Lag 00	1+ Billion
32.	CATS2D Donor-Negative at Lag 01	1+ Billion
33.	CATS2D Donor-Negative at Lag 02	1+ Billion
34.	CATS2D Donor-Negative at Lag 03	1+ Billion
35.	CATS2D Donor-Negative at Lag 04	1+ Billion
36.	CATS2D Donor-Negative at Lag 05	1+ Billion
37.	CATS2D Donor-Negative at Lag 06	1+ Billion
38.	CATS2D Donor-Negative at Lag 07	1+ Billion
39.	CATS2D Donor-Negative at Lag 08	1+ Billion
40.	CATS2D Donor-Negative at Lag 09	1+ Billion
41.	CATS2D Donor-Lipophilic at Lag 00	1+ Billion
42.	CATS2D Donor-Lipophilic at Lag 01	1+ Billion
43.	CATS2D Donor-Lipophilic at Lag 02	1+ Billion
44.	CATS2D Donor-Lipophilic at Lag 03	1+ Billion
45.	CATS2D Donor-Lipophilic at Lag 04	1+ Billion
46.	CATS2D Donor-Lipophilic at Lag 05	1+ Billion
47.	CATS2D Donor-Lipophilic at Lag 06	1+ Billion
48.	CATS2D Donor-Lipophilic at Lag 07	1+ Billion
49.	CATS2D Donor-Lipophilic at Lag 08	1+ Billion
50.	CATS2D Donor-Lipophilic at Lag 09	1+ Billion
51.	CATS2D Acceptor-Acceptor at Lag 00	1+ Billion
52.	CATS2D Acceptor-Acceptor at Lag 01	1+ Billion





1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

53.	CATS2D Acceptor-Acceptor at Lag 02	1+ Billion
54.	CATS2D Acceptor-Acceptor at Lag 03	1+ Billion
55.	CATS2D Acceptor-Acceptor at Lag 04	1+ Billion
56.	CATS2D Acceptor-Acceptor at Lag 05	1+ Billion
57.	CATS2D Acceptor-Acceptor at Lag 06	1+ Billion
58.	CATS2D Acceptor-Acceptor at Lag 07	1+ Billion
59.	CATS2D Acceptor-Acceptor at Lag 08	1+ Billion
60.	CATS2D Acceptor-Acceptor at Lag 09	1+ Billion
61.	CATS2D Acceptor-Positive at Lag 00	1+ Billion
62.	CATS2D Acceptor-Positive at Lag 01	1+ Billion
63.	CATS2D Acceptor-Positive at Lag 02	1+ Billion
64.	CATS2D Acceptor-Positive at Lag 03	1+ Billion
65.	CATS2D Acceptor-Positive at Lag 04	1+ Billion
66.	CATS2D Acceptor-Positive at Lag 05	1+ Billion
67.	CATS2D Acceptor-Positive at Lag 06	1+ Billion
68.	CATS2D Acceptor-Positive at Lag 07	1+ Billion
69.	CATS2D Acceptor-Positive at Lag 08	1+ Billion
70.	CATS2D Acceptor-Positive at Lag 09	1+ Billion
71.	CATS2D Acceptor-Negative at Lag 00	1+ Billion
72.	CATS2D Acceptor-Negative at Lag 01	1+ Billion
73.	CATS2D Acceptor-Negative at Lag 02	1+ Billion
74.	CATS2D Acceptor-Negative at Lag 03	1+ Billion
75.	CATS2D Acceptor-Negative at Lag 04	1+ Billion
76.	CATS2D Acceptor-Negative at Lag 05	1+ Billion
77.	CATS2D Acceptor-Negative at Lag 06	1+ Billion
78.	CATS2D Acceptor-Negative at Lag 07	1+ Billion

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79.	CATS2D Acceptor-Negative at Lag 08	1+ Billion
80.	CATS2D Acceptor-Negative at Lag 09	1+ Billion
81.	CATS2D Acceptor-Lipophilic at Lag 00	1+ Billion
82.	CATS2D Acceptor-Lipophilic at Lag 01	1+ Billion
83.	CATS2D Acceptor-Lipophilic at Lag 02	1+ Billion
84.	CATS2D Acceptor-Lipophilic at Lag 03	1+ Billion
85.	CATS2D Acceptor-Lipophilic at Lag 04	1+ Billion
86.	CATS2D Acceptor-Lipophilic at Lag 05	1+ Billion
87.	CATS2D Acceptor-Lipophilic at Lag 06	1+ Billion
88.	CATS2D Acceptor-Lipophilic at Lag 07	1+ Billion
89.	CATS2D Acceptor-Lipophilic at Lag 08	1+ Billion
90.	CATS2D Acceptor-Lipophilic at Lag 09	1+ Billion
91.	CATS2D Positive-Positive at Lag 00	1+ Billion
92.	CATS2D Positive-Positive at Lag 01	1+ Billion
93.	CATS2D Positive-Positive at Lag 02	1+ Billion
94.	CATS2D Positive-Positive at Lag 03	1+ Billion
95.	CATS2D Positive-Positive at Lag 04	1+ Billion
96.	CATS2D Positive-Positive at Lag 05	1+ Billion
97.	CATS2D Positive-Positive at Lag 06	1+ Billion
98.	CATS2D Positive-Positive at Lag 07	1+ Billion
99.	CATS2D Positive-Positive at Lag 08	1+ Billion
100.	CATS2D Positive-Positive at Lag 09	1+ Billion
101.	CATS2D Positive-Negative at Lag 00	1+ Billion
102.	CATS2D Positive-Negative at Lag 01	1+ Billion
103.	CATS2D Positive-Negative at Lag 02	1+ Billion
104.	CATS2D Positive-Negative at Lag 03	1+ Billion





105. CATS2D Positive-Negative at Lag 04	1+ Billion
106. CATS2D Positive-Negative at Lag 05	1+ Billion
107. CATS2D Positive-Negative at Lag 06	1+ Billion
108. CATS2D Positive-Negative at Lag 07	1+ Billion
109. CATS2D Positive-Negative at Lag 08	1+ Billion
110. CATS2D Positive-Negative at Lag 09	1+ Billion
111. CATS2D Positive-Lipophilic at Lag 00	1+ Billion
112. CATS2D Positive-Lipophilic at Lag 01	1+ Billion
113. CATS2D Positive-Lipophilic at Lag 02	1+ Billion
114. CATS2D Positive-Lipophilic at Lag 03	1+ Billion
115. CATS2D Positive-Lipophilic at Lag 04	1+ Billion
116. CATS2D Positive-Lipophilic at Lag 05	1+ Billion
117. CATS2D Positive-Lipophilic at Lag 06	1+ Billion
118. CATS2D Positive-Lipophilic at Lag 07	1+ Billion
119. CATS2D Positive-Lipophilic at Lag 08	1+ Billion
120. CATS2D Positive-Lipophilic at Lag 09	1+ Billion
121. CATS2D Negative-Negative at Lag 00	1+ Billion
122. CATS2D Negative-Negative at Lag 01	1+ Billion
123. CATS2D Negative-Negative at Lag 02	1+ Billion
124. CATS2D Negative-Negative at Lag 03	1+ Billion
125. CATS2D Negative-Negative at Lag 04	1+ Billion
126. CATS2D Negative-Negative at Lag 05	1+ Billion
127. CATS2D Negative-Negative at Lag 06	1+ Billion
128. CATS2D Negative-Negative at Lag 07	1+ Billion
129. CATS2D Negative-Negative at Lag 08	1+ Billion
130. CATS2D Negative-Negative at Lag 09	1+ Billion





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131. CATS2D Negative-Lipophilic at Lag 00	1+ Billion
132. CATS2D Negative-Lipophilic at Lag 01	1+ Billion
133. CATS2D Negative-Lipophilic at Lag 02	1+ Billion
134. CATS2D Negative-Lipophilic at Lag 03	1+ Billion
135. CATS2D Negative-Lipophilic at Lag 04	1+ Billion
136. CATS2D Negative-Lipophilic at Lag 05	1+ Billion
137. CATS2D Negative-Lipophilic at Lag 06	1+ Billion
138. CATS2D Negative-Lipophilic at Lag 07	1+ Billion
139. CATS2D Negative-Lipophilic at Lag 08	1+ Billion
140. CATS2D Negative-Lipophilic at Lag 09	1+ Billion
141. CATS2D Lipophilic-Lipophilic at Lag 00	1+ Billion
142. CATS2D Lipophilic-Lipophilic at Lag 01	1+ Billion
143. CATS2D Lipophilic-Lipophilic at Lag 02	1+ Billion
144. CATS2D Lipophilic-Lipophilic at Lag 03	1+ Billion
145. CATS2D Lipophilic-Lipophilic at Lag 04	1+ Billion
146. CATS2D Lipophilic-Lipophilic at Lag 05	1+ Billion
147. CATS2D Lipophilic-Lipophilic at Lag 06	1+ Billion
148. CATS2D Lipophilic-Lipophilic at Lag 07	1+ Billion
149. CATS2D Lipophilic-Lipophilic at Lag 08	1+ Billion
150. CATS2D Lipophilic-Lipophilic at Lag 09	1+ Billion

# > 2D Atom Pair Descriptors (1596)





1.	Sum of Topological Distances between NN	1+ Billion
2.	Sum of Topological Distances between NO	1+ Billion
3.	Sum of Topological Distances between NS	1+ Billion
4.	Sum of Topological Distances between NP	1+ Billion
5.	Sum of Topological Distances between NF	1+ Billion
6.	Sum of Topological Distances between NCl	1+ Billion
7.	Sum of Topological Distances between NBr	1+ Billion
8.	Sum of Topological Distances between NI	1+ Billion
9.	Sum of Topological Distances between OO	1+ Billion
10.	Sum of Topological Distances between OS	1+ Billion
11.	Sum of Topological Distances between OP	1+ Billion
12.	Sum of Topological Distances between OF	1+ Billion
13.	Sum of Topological Distances between OCl	1+ Billion
14.	Sum of Topological Distances between OBr	1+ Billion
15.	Sum of Topological Distances between OI	1+ Billion
16.	Sum of Topological Distances between SS	1+ Billion
17.	Sum of Topological Distances between SP	1+ Billion
18.	Sum of Topological Distances between SF	1+ Billion
19.	Sum of Topological Distances between SCl	1+ Billion
20.	Sum of Topological Distances between SBr	1+ Billion
21.	Sum of Topological Distances between SI	1+ Billion
22.	Sum of Topological Distances between PP	1+ Billion
23.	Sum of Topological Distances between PF	1+ Billion
24.	Sum of Topological Distances between PCl	1+ Billion
25.	Sum of Topological Distances between PBr	1+ Billion
26.	Sum of Topological Distances between PI	1+ Billion





27.	Sum of Topological Distances between FF	1+ Billion
28.	Sum of Topological Distances between FCl	1+ Billion
29.	Sum of Topological Distances between FBr	1+ Billion
30.	Sum of Topological Distances between FI	1+ Billion
31.	Sum of Topological Distances between ClCl	1+ Billion
32.	Sum of Topological Distances between ClBr	1+ Billion
33.	Sum of Topological Distances between ClI	1+ Billion
34.	Sum of Topological Distances between BrBr	1+ Billion
35.	Sum of Topological Distances between BrI	1+ Billion
36.	Sum of Topological Distances between II	1+ Billion
37.	Presence/Absence of C - C at Topological Distance 1	1+ Billion
38.	Presence/Absence of C - N at Topological Distance 1	1+ Billion
39.	Presence/Absence of C - O at Topological Distance 1	1+ Billion
40.	Presence/Absence of C - S at Topological Distance 1	1+ Billion
41.	Presence/Absence of C - P at Topological Distance 1	1+ Billion
42.	Presence/Absence of C - F at Topological Distance 1	1+ Billion
43.	Presence/Absence of C - Cl at Topological Distance 1	1+ Billion
44.	Presence/Absence of C - Br at Topological Distance 1	1+ Billion
45.	Presence/Absence of C - I at Topological Distance 1	1+ Billion
46.	Presence/Absence of C - B at Topological Distance 1	1+ Billion
47.	Presence/Absence of C - Si at Topological Distance 1	1+ Billion
48.	Presence/Absence of C - X at Topological Distance 1	1+ Billion
49.	Presence/Absence of N - N at Topological Distance 1	1+ Billion
50.	Presence/Absence of N - O at Topological Distance 1	1+ Billion
51.	Presence/Absence of N - S at Topological Distance 1	1+ Billion
52.	Presence/Absence of N - P at Topological Distance 1	1+ Billion





53.	Presence/Absence of N - F at Topological Distance 1	1+ Billion
54.	Presence/Absence of N - Cl at Topological Distance 1	1+ Billion
55.	Presence/Absence of N - Br at Topological Distance 1	1+ Billion
56.	Presence/Absence of N - I at Topological Distance 1	1+ Billion
57.	Presence/Absence of N - B at Topological Distance 1	1+ Billion
58.	Presence/Absence of N - Si at Topological Distance 1	1+ Billion
59.	Presence/Absence of N - X at Topological Distance 1	1+ Billion
60.	Presence/Absence of O - O at Topological Distance 1	1+ Billion
61.	Presence/Absence of O - S at Topological Distance 1	1+ Billion
62.	Presence/Absence of O - P at Topological Distance 1	1+ Billion
63.	Presence/Absence of O - F at Topological Distance 1	1+ Billion
64.	Presence/Absence of O - Cl at Topological Distance 1	1+ Billion
65.	Presence/Absence of O - Br at Topological Distance 1	1+ Billion
66.	Presence/Absence of O - I at Topological Distance 1	1+ Billion
67.	Presence/Absence of O - B at Topological Distance 1	1+ Billion
68.	Presence/Absence of O - Si at Topological Distance 1	1+ Billion
69.	Presence/Absence of O - X at Topological Distance 1	1+ Billion
70.	Presence/Absence of S - S at Topological Distance 1	1+ Billion
71.	Presence/Absence of S - P at Topological Distance 1	1+ Billion
72.	Presence/Absence of S - F at Topological Distance 1	1+ Billion
73.	Presence/Absence of S - Cl at Topological Distance 1	1+ Billion
74.	Presence/Absence of S - Br at Topological Distance 1	1+ Billion
75.	Presence/Absence of S - I at Topological Distance 1	1+ Billion
76.	Presence/Absence of S - B at Topological Distance 1	1+ Billion
77.	Presence/Absence of S - Si at Topological Distance 1	1+ Billion
78.	Presence/Absence of S - X at Topological Distance 1	1+ Billion





79.	Presence/Absence of P - P at Topological Distance 1	1+ Billion
80.	Presence/Absence of P - F at Topological Distance 1	1+ Billion
81.	Presence/Absence of P - Cl at Topological Distance 1	1+ Billion
82.	Presence/Absence of P - Br at Topological Distance 1	1+ Billion
83.	Presence/Absence of P - I at Topological Distance 1	1+ Billion
84.	Presence/Absence of P - B at Topological Distance 1	1+ Billion
85.	Presence/Absence of P - Si at Topological Distance 1	1+ Billion
86.	Presence/Absence of P - X at Topological Distance 1	1+ Billion
87.	Presence/Absence of F - F at Topological Distance 1	1+ Billion
88.	Presence/Absence of F - Cl at Topological Distance 1	1+ Billion
89.	Presence/Absence of F - Br at Topological Distance 1	1+ Billion
90.	Presence/Absence of F - I at Topological Distance 1	1+ Billion
91.	Presence/Absence of F - B at Topological Distance 1	1+ Billion
92.	Presence/Absence of F - Si at Topological Distance 1	1+ Billion
93.	Presence/Absence of F - X at Topological Distance 1	1+ Billion
94.	Presence/Absence of Cl - Cl at Topological Distance 1	1+ Billion
95.	Presence/Absence of Cl - Br at Topological Distance 1	1+ Billion
96.	Presence/Absence of Cl - I at Topological Distance 1	1+ Billion
97.	Presence/Absence of Cl - B at Topological Distance 1	1+ Billion
98.	Presence/Absence of Cl - Si at Topological Distance 1	1+ Billion
99.	Presence/Absence of Cl - X at Topological Distance 1	1+ Billion
100.	Presence/Absence of Br - Br at Topological Distance 1	1+ Billion
101.	Presence/Absence of Br - I at Topological Distance 1	1+ Billion
102.	Presence/Absence of Br - B at Topological Distance 1	1+ Billion
103.	Presence/Absence of Br - Si at Topological Distance 1	1+ Billion
104.	Presence/Absence of Br - X at Topological Distance 1	1+ Billion





105. Presence/Absence of I - I at Topological Distance 1	1+ Billion
106. Presence/Absence of I - B at Topological Distance 1	1+ Billion
107. Presence/Absence of I - Si at Topological Distance 1	1+ Billion
108. Presence/Absence of I - X at Topological Distance 1	1+ Billion
109. Presence/Absence of B - B at Topological Distance 1	1+ Billion
110. Presence/Absence of B - Si at Topological Distance 1	1+ Billion
111. Presence/Absence of B - X at Topological Distance 1	1+ Billion
112. Presence/Absence of Si - Si at Topological Distance 1	1+ Billion
113. Presence/Absence of Si - X at Topological Distance 1	1+ Billion
114. Presence/Absence of X - X at Topological Distance 1	1+ Billion
115. Presence/Absence of C - C at Topological Distance 2	1+ Billion
116. Presence/Absence of C - N at Topological Distance 2	1+ Billion
117. Presence/Absence of C - O at Topological Distance 2	1+ Billion
118. Presence/Absence of C - S at Topological Distance 2	1+ Billion
119. Presence/Absence of C - P at Topological Distance 2	1+ Billion
120. Presence/Absence of C - F at Topological Distance 2	1+ Billion
121. Presence/Absence of C - Cl at Topological Distance 2	1+ Billion
122. Presence/Absence of C - Br at Topological Distance 2	1+ Billion
123. Presence/Absence of C - I at Topological Distance 2	1+ Billion
124. Presence/Absence of C - B at Topological Distance 2	1+ Billion
125. Presence/Absence of C - Si at Topological Distance 2	1+ Billion
126. Presence/Absence of C - X at Topological Distance 2	1+ Billion
127. Presence/Absence of N - N at Topological Distance 2	1+ Billion
128. Presence/Absence of N - O at Topological Distance 2	1+ Billion
129. Presence/Absence of N - S at Topological Distance 2	1+ Billion
130. Presence/Absence of N - P at Topological Distance 2	1+ Billion





131. Presence/Absence of N - F at Topological Distance 2	1+ Billion
132. Presence/Absence of N - Cl at Topological Distance 2	1+ Billion
133. Presence/Absence of N - Br at Topological Distance 2	1+ Billion
134. Presence/Absence of N - I at Topological Distance 2	1+ Billion
135. Presence/Absence of N - B at Topological Distance 2	1+ Billion
136. Presence/Absence of N - Si at Topological Distance 2	1+ Billion
137. Presence/Absence of N - X at Topological Distance 2	1+ Billion
138. Presence/Absence of O - O at Topological Distance 2	1+ Billion
139. Presence/Absence of O - S at Topological Distance 2	1+ Billion
140. Presence/Absence of O - P at Topological Distance 2	1+ Billion
141. Presence/Absence of O - F at Topological Distance 2	1+ Billion
142. Presence/Absence of O - Cl at Topological Distance 2	1+ Billion
143. Presence/Absence of O - Br at Topological Distance 2	1+ Billion
144. Presence/Absence of O - I at Topological Distance 2	1+ Billion
145. Presence/Absence of O - B at Topological Distance 2	1+ Billion
146. Presence/Absence of O - Si at Topological Distance 2	1+ Billion
147. Presence/Absence of O - X at Topological Distance 2	1+ Billion
148. Presence/Absence of S - S at Topological Distance 2	1+ Billion
149. Presence/Absence of S - P at Topological Distance 2	1+ Billion
150. Presence/Absence of S - F at Topological Distance 2	1+ Billion
151. Presence/Absence of S - Cl at Topological Distance 2	1+ Billion
152. Presence/Absence of S - Br at Topological Distance 2	1+ Billion
153. Presence/Absence of S - I at Topological Distance 2	1+ Billion
154. Presence/Absence of S - B at Topological Distance 2	1+ Billion
155. Presence/Absence of S - Si at Topological Distance 2	1+ Billion
156. Presence/Absence of S - X at Topological Distance 2	1+ Billion





157. Presence/Absence of P - P at Topological Distance 2	1+ Billion
158. Presence/Absence of P - F at Topological Distance 2	1+ Billion
159. Presence/Absence of P - Cl at Topological Distance 2	1+ Billion
160. Presence/Absence of P - Br at Topological Distance 2	1+ Billion
161. Presence/Absence of P - I at Topological Distance 2	1+ Billion
162. Presence/Absence of P - B at Topological Distance 2	1+ Billion
163. Presence/Absence of P - Si at Topological Distance 2	1+ Billion
164. Presence/Absence of P - X at Topological Distance 2	1+ Billion
165. Presence/Absence of F - F at Topological Distance 2	1+ Billion
166. Presence/Absence of F - Cl at Topological Distance 2	1+ Billion
167. Presence/Absence of F - Br at Topological Distance 2	1+ Billion
168. Presence/Absence of F - I at Topological Distance 2	1+ Billion
169. Presence/Absence of F - B at Topological Distance 2	1+ Billion
170. Presence/Absence of F - Si at Topological Distance 2	1+ Billion
171. Presence/Absence of F - X at Topological Distance 2	1+ Billion
172. Presence/Absence of Cl - Cl at Topological Distance 2	1+ Billion
173. Presence/Absence of Cl - Br at Topological Distance 2	1+ Billion
174. Presence/Absence of Cl - I at Topological Distance 2	1+ Billion
175. Presence/Absence of Cl - B at Topological Distance 2	1+ Billion
176. Presence/Absence of Cl - Si at Topological Distance 2	1+ Billion
177. Presence/Absence of Cl - X at Topological Distance 2	1+ Billion
178. Presence/Absence of Br - Br at Topological Distance 2	1+ Billion
179. Presence/Absence of Br - I at Topological Distance 2	1+ Billion
180. Presence/Absence of Br - B at Topological Distance 2	1+ Billion
181. Presence/Absence of Br - Si at Topological Distance 2	1+ Billion
182. Presence/Absence of Br - X at Topological Distance 2	1+ Billion





183. Presence/Absence of I - I at Topological Distance 2	1+ Billion
184. Presence/Absence of I - B at Topological Distance 2	1+ Billion
185. Presence/Absence of I - Si at Topological Distance 2	1+ Billion
186. Presence/Absence of I - X at Topological Distance 2	1+ Billion
187. Presence/Absence of B - B at Topological Distance 2	1+ Billion
188. Presence/Absence of B - Si at Topological Distance 2	1+ Billion
189. Presence/Absence of B - X at Topological Distance 2	1+ Billion
190. Presence/Absence of Si - Si at Topological Distance 2	1+ Billion
191. Presence/Absence of Si - X at Topological Distance 2	1+ Billion
192. Presence/Absence of X - X at Topological Distance 2	1+ Billion
193. Presence/Absence of C - C at Topological Distance 3	1+ Billion
194. Presence/Absence of C - N at Topological Distance 3	1+ Billion
195. Presence/Absence of C - O at Topological Distance 3	1+ Billion
196. Presence/Absence of C - S at Topological Distance 3	1+ Billion
197. Presence/Absence of C - P at Topological Distance 3	1+ Billion
198. Presence/Absence of C - F at Topological Distance 3	1+ Billion
199. Presence/Absence of C - Cl at Topological Distance 3	1+ Billion
200. Presence/Absence of C - Br at Topological Distance 3	1+ Billion
201. Presence/Absence of C - I at Topological Distance 3	1+ Billion
202. Presence/Absence of C - B at Topological Distance 3	1+ Billion
203. Presence/Absence of C - Si at Topological Distance 3	1+ Billion
204. Presence/Absence of C - X at Topological Distance 3	1+ Billion
205. Presence/Absence of N - N at Topological Distance 3	1+ Billion
206. Presence/Absence of N - O at Topological Distance 3	1+ Billion
207. Presence/Absence of N - S at Topological Distance 3	1+ Billion
208. Presence/Absence of N - P at Topological Distance 3	1+ Billion





209. Presence/Absence of N - F at Topological Distance 3	1+ Billion
210. Presence/Absence of N - Cl at Topological Distance 3	1+ Billion
211. Presence/Absence of N - Br at Topological Distance 3	1+ Billion
212. Presence/Absence of N - I at Topological Distance 3	1+ Billion
213. Presence/Absence of N - B at Topological Distance 3	1+ Billion
214. Presence/Absence of N - Si at Topological Distance 3	1+ Billion
215. Presence/Absence of N - X at Topological Distance 3	1+ Billion
216. Presence/Absence of O - O at Topological Distance 3	1+ Billion
217. Presence/Absence of O - S at Topological Distance 3	1+ Billion
218. Presence/Absence of O - P at Topological Distance 3	1+ Billion
219. Presence/Absence of O - F at Topological Distance 3	1+ Billion
220. Presence/Absence of O - Cl at Topological Distance 3	1+ Billion
221. Presence/Absence of O - Br at Topological Distance 3	1+ Billion
222. Presence/Absence of O - I at Topological Distance 3	1+ Billion
223. Presence/Absence of O - B at Topological Distance 3	1+ Billion
224. Presence/Absence of O - Si at Topological Distance 3	1+ Billion
225. Presence/Absence of O - X at Topological Distance 3	1+ Billion
226. Presence/Absence of S - S at Topological Distance 3	1+ Billion
227. Presence/Absence of S - P at Topological Distance 3	1+ Billion
228. Presence/Absence of S - F at Topological Distance 3	1+ Billion
229. Presence/Absence of S - Cl at Topological Distance 3	1+ Billion
230. Presence/Absence of S - Br at Topological Distance 3	1+ Billion
231. Presence/Absence of S - I at Topological Distance 3	1+ Billion
232. Presence/Absence of S - B at Topological Distance 3	1+ Billion
233. Presence/Absence of S - Si at Topological Distance 3	1+ Billion
234. Presence/Absence of S - X at Topological Distance 3	1+ Billion





235. Presence/Absence of P - P at Topological Distance 3	1+ Billion
236. Presence/Absence of P - F at Topological Distance 3	1+ Billion
237. Presence/Absence of P - Cl at Topological Distance 3	1+ Billion
238. Presence/Absence of P - Br at Topological Distance 3	1+ Billion
239. Presence/Absence of P - I at Topological Distance 3	1+ Billion
240. Presence/Absence of P - B at Topological Distance 3	1+ Billion
241. Presence/Absence of P - Si at Topological Distance 3	1+ Billion
242. Presence/Absence of P - X at Topological Distance 3	1+ Billion
243. Presence/Absence of F - F at Topological Distance 3	1+ Billion
244. Presence/Absence of F - Cl at Topological Distance 3	1+ Billion
245. Presence/Absence of F - Br at Topological Distance 3	1+ Billion
246. Presence/Absence of F - I at Topological Distance 3	1+ Billion
247. Presence/Absence of F - B at Topological Distance 3	1+ Billion
248. Presence/Absence of F - Si at Topological Distance 3	1+ Billion
249. Presence/Absence of F - X at Topological Distance 3	1+ Billion
250. Presence/Absence of Cl - Cl at Topological Distance 3	1+ Billion
251. Presence/Absence of Cl - Br at Topological Distance 3	1+ Billion
252. Presence/Absence of Cl - I at Topological Distance 3	1+ Billion
253. Presence/Absence of Cl - B at Topological Distance 3	1+ Billion
254. Presence/Absence of Cl - Si at Topological Distance 3	1+ Billion
255. Presence/Absence of Cl - X at Topological Distance 3	1+ Billion
256. Presence/Absence of Br - Br at Topological Distance 3	1+ Billion
257. Presence/Absence of Br - I at Topological Distance 3	1+ Billion
258. Presence/Absence of Br - B at Topological Distance 3	1+ Billion
259. Presence/Absence of Br - Si at Topological Distance 3	1+ Billion
260. Presence/Absence of Br - X at Topological Distance 3	1+ Billion





261. Presence/Absence of I - I at Topological Distance 3	1+ Billion
262. Presence/Absence of I - B at Topological Distance 3	1+ Billion
263. Presence/Absence of I - Si at Topological Distance 3	1+ Billion
264. Presence/Absence of I - X at Topological Distance 3	1+ Billion
265. Presence/Absence of B - B at Topological Distance 3	1+ Billion
266. Presence/Absence of B - Si at Topological Distance 3	1+ Billion
267. Presence/Absence of B - X at Topological Distance 3	1+ Billion
268. Presence/Absence of Si - Si at Topological Distance 3	1+ Billion
269. Presence/Absence of Si - X at Topological Distance 3	1+ Billion
270. Presence/Absence of X - X at Topological Distance 3	1+ Billion
271. Presence/Absence of C - C at Topological Distance 4	1+ Billion
272. Presence/Absence of C - N at Topological Distance 4	1+ Billion
273. Presence/Absence of C - O at Topological Distance 4	1+ Billion
274. Presence/Absence of C - S at Topological Distance 4	1+ Billion
275. Presence/Absence of C - P at Topological Distance 4	1+ Billion
276. Presence/Absence of C - F at Topological Distance 4	1+ Billion
277. Presence/Absence of C - Cl at Topological Distance 4	1+ Billion
278. Presence/Absence of C - Br at Topological Distance 4	1+ Billion
279. Presence/Absence of C - I at Topological Distance 4	1+ Billion
280. Presence/Absence of C - B at Topological Distance 4	1+ Billion
281. Presence/Absence of C - Si at Topological Distance 4	1+ Billion
282. Presence/Absence of C - X at Topological Distance 4	1+ Billion
283. Presence/Absence of N - N at Topological Distance 4	1+ Billion
284. Presence/Absence of N - O at Topological Distance 4	1+ Billion
285. Presence/Absence of N - S at Topological Distance 4	1+ Billion
286. Presence/Absence of N - P at Topological Distance 4	1+ Billion





287. Presence/Absence of N - F at Topological Distance 4	1+ Billion
288. Presence/Absence of N - Cl at Topological Distance 4	1+ Billion
289. Presence/Absence of N - Br at Topological Distance 4	1+ Billion
290. Presence/Absence of N - I at Topological Distance 4	1+ Billion
291. Presence/Absence of N - B at Topological Distance 4	1+ Billion
292. Presence/Absence of N - Si at Topological Distance 4	1+ Billion
293. Presence/Absence of N - X at Topological Distance 4	1+ Billion
294. Presence/Absence of O - O at Topological Distance 4	1+ Billion
295. Presence/Absence of O - S at Topological Distance 4	1+ Billion
296. Presence/Absence of O - P at Topological Distance 4	1+ Billion
297. Presence/Absence of O - F at Topological Distance 4	1+ Billion
298. Presence/Absence of O - Cl at Topological Distance 4	1+ Billion
299. Presence/Absence of O - Br at Topological Distance 4	1+ Billion
300. Presence/Absence of O - I at Topological Distance 4	1+ Billion
301. Presence/Absence of O - B at Topological Distance 4	1+ Billion
302. Presence/Absence of O - Si at Topological Distance 4	1+ Billion
303. Presence/Absence of O - X at Topological Distance 4	1+ Billion
304. Presence/Absence of S - S at Topological Distance 4	1+ Billion
305. Presence/Absence of S - P at Topological Distance 4	1+ Billion
306. Presence/Absence of S - F at Topological Distance 4	1+ Billion
307. Presence/Absence of S - Cl at Topological Distance 4	1+ Billion
308. Presence/Absence of S - Br at Topological Distance 4	1+ Billion
309. Presence/Absence of S - I at Topological Distance 4	1+ Billion
310. Presence/Absence of S - B at Topological Distance 4	1+ Billion
311. Presence/Absence of S - Si at Topological Distance 4	1+ Billion
312. Presence/Absence of S - X at Topological Distance 4	1+ Billion





313. Presence/Absence of P - P at Topological Distance 4	1+ Billion
314. Presence/Absence of P - F at Topological Distance 4	1+ Billion
315. Presence/Absence of P - Cl at Topological Distance 4	1+ Billion
316. Presence/Absence of P - Br at Topological Distance 4	1+ Billion
317. Presence/Absence of P - I at Topological Distance 4	1+ Billion
318. Presence/Absence of P - B at Topological Distance 4	1+ Billion
319. Presence/Absence of P - Si at Topological Distance 4	1+ Billion
320. Presence/Absence of P - X at Topological Distance 4	1+ Billion
321. Presence/Absence of F - F at Topological Distance 4	1+ Billion
322. Presence/Absence of F - Cl at Topological Distance 4	1+ Billion
323. Presence/Absence of F - Br at Topological Distance 4	1+ Billion
324. Presence/Absence of F - I at Topological Distance 4	1+ Billion
325. Presence/Absence of F - B at Topological Distance 4	1+ Billion
326. Presence/Absence of F - Si at Topological Distance 4	1+ Billion
327. Presence/Absence of F - X at Topological Distance 4	1+ Billion
328. Presence/Absence of Cl - Cl at Topological Distance 4	1+ Billion
329. Presence/Absence of Cl - Br at Topological Distance 4	1+ Billion
330. Presence/Absence of Cl - I at Topological Distance 4	1+ Billion
331. Presence/Absence of Cl - B at Topological Distance 4	1+ Billion
332. Presence/Absence of Cl - Si at Topological Distance 4	1+ Billion
333. Presence/Absence of Cl - X at Topological Distance 4	1+ Billion
334. Presence/Absence of Br - Br at Topological Distance 4	1+ Billion
335. Presence/Absence of Br - I at Topological Distance 4	1+ Billion
336. Presence/Absence of Br - B at Topological Distance 4	1+ Billion
337. Presence/Absence of Br - Si at Topological Distance 4	1+ Billion
338. Presence/Absence of Br - X at Topological Distance 4	1+ Billion





339. Pi	resence/Absence of I - I at Topological Distance 4	1+ Billion
340. Pi	resence/Absence of I - B at Topological Distance 4	1+ Billion
341. Pi	resence/Absence of I - Si at Topological Distance 4	1+ Billion
342. Pi	resence/Absence of I - X at Topological Distance 4	1+ Billion
343. Pi	resence/Absence of B - B at Topological Distance 4	1+ Billion
344. Pi	resence/Absence of B - Si at Topological Distance 4	1+ Billion
345. Pi	resence/Absence of B - X at Topological Distance 4	1+ Billion
346. Pi	resence/Absence of Si - Si at Topological Distance 4	1+ Billion
347. Pi	resence/Absence of Si - X at Topological Distance 4	1+ Billion
348. Pi	resence/Absence of X - X at Topological Distance 4	1+ Billion
349. Pi	resence/Absence of C - C at Topological Distance 5	1+ Billion
350. Pi	resence/Absence of C - N at Topological Distance 5	1+ Billion
351. Pi	resence/Absence of C - O at Topological Distance 5	1+ Billion
352. Pi	resence/Absence of C - S at Topological Distance 5	1+ Billion
353. Pi	resence/Absence of C - P at Topological Distance 5	1+ Billion
354. Pi	resence/Absence of C - F at Topological Distance 5	1+ Billion
355. Pi	resence/Absence of C - Cl at Topological Distance 5	1+ Billion
356. Pi	resence/Absence of C - Br at Topological Distance 5	1+ Billion
357. Pi	resence/Absence of C - I at Topological Distance 5	1+ Billion
358. Pi	resence/Absence of C - B at Topological Distance 5	1+ Billion
359. Pi	resence/Absence of C - Si at Topological Distance 5	1+ Billion
360. Pi	resence/Absence of C - X at Topological Distance 5	1+ Billion
361. P	resence/Absence of N - N at Topological Distance 5	1+ Billion
362. P	resence/Absence of N - O at Topological Distance 5	1+ Billion
363. Pi	resence/Absence of N - S at Topological Distance 5	1+ Billion
364. P	resence/Absence of N - P at Topological Distance 5	1+ Billion





365. Presence/Absence of N - F at Topological Distance 5	1+ Billion
366. Presence/Absence of N - Cl at Topological Distance 5	1+ Billion
367. Presence/Absence of N - Br at Topological Distance 5	1+ Billion
368. Presence/Absence of N - I at Topological Distance 5	1+ Billion
369. Presence/Absence of N - B at Topological Distance 5	1+ Billion
370. Presence/Absence of N - Si at Topological Distance 5	1+ Billion
371. Presence/Absence of N - X at Topological Distance 5	1+ Billion
372. Presence/Absence of O - O at Topological Distance 5	1+ Billion
373. Presence/Absence of O - S at Topological Distance 5	1+ Billion
374. Presence/Absence of O - P at Topological Distance 5	1+ Billion
375. Presence/Absence of O - F at Topological Distance 5	1+ Billion
376. Presence/Absence of O - Cl at Topological Distance 5	1+ Billion
377. Presence/Absence of O - Br at Topological Distance 5	1+ Billion
378. Presence/Absence of O - I at Topological Distance 5	1+ Billion
379. Presence/Absence of O - B at Topological Distance 5	1+ Billion
380. Presence/Absence of O - Si at Topological Distance 5	1+ Billion
381. Presence/Absence of O - X at Topological Distance 5	1+ Billion
382. Presence/Absence of S - S at Topological Distance 5	1+ Billion
383. Presence/Absence of S - P at Topological Distance 5	1+ Billion
384. Presence/Absence of S - F at Topological Distance 5	1+ Billion
385. Presence/Absence of S - Cl at Topological Distance 5	1+ Billion
386. Presence/Absence of S - Br at Topological Distance 5	1+ Billion
387. Presence/Absence of S - I at Topological Distance 5	1+ Billion
388. Presence/Absence of S - B at Topological Distance 5	1+ Billion
389. Presence/Absence of S - Si at Topological Distance 5	1+ Billion
390. Presence/Absence of S - X at Topological Distance 5	1+ Billion





391. Presence/Absence of P - P at Topological Distance 5	1+ Billion
392. Presence/Absence of P - F at Topological Distance 5	1+ Billion
393. Presence/Absence of P - Cl at Topological Distance 5	1+ Billion
394. Presence/Absence of P - Br at Topological Distance 5	1+ Billion
395. Presence/Absence of P - I at Topological Distance 5	1+ Billion
396. Presence/Absence of P - B at Topological Distance 5	1+ Billion
397. Presence/Absence of P - Si at Topological Distance 5	1+ Billion
398. Presence/Absence of P - X at Topological Distance 5	1+ Billion
399. Presence/Absence of F - F at Topological Distance 5	1+ Billion
400. Presence/Absence of F - Cl at Topological Distance 5	1+ Billion
401. Presence/Absence of F - Br at Topological Distance 5	1+ Billion
402. Presence/Absence of F - I at Topological Distance 5	1+ Billion
403. Presence/Absence of F - B at Topological Distance 5	1+ Billion
404. Presence/Absence of F - Si at Topological Distance 5	1+ Billion
405. Presence/Absence of F - X at Topological Distance 5	1+ Billion
406. Presence/Absence of Cl - Cl at Topological Distance 5	1+ Billion
407. Presence/Absence of Cl - Br at Topological Distance 5	1+ Billion
408. Presence/Absence of Cl - I at Topological Distance 5	1+ Billion
409. Presence/Absence of Cl - B at Topological Distance 5	1+ Billion
410. Presence/Absence of Cl - Si at Topological Distance 5	1+ Billion
411. Presence/Absence of Cl - X at Topological Distance 5	1+ Billion
412. Presence/Absence of Br - Br at Topological Distance 5	1+ Billion
413. Presence/Absence of Br - I at Topological Distance 5	1+ Billion
414. Presence/Absence of Br - B at Topological Distance 5	1+ Billion
415. Presence/Absence of Br - Si at Topological Distance 5	1+ Billion
416. Presence/Absence of Br - X at Topological Distance 5	1+ Billion





1+ Billion
1+ Billion





443. Presence/Absence of N - F at Topological Distance 6	1+ Billion
444. Presence/Absence of N - Cl at Topological Distance 6	1+ Billion
445. Presence/Absence of N - Br at Topological Distance 6	1+ Billion
446. Presence/Absence of N - I at Topological Distance 6	1+ Billion
447. Presence/Absence of N - B at Topological Distance 6	1+ Billion
448. Presence/Absence of N - Si at Topological Distance 6	1+ Billion
449. Presence/Absence of N - X at Topological Distance 6	1+ Billion
450. Presence/Absence of O - O at Topological Distance 6	1+ Billion
451. Presence/Absence of O - S at Topological Distance 6	1+ Billion
452. Presence/Absence of O - P at Topological Distance 6	1+ Billion
453. Presence/Absence of O - F at Topological Distance 6	1+ Billion
454. Presence/Absence of O - Cl at Topological Distance 6	1+ Billion
455. Presence/Absence of O - Br at Topological Distance 6	1+ Billion
456. Presence/Absence of O - I at Topological Distance 6	1+ Billion
457. Presence/Absence of O - B at Topological Distance 6	1+ Billion
458. Presence/Absence of O - Si at Topological Distance 6	1+ Billion
459. Presence/Absence of O - X at Topological Distance 6	1+ Billion
460. Presence/Absence of S - S at Topological Distance 6	1+ Billion
461. Presence/Absence of S - P at Topological Distance 6	1+ Billion
462. Presence/Absence of S - F at Topological Distance 6	1+ Billion
463. Presence/Absence of S - Cl at Topological Distance 6	1+ Billion
464. Presence/Absence of S - Br at Topological Distance 6	1+ Billion
465. Presence/Absence of S - I at Topological Distance 6	1+ Billion
466. Presence/Absence of S - B at Topological Distance 6	1+ Billion
467. Presence/Absence of S - Si at Topological Distance 6	1+ Billion
468. Presence/Absence of S - X at Topological Distance 6	1+ Billion





469. Presence/Absence of P - P at Topological Distance 6	1+ Billion
470. Presence/Absence of P - F at Topological Distance 6	1+ Billion
471. Presence/Absence of P - Cl at Topological Distance 6	1+ Billion
472. Presence/Absence of P - Br at Topological Distance 6	1+ Billion
473. Presence/Absence of P - I at Topological Distance 6	1+ Billion
474. Presence/Absence of P - B at Topological Distance 6	1+ Billion
475. Presence/Absence of P - Si at Topological Distance 6	1+ Billion
476. Presence/Absence of P - X at Topological Distance 6	1+ Billion
477. Presence/Absence of F - F at Topological Distance 6	1+ Billion
478. Presence/Absence of F - Cl at Topological Distance 6	1+ Billion
479. Presence/Absence of F - Br at Topological Distance 6	1+ Billion
480. Presence/Absence of F - I at Topological Distance 6	1+ Billion
481. Presence/Absence of F - B at Topological Distance 6	1+ Billion
482. Presence/Absence of F - Si at Topological Distance 6	1+ Billion
483. Presence/Absence of F - X at Topological Distance 6	1+ Billion
484. Presence/Absence of Cl - Cl at Topological Distance 6	1+ Billion
485. Presence/Absence of Cl - Br at Topological Distance 6	1+ Billion
486. Presence/Absence of Cl - I at Topological Distance 6	1+ Billion
487. Presence/Absence of Cl - B at Topological Distance 6	1+ Billion
488. Presence/Absence of Cl - Si at Topological Distance 6	1+ Billion
489. Presence/Absence of Cl - X at Topological Distance 6	1+ Billion
490. Presence/Absence of Br - Br at Topological Distance 6	1+ Billion
491. Presence/Absence of Br - I at Topological Distance 6	1+ Billion
492. Presence/Absence of Br - B at Topological Distance 6	1+ Billion
493. Presence/Absence of Br - Si at Topological Distance 6	1+ Billion
494. Presence/Absence of Br - X at Topological Distance 6	1+ Billion





495. Presence/Absence of I - I at Topological Distance 6	1+ Billion
496. Presence/Absence of I - B at Topological Distance 6	1+ Billion
497. Presence/Absence of I - Si at Topological Distance 6	1+ Billion
498. Presence/Absence of I - X at Topological Distance 6	1+ Billion
499. Presence/Absence of B - B at Topological Distance 6	1+ Billion
500. Presence/Absence of B - Si at Topological Distance 6	1+ Billion
501. Presence/Absence of B - X at Topological Distance 6	1+ Billion
502. Presence/Absence of Si - Si at Topological Distance 6	1+ Billion
503. Presence/Absence of Si - X at Topological Distance 6	1+ Billion
504. Presence/Absence of X - X at Topological Distance 6	1+ Billion
505. Presence/Absence of C - C at Topological Distance 7	1+ Billion
506. Presence/Absence of C - N at Topological Distance 7	1+ Billion
507. Presence/Absence of C - O at Topological Distance 7	1+ Billion
508. Presence/Absence of C - S at Topological Distance 7	1+ Billion
509. Presence/Absence of C - P at Topological Distance 7	1+ Billion
510. Presence/Absence of C - F at Topological Distance 7	1+ Billion
511. Presence/Absence of C - Cl at Topological Distance 7	1+ Billion
512. Presence/Absence of C - Br at Topological Distance 7	1+ Billion
513. Presence/Absence of C - I at Topological Distance 7	1+ Billion
514. Presence/Absence of C - B at Topological Distance 7	1+ Billion
515. Presence/Absence of C - Si at Topological Distance 7	1+ Billion
516. Presence/Absence of C - X at Topological Distance 7	1+ Billion
517. Presence/Absence of N - N at Topological Distance 7	1+ Billion
518. Presence/Absence of N - O at Topological Distance 7	1+ Billion
519. Presence/Absence of N - S at Topological Distance 7	1+ Billion
520. Presence/Absence of N - P at Topological Distance 7	1+ Billion





ļ	521. Presence/Absence of N - F at Topological Distance 7	1+ Billion
ļ	522. Presence/Absence of N - Cl at Topological Distance 7	1+ Billion
ļ	523. Presence/Absence of N - Br at Topological Distance 7	1+ Billion
ļ	524. Presence/Absence of N - I at Topological Distance 7	1+ Billion
ļ	525. Presence/Absence of N - B at Topological Distance 7	1+ Billion
ļ	526. Presence/Absence of N - Si at Topological Distance 7	1+ Billion
ļ	527. Presence/Absence of N - X at Topological Distance 7	1+ Billion
ļ	528. Presence/Absence of O - O at Topological Distance 7	1+ Billion
ļ	529. Presence/Absence of O - S at Topological Distance 7	1+ Billion
ļ	530. Presence/Absence of O - P at Topological Distance 7	1+ Billion
ļ	531. Presence/Absence of O - F at Topological Distance 7	1+ Billion
ļ	532. Presence/Absence of O - Cl at Topological Distance 7	1+ Billion
ļ	533. Presence/Absence of O - Br at Topological Distance 7	1+ Billion
ļ	534. Presence/Absence of O - I at Topological Distance 7	1+ Billion
ļ	535. Presence/Absence of O - B at Topological Distance 7	1+ Billion
ļ	536. Presence/Absence of O - Si at Topological Distance 7	1+ Billion
ļ	537. Presence/Absence of O - X at Topological Distance 7	1+ Billion
ļ	538. Presence/Absence of S - S at Topological Distance 7	1+ Billion
ļ	539. Presence/Absence of S - P at Topological Distance 7	1+ Billion
ļ	540. Presence/Absence of S - F at Topological Distance 7	1+ Billion
ļ	541. Presence/Absence of S - Cl at Topological Distance 7	1+ Billion
ļ	542. Presence/Absence of S - Br at Topological Distance 7	1+ Billion
ļ	543. Presence/Absence of S - I at Topological Distance 7	1+ Billion
ļ	544. Presence/Absence of S - B at Topological Distance 7	1+ Billion
ļ	545. Presence/Absence of S - Si at Topological Distance 7	1+ Billion
ļ	546. Presence/Absence of S - X at Topological Distance 7	1+ Billion





547.	Presence/Absence of P - P at Topological Distance 7	1+ Billion
548.	Presence/Absence of P - F at Topological Distance 7	1+ Billion
549.	Presence/Absence of P - Cl at Topological Distance 7	1+ Billion
550.	Presence/Absence of P - Br at Topological Distance 7	1+ Billion
551.	Presence/Absence of P - I at Topological Distance 7	1+ Billion
552.	Presence/Absence of P - B at Topological Distance 7	1+ Billion
553.	Presence/Absence of P - Si at Topological Distance 7	1+ Billion
554.	Presence/Absence of P - X at Topological Distance 7	1+ Billion
555.	Presence/Absence of F - F at Topological Distance 7	1+ Billion
556.	Presence/Absence of F - Cl at Topological Distance 7	1+ Billion
557.	Presence/Absence of F - Br at Topological Distance 7	1+ Billion
558.	Presence/Absence of F - I at Topological Distance 7	1+ Billion
559.	Presence/Absence of F - B at Topological Distance 7	1+ Billion
560.	Presence/Absence of F - Si at Topological Distance 7	1+ Billion
561.	Presence/Absence of F - X at Topological Distance 7	1+ Billion
562.	Presence/Absence of Cl - Cl at Topological Distance 7	1+ Billion
563.	Presence/Absence of Cl - Br at Topological Distance 7	1+ Billion
564.	Presence/Absence of Cl - I at Topological Distance 7	1+ Billion
565.	Presence/Absence of Cl - B at Topological Distance 7	1+ Billion
566.	Presence/Absence of Cl - Si at Topological Distance 7	1+ Billion
567.	Presence/Absence of Cl - X at Topological Distance 7	1+ Billion
568.	Presence/Absence of Br - Br at Topological Distance 7	1+ Billion
569.	Presence/Absence of Br - I at Topological Distance 7	1+ Billion
570.	Presence/Absence of Br - B at Topological Distance 7	1+ Billion
571.	Presence/Absence of Br - Si at Topological Distance 7	1+ Billion
572.	Presence/Absence of Br - X at Topological Distance 7	1+ Billion





573. Presei	nce/Absence of I - I at Topological Distance 7	1+ Billion
574. Presei	nce/Absence of I - B at Topological Distance 7	1+ Billion
575. Presei	nce/Absence of I - Si at Topological Distance 7	1+ Billion
576. Presei	nce/Absence of I - X at Topological Distance 7	1+ Billion
577. Presei	nce/Absence of B - B at Topological Distance 7	1+ Billion
578. Presei	nce/Absence of B - Si at Topological Distance 7	1+ Billion
579. Presei	nce/Absence of B - X at Topological Distance 7	1+ Billion
580. Presei	nce/Absence of Si - Si at Topological Distance 7	1+ Billion
581. Presei	nce/Absence of Si - X at Topological Distance 7	1+ Billion
582. Presei	nce/Absence of X - X at Topological Distance 7	1+ Billion
583. Presei	nce/Absence of C - C at Topological Distance 8	1+ Billion
584. Presei	nce/Absence of C - N at Topological Distance 8	1+ Billion
585. Presei	nce/Absence of C - O at Topological Distance 8	1+ Billion
586. Presei	nce/Absence of C - S at Topological Distance 8	1+ Billion
587. Presei	nce/Absence of C - P at Topological Distance 8	1+ Billion
588. Presei	nce/Absence of C - F at Topological Distance 8	1+ Billion
589. Presei	nce/Absence of C - Cl at Topological Distance 8	1+ Billion
590. Presei	nce/Absence of C - Br at Topological Distance 8	1+ Billion
591. Presei	nce/Absence of C - I at Topological Distance 8	1+ Billion
592. Presei	nce/Absence of C - B at Topological Distance 8	1+ Billion
593. Preser	nce/Absence of C - Si at Topological Distance 8	1+ Billion
594. Preser	nce/Absence of C - X at Topological Distance 8	1+ Billion
595. Presei	nce/Absence of N - N at Topological Distance 8	1+ Billion
596. Presei	nce/Absence of N - O at Topological Distance 8	1+ Billion
597. Prese	nce/Absence of N - S at Topological Distance 8	1+ Billion
598. Presei	nce/Absence of N - P at Topological Distance 8	1+ Billion





599. Presence/Absence of N - F at Topological Distance 8	1+ Billion
600. Presence/Absence of N - Cl at Topological Distance 8	1+ Billion
601. Presence/Absence of N - Br at Topological Distance 8	1+ Billion
602. Presence/Absence of N - I at Topological Distance 8	1+ Billion
603. Presence/Absence of N - B at Topological Distance 8	1+ Billion
604. Presence/Absence of N - Si at Topological Distance 8	1+ Billion
605. Presence/Absence of N - X at Topological Distance 8	1+ Billion
606. Presence/Absence of O - O at Topological Distance 8	1+ Billion
607. Presence/Absence of O - S at Topological Distance 8	1+ Billion
608. Presence/Absence of O - P at Topological Distance 8	1+ Billion
609. Presence/Absence of O - F at Topological Distance 8	1+ Billion
610. Presence/Absence of O - Cl at Topological Distance 8	1+ Billion
611. Presence/Absence of O - Br at Topological Distance 8	1+ Billion
612. Presence/Absence of O - I at Topological Distance 8	1+ Billion
613. Presence/Absence of O - B at Topological Distance 8	1+ Billion
614. Presence/Absence of O - Si at Topological Distance 8	1+ Billion
615. Presence/Absence of O - X at Topological Distance 8	1+ Billion
616. Presence/Absence of S - S at Topological Distance 8	1+ Billion
617. Presence/Absence of S - P at Topological Distance 8	1+ Billion
618. Presence/Absence of S - F at Topological Distance 8	1+ Billion
619. Presence/Absence of S - Cl at Topological Distance 8	1+ Billion
620. Presence/Absence of S - Br at Topological Distance 8	1+ Billion
621. Presence/Absence of S - I at Topological Distance 8	1+ Billion
622. Presence/Absence of S - B at Topological Distance 8	1+ Billion
623. Presence/Absence of S - Si at Topological Distance 8	1+ Billion
624. Presence/Absence of S - X at Topological Distance 8	1+ Billion





625. Presence/Absence of P - P at Topological Distance 8	1+ Billion
626. Presence/Absence of P - F at Topological Distance 8	1+ Billion
627. Presence/Absence of P - Cl at Topological Distance 8	1+ Billion
628. Presence/Absence of P - Br at Topological Distance 8	1+ Billion
629. Presence/Absence of P - I at Topological Distance 8	1+ Billion
630. Presence/Absence of P - B at Topological Distance 8	1+ Billion
631. Presence/Absence of P - Si at Topological Distance 8	1+ Billion
632. Presence/Absence of P - X at Topological Distance 8	1+ Billion
633. Presence/Absence of F - F at Topological Distance 8	1+ Billion
634. Presence/Absence of F - Cl at Topological Distance 8	1+ Billion
635. Presence/Absence of F - Br at Topological Distance 8	1+ Billion
636. Presence/Absence of F - I at Topological Distance 8	1+ Billion
637. Presence/Absence of F - B at Topological Distance 8	1+ Billion
638. Presence/Absence of F - Si at Topological Distance 8	1+ Billion
639. Presence/Absence of F - X at Topological Distance 8	1+ Billion
640. Presence/Absence of Cl - Cl at Topological Distance 8	1+ Billion
641. Presence/Absence of Cl - Br at Topological Distance 8	1+ Billion
642. Presence/Absence of Cl - I at Topological Distance 8	1+ Billion
643. Presence/Absence of Cl - B at Topological Distance 8	1+ Billion
644. Presence/Absence of Cl - Si at Topological Distance 8	1+ Billion
645. Presence/Absence of Cl - X at Topological Distance 8	1+ Billion
646. Presence/Absence of Br - Br at Topological Distance 8	1+ Billion
647. Presence/Absence of Br - I at Topological Distance 8	1+ Billion
648. Presence/Absence of Br - B at Topological Distance 8	1+ Billion
649. Presence/Absence of Br - Si at Topological Distance 8	1+ Billion
650. Presence/Absence of Br - X at Topological Distance 8	1+ Billion





651. Presence/Absence of I - I at Topological Distance 8	1+ Billion
652. Presence/Absence of I - B at Topological Distance 8	1+ Billion
653. Presence/Absence of I - Si at Topological Distance 8	1+ Billion
654. Presence/Absence of I - X at Topological Distance 8	1+ Billion
655. Presence/Absence of B - B at Topological Distance 8	1+ Billion
656. Presence/Absence of B - Si at Topological Distance 8	1+ Billion
657. Presence/Absence of B - X at Topological Distance 8	1+ Billion
658. Presence/Absence of Si - Si at Topological Distance 8	1+ Billion
659. Presence/Absence of Si - X at Topological Distance 8	1+ Billion
660. Presence/Absence of X - X at Topological Distance 8	1+ Billion
661. Presence/Absence of C - C at Topological Distance 9	1+ Billion
662. Presence/Absence of C - N at Topological Distance 9	1+ Billion
663. Presence/Absence of C - O at Topological Distance 9	1+ Billion
664. Presence/Absence of C - S at Topological Distance 9	1+ Billion
665. Presence/Absence of C - P at Topological Distance 9	1+ Billion
666. Presence/Absence of C - F at Topological Distance 9	1+ Billion
667. Presence/Absence of C - Cl at Topological Distance 9	1+ Billion
668. Presence/Absence of C - Br at Topological Distance 9	1+ Billion
669. Presence/Absence of C - I at Topological Distance 9	1+ Billion
670. Presence/Absence of C - B at Topological Distance 9	1+ Billion
671. Presence/Absence of C - Si at Topological Distance 9	1+ Billion
672. Presence/Absence of C - X at Topological Distance 9	1+ Billion
673. Presence/Absence of N - N at Topological Distance 9	1+ Billion
674. Presence/Absence of N - O at Topological Distance 9	1+ Billion
675. Presence/Absence of N - S at Topological Distance 9	1+ Billion
676. Presence/Absence of N - P at Topological Distance 9	1+ Billion





67	7. Presence/Absence of N - F at Topological Distance 9	1+ Billion
67	8. Presence/Absence of N - Cl at Topological Distance 9	1+ Billion
67	9. Presence/Absence of N - Br at Topological Distance 9	1+ Billion
68	0. Presence/Absence of N - I at Topological Distance 9	1+ Billion
68	1. Presence/Absence of N - B at Topological Distance 9	1+ Billion
68	2. Presence/Absence of N - Si at Topological Distance 9	1+ Billion
68	3. Presence/Absence of N - X at Topological Distance 9	1+ Billion
68	4. Presence/Absence of O - O at Topological Distance 9	1+ Billion
68	5. Presence/Absence of O - S at Topological Distance 9	1+ Billion
68	6. Presence/Absence of O - P at Topological Distance 9	1+ Billion
68	7. Presence/Absence of O - F at Topological Distance 9	1+ Billion
68	8. Presence/Absence of O - Cl at Topological Distance 9	1+ Billion
68	9. Presence/Absence of O - Br at Topological Distance 9	1+ Billion
69	0. Presence/Absence of O - I at Topological Distance 9	1+ Billion
69	1. Presence/Absence of O - B at Topological Distance 9	1+ Billion
69	2. Presence/Absence of O - Si at Topological Distance 9	1+ Billion
69	3. Presence/Absence of O - X at Topological Distance 9	1+ Billion
69	4. Presence/Absence of S - S at Topological Distance 9	1+ Billion
69	5. Presence/Absence of S - P at Topological Distance 9	1+ Billion
69	6. Presence/Absence of S - F at Topological Distance 9	1+ Billion
69	7. Presence/Absence of S - Cl at Topological Distance 9	1+ Billion
69	8. Presence/Absence of S - Br at Topological Distance 9	1+ Billion
69	9. Presence/Absence of S - I at Topological Distance 9	1+ Billion
70	0. Presence/Absence of S - B at Topological Distance 9	1+ Billion
70	1. Presence/Absence of S - Si at Topological Distance 9	1+ Billion
70	2. Presence/Absence of S - X at Topological Distance 9	1+ Billion



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703. Presence/Absence of P - P at Topological Distance 9	1+ Billion
704. Presence/Absence of P - F at Topological Distance 9	1+ Billion
705. Presence/Absence of P - Cl at Topological Distance 9	1+ Billion
706. Presence/Absence of P - Br at Topological Distance 9	1+ Billion
707. Presence/Absence of P - I at Topological Distance 9	1+ Billion
708. Presence/Absence of P - B at Topological Distance 9	1+ Billion
709. Presence/Absence of P - Si at Topological Distance 9	1+ Billion
710. Presence/Absence of P - X at Topological Distance 9	1+ Billion
711. Presence/Absence of F - F at Topological Distance 9	1+ Billion
712. Presence/Absence of F - Cl at Topological Distance 9	1+ Billion
713. Presence/Absence of F - Br at Topological Distance 9	1+ Billion
714. Presence/Absence of F - I at Topological Distance 9	1+ Billion
715. Presence/Absence of F - B at Topological Distance 9	1+ Billion
716. Presence/Absence of F - Si at Topological Distance 9	1+ Billion
717. Presence/Absence of F - X at Topological Distance 9	1+ Billion
718. Presence/Absence of Cl - Cl at Topological Distance 9	1+ Billion
719. Presence/Absence of Cl - Br at Topological Distance 9	1+ Billion
720. Presence/Absence of Cl - I at Topological Distance 9	1+ Billion
721. Presence/Absence of Cl - B at Topological Distance 9	1+ Billion
722. Presence/Absence of Cl - Si at Topological Distance 9	1+ Billion
723. Presence/Absence of Cl - X at Topological Distance 9	1+ Billion
724. Presence/Absence of Br - Br at Topological Distance 9	1+ Billion
725. Presence/Absence of Br - I at Topological Distance 9	1+ Billion
726. Presence/Absence of Br - B at Topological Distance 9	1+ Billion
727. Presence/Absence of Br - Si at Topological Distance 9	1+ Billion
728. Presence/Absence of Br - X at Topological Distance 9	1+ Billion





729. Presence/Absence of I - I at Topological Distance 9	1+ Billion
730. Presence/Absence of I - B at Topological Distance 9	1+ Billion
731. Presence/Absence of I - Si at Topological Distance 9	1+ Billion
732. Presence/Absence of I - X at Topological Distance 9	1+ Billion
733. Presence/Absence of B - B at Topological Distance 9	1+ Billion
734. Presence/Absence of B - Si at Topological Distance 9	1+ Billion
735. Presence/Absence of B - X at Topological Distance 9	1+ Billion
736. Presence/Absence of Si - Si at Topological Distance 9	1+ Billion
737. Presence/Absence of Si - X at Topological Distance 9	1+ Billion
738. Presence/Absence of X - X at Topological Distance 9	1+ Billion
739. Presence/Absence of C - C at Topological Distance 10	1+ Billion
740. Presence/Absence of C - N at Topological Distance 10	1+ Billion
741. Presence/Absence of C - O at Topological Distance 10	1+ Billion
742. Presence/Absence of C - S at Topological Distance 10	1+ Billion
743. Presence/Absence of C - P at Topological Distance 10	1+ Billion
744. Presence/Absence of C - F at Topological Distance 10	1+ Billion
745. Presence/Absence of C - Cl at Topological Distance 10	1+ Billion
746. Presence/Absence of C - Br at Topological Distance 10	1+ Billion
747. Presence/Absence of C - I at Topological Distance 10	1+ Billion
748. Presence/Absence of C - B at Topological Distance 10	1+ Billion
749. Presence/Absence of C - Si at Topological Distance 10	1+ Billion
750. Presence/Absence of C - X at Topological Distance 10	1+ Billion
751. Presence/Absence of N - N at Topological Distance 10	1+ Billion
752. Presence/Absence of N - O at Topological Distance 10	1+ Billion
753. Presence/Absence of N - S at Topological Distance 10	1+ Billion
754. Presence/Absence of N - P at Topological Distance 10	1+ Billion





755. Presence/Absence of N - F at Topological Distance 10	1+ Billion
756. Presence/Absence of N - Cl at Topological Distance 10	1+ Billion
757. Presence/Absence of N - Br at Topological Distance 10	1+ Billion
758. Presence/Absence of N - I at Topological Distance 10	1+ Billion
759. Presence/Absence of N - B at Topological Distance 10	1+ Billion
760. Presence/Absence of N - Si at Topological Distance 10	1+ Billion
761. Presence/Absence of N - X at Topological Distance 10	1+ Billion
762. Presence/Absence of O - O at Topological Distance 10	1+ Billion
763. Presence/Absence of O - S at Topological Distance 10	1+ Billion
764. Presence/Absence of O - P at Topological Distance 10	1+ Billion
765. Presence/Absence of O - F at Topological Distance 10	1+ Billion
766. Presence/Absence of O - Cl at Topological Distance 10	1+ Billion
767. Presence/Absence of O - Br at Topological Distance 10	1+ Billion
768. Presence/Absence of O - I at Topological Distance 10	1+ Billion
769. Presence/Absence of O - B at Topological Distance 10	1+ Billion
770. Presence/Absence of O - Si at Topological Distance 10	1+ Billion
771. Presence/Absence of O - X at Topological Distance 10	1+ Billion
772. Presence/Absence of S - S at Topological Distance 10	1+ Billion
773. Presence/Absence of S - P at Topological Distance 10	1+ Billion
774. Presence/Absence of S - F at Topological Distance 10	1+ Billion
775. Presence/Absence of S - Cl at Topological Distance 10	1+ Billion
776. Presence/Absence of S - Br at Topological Distance 10	1+ Billion
777. Presence/Absence of S - I at Topological Distance 10	1+ Billion
778. Presence/Absence of S - B at Topological Distance 10	1+ Billion
779. Presence/Absence of S - Si at Topological Distance 10	1+ Billion
780. Presence/Absence of S - X at Topological Distance 10	1+ Billion



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781. Presence/Absence of P - P at Topological Distance 10	1+ Billion
782. Presence/Absence of P - F at Topological Distance 10	1+ Billion
783. Presence/Absence of P - Cl at Topological Distance 10	1+ Billion
784. Presence/Absence of P - Br at Topological Distance 10	1+ Billion
785. Presence/Absence of P - I at Topological Distance 10	1+ Billion
786. Presence/Absence of P - B at Topological Distance 10	1+ Billion
787. Presence/Absence of P - Si at Topological Distance 10	1+ Billion
788. Presence/Absence of P - X at Topological Distance 10	1+ Billion
789. Presence/Absence of F - F at Topological Distance 10	1+ Billion
790. Presence/Absence of F - Cl at Topological Distance 10	1+ Billion
791. Presence/Absence of F - Br at Topological Distance 10	1+ Billion
792. Presence/Absence of F - I at Topological Distance 10	1+ Billion
793. Presence/Absence of F - B at Topological Distance 10	1+ Billion
794. Presence/Absence of F - Si at Topological Distance 10	1+ Billion
795. Presence/Absence of F - X at Topological Distance 10	1+ Billion
796. Presence/Absence of Cl - Cl at Topological Distance 10	1+ Billion
797. Presence/Absence of Cl - Br at Topological Distance 10	1+ Billion
798. Presence/Absence of Cl - I at Topological Distance 10	1+ Billion
799. Presence/Absence of Cl - B at Topological Distance 10	1+ Billion
800. Presence/Absence of Cl - Si at Topological Distance 10	1+ Billion
801. Presence/Absence of Cl - X at Topological Distance 10	1+ Billion
802. Presence/Absence of Br - Br at Topological Distance 10	1+ Billion
803. Presence/Absence of Br - I at Topological Distance 10	1+ Billion
804. Presence/Absence of Br - B at Topological Distance 10	1+ Billion
805. Presence/Absence of Br - Si at Topological Distance 10	1+ Billion
806. Presence/Absence of Br - X at Topological Distance 10	1+ Billion





807. Presence/Absence of I - I at Topological Distance 10	1+ Billion
808. Presence/Absence of I - B at Topological Distance 10	1+ Billion
809. Presence/Absence of I - Si at Topological Distance 10	1+ Billion
810. Presence/Absence of I - X at Topological Distance 10	1+ Billion
811. Presence/Absence of B - B at Topological Distance 10	1+ Billion
812. Presence/Absence of B - Si at Topological Distance 10	1+ Billion
813. Presence/Absence of B - X at Topological Distance 10	1+ Billion
814. Presence/Absence of Si - Si at Topological Distance 10	1+ Billion
815. Presence/Absence of Si - X at Topological Distance 10	1+ Billion
816. Presence/Absence of X - X at Topological Distance 10	1+ Billion
817. Frequency of C - C at Topological Distance 1	1+ Billion
818. Frequency of C - N at Topological Distance 1	1+ Billion
819. Frequency of C - O at Topological Distance 1	1+ Billion
820. Frequency of C - S at Topological Distance 1	1+ Billion
821. Frequency of C - P at Topological Distance 1	1+ Billion
822. Frequency of C - F at Topological Distance 1	1+ Billion
823. Frequency of C - Cl at Topological Distance 1	1+ Billion
824. Frequency of C - Br at Topological Distance 1	1+ Billion
825. Frequency of C - I at Topological Distance 1	1+ Billion
826. Frequency of C - B at Topological Distance 1	1+ Billion
827. Frequency of C - Si at Topological Distance 1	1+ Billion
828. Frequency of C - X at Topological Distance 1	1+ Billion
829. Frequency of N - N at Topological Distance 1	1+ Billion
830. Frequency of N - O at Topological Distance 1	1+ Billion
831. Frequency of N - S at Topological Distance 1	1+ Billion
832. Frequency of N - P at Topological Distance 1	1+ Billion





833. Frequency of N - F at Topological Distance 1	1+ Billion
834. Frequency of N - Cl at Topological Distance 1	1+ Billion
835. Frequency of N - Br at Topological Distance 1	1+ Billion
836. Frequency of N - I at Topological Distance 1	1+ Billion
837. Frequency of N - B at Topological Distance 1	1+ Billion
838. Frequency of N - Si at Topological Distance 1	1+ Billion
839. Frequency of N - X at Topological Distance 1	1+ Billion
840. Frequency of O - O at Topological Distance 1	1+ Billion
841. Frequency of O - S at Topological Distance 1	1+ Billion
842. Frequency of O - P at Topological Distance 1	1+ Billion
843. Frequency of O - F at Topological Distance 1	1+ Billion
844. Frequency of O - Cl at Topological Distance 1	1+ Billion
845. Frequency of O - Br at Topological Distance 1	1+ Billion
846. Frequency of O - I at Topological Distance 1	1+ Billion
847. Frequency of O - B at Topological Distance 1	1+ Billion
848. Frequency of O - Si at Topological Distance 1	1+ Billion
849. Frequency of O - X at Topological Distance 1	1+ Billion
850. Frequency of S - S at Topological Distance 1	1+ Billion
851. Frequency of S - P at Topological Distance 1	1+ Billion
852. Frequency of S - F at Topological Distance 1	1+ Billion
853. Frequency of S - Cl at Topological Distance 1	1+ Billion
854. Frequency of S - Br at Topological Distance 1	1+ Billion
855. Frequency of S - I at Topological Distance 1	1+ Billion
856. Frequency of S - B at Topological Distance 1	1+ Billion
857. Frequency of S - Si at Topological Distance 1	1+ Billion
858. Frequency of S - X at Topological Distance 1	1+ Billion



C h e m E s s e n , l n c .

859. Frequency of P - P at Topological Distance 1	1+ Billion
860. Frequency of P - F at Topological Distance 1	1+ Billion
861. Frequency of P - Cl at Topological Distance 1	1+ Billion
862. Frequency of P - Br at Topological Distance 1	1+ Billion
863. Frequency of P - I at Topological Distance 1	1+ Billion
864. Frequency of P - B at Topological Distance 1	1+ Billion
865. Frequency of P - Si at Topological Distance 1	1+ Billion
866. Frequency of P - X at Topological Distance 1	1+ Billion
867. Frequency of F - F at Topological Distance 1	1+ Billion
868. Frequency of F - Cl at Topological Distance 1	1+ Billion
869. Frequency of F - Br at Topological Distance 1	1+ Billion
870. Frequency of F - I at Topological Distance 1	1+ Billion
871. Frequency of F - B at Topological Distance 1	1+ Billion
872. Frequency of F - Si at Topological Distance 1	1+ Billion
873. Frequency of F - X at Topological Distance 1	1+ Billion
874. Frequency of Cl - Cl at Topological Distance 1	1+ Billion
875. Frequency of Cl - Br at Topological Distance 1	1+ Billion
876. Frequency of Cl - I at Topological Distance 1	1+ Billion
877. Frequency of Cl - B at Topological Distance 1	1+ Billion
878. Frequency of Cl - Si at Topological Distance 1	1+ Billion
879. Frequency of Cl - X at Topological Distance 1	1+ Billion
880. Frequency of Br - Br at Topological Distance 1	1+ Billion
881. Frequency of Br - I at Topological Distance 1	1+ Billion
882. Frequency of Br - B at Topological Distance 1	1+ Billion
883. Frequency of Br - Si at Topological Distance 1	1+ Billion
884. Frequency of Br - X at Topological Distance 1	1+ Billion



C h e m E s s e n , l n c .

885. Frequency of I - I at Topological Distance 1	1+ Billion
886. Frequency of I - B at Topological Distance 1	1+ Billion
887. Frequency of I - Si at Topological Distance 1	1+ Billion
888. Frequency of I - X at Topological Distance 1	1+ Billion
889. Frequency of B - B at Topological Distance 1	1+ Billion
890. Frequency of B - Si at Topological Distance 1	1+ Billion
891. Frequency of B - X at Topological Distance 1	1+ Billion
892. Frequency of Si - Si at Topological Distance 1	1+ Billion
893. Frequency of Si - X at Topological Distance 1	1+ Billion
894. Frequency of X - X at Topological Distance 1	1+ Billion
895. Frequency of C - C at Topological Distance 2	1+ Billion
896. Frequency of C - N at Topological Distance 2	1+ Billion
897. Frequency of C - O at Topological Distance 2	1+ Billion
898. Frequency of C - S at Topological Distance 2	1+ Billion
899. Frequency of C - P at Topological Distance 2	1+ Billion
900. Frequency of C - F at Topological Distance 2	1+ Billion
901. Frequency of C - Cl at Topological Distance 2	1+ Billion
902. Frequency of C - Br at Topological Distance 2	1+ Billion
903. Frequency of C - I at Topological Distance 2	1+ Billion
904. Frequency of C - B at Topological Distance 2	1+ Billion
905. Frequency of C - Si at Topological Distance 2	1+ Billion
906. Frequency of C - X at Topological Distance 2	1+ Billion
907. Frequency of N - N at Topological Distance 2	1+ Billion
908. Frequency of N - O at Topological Distance 2	1+ Billion
909. Frequency of N - S at Topological Distance 2	1+ Billion
910. Frequency of N - P at Topological Distance 2	1+ Billion





911. Frequency of N - F at Topological Distance 2	1+ Billion
912. Frequency of N - Cl at Topological Distance 2	1+ Billion
913. Frequency of N - Br at Topological Distance 2	1+ Billion
914. Frequency of N - I at Topological Distance 2	1+ Billion
915. Frequency of N - B at Topological Distance 2	1+ Billion
916. Frequency of N - Si at Topological Distance 2	1+ Billion
917. Frequency of N - X at Topological Distance 2	1+ Billion
918. Frequency of O - O at Topological Distance 2	1+ Billion
919. Frequency of O - S at Topological Distance 2	1+ Billion
920. Frequency of O - P at Topological Distance 2	1+ Billion
921. Frequency of O - F at Topological Distance 2	1+ Billion
922. Frequency of O - Cl at Topological Distance 2	1+ Billion
923. Frequency of O - Br at Topological Distance 2	1+ Billion
924. Frequency of O - I at Topological Distance 2	1+ Billion
925. Frequency of O - B at Topological Distance 2	1+ Billion
926. Frequency of O - Si at Topological Distance 2	1+ Billion
927. Frequency of O - X at Topological Distance 2	1+ Billion
928. Frequency of S - S at Topological Distance 2	1+ Billion
929. Frequency of S - P at Topological Distance 2	1+ Billion
930. Frequency of S - F at Topological Distance 2	1+ Billion
931. Frequency of S - Cl at Topological Distance 2	1+ Billion
932. Frequency of S - Br at Topological Distance 2	1+ Billion
933. Frequency of S - I at Topological Distance 2	1+ Billion
934. Frequency of S - B at Topological Distance 2	1+ Billion
935. Frequency of S - Si at Topological Distance 2	1+ Billion
936. Frequency of S - X at Topological Distance 2	1+ Billion



C h e m E s s e n , l n c .

937. Frequency of P - P at Topological Distance 2	1+ Billion
938. Frequency of P - F at Topological Distance 2	1+ Billion
939. Frequency of P - Cl at Topological Distance 2	1+ Billion
940. Frequency of P - Br at Topological Distance 2	1+ Billion
941. Frequency of P - I at Topological Distance 2	1+ Billion
942. Frequency of P - B at Topological Distance 2	1+ Billion
943. Frequency of P - Si at Topological Distance 2	1+ Billion
944. Frequency of P - X at Topological Distance 2	1+ Billion
945. Frequency of F - F at Topological Distance 2	1+ Billion
946. Frequency of F - Cl at Topological Distance 2	1+ Billion
947. Frequency of F - Br at Topological Distance 2	1+ Billion
948. Frequency of F - I at Topological Distance 2	1+ Billion
949. Frequency of F - B at Topological Distance 2	1+ Billion
950. Frequency of F - Si at Topological Distance 2	1+ Billion
951. Frequency of F - X at Topological Distance 2	1+ Billion
952. Frequency of Cl - Cl at Topological Distance 2	1+ Billion
953. Frequency of Cl - Br at Topological Distance 2	1+ Billion
954. Frequency of Cl - I at Topological Distance 2	1+ Billion
955. Frequency of Cl - B at Topological Distance 2	1+ Billion
956. Frequency of Cl - Si at Topological Distance 2	1+ Billion
957. Frequency of Cl - X at Topological Distance 2	1+ Billion
958. Frequency of Br - Br at Topological Distance 2	1+ Billion
959. Frequency of Br - I at Topological Distance 2	1+ Billion
960. Frequency of Br - B at Topological Distance 2	1+ Billion
961. Frequency of Br - Si at Topological Distance 2	1+ Billion
962. Frequency of Br - X at Topological Distance 2	1+ Billion





963. Frequency of I - I at Topological Distance 2	1+ Billion
964. Frequency of I - B at Topological Distance 2	1+ Billion
965. Frequency of I - Si at Topological Distance 2	1+ Billion
966. Frequency of I - X at Topological Distance 2	1+ Billion
967. Frequency of B - B at Topological Distance 2	1+ Billion
968. Frequency of B - Si at Topological Distance 2	1+ Billion
969. Frequency of B - X at Topological Distance 2	1+ Billion
970. Frequency of Si - Si at Topological Distance 2	1+ Billion
971. Frequency of Si - X at Topological Distance 2	1+ Billion
972. Frequency of X - X at Topological Distance 2	1+ Billion
973. Frequency of C - C at Topological Distance 3	1+ Billion
974. Frequency of C - N at Topological Distance 3	1+ Billion
975. Frequency of C - O at Topological Distance 3	1+ Billion
976. Frequency of C - S at Topological Distance 3	1+ Billion
977. Frequency of C - P at Topological Distance 3	1+ Billion
978. Frequency of C - F at Topological Distance 3	1+ Billion
979. Frequency of C - Cl at Topological Distance 3	1+ Billion
980. Frequency of C - Br at Topological Distance 3	1+ Billion
981. Frequency of C - I at Topological Distance 3	1+ Billion
982. Frequency of C - B at Topological Distance 3	1+ Billion
983. Frequency of C - Si at Topological Distance 3	1+ Billion
984. Frequency of C - X at Topological Distance 3	1+ Billion
985. Frequency of N - N at Topological Distance 3	1+ Billion
986. Frequency of N - O at Topological Distance 3	1+ Billion
987. Frequency of N - S at Topological Distance 3	1+ Billion
988. Frequency of N - P at Topological Distance 3	1+ Billion





989. Fre	quency of N - F at Topological Distance 3	1+ Billion
990. Fre	quency of N - Cl at Topological Distance 3	1+ Billion
991. Fre	quency of N - Br at Topological Distance 3	1+ Billion
992. Fre	quency of N - I at Topological Distance 3	1+ Billion
993. Fre	quency of N - B at Topological Distance 3	1+ Billion
994. Fre	quency of N - Si at Topological Distance 3	1+ Billion
995. Fre	quency of N - X at Topological Distance 3	1+ Billion
996. Fre	quency of O - O at Topological Distance 3	1+ Billion
997. Fre	quency of O - S at Topological Distance 3	1+ Billion
998. Fre	quency of O - P at Topological Distance 3	1+ Billion
999. Fre	quency of O - F at Topological Distance 3	1+ Billion
1000.	Frequency of O - Cl at Topological Distance 3	1+ Billion
1001.	Frequency of O - Br at Topological Distance 3	1+ Billion
1002.	Frequency of O - I at Topological Distance 3	1+ Billion
1003.	Frequency of O - B at Topological Distance 3	1+ Billion
1004.	Frequency of O - Si at Topological Distance 3	1+ Billion
1005.	Frequency of O - X at Topological Distance 3	1+ Billion
1006.	Frequency of S - S at Topological Distance 3	1+ Billion
1007.	Frequency of S - P at Topological Distance 3	1+ Billion
1008.	Frequency of S - F at Topological Distance 3	1+ Billion
1009.	Frequency of S - Cl at Topological Distance 3	1+ Billion
1010.	Frequency of S - Br at Topological Distance 3	1+ Billion
1011.	Frequency of S - I at Topological Distance 3	1+ Billion
1012.	Frequency of S - B at Topological Distance 3	1+ Billion
1013.	Frequency of S - Si at Topological Distance 3	1+ Billion
1014.	Frequency of S - X at Topological Distance 3	1+ Billion





1015.	Frequency of P - P at Topological Distance 3	1+ Billion
1016.	Frequency of P - F at Topological Distance 3	1+ Billion
1017.	Frequency of P - Cl at Topological Distance 3	1+ Billion
1018.	Frequency of P - Br at Topological Distance 3	1+ Billion
1019.	Frequency of P - I at Topological Distance 3	1+ Billion
1020.	Frequency of P - B at Topological Distance 3	1+ Billion
1021.	Frequency of P - Si at Topological Distance 3	1+ Billion
1022.	Frequency of P - X at Topological Distance 3	1+ Billion
1023.	Frequency of F - F at Topological Distance 3	1+ Billion
1024.	Frequency of F - Cl at Topological Distance 3	1+ Billion
1025.	Frequency of F - Br at Topological Distance 3	1+ Billion
1026.	Frequency of F - I at Topological Distance 3	1+ Billion
1027.	Frequency of F - B at Topological Distance 3	1+ Billion
1028.	Frequency of F - Si at Topological Distance 3	1+ Billion
1029.	Frequency of F - X at Topological Distance 3	1+ Billion
1030.	Frequency of Cl - Cl at Topological Distance 3	1+ Billion
1031.	Frequency of Cl - Br at Topological Distance 3	1+ Billion
1032.	Frequency of Cl - I at Topological Distance 3	1+ Billion
1033.	Frequency of Cl - B at Topological Distance 3	1+ Billion
1034.	Frequency of Cl - Si at Topological Distance 3	1+ Billion
1035.	Frequency of Cl - X at Topological Distance 3	1+ Billion
1036.	Frequency of Br - Br at Topological Distance 3	1+ Billion
1037.	Frequency of Br - I at Topological Distance 3	1+ Billion
1038.	Frequency of Br - B at Topological Distance 3	1+ Billion
1039.	Frequency of Br - Si at Topological Distance 3	1+ Billion
1040.	Frequency of Br - X at Topological Distance 3	1+ Billion





1041.	Frequency of I - I at Topological Distance 3	1+ Billion
1042.	Frequency of I - B at Topological Distance 3	1+ Billion
1043.	Frequency of I - Si at Topological Distance 3	1+ Billion
1044.	Frequency of I - X at Topological Distance 3	1+ Billion
1045.	Frequency of B - B at Topological Distance 3	1+ Billion
1046.	Frequency of B - Si at Topological Distance 3	1+ Billion
1047.	Frequency of B - X at Topological Distance 3	1+ Billion
1048.	Frequency of Si - Si at Topological Distance 3	1+ Billion
1049.	Frequency of Si - X at Topological Distance 3	1+ Billion
1050.	Frequency of X - X at Topological Distance 3	1+ Billion
1051.	Frequency of C - C at Topological Distance 4	1+ Billion
1052.	Frequency of C - N at Topological Distance 4	1+ Billion
1053.	Frequency of C - O at Topological Distance 4	1+ Billion
1054.	Frequency of C - S at Topological Distance 4	1+ Billion
1055.	Frequency of C - P at Topological Distance 4	1+ Billion
1056.	Frequency of C - F at Topological Distance 4	1+ Billion
1057.	Frequency of C - Cl at Topological Distance 4	1+ Billion
1058.	Frequency of C - Br at Topological Distance 4	1+ Billion
1059.	Frequency of C - I at Topological Distance 4	1+ Billion
1060.	Frequency of C - B at Topological Distance 4	1+ Billion
1061.	Frequency of C - Si at Topological Distance 4	1+ Billion
1062.	Frequency of C - X at Topological Distance 4	1+ Billion
1063.	Frequency of N - N at Topological Distance 4	1+ Billion
1064.	Frequency of N - O at Topological Distance 4	1+ Billion
1065.	Frequency of N - S at Topological Distance 4	1+ Billion
1066.	Frequency of N - P at Topological Distance 4	1+ Billion





1067.	Frequency of N - F at Topological Distance 4	1+ Billion
1068.	Frequency of N - Cl at Topological Distance 4	1+ Billion
1069.	Frequency of N - Br at Topological Distance 4	1+ Billion
1070.	Frequency of N - I at Topological Distance 4	1+ Billion
1071.	Frequency of N - B at Topological Distance 4	1+ Billion
1072.	Frequency of N - Si at Topological Distance 4	1+ Billion
1073.	Frequency of N - X at Topological Distance 4	1+ Billion
1074.	Frequency of O - O at Topological Distance 4	1+ Billion
1075.	Frequency of O - S at Topological Distance 4	1+ Billion
1076.	Frequency of O - P at Topological Distance 4	1+ Billion
1077.	Frequency of O - F at Topological Distance 4	1+ Billion
1078.	Frequency of O - Cl at Topological Distance 4	1+ Billion
1079.	Frequency of O - Br at Topological Distance 4	1+ Billion
1080.	Frequency of O - I at Topological Distance 4	1+ Billion
1081.	Frequency of O - B at Topological Distance 4	1+ Billion
1082.	Frequency of O - Si at Topological Distance 4	1+ Billion
1083.	Frequency of O - X at Topological Distance 4	1+ Billion
1084.	Frequency of S - S at Topological Distance 4	1+ Billion
1085.	Frequency of S - P at Topological Distance 4	1+ Billion
1086.	Frequency of S - F at Topological Distance 4	1+ Billion
1087.	Frequency of S - Cl at Topological Distance 4	1+ Billion
1088.	Frequency of S - Br at Topological Distance 4	1+ Billion
1089.	Frequency of S - I at Topological Distance 4	1+ Billion
1090.	Frequency of S - B at Topological Distance 4	1+ Billion
1091.	Frequency of S - Si at Topological Distance 4	1+ Billion
1092.	Frequency of S - X at Topological Distance 4	1+ Billion





1093.	Frequency of P - P at Topological Distance 4	1+ Billion
1094.	Frequency of P - F at Topological Distance 4	1+ Billion
1095.	Frequency of P - Cl at Topological Distance 4	1+ Billion
1096.	Frequency of P - Br at Topological Distance 4	1+ Billion
1097.	Frequency of P - I at Topological Distance 4	1+ Billion
1098.	Frequency of P - B at Topological Distance 4	1+ Billion
1099.	Frequency of P - Si at Topological Distance 4	1+ Billion
1100.	Frequency of P - X at Topological Distance 4	1+ Billion
1101.	Frequency of F - F at Topological Distance 4	1+ Billion
1102.	Frequency of F - Cl at Topological Distance 4	1+ Billion
1103.	Frequency of F - Br at Topological Distance 4	1+ Billion
1104.	Frequency of F - I at Topological Distance 4	1+ Billion
1105.	Frequency of F - B at Topological Distance 4	1+ Billion
1106.	Frequency of F - Si at Topological Distance 4	1+ Billion
1107.	Frequency of F - X at Topological Distance 4	1+ Billion
1108.	Frequency of Cl - Cl at Topological Distance 4	1+ Billion
1109.	Frequency of Cl - Br at Topological Distance 4	1+ Billion
1110.	Frequency of Cl - I at Topological Distance 4	1+ Billion
1111.	Frequency of Cl - B at Topological Distance 4	1+ Billion
1112.	Frequency of Cl - Si at Topological Distance 4	1+ Billion
1113.	Frequency of Cl - X at Topological Distance 4	1+ Billion
1114.	Frequency of Br - Br at Topological Distance 4	1+ Billion
1115.	Frequency of Br - I at Topological Distance 4	1+ Billion
1116.	Frequency of Br - B at Topological Distance 4	1+ Billion
1117.	Frequency of Br - Si at Topological Distance 4	1+ Billion
1118.	Frequency of Br - X at Topological Distance 4	1+ Billion





1119.	Frequency of I - I at Topological Distance 4	1+ Billion
1120.	Frequency of I - B at Topological Distance 4	1+ Billion
1121.	Frequency of I - Si at Topological Distance 4	1+ Billion
1122.	Frequency of I - X at Topological Distance 4	1+ Billion
1123.	Frequency of B - B at Topological Distance 4	1+ Billion
1124.	Frequency of B - Si at Topological Distance 4	1+ Billion
1125.	Frequency of B - X at Topological Distance 4	1+ Billion
1126.	Frequency of Si - Si at Topological Distance 4	1+ Billion
1127.	Frequency of Si - X at Topological Distance 4	1+ Billion
1128.	Frequency of X - X at Topological Distance 4	1+ Billion
1129.	Frequency of C - C at Topological Distance 5	1+ Billion
1130.	Frequency of C - N at Topological Distance 5	1+ Billion
1131.	Frequency of C - O at Topological Distance 5	1+ Billion
1132.	Frequency of C - S at Topological Distance 5	1+ Billion
1133.	Frequency of C - P at Topological Distance 5	1+ Billion
1134.	Frequency of C - F at Topological Distance 5	1+ Billion
1135.	Frequency of C - Cl at Topological Distance 5	1+ Billion
1136.	Frequency of C - Br at Topological Distance 5	1+ Billion
1137.	Frequency of C - I at Topological Distance 5	1+ Billion
1138.	Frequency of C - B at Topological Distance 5	1+ Billion
1139.	Frequency of C - Si at Topological Distance 5	1+ Billion
1140.	Frequency of C - X at Topological Distance 5	1+ Billion
1141.	Frequency of N - N at Topological Distance 5	1+ Billion
1142.	Frequency of N - O at Topological Distance 5	1+ Billion
1143.	Frequency of N - S at Topological Distance 5	1+ Billion
1144.	Frequency of N - P at Topological Distance 5	1+ Billion





1145.	Frequency of N - F at Topological Distance 5	1+ Billion
1146.	Frequency of N - Cl at Topological Distance 5	1+ Billion
1147.	Frequency of N - Br at Topological Distance 5	1+ Billion
1148.	Frequency of N - I at Topological Distance 5	1+ Billion
1149.	Frequency of N - B at Topological Distance 5	1+ Billion
1150.	Frequency of N - Si at Topological Distance 5	1+ Billion
1151.	Frequency of N - X at Topological Distance 5	1+ Billion
1152.	Frequency of O - O at Topological Distance 5	1+ Billion
1153.	Frequency of O - S at Topological Distance 5	1+ Billion
1154.	Frequency of O - P at Topological Distance 5	1+ Billion
1155.	Frequency of O - F at Topological Distance 5	1+ Billion
1156.	Frequency of O - Cl at Topological Distance 5	1+ Billion
1157.	Frequency of O - Br at Topological Distance 5	1+ Billion
1158.	Frequency of O - I at Topological Distance 5	1+ Billion
1159.	Frequency of O - B at Topological Distance 5	1+ Billion
1160.	Frequency of O - Si at Topological Distance 5	1+ Billion
1161.	Frequency of O - X at Topological Distance 5	1+ Billion
1162.	Frequency of S - S at Topological Distance 5	1+ Billion
1163.	Frequency of S - P at Topological Distance 5	1+ Billion
1164.	Frequency of S - F at Topological Distance 5	1+ Billion
1165.	Frequency of S - Cl at Topological Distance 5	1+ Billion
1166.	Frequency of S - Br at Topological Distance 5	1+ Billion
1167.	Frequency of S - I at Topological Distance 5	1+ Billion
1168.	Frequency of S - B at Topological Distance 5	1+ Billion
1169.	Frequency of S - Si at Topological Distance 5	1+ Billion
1170.	Frequency of S - X at Topological Distance 5	1+ Billion





1171.	Frequency of P - P at Topological Distance 5	1+ Billion
1172.	Frequency of P - F at Topological Distance 5	1+ Billion
1173.	Frequency of P - Cl at Topological Distance 5	1+ Billion
1174.	Frequency of P - Br at Topological Distance 5	1+ Billion
1175.	Frequency of P - I at Topological Distance 5	1+ Billion
1176.	Frequency of P - B at Topological Distance 5	1+ Billion
1177.	Frequency of P - Si at Topological Distance 5	1+ Billion
1178.	Frequency of P - X at Topological Distance 5	1+ Billion
1179.	Frequency of F - F at Topological Distance 5	1+ Billion
1180.	Frequency of F - Cl at Topological Distance 5	1+ Billion
1181.	Frequency of F - Br at Topological Distance 5	1+ Billion
1182.	Frequency of F - I at Topological Distance 5	1+ Billion
1183.	Frequency of F - B at Topological Distance 5	1+ Billion
1184.	Frequency of F - Si at Topological Distance 5	1+ Billion
1185.	Frequency of F - X at Topological Distance 5	1+ Billion
1186.	Frequency of Cl - Cl at Topological Distance 5	1+ Billion
1187.	Frequency of Cl - Br at Topological Distance 5	1+ Billion
1188.	Frequency of Cl - I at Topological Distance 5	1+ Billion
1189.	Frequency of Cl - B at Topological Distance 5	1+ Billion
1190.	Frequency of Cl - Si at Topological Distance 5	1+ Billion
1191.	Frequency of Cl - X at Topological Distance 5	1+ Billion
1192.	Frequency of Br - Br at Topological Distance 5	1+ Billion
1193.	Frequency of Br - I at Topological Distance 5	1+ Billion
1194.	Frequency of Br - B at Topological Distance 5	1+ Billion
1195.	Frequency of Br - Si at Topological Distance 5	1+ Billion
1196.	Frequency of Br - X at Topological Distance 5	1+ Billion





1197.	Frequency of I - I at Topological Distance 5	1+ Billion
1198.	Frequency of I - B at Topological Distance 5	1+ Billion
1199.	Frequency of I - Si at Topological Distance 5	1+ Billion
1200.	Frequency of I - X at Topological Distance 5	1+ Billion
1201.	Frequency of B - B at Topological Distance 5	1+ Billion
1202.	Frequency of B - Si at Topological Distance 5	1+ Billion
1203.	Frequency of B - X at Topological Distance 5	1+ Billion
1204.	Frequency of Si - Si at Topological Distance 5	1+ Billion
1205.	Frequency of Si - X at Topological Distance 5	1+ Billion
1206.	Frequency of X - X at Topological Distance 5	1+ Billion
1207.	Frequency of C - C at Topological Distance 6	1+ Billion
1208.	Frequency of C - N at Topological Distance 6	1+ Billion
1209.	Frequency of C - O at Topological Distance 6	1+ Billion
1210.	Frequency of C - S at Topological Distance 6	1+ Billion
1211.	Frequency of C - P at Topological Distance 6	1+ Billion
1212.	Frequency of C - F at Topological Distance 6	1+ Billion
1213.	Frequency of C - Cl at Topological Distance 6	1+ Billion
1214.	Frequency of C - Br at Topological Distance 6	1+ Billion
1215.	Frequency of C - I at Topological Distance 6	1+ Billion
1216.	Frequency of C - B at Topological Distance 6	1+ Billion
1217.	Frequency of C - Si at Topological Distance 6	1+ Billion
1218.	Frequency of C - X at Topological Distance 6	1+ Billion
1219.	Frequency of N - N at Topological Distance 6	1+ Billion
1220.	Frequency of N - O at Topological Distance 6	1+ Billion
1221.	Frequency of N - S at Topological Distance 6	1+ Billion
1222.	Frequency of N - P at Topological Distance 6	1+ Billion





1223.	Frequency of N - F at Topological Distance 6	1+ Billion
1224.	Frequency of N - Cl at Topological Distance 6	1+ Billion
1225.	Frequency of N - Br at Topological Distance 6	1+ Billion
1226.	Frequency of N - I at Topological Distance 6	1+ Billion
1227.	Frequency of N - B at Topological Distance 6	1+ Billion
1228.	Frequency of N - Si at Topological Distance 6	1+ Billion
1229.	Frequency of N - X at Topological Distance 6	1+ Billion
1230.	Frequency of O - O at Topological Distance 6	1+ Billion
1231.	Frequency of O - S at Topological Distance 6	1+ Billion
1232.	Frequency of O - P at Topological Distance 6	1+ Billion
1233.	Frequency of O - F at Topological Distance 6	1+ Billion
1234.	Frequency of O - Cl at Topological Distance 6	1+ Billion
1235.	Frequency of O - Br at Topological Distance 6	1+ Billion
1236.	Frequency of O - I at Topological Distance 6	1+ Billion
1237.	Frequency of O - B at Topological Distance 6	1+ Billion
1238.	Frequency of O - Si at Topological Distance 6	1+ Billion
1239.	Frequency of O - X at Topological Distance 6	1+ Billion
1240.	Frequency of S - S at Topological Distance 6	1+ Billion
1241.	Frequency of S - P at Topological Distance 6	1+ Billion
1242.	Frequency of S - F at Topological Distance 6	1+ Billion
1243.	Frequency of S - Cl at Topological Distance 6	1+ Billion
1244.	Frequency of S - Br at Topological Distance 6	1+ Billion
1245.	Frequency of S - I at Topological Distance 6	1+ Billion
1246.	Frequency of S - B at Topological Distance 6	1+ Billion
1247.	Frequency of S - Si at Topological Distance 6	1+ Billion
1248.	Frequency of S - X at Topological Distance 6	1+ Billion





1249.	Frequency of P - P at Topological Distance 6	1+ Billion
1250.	Frequency of P - F at Topological Distance 6	1+ Billion
1251.	Frequency of P - Cl at Topological Distance 6	1+ Billion
1252.	Frequency of P - Br at Topological Distance 6	1+ Billion
1253.	Frequency of P - I at Topological Distance 6	1+ Billion
1254.	Frequency of P - B at Topological Distance 6	1+ Billion
1255.	Frequency of P - Si at Topological Distance 6	1+ Billion
1256.	Frequency of P - X at Topological Distance 6	1+ Billion
1257.	Frequency of F - F at Topological Distance 6	1+ Billion
1258.	Frequency of F - Cl at Topological Distance 6	1+ Billion
1259.	Frequency of F - Br at Topological Distance 6	1+ Billion
1260.	Frequency of F - I at Topological Distance 6	1+ Billion
1261.	Frequency of F - B at Topological Distance 6	1+ Billion
1262.	Frequency of F - Si at Topological Distance 6	1+ Billion
1263.	Frequency of F - X at Topological Distance 6	1+ Billion
1264.	Frequency of Cl - Cl at Topological Distance 6	1+ Billion
1265.	Frequency of Cl - Br at Topological Distance 6	1+ Billion
1266.	Frequency of Cl - I at Topological Distance 6	1+ Billion
1267.	Frequency of Cl - B at Topological Distance 6	1+ Billion
1268.	Frequency of Cl - Si at Topological Distance 6	1+ Billion
1269.	Frequency of Cl - X at Topological Distance 6	1+ Billion
1270.	Frequency of Br - Br at Topological Distance 6	1+ Billion
1271.	Frequency of Br - I at Topological Distance 6	1+ Billion
1272.	Frequency of Br - B at Topological Distance 6	1+ Billion
1273.	Frequency of Br - Si at Topological Distance 6	1+ Billion
1274.	Frequency of Br - X at Topological Distance 6	1+ Billion





1275.	Frequency of I - I at Topological Distance 6	1+ Billion
1276.	Frequency of I - B at Topological Distance 6	1+ Billion
1277.	Frequency of I - Si at Topological Distance 6	1+ Billion
1278.	Frequency of I - X at Topological Distance 6	1+ Billion
1279.	Frequency of B - B at Topological Distance 6	1+ Billion
1280.	Frequency of B - Si at Topological Distance 6	1+ Billion
1281.	Frequency of B - X at Topological Distance 6	1+ Billion
1282.	Frequency of Si - Si at Topological Distance 6	1+ Billion
1283.	Frequency of Si - X at Topological Distance 6	1+ Billion
1284.	Frequency of X - X at Topological Distance 6	1+ Billion
1285.	Frequency of C - C at Topological Distance 7	1+ Billion
1286.	Frequency of C - N at Topological Distance 7	1+ Billion
1287.	Frequency of C - O at Topological Distance 7	1+ Billion
1288.	Frequency of C - S at Topological Distance 7	1+ Billion
1289.	Frequency of C - P at Topological Distance 7	1+ Billion
1290.	Frequency of C - F at Topological Distance 7	1+ Billion
1291.	Frequency of C - Cl at Topological Distance 7	1+ Billion
1292.	Frequency of C - Br at Topological Distance 7	1+ Billion
1293.	Frequency of C - I at Topological Distance 7	1+ Billion
1294.	Frequency of C - B at Topological Distance 7	1+ Billion
1295.	Frequency of C - Si at Topological Distance 7	1+ Billion
1296.	Frequency of C - X at Topological Distance 7	1+ Billion
1297.	Frequency of N - N at Topological Distance 7	1+ Billion
1298.	Frequency of N - O at Topological Distance 7	1+ Billion
1299.	Frequency of N - S at Topological Distance 7	1+ Billion
1300.	Frequency of N - P at Topological Distance 7	1+ Billion





1301.	Frequency of N - F at Topological Distance 7	1+ Billion
1302.	Frequency of N - Cl at Topological Distance 7	1+ Billion
1303.	Frequency of N - Br at Topological Distance 7	1+ Billion
1304.	Frequency of N - I at Topological Distance 7	1+ Billion
1305.	Frequency of N - B at Topological Distance 7	1+ Billion
1306.	Frequency of N - Si at Topological Distance 7	1+ Billion
1307.	Frequency of N - X at Topological Distance 7	1+ Billion
1308.	Frequency of O - O at Topological Distance 7	1+ Billion
1309.	Frequency of O - S at Topological Distance 7	1+ Billion
1310.	Frequency of O - P at Topological Distance 7	1+ Billion
1311.	Frequency of O - F at Topological Distance 7	1+ Billion
1312.	Frequency of O - Cl at Topological Distance 7	1+ Billion
1313.	Frequency of O - Br at Topological Distance 7	1+ Billion
1314.	Frequency of O - I at Topological Distance 7	1+ Billion
1315.	Frequency of O - B at Topological Distance 7	1+ Billion
1316.	Frequency of O - Si at Topological Distance 7	1+ Billion
1317.	Frequency of O - X at Topological Distance 7	1+ Billion
1318.	Frequency of S - S at Topological Distance 7	1+ Billion
1319.	Frequency of S - P at Topological Distance 7	1+ Billion
1320.	Frequency of S - F at Topological Distance 7	1+ Billion
1321.	Frequency of S - Cl at Topological Distance 7	1+ Billion
1322.	Frequency of S - Br at Topological Distance 7	1+ Billion
1323.	Frequency of S - I at Topological Distance 7	1+ Billion
1324.	Frequency of S - B at Topological Distance 7	1+ Billion
1325.	Frequency of S - Si at Topological Distance 7	1+ Billion
1326.	Frequency of S - X at Topological Distance 7	1+ Billion





1327.	Frequency of P - P at Topological Distance 7	1+ Billion
1328.	Frequency of P - F at Topological Distance 7	1+ Billion
1329.	Frequency of P - Cl at Topological Distance 7	1+ Billion
1330.	Frequency of P - Br at Topological Distance 7	1+ Billion
1331.	Frequency of P - I at Topological Distance 7	1+ Billion
1332.	Frequency of P - B at Topological Distance 7	1+ Billion
1333.	Frequency of P - Si at Topological Distance 7	1+ Billion
1334.	Frequency of P - X at Topological Distance 7	1+ Billion
1335.	Frequency of F - F at Topological Distance 7	1+ Billion
1336.	Frequency of F - Cl at Topological Distance 7	1+ Billion
1337.	Frequency of F - Br at Topological Distance 7	1+ Billion
1338.	Frequency of F - I at Topological Distance 7	1+ Billion
1339.	Frequency of F - B at Topological Distance 7	1+ Billion
1340.	Frequency of F - Si at Topological Distance 7	1+ Billion
1341.	Frequency of F - X at Topological Distance 7	1+ Billion
1342.	Frequency of Cl - Cl at Topological Distance 7	1+ Billion
1343.	Frequency of Cl - Br at Topological Distance 7	1+ Billion
1344.	Frequency of Cl - I at Topological Distance 7	1+ Billion
1345.	Frequency of Cl - B at Topological Distance 7	1+ Billion
1346.	Frequency of Cl - Si at Topological Distance 7	1+ Billion
1347.	Frequency of Cl - X at Topological Distance 7	1+ Billion
1348.	Frequency of Br - Br at Topological Distance 7	1+ Billion
1349.	Frequency of Br - I at Topological Distance 7	1+ Billion
1350.	Frequency of Br - B at Topological Distance 7	1+ Billion
1351.	Frequency of Br - Si at Topological Distance 7	1+ Billion
1352.	Frequency of Br - X at Topological Distance 7	1+ Billion





1353.	Frequency of I - I at Topological Distance 7	1+ Billion
1354.	Frequency of I - B at Topological Distance 7	1+ Billion
1355.	Frequency of I - Si at Topological Distance 7	1+ Billion
1356.	Frequency of I - X at Topological Distance 7	1+ Billion
1357.	Frequency of B - B at Topological Distance 7	1+ Billion
1358.	Frequency of B - Si at Topological Distance 7	1+ Billion
1359.	Frequency of B - X at Topological Distance 7	1+ Billion
1360.	Frequency of Si - Si at Topological Distance 7	1+ Billion
1361.	Frequency of Si - X at Topological Distance 7	1+ Billion
1362.	Frequency of X - X at Topological Distance 7	1+ Billion
1363.	Frequency of C - C at Topological Distance 8	1+ Billion
1364.	Frequency of C - N at Topological Distance 8	1+ Billion
1365.	Frequency of C - O at Topological Distance 8	1+ Billion
1366.	Frequency of C - S at Topological Distance 8	1+ Billion
1367.	Frequency of C - P at Topological Distance 8	1+ Billion
1368.	Frequency of C - F at Topological Distance 8	1+ Billion
1369.	Frequency of C - Cl at Topological Distance 8	1+ Billion
1370.	Frequency of C - Br at Topological Distance 8	1+ Billion
1371.	Frequency of C - I at Topological Distance 8	1+ Billion
1372.	Frequency of C - B at Topological Distance 8	1+ Billion
1373.	Frequency of C - Si at Topological Distance 8	1+ Billion
1374.	Frequency of C - X at Topological Distance 8	1+ Billion
1375.	Frequency of N - N at Topological Distance 8	1+ Billion
1376.	Frequency of N - O at Topological Distance 8	1+ Billion
1377.	Frequency of N - S at Topological Distance 8	1+ Billion
1378.	Frequency of N - P at Topological Distance 8	1+ Billion





1379.	Frequency of N - F at Topological Distance 8	1+ Billion
1380.	Frequency of N - Cl at Topological Distance 8	1+ Billion
1381.	Frequency of N - Br at Topological Distance 8	1+ Billion
1382.	Frequency of N - I at Topological Distance 8	1+ Billion
1383.	Frequency of N - B at Topological Distance 8	1+ Billion
1384.	Frequency of N - Si at Topological Distance 8	1+ Billion
1385.	Frequency of N - X at Topological Distance 8	1+ Billion
1386.	Frequency of O - O at Topological Distance 8	1+ Billion
1387.	Frequency of O - S at Topological Distance 8	1+ Billion
1388.	Frequency of O - P at Topological Distance 8	1+ Billion
1389.	Frequency of O - F at Topological Distance 8	1+ Billion
1390.	Frequency of O - Cl at Topological Distance 8	1+ Billion
1391.	Frequency of O - Br at Topological Distance 8	1+ Billion
1392.	Frequency of O - I at Topological Distance 8	1+ Billion
1393.	Frequency of O - B at Topological Distance 8	1+ Billion
1394.	Frequency of O - Si at Topological Distance 8	1+ Billion
1395.	Frequency of O - X at Topological Distance 8	1+ Billion
1396.	Frequency of S - S at Topological Distance 8	1+ Billion
1397.	Frequency of S - P at Topological Distance 8	1+ Billion
1398.	Frequency of S - F at Topological Distance 8	1+ Billion
1399.	Frequency of S - Cl at Topological Distance 8	1+ Billion
1400.	Frequency of S - Br at Topological Distance 8	1+ Billion
1401.	Frequency of S - I at Topological Distance 8	1+ Billion
1402.	Frequency of S - B at Topological Distance 8	1+ Billion
1403.	Frequency of S - Si at Topological Distance 8	1+ Billion
1404.	Frequency of S - X at Topological Distance 8	1+ Billion





1405.	Frequency of P - P at Topological Distance 8	1+ Billion
1406.	Frequency of P - F at Topological Distance 8	1+ Billion
1407.	Frequency of P - Cl at Topological Distance 8	1+ Billion
1408.	Frequency of P - Br at Topological Distance 8	1+ Billion
1409.	Frequency of P - I at Topological Distance 8	1+ Billion
1410.	Frequency of P - B at Topological Distance 8	1+ Billion
1411.	Frequency of P - Si at Topological Distance 8	1+ Billion
1412.	Frequency of P - X at Topological Distance 8	1+ Billion
1413.	Frequency of F - F at Topological Distance 8	1+ Billion
1414.	Frequency of F - Cl at Topological Distance 8	1+ Billion
1415.	Frequency of F - Br at Topological Distance 8	1+ Billion
1416.	Frequency of F - I at Topological Distance 8	1+ Billion
1417.	Frequency of F - B at Topological Distance 8	1+ Billion
1418.	Frequency of F - Si at Topological Distance 8	1+ Billion
1419.	Frequency of F - X at Topological Distance 8	1+ Billion
1420.	Frequency of Cl - Cl at Topological Distance 8	1+ Billion
1421.	Frequency of Cl - Br at Topological Distance 8	1+ Billion
1422.	Frequency of Cl - I at Topological Distance 8	1+ Billion
1423.	Frequency of Cl - B at Topological Distance 8	1+ Billion
1424.	Frequency of Cl - Si at Topological Distance 8	1+ Billion
1425.	Frequency of Cl - X at Topological Distance 8	1+ Billion
1426.	Frequency of Br - Br at Topological Distance 8	1+ Billion
1427.	Frequency of Br - I at Topological Distance 8	1+ Billion
1428.	Frequency of Br - B at Topological Distance 8	1+ Billion
1429.	Frequency of Br - Si at Topological Distance 8	1+ Billion
1430.	Frequency of Br - X at Topological Distance 8	1+ Billion





1431.	Frequency of I - I at Topological Distance 8	1+ Billion
1432.	Frequency of I - B at Topological Distance 8	1+ Billion
1433.	Frequency of I - Si at Topological Distance 8	1+ Billion
1434.	Frequency of I - X at Topological Distance 8	1+ Billion
1435.	Frequency of B - B at Topological Distance 8	1+ Billion
1436.	Frequency of B - Si at Topological Distance 8	1+ Billion
1437.	Frequency of B - X at Topological Distance 8	1+ Billion
1438.	Frequency of Si - Si at Topological Distance 8	1+ Billion
1439.	Frequency of Si - X at Topological Distance 8	1+ Billion
1440.	Frequency of X - X at Topological Distance 8	1+ Billion
1441.	Frequency of C - C at Topological Distance 9	1+ Billion
1442.	Frequency of C - N at Topological Distance 9	1+ Billion
1443.	Frequency of C - O at Topological Distance 9	1+ Billion
1444.	Frequency of C - S at Topological Distance 9	1+ Billion
1445.	Frequency of C - P at Topological Distance 9	1+ Billion
1446.	Frequency of C - F at Topological Distance 9	1+ Billion
1447.	Frequency of C - Cl at Topological Distance 9	1+ Billion
1448.	Frequency of C - Br at Topological Distance 9	1+ Billion
1449.	Frequency of C - I at Topological Distance 9	1+ Billion
1450.	Frequency of C - B at Topological Distance 9	1+ Billion
1451.	Frequency of C - Si at Topological Distance 9	1+ Billion
1452.	Frequency of C - X at Topological Distance 9	1+ Billion
1453.	Frequency of N - N at Topological Distance 9	1+ Billion
1454.	Frequency of N - O at Topological Distance 9	1+ Billion
1455.	Frequency of N - S at Topological Distance 9	1+ Billion
1456.	Frequency of N - P at Topological Distance 9	1+ Billion





1457.	Frequency of N - F at Topological Distance 9	1+ Billion
1458.	Frequency of N - Cl at Topological Distance 9	1+ Billion
1459.	Frequency of N - Br at Topological Distance 9	1+ Billion
1460.	Frequency of N - I at Topological Distance 9	1+ Billion
1461.	Frequency of N - B at Topological Distance 9	1+ Billion
1462.	Frequency of N - Si at Topological Distance 9	1+ Billion
1463.	Frequency of N - X at Topological Distance 9	1+ Billion
1464.	Frequency of O - O at Topological Distance 9	1+ Billion
1465.	Frequency of O - S at Topological Distance 9	1+ Billion
1466.	Frequency of O - P at Topological Distance 9	1+ Billion
1467.	Frequency of O - F at Topological Distance 9	1+ Billion
1468.	Frequency of O - Cl at Topological Distance 9	1+ Billion
1469.	Frequency of O - Br at Topological Distance 9	1+ Billion
1470.	Frequency of O - I at Topological Distance 9	1+ Billion
1471.	Frequency of O - B at Topological Distance 9	1+ Billion
1472.	Frequency of O - Si at Topological Distance 9	1+ Billion
1473.	Frequency of O - X at Topological Distance 9	1+ Billion
1474.	Frequency of S - S at Topological Distance 9	1+ Billion
1475.	Frequency of S - P at Topological Distance 9	1+ Billion
1476.	Frequency of S - F at Topological Distance 9	1+ Billion
1477.	Frequency of S - Cl at Topological Distance 9	1+ Billion
1478.	Frequency of S - Br at Topological Distance 9	1+ Billion
1479.	Frequency of S - I at Topological Distance 9	1+ Billion
1480.	Frequency of S - B at Topological Distance 9	1+ Billion
1481.	Frequency of S - Si at Topological Distance 9	1+ Billion
1482.	Frequency of S - X at Topological Distance 9	1+ Billion





1483.	Frequency of P - P at Topological Distance 9	1+ Billion
1484.	Frequency of P - F at Topological Distance 9	1+ Billion
1485.	Frequency of P - Cl at Topological Distance 9	1+ Billion
1486.	Frequency of P - Br at Topological Distance 9	1+ Billion
1487.	Frequency of P - I at Topological Distance 9	1+ Billion
1488.	Frequency of P - B at Topological Distance 9	1+ Billion
1489.	Frequency of P - Si at Topological Distance 9	1+ Billion
1490.	Frequency of P - X at Topological Distance 9	1+ Billion
1491.	Frequency of F - F at Topological Distance 9	1+ Billion
1492.	Frequency of F - Cl at Topological Distance 9	1+ Billion
1493.	Frequency of F - Br at Topological Distance 9	1+ Billion
1494.	Frequency of F - I at Topological Distance 9	1+ Billion
1495.	Frequency of F - B at Topological Distance 9	1+ Billion
1496.	Frequency of F - Si at Topological Distance 9	1+ Billion
1497.	Frequency of F - X at Topological Distance 9	1+ Billion
1498.	Frequency of Cl - Cl at Topological Distance 9	1+ Billion
1499.	Frequency of Cl - Br at Topological Distance 9	1+ Billion
1500.	Frequency of Cl - I at Topological Distance 9	1+ Billion
1501.	Frequency of Cl - B at Topological Distance 9	1+ Billion
1502.	Frequency of Cl - Si at Topological Distance 9	1+ Billion
1503.	Frequency of Cl - X at Topological Distance 9	1+ Billion
1504.	Frequency of Br - Br at Topological Distance 9	1+ Billion
1505.	Frequency of Br - I at Topological Distance 9	1+ Billion
1506.	Frequency of Br - B at Topological Distance 9	1+ Billion
1507.	Frequency of Br - Si at Topological Distance 9	1+ Billion
1508.	Frequency of Br - X at Topological Distance 9	1+ Billion





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1509.	Frequency of I - I at Topological Distance 9	1+ Billion
1510.	Frequency of I - B at Topological Distance 9	1+ Billion
1511.	Frequency of I - Si at Topological Distance 9	1+ Billion
1512.	Frequency of I - X at Topological Distance 9	1+ Billion
1513.	Frequency of B - B at Topological Distance 9	1+ Billion
1514.	Frequency of B - Si at Topological Distance 9	1+ Billion
1515.	Frequency of B - X at Topological Distance 9	1+ Billion
1516.	Frequency of Si - Si at Topological Distance 9	1+ Billion
1517.	Frequency of Si - X at Topological Distance 9	1+ Billion
1518.	Frequency of X - X at Topological Distance 9	1+ Billion
1519.	Frequency of C - C at Topological Distance 10	1+ Billion
1520.	Frequency of C - N at Topological Distance 10	1+ Billion
1521.	Frequency of C - O at Topological Distance 10	1+ Billion
1522.	Frequency of C - S at Topological Distance 10	1+ Billion
1523.	Frequency of C - P at Topological Distance 10	1+ Billion
1524.	Frequency of C - F at Topological Distance 10	1+ Billion
1525.	Frequency of C - Cl at Topological Distance 10	1+ Billion
1526.	Frequency of C - Br at Topological Distance 10	1+ Billion
1527.	Frequency of C - I at Topological Distance 10	1+ Billion
1528.	Frequency of C - B at Topological Distance 10	1+ Billion
1529.	Frequency of C - Si at Topological Distance 10	1+ Billion
1530.	Frequency of C - X at Topological Distance 10	1+ Billion
1531.	Frequency of N - N at Topological Distance 10	1+ Billion
1532.	Frequency of N - O at Topological Distance 10	1+ Billion
1533.	Frequency of N - S at Topological Distance 10	1+ Billion
1534.	Frequency of N - P at Topological Distance 10	1+ Billion

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1535.	Frequency of N - F at Topological Distance 10	1+ Billion
1536.	Frequency of N - Cl at Topological Distance 10	1+ Billion
1537.	Frequency of N - Br at Topological Distance 10	1+ Billion
1538.	Frequency of N - I at Topological Distance 10	1+ Billion
1539.	Frequency of N - B at Topological Distance 10	1+ Billion
1540.	Frequency of N - Si at Topological Distance 10	1+ Billion
1541.	Frequency of N - X at Topological Distance 10	1+ Billion
1542.	Frequency of O - O at Topological Distance 10	1+ Billion
1543.	Frequency of O - S at Topological Distance 10	1+ Billion
1544.	Frequency of O - P at Topological Distance 10	1+ Billion
1545.	Frequency of O - F at Topological Distance 10	1+ Billion
1546.	Frequency of O - Cl at Topological Distance 10	1+ Billion
1547.	Frequency of O - Br at Topological Distance 10	1+ Billion
1548.	Frequency of O - I at Topological Distance 10	1+ Billion
1549.	Frequency of O - B at Topological Distance 10	1+ Billion
1550.	Frequency of O - Si at Topological Distance 10	1+ Billion
1551.	Frequency of O - X at Topological Distance 10	1+ Billion
1552.	Frequency of S - S at Topological Distance 10	1+ Billion
1553.	Frequency of S - P at Topological Distance 10	1+ Billion
1554.	Frequency of S - F at Topological Distance 10	1+ Billion
1555.	Frequency of S - Cl at Topological Distance 10	1+ Billion
1556.	Frequency of S - Br at Topological Distance 10	1+ Billion
1557.	Frequency of S - I at Topological Distance 10	1+ Billion
1558.	Frequency of S - B at Topological Distance 10	1+ Billion
1559.	Frequency of S - Si at Topological Distance 10	1+ Billion
1560.	Frequency of S - X at Topological Distance 10	1+ Billion





1561.	Frequency of P - P at Topological Distance 10	1+ Billion
1562.	Frequency of P - F at Topological Distance 10	1+ Billion
1563.	Frequency of P - Cl at Topological Distance 10	1+ Billion
1564.	Frequency of P - Br at Topological Distance 10	1+ Billion
1565.	Frequency of P - I at Topological Distance 10	1+ Billion
1566.	Frequency of P - B at Topological Distance 10	1+ Billion
1567.	Frequency of P - Si at Topological Distance 10	1+ Billion
1568.	Frequency of P - X at Topological Distance 10	1+ Billion
1569.	Frequency of F - F at Topological Distance 10	1+ Billion
1570.	Frequency of F - Cl at Topological Distance 10	1+ Billion
1571.	Frequency of F - Br at Topological Distance 10	1+ Billion
1572.	Frequency of F - I at Topological Distance 10	1+ Billion
1573.	Frequency of F - B at Topological Distance 10	1+ Billion
1574.	Frequency of F - Si at Topological Distance 10	1+ Billion
1575.	Frequency of F - X at Topological Distance 10	1+ Billion
1576.	Frequency of Cl - Cl at Topological Distance 10	1+ Billion
1577.	Frequency of Cl - Br at Topological Distance 10	1+ Billion
1578.	Frequency of Cl - I at Topological Distance 10	1+ Billion
1579.	Frequency of Cl - B at Topological Distance 10	1+ Billion
1580.	Frequency of Cl - Si at Topological Distance 10	1+ Billion
1581.	Frequency of Cl - X at Topological Distance 10	1+ Billion
1582.	Frequency of Br - Br at Topological Distance 10	1+ Billion
1583.	Frequency of Br - I at Topological Distance 10	1+ Billion
1584.	Frequency of Br - B at Topological Distance 10	1+ Billion
1585.	Frequency of Br - Si at Topological Distance 10	1+ Billion
1586.	Frequency of Br - X at Topological Distance 10	1+ Billion





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1587.	Frequency of I - I at Topological Distance 10	1+ Billion
1588.	Frequency of I - B at Topological Distance 10	1+ Billion
1589.	Frequency of I - Si at Topological Distance 10	1+ Billion
1590.	Frequency of I - X at Topological Distance 10	1+ Billion
1591.	Frequency of B - B at Topological Distance 10	1+ Billion
1592.	Frequency of B - Si at Topological Distance 10	1+ Billion
1593.	Frequency of B - X at Topological Distance 10	1+ Billion
1594.	Frequency of Si - Si at Topological Distance 10	1+ Billion
1595.	Frequency of Si - X at Topological Distance 10	1+ Billion
1596.	Frequency of X - X at Topological Distance 10	1+ Billion

## Charge Descriptors (15)

	Charge Descriptors	Number of Compounds
1.	Maximum Positive Charge	1+ Billion
2.	Maximum Negative Charge	1+ Billion
3.	Total Positive Charge	1+ Billion
4.	Total Negative Charge	1+ Billion
5.	Total Absolute Charge (Electronic Charge Index - ECI)	1+ Billion
6.	Mean Absolute Charge (Charge Polarization)	1+ Billion
7.	Total Squared Charge	1+ Billion
8.	Relative Positive Charge	1+ Billion
9.	Relative Negative Charge	1+ Billion
10.	Submolecular Polarity Parameter	1+ Billion



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11.	Topographic Electronic Descriptor	1+ Billion
12.	Topographic Electronic Descriptor (Bond Restricted)	1+ Billion
13.	Partial Charge Weighted Topological Electronic Index	1+ Billion
14.	Partial Charge Weighted Topological Electronic Index (Bond Restricted)	1+ Billion
15.	Local Dipole Index	1+ Billion

## Molecular Properties (20)

	Molecular Properties	Number of Compounds
1.	Unsaturation Count	1+ Billion
2.	Unsaturation Index	1+ Billion
3.	Hydrophilic Factor	1+ Billion
4.	Ghose-Crippen Molar Refractivity	1+ Billion
5.	Topological Polar Surface Area Using N,O Polar Contributions	1+ Billion
6.	Topological Polar Surface Area Using N,O,S,P Polar Contributions	1+ Billion
7.	Moriguchi Octanol-Water Partition Coeff. (LogP)	1+ Billion
8.	Squared Moriguchi Octanol-Water Partition Coeff. (LogP^2)	1+ Billion
9.	Ghose-Crippen Octanol-Water Partition Coeff. (LogP)	1+ Billion
10.	Squared Ghose-Crippen Octanol-Water Partition Coeff. (LogP^2)	1+ Billion
11.	Total Surface Area from P_VSA-Like Descriptors	1+ Billion
12.	Surface Area Of Acceptor Atoms from P_VSA-Like Descriptors	1+ Billion
13.	Surface Area Of Donor Atoms from P_VSA-Like Descriptors	1+ Billion
14.	McGowan Volume	1+ Billion
15.	van der Waals Volume from McGowan Volume	1+ Billion
16.	van der Waals Volume from Zhao-Abraham-Zissimos Equation	1+ Billion



1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil, Yeongdeungpo-gu,07282 Seoul, Republic of Korea Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920 www.chemessen.com

17.	Packing Density Index	1+ Billion
18.	Verhaar Fish Base-Line Toxicity from MLOGP (mmol/L)	1+ Billion
19.	Verhaar Daphnia Base-Line Toxicity from MLOGP (mmol/L)	1+ Billion
20.	Verhaar Algae Base-Line Toxicity from MLOGP (mmol/L)	1+ Billion

## Drug-Like Indices (27)

	Drug-Like Indices	Number of Compounds
1.	Complementary Lipinski Alert Index	1+ Billion
2.	Modified Drug-Like Score from Lipinski (4 Rules)	1+ Billion
3.	Modified Drug-Like Score from Oprea et al. (6 Rules)	1+ Billion
4.	Modified Drug-Like Score from Walters et al. (6 Rules)	1+ Billion
5.	Modified Drug-Like Score from Chen et al. (7 Rules)	1+ Billion
6.	Modified Drug-Like Score from Zheng et al. (2 Rules)	1+ Billion
7.	Modified Drug-Like Score from Rishton (6 Rules)	1+ Billion
8.	Modified Drug-Like Score from Veber et al. (2 Rules)	1+ Billion
9.	DRAGON Consensus Drug-Like Score	1+ Billion
10.	Modified Lead-Like Score from Congreve et al. (6 Rules)	1+ Billion
11.	Modified Lead-Like Score from Monge et al. (8 Rules)	1+ Billion
12.	Ghose-Viswanadhan-Wendoloski CMC Drug-Like Index at 80%	1+ Billion
13.	Ghose-Viswanadhan-Wendoloski CMC Drug-Like Index at 50%	1+ Billion
14.	Ghose-Viswanadhan-Wendoloski Antiinflammatory-Like Index at 80%	1+ Billion
15.	Ghose-Viswanadhan-Wendoloski Antiinflammatory-Like Index at 50%	1+ Billion
16.	Ghose-Viswanadhan-Wendoloski Antidepressant-Like Index at 80%	1+ Billion





17.	Ghose-Viswanadhan-Wendoloski Antidepressant-Like Index at 50%	1+ Billion
18.	Ghose-Viswanadhan-Wendoloski Antipsychotic-Like Index at 80%	1+ Billion
19.	Ghose-Viswanadhan-Wendoloski Antipsychotic-Like Index at 50%	1+ Billion
20.	Ghose-Viswanadhan-Wendoloski Antihypertensive-Like Index at 80%	1+ Billion
21.	Ghose-Viswanadhan-Wendoloski Antihypertensive-Like Index at 50%	1+ Billion
22.	Ghose-Viswanadhan-Wendoloski Hypnotic-Like Index at 80%	1+ Billion
23.	Ghose-Viswanadhan-Wendoloski Hypnotic-Like Index at 50%	1+ Billion
24.	Ghose-Viswanadhan-Wendoloski Antineoplastic-Like Index at 80%	1+ Billion
25.	Ghose-Viswanadhan-Wendoloski Antineoplastic-Like Index at 50%	1+ Billion
26.	Ghose-Viswanadhan-Wendoloski Antiinfective-Like Index at 80%	1+ Billion
27.	Ghose-Viswanadhan-Wendoloski Antiinfective-Like Index at 50%	1+ Billion