Descriptor List

preset descriptors

```
calc = Calculator(descriptors)
```

Descriptor list

#	module	name	constructor	dim	description
1	ABCIndex	ABC	ABCIndex ()	2D	atom-bond connectivity index
2		ABCGG	ABCGGIndex ()	2D	Graovac-Ghorbani atom-bond connectivity index
3	AcidBase	nAcid	AcidicGroupCount ()	2D	acidic group count
4		nBase	BasicGroupCount ()	2D	basic group count
5	AdjacencyMatrix	SpAbs_A	AdjacencyMatrix ('SpAbs')	2D	SpAbs of adjacency matrix
6		SpMax_A	AdjacencyMatrix ('SpMax')	2D	SpMax of adjacency matrix
7		SpDiam_A	AdjacencyMatrix ('SpDiam')	2D	SpDiam of adjacency matrix
8		SpAD_A	AdjacencyMatrix ('SpAD')	2D	SpAD of adjacency matrix
9		SpMAD_A	AdjacencyMatrix ('SpMAD')	2D	SpMAD of adjacency matrix
10		LogEE_A	AdjacencyMatrix ('LogEE')	2D	LogEE of adjacency matrix
11		VE1_A	AdjacencyMatrix ('VE1')	2D	VE1 of adjacency matrix
12		VE2_A	AdjacencyMatrix ('VE2')	2D	VE2 of adjacency matrix
13		VE3_A	AdjacencyMatrix ('VE3')	2D	VE3 of adjacency matrix
14		VR1_A	AdjacencyMatrix ('VR1')	2D	VR1 of adjacency matrix

#	module	name	constructor	dim	description
15		VR2_A	AdjacencyMatrix ('VR2')	2D	VR2 of adjacency matrix
16		VR3_A	AdjacencyMatrix ('VR3')	2D	VR3 of adjacency matrix
17	Aromatic	nAromAtom	AromaticAtomsCount ()	2D	aromatic atoms count
18		nAromBond	AromaticBondsCount ()	2D	aromatic bonds count
19	AtomCount	nAtom	AtomCount ('Atom')	2D	number of all atoms
20		nHeavyAtom	AtomCount ('HeavyAtom')	2D	number of heavy atoms
21		nSpiro	AtomCount ('Spiro')	2D	number of spiro atoms
22		nBridgehead	AtomCount ('Bridgehead')	2D	number of bridgehead atoms
23		nHetero	AtomCount ('Hetero')	2D	number of hetero atoms
24		nH	AtomCount ('H')	2D	number of H atoms
25		nB	AtomCount ('B')	2D	number of B atoms
26		nC	AtomCount ('C')	2D	number of C atoms
27		nN	AtomCount ('N')	2D	number of N atoms
28		nO	AtomCount ('O')	2D	number of O atoms
29		nS	AtomCount ('S')	2D	number of S atoms
30		nP	AtomCount ('P')	2D	number of P atoms
31		nF	AtomCount ('F')	2D	number of F atoms
32		nCl	AtomCount ('Cl')	2D	number of Cl atoms
33		nBr	AtomCount ('Br')	2D	number of Br atoms
34		nI	AtomCount ('I')	2D	number of I atoms
35		nX	AtomCount ('X')	2D	number of halogen atoms

#	module	name	constructor	dim	description
36	Autocorrelation	ATS0dv	ATS (0, ‘dv’)	2D	moreau-broto autocorrelation of lag 0 weighted by valence electrons
37		ATS1dv	ATS (1, ‘dv’)	2D	moreau-broto autocorrelation of lag 1 weighted by valence electrons
38		ATS2dv	ATS (2, ‘dv’)	2D	moreau-broto autocorrelation of lag 2 weighted by valence electrons
39		ATS3dv	ATS (3, ‘dv’)	2D	moreau-broto autocorrelation of lag 3 weighted by valence electrons
40		ATS4dv	ATS (4, ‘dv’)	2D	moreau-broto autocorrelation of lag 4 weighted by valence electrons
41		ATS5dv	ATS (5, ‘dv’)	2D	moreau-broto autocorrelation of lag 5 weighted by valence electrons
42		ATS6dv	ATS (6, ‘dv’)	2D	moreau-broto autocorrelation of lag 6 weighted by valence electrons
43		ATS7dv	ATS (7, ‘dv’)	2D	moreau-broto autocorrelation of lag 7 weighted by valence electrons

#	module	name	constructor	dim	description
44		ATS8dv	ATS (8, ‘dv’)	2D	moreau-broto autocorrelation of lag 8 weighted by valence electrons
45		ATS0d	ATS (0, ‘d’)	2D	moreau-broto autocorrelation of lag 0 weighted by sigma electrons
46		ATS1d	ATS (1, ‘d’)	2D	moreau-broto autocorrelation of lag 1 weighted by sigma electrons
47		ATS2d	ATS (2, ‘d’)	2D	moreau-broto autocorrelation of lag 2 weighted by sigma electrons
48		ATS3d	ATS (3, ‘d’)	2D	moreau-broto autocorrelation of lag 3 weighted by sigma electrons
49		ATS4d	ATS (4, ‘d’)	2D	moreau-broto autocorrelation of lag 4 weighted by sigma electrons
50		ATS5d	ATS (5, ‘d’)	2D	moreau-broto autocorrelation of lag 5 weighted by sigma electrons
51		ATS6d	ATS (6, ‘d’)	2D	moreau-broto autocorrelation of lag 6 weighted by sigma electrons

#	module	name	constructor	dim	description
52		ATS7d	ATS (7, ‘d’)	2D	moreau-broto autocorrelation of lag 7 weighted by sigma electrons
53		ATS8d	ATS (8, ‘d’)	2D	moreau-broto autocorrelation of lag 8 weighted by sigma electrons
54		ATS0s	ATS (0, ‘s’)	2D	moreau-broto autocorrelation of lag 0 weighted by intrinsic state
55		ATS1s	ATS (1, ‘s’)	2D	moreau-broto autocorrelation of lag 1 weighted by intrinsic state
56		ATS2s	ATS (2, ‘s’)	2D	moreau-broto autocorrelation of lag 2 weighted by intrinsic state
57		ATS3s	ATS (3, ‘s’)	2D	moreau-broto autocorrelation of lag 3 weighted by intrinsic state
58		ATS4s	ATS (4, ‘s’)	2D	moreau-broto autocorrelation of lag 4 weighted by intrinsic state
59		ATS5s	ATS (5, ‘s’)	2D	moreau-broto autocorrelation of lag 5 weighted by intrinsic state
60		ATS6s	ATS (6, ‘s’)	2D	moreau-broto autocorrelation of lag 6 weighted by intrinsic state
61		ATS7s	ATS (7, ‘s’)	2D	moreau-broto autocorrelation of lag 7 weighted by intrinsic state

#	module	name	constructor	dim	description
62		ATS8s	ATS (8, ‘s’)	2D	moreau-broto autocorrelation of lag 8 weighted by intrinsic state
63		ATS0Z	ATS (0, ‘Z’)	2D	moreau-broto autocorrelation of lag 0 weighted by atomic number
64		ATS1Z	ATS (1, ‘Z’)	2D	moreau-broto autocorrelation of lag 1 weighted by atomic number
65		ATS2Z	ATS (2, ‘Z’)	2D	moreau-broto autocorrelation of lag 2 weighted by atomic number
66		ATS3Z	ATS (3, ‘Z’)	2D	moreau-broto autocorrelation of lag 3 weighted by atomic number
67		ATS4Z	ATS (4, ‘Z’)	2D	moreau-broto autocorrelation of lag 4 weighted by atomic number
68		ATS5Z	ATS (5, ‘Z’)	2D	moreau-broto autocorrelation of lag 5 weighted by atomic number
69		ATS6Z	ATS (6, ‘Z’)	2D	moreau-broto autocorrelation of lag 6 weighted by atomic number
70		ATS7Z	ATS (7, ‘Z’)	2D	moreau-broto autocorrelation of lag 7 weighted by atomic number
71		ATS8Z	ATS (8, ‘Z’)	2D	moreau-broto autocorrelation of lag 8 weighted by atomic number

#	module	name	constructor	dim	description
72		ATS0m	ATS (0, ‘m’)	2D	moreau-broto autocorrelation of lag 0 weighted by mass
73		ATS1m	ATS (1, ‘m’)	2D	moreau-broto autocorrelation of lag 1 weighted by mass
74		ATS2m	ATS (2, ‘m’)	2D	moreau-broto autocorrelation of lag 2 weighted by mass
75		ATS3m	ATS (3, ‘m’)	2D	moreau-broto autocorrelation of lag 3 weighted by mass
76		ATS4m	ATS (4, ‘m’)	2D	moreau-broto autocorrelation of lag 4 weighted by mass
77		ATS5m	ATS (5, ‘m’)	2D	moreau-broto autocorrelation of lag 5 weighted by mass
78		ATS6m	ATS (6, ‘m’)	2D	moreau-broto autocorrelation of lag 6 weighted by mass
79		ATS7m	ATS (7, ‘m’)	2D	moreau-broto autocorrelation of lag 7 weighted by mass
80		ATS8m	ATS (8, ‘m’)	2D	moreau-broto autocorrelation of lag 8 weighted by mass
81		ATS0v	ATS (0, ‘v’)	2D	moreau-broto autocorrelation of lag 0 weighted by vdw volume

#	module	name	constructor	dim	description
82		ATS1v	ATS (1, ‘v’)	2D	moreau-broto autocorrelation of lag 1 weighted by vdw volume
83		ATS2v	ATS (2, ‘v’)	2D	moreau-broto autocorrelation of lag 2 weighted by vdw volume
84		ATS3v	ATS (3, ‘v’)	2D	moreau-broto autocorrelation of lag 3 weighted by vdw volume
85		ATS4v	ATS (4, ‘v’)	2D	moreau-broto autocorrelation of lag 4 weighted by vdw volume
86		ATS5v	ATS (5, ‘v’)	2D	moreau-broto autocorrelation of lag 5 weighted by vdw volume
87		ATS6v	ATS (6, ‘v’)	2D	moreau-broto autocorrelation of lag 6 weighted by vdw volume
88		ATS7v	ATS (7, ‘v’)	2D	moreau-broto autocorrelation of lag 7 weighted by vdw volume
89		ATS8v	ATS (8, ‘v’)	2D	moreau-broto autocorrelation of lag 8 weighted by vdw volume
90		ATS0se	ATS (0, ‘se’)	2D	moreau-broto autocorrelation of lag 0 weighted by sanderson EN
91		ATS1se	ATS (1, ‘se’)	2D	moreau-broto autocorrelation of lag 1 weighted by sanderson EN

#	module	name	constructor	dim	description
92		ATS2se	ATS (2, ‘se’)	2D	moreau-broto autocorrelation of lag 2 weighted by sanderson EN
93		ATS3se	ATS (3, ‘se’)	2D	moreau-broto autocorrelation of lag 3 weighted by sanderson EN
94		ATS4se	ATS (4, ‘se’)	2D	moreau-broto autocorrelation of lag 4 weighted by sanderson EN
95		ATS5se	ATS (5, ‘se’)	2D	moreau-broto autocorrelation of lag 5 weighted by sanderson EN
96		ATS6se	ATS (6, ‘se’)	2D	moreau-broto autocorrelation of lag 6 weighted by sanderson EN
97		ATS7se	ATS (7, ‘se’)	2D	moreau-broto autocorrelation of lag 7 weighted by sanderson EN
98		ATS8se	ATS (8, ‘se’)	2D	moreau-broto autocorrelation of lag 8 weighted by sanderson EN
99		ATS0pe	ATS (0, ‘pe’)	2D	moreau-broto autocorrelation of lag 0 weighted by pauling EN
100		ATS1pe	ATS (1, ‘pe’)	2D	moreau-broto autocorrelation of lag 1 weighted by pauling EN
101		ATS2pe	ATS (2, ‘pe’)	2D	moreau-broto autocorrelation of lag 2 weighted by pauling EN

#	module	name	constructor	dim	description
102		ATS3pe	ATS (3, ‘pe’)	2D	moreau-broto autocorrelation of lag 3 weighted by pauling EN
103		ATS4pe	ATS (4, ‘pe’)	2D	moreau-broto autocorrelation of lag 4 weighted by pauling EN
104		ATS5pe	ATS (5, ‘pe’)	2D	moreau-broto autocorrelation of lag 5 weighted by pauling EN
105		ATS6pe	ATS (6, ‘pe’)	2D	moreau-broto autocorrelation of lag 6 weighted by pauling EN
106		ATS7pe	ATS (7, ‘pe’)	2D	moreau-broto autocorrelation of lag 7 weighted by pauling EN
107		ATS8pe	ATS (8, ‘pe’)	2D	moreau-broto autocorrelation of lag 8 weighted by pauling EN
108		ATS0are	ATS (0, ‘are’)	2D	moreau-broto autocorrelation of lag 0 weighted by allred-rocow EN
109		ATS1are	ATS (1, ‘are’)	2D	moreau-broto autocorrelation of lag 1 weighted by allred-rocow EN
110		ATS2are	ATS (2, ‘are’)	2D	moreau-broto autocorrelation of lag 2 weighted by allred-rocow EN

#	module	name	constructor	dim	description
111		ATS3are	ATS (3, 'are')	2D	moreau-broto autocorrelation of lag 3 weighted by allred-rocow EN
112		ATS4are	ATS (4, 'are')	2D	moreau-broto autocorrelation of lag 4 weighted by allred-rocow EN
113		ATS5are	ATS (5, 'are')	2D	moreau-broto autocorrelation of lag 5 weighted by allred-rocow EN
114		ATS6are	ATS (6, 'are')	2D	moreau-broto autocorrelation of lag 6 weighted by allred-rocow EN
115		ATS7are	ATS (7, 'are')	2D	moreau-broto autocorrelation of lag 7 weighted by allred-rocow EN
116		ATS8are	ATS (8, 'are')	2D	moreau-broto autocorrelation of lag 8 weighted by allred-rocow EN
117		ATS0p	ATS (0, 'p')	2D	moreau-broto autocorrelation of lag 0 weighted by polarizability
118		ATS1p	ATS (1, 'p')	2D	moreau-broto autocorrelation of lag 1 weighted by polarizability
119		ATS2p	ATS (2, 'p')	2D	moreau-broto autocorrelation of lag 2 weighted by polarizability

#	module	name	constructor	dim	description
120		ATS3p	ATS (3, ‘p’)	2D	moreau-broto autocorrelation of lag 3 weighted by polarizability
121		ATS4p	ATS (4, ‘p’)	2D	moreau-broto autocorrelation of lag 4 weighted by polarizability
122		ATS5p	ATS (5, ‘p’)	2D	moreau-broto autocorrelation of lag 5 weighted by polarizability
123		ATS6p	ATS (6, ‘p’)	2D	moreau-broto autocorrelation of lag 6 weighted by polarizability
124		ATS7p	ATS (7, ‘p’)	2D	moreau-broto autocorrelation of lag 7 weighted by polarizability
125		ATS8p	ATS (8, ‘p’)	2D	moreau-broto autocorrelation of lag 8 weighted by polarizability
126		ATS0i	ATS (0, ‘i’)	2D	moreau-broto autocorrelation of lag 0 weighted by ionization potential
127		ATS1i	ATS (1, ‘i’)	2D	moreau-broto autocorrelation of lag 1 weighted by ionization potential
128		ATS2i	ATS (2, ‘i’)	2D	moreau-broto autocorrelation of lag 2 weighted by ionization potential

#	module	name	constructor	dim	description
129		ATS3i	ATS (3, 'i')	2D	moreau-broto autocorrelation of lag 3 weighted by ionization potential
130		ATS4i	ATS (4, 'i')	2D	moreau-broto autocorrelation of lag 4 weighted by ionization potential
131		ATS5i	ATS (5, 'i')	2D	moreau-broto autocorrelation of lag 5 weighted by ionization potential
132		ATS6i	ATS (6, 'i')	2D	moreau-broto autocorrelation of lag 6 weighted by ionization potential
133		ATS7i	ATS (7, 'i')	2D	moreau-broto autocorrelation of lag 7 weighted by ionization potential
134		ATS8i	ATS (8, 'i')	2D	moreau-broto autocorrelation of lag 8 weighted by ionization potential
135		AATS0dv	AATS (0, 'dv')	2D	averaged moreau-broto autocorrelation of lag 0 weighted by valence electrons
136		AATS1dv	AATS (1, 'dv')	2D	averaged moreau-broto autocorrelation of lag 1 weighted by valence electrons

#	module	name	constructor	dim	description
137		AATS2dv	AATS (2, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by valence electrons
138		AATS3dv	AATS (3, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by valence electrons
139		AATS4dv	AATS (4, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by valence electrons
140		AATS5dv	AATS (5, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by valence electrons
141		AATS6dv	AATS (6, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by valence electrons
142		AATS7dv	AATS (7, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by valence electrons
143		AATS8dv	AATS (8, ‘dv’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by valence electrons

#	module	name	constructor	dim	description
144		AATS0d	AATS (0, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by sigma electrons
145		AATS1d	AATS (1, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by sigma electrons
146		AATS2d	AATS (2, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by sigma electrons
147		AATS3d	AATS (3, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by sigma electrons
148		AATS4d	AATS (4, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by sigma electrons
149		AATS5d	AATS (5, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by sigma electrons
150		AATS6d	AATS (6, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by sigma electrons

#	module	name	constructor	dim	description
151		AATS7d	AATS (7, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by sigma electrons
152		AATS8d	AATS (8, ‘d’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by sigma electrons
153		AATS0s	AATS (0, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by intrinsic state
154		AATS1s	AATS (1, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by intrinsic state
155		AATS2s	AATS (2, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by intrinsic state
156		AATS3s	AATS (3, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by intrinsic state
157		AATS4s	AATS (4, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by intrinsic state
158		AATS5s	AATS (5, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by intrinsic state

#	module	name	constructor	dim	description
159		AATS6s	AATS (6, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by intrinsic state
160		AATS7s	AATS (7, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by intrinsic state
161		AATS8s	AATS (8, ‘s’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by intrinsic state
162		AATS0Z	AATS (0, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by atomic number
163		AATS1Z	AATS (1, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by atomic number
164		AATS2Z	AATS (2, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by atomic number
165		AATS3Z	AATS (3, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by atomic number
166		AATS4Z	AATS (4, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by atomic number

#	module	name	constructor	dim	description
167		AATS5Z	AATS (5, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by atomic number
168		AATS6Z	AATS (6, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by atomic number
169		AATS7Z	AATS (7, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by atomic number
170		AATS8Z	AATS (8, ‘Z’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by atomic number
171		AATS0m	AATS (0, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by mass
172		AATS1m	AATS (1, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by mass
173		AATS2m	AATS (2, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by mass
174		AATS3m	AATS (3, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by mass

#	module	name	constructor	dim	description
175		AATS4m	AATS (4, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by mass
176		AATS5m	AATS (5, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by mass
177		AATS6m	AATS (6, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by mass
178		AATS7m	AATS (7, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by mass
179		AATS8m	AATS (8, ‘m’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by mass
180		AATS0v	AATS (0, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by vdw volume
181		AATS1v	AATS (1, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by vdw volume
182		AATS2v	AATS (2, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by vdw volume

#	module	name	constructor	dim	description
183		AATS3v	AATS (3, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by vdw volume
184		AATS4v	AATS (4, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by vdw volume
185		AATS5v	AATS (5, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by vdw volume
186		AATS6v	AATS (6, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by vdw volume
187		AATS7v	AATS (7, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by vdw volume
188		AATS8v	AATS (8, ‘v’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by vdw volume
189		AATS0se	AATS (0, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by sanderson EN
190		AATS1se	AATS (1, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by sanderson EN

#	module	name	constructor	dim	description
191		AATS2se	AATS (2, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by sanderson EN
192		AATS3se	AATS (3, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by sanderson EN
193		AATS4se	AATS (4, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by sanderson EN
194		AATS5se	AATS (5, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by sanderson EN
195		AATS6se	AATS (6, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by sanderson EN
196		AATS7se	AATS (7, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by sanderson EN
197		AATS8se	AATS (8, ‘se’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by sanderson EN
198		AATS0pe	AATS (0, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by pauling EN

#	module	name	constructor	dim	description
199		AATS1pe	AATS (1, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by pauling EN
200		AATS2pe	AATS (2, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by pauling EN
201		AATS3pe	AATS (3, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by pauling EN
202		AATS4pe	AATS (4, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by pauling EN
203		AATS5pe	AATS (5, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by pauling EN
204		AATS6pe	AATS (6, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by pauling EN
205		AATS7pe	AATS (7, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by pauling EN
206		AATS8pe	AATS (8, ‘pe’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by pauling EN

#	module	name	constructor	dim	description
207		AATS0are	AATS (0, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by allred-rocow EN
208		AATS1are	AATS (1, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by allred-rocow EN
209		AATS2are	AATS (2, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by allred-rocow EN
210		AATS3are	AATS (3, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by allred-rocow EN
211		AATS4are	AATS (4, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by allred-rocow EN
212		AATS5are	AATS (5, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by allred-rocow EN
213		AATS6are	AATS (6, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by allred-rocow EN

#	module	name	constructor	dim	description
214		AATS7are	AATS (7, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by allred-rocow EN
215		AATS8are	AATS (8, ‘are’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by allred-rocow EN
216		AATS0p	AATS (0, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by polarizability
217		AATS1p	AATS (1, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by polarizability
218		AATS2p	AATS (2, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by polarizability
219		AATS3p	AATS (3, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by polarizability
220		AATS4p	AATS (4, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by polarizability
221		AATS5p	AATS (5, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by polarizability

#	module	name	constructor	dim	description
222		AATS6p	AATS (6, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by polarizability
223		AATS7p	AATS (7, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by polarizability
224		AATS8p	AATS (8, ‘p’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by polarizability
225		AATS0i	AATS (0, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 0 weighted by ionization potential
226		AATS1i	AATS (1, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 1 weighted by ionization potential
227		AATS2i	AATS (2, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 2 weighted by ionization potential
228		AATS3i	AATS (3, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 3 weighted by ionization potential
229		AATS4i	AATS (4, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 4 weighted by ionization potential

#	module	name	constructor	dim	description
230		AATS5i	AATS (5, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 5 weighted by ionization potential
231		AATS6i	AATS (6, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 6 weighted by ionization potential
232		AATS7i	AATS (7, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 7 weighted by ionization potential
233		AATS8i	AATS (8, ‘i’)	2D	averaged moreau-broto autocorrelation of lag 8 weighted by ionization potential
234		ATSC0c	ATSC (0, ‘c’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by gasteiger charge
235		ATSC1c	ATSC (1, ‘c’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by gasteiger charge
236		ATSC2c	ATSC (2, ‘c’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by gasteiger charge

#	module	name	constructor	dim	description
237		ATSC3c	ATSC (3, ‘c’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by gasteiger charge
238		ATSC4c	ATSC (4, ‘c’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by gasteiger charge
239		ATSC5c	ATSC (5, ‘c’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by gasteiger charge
240		ATSC6c	ATSC (6, ‘c’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by gasteiger charge
241		ATSC7c	ATSC (7, ‘c’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by gasteiger charge
242		ATSC8c	ATSC (8, ‘c’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by gasteiger charge
243		ATSC0dv	ATSC (0, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by valence electrons

#	module	name	constructor	dim	description
244		ATSC1dv	ATSC (1, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by valence electrons
245		ATSC2dv	ATSC (2, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by valence electrons
246		ATSC3dv	ATSC (3, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by valence electrons
247		ATSC4dv	ATSC (4, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by valence electrons
248		ATSC5dv	ATSC (5, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by valence electrons
249		ATSC6dv	ATSC (6, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by valence electrons
250		ATSC7dv	ATSC (7, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by valence electrons

#	module	name	constructor	dim	description
251		ATSC8dv	ATSC (8, ‘dv’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by valence electrons
252		ATSC0d	ATSC (0, ‘d’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by sigma electrons
253		ATSC1d	ATSC (1, ‘d’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by sigma electrons
254		ATSC2d	ATSC (2, ‘d’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by sigma electrons
255		ATSC3d	ATSC (3, ‘d’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by sigma electrons
256		ATSC4d	ATSC (4, ‘d’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by sigma electrons
257		ATSC5d	ATSC (5, ‘d’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by sigma electrons

#	module	name	constructor	dim	description
258		ATSC6d	ATSC (6, ‘d’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by sigma electrons
259		ATSC7d	ATSC (7, ‘d’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by sigma electrons
260		ATSC8d	ATSC (8, ‘d’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by sigma electrons
261		ATSC0s	ATSC (0, ‘s’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by intrinsic state
262		ATSC1s	ATSC (1, ‘s’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by intrinsic state
263		ATSC2s	ATSC (2, ‘s’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by intrinsic state
264		ATSC3s	ATSC (3, ‘s’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by intrinsic state
265		ATSC4s	ATSC (4, ‘s’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by intrinsic state

#	module	name	constructor	dim	description
266		ATSC5s	ATSC (5, ‘s’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by intrinsic state
267		ATSC6s	ATSC (6, ‘s’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by intrinsic state
268		ATSC7s	ATSC (7, ‘s’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by intrinsic state
269		ATSC8s	ATSC (8, ‘s’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by intrinsic state
270		ATSC0Z	ATSC (0, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by atomic number
271		ATSC1Z	ATSC (1, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by atomic number
272		ATSC2Z	ATSC (2, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by atomic number
273		ATSC3Z	ATSC (3, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by atomic number

#	module	name	constructor	dim	description
274		ATSC4Z	ATSC (4, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by atomic number
275		ATSC5Z	ATSC (5, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by atomic number
276		ATSC6Z	ATSC (6, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by atomic number
277		ATSC7Z	ATSC (7, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by atomic number
278		ATSC8Z	ATSC (8, ‘Z’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by atomic number
279		ATSC0m	ATSC (0, ‘m’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by mass
280		ATSC1m	ATSC (1, ‘m’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by mass
281		ATSC2m	ATSC (2, ‘m’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by mass

#	module	name	constructor	dim	description
282		ATSC3m	ATSC (3, ‘m’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by mass
283		ATSC4m	ATSC (4, ‘m’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by mass
284		ATSC5m	ATSC (5, ‘m’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by mass
285		ATSC6m	ATSC (6, ‘m’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by mass
286		ATSC7m	ATSC (7, ‘m’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by mass
287		ATSC8m	ATSC (8, ‘m’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by mass
288		ATSC0v	ATSC (0, ‘v’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by vdw volume
289		ATSC1v	ATSC (1, ‘v’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by vdw volume

#	module	name	constructor	dim	description
290		ATSC2v	ATSC (2, ‘v’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by vdw volume
291		ATSC3v	ATSC (3, ‘v’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by vdw volume
292		ATSC4v	ATSC (4, ‘v’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by vdw volume
293		ATSC5v	ATSC (5, ‘v’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by vdw volume
294		ATSC6v	ATSC (6, ‘v’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by vdw volume
295		ATSC7v	ATSC (7, ‘v’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by vdw volume
296		ATSC8v	ATSC (8, ‘v’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by vdw volume
297		ATSC0se	ATSC (0, ‘se’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by sanderson EN

#	module	name	constructor	dim	description
298		ATSC1se	ATSC (1, ‘se’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by sanderson EN
299		ATSC2se	ATSC (2, ‘se’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by sanderson EN
300		ATSC3se	ATSC (3, ‘se’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by sanderson EN
301		ATSC4se	ATSC (4, ‘se’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by sanderson EN
302		ATSC5se	ATSC (5, ‘se’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by sanderson EN
303		ATSC6se	ATSC (6, ‘se’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by sanderson EN
304		ATSC7se	ATSC (7, ‘se’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by sanderson EN
305		ATSC8se	ATSC (8, ‘se’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by sanderson EN

#	module	name	constructor	dim	description
306		ATSC0pe	ATSC (0, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by pauling EN
307		ATSC1pe	ATSC (1, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by pauling EN
308		ATSC2pe	ATSC (2, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by pauling EN
309		ATSC3pe	ATSC (3, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by pauling EN
310		ATSC4pe	ATSC (4, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by pauling EN
311		ATSC5pe	ATSC (5, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by pauling EN
312		ATSC6pe	ATSC (6, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by pauling EN
313		ATSC7pe	ATSC (7, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by pauling EN

#	module	name	constructor	dim	description
314		ATSC8pe	ATSC (8, ‘pe’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by pauling EN
315		ATSC0are	ATSC (0, ‘are’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by allred-rocow EN
316		ATSC1are	ATSC (1, ‘are’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by allred-rocow EN
317		ATSC2are	ATSC (2, ‘are’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by allred-rocow EN
318		ATSC3are	ATSC (3, ‘are’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by allred-rocow EN
319		ATSC4are	ATSC (4, ‘are’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by allred-rocow EN
320		ATSC5are	ATSC (5, ‘are’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by allred-rocow EN

#	module	name	constructor	dim	description
321		ATSC6are	ATSC (6, ‘are’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by allred-rocow EN
322		ATSC7are	ATSC (7, ‘are’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by allred-rocow EN
323		ATSC8are	ATSC (8, ‘are’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by allred-rocow EN
324		ATSC0p	ATSC (0, ‘p’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by polarizability
325		ATSC1p	ATSC (1, ‘p’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by polarizability
326		ATSC2p	ATSC (2, ‘p’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by polarizability
327		ATSC3p	ATSC (3, ‘p’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by polarizability
328		ATSC4p	ATSC (4, ‘p’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by polarizability

#	module	name	constructor	dim	description
329		ATSC5p	ATSC (5, ‘p’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by polarizability
330		ATSC6p	ATSC (6, ‘p’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by polarizability
331		ATSC7p	ATSC (7, ‘p’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by polarizability
332		ATSC8p	ATSC (8, ‘p’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by polarizability
333		ATSC0i	ATSC (0, ‘i’)	2D	centered moreau-broto autocorrelation of lag 0 weighted by ionization potential
334		ATSC1i	ATSC (1, ‘i’)	2D	centered moreau-broto autocorrelation of lag 1 weighted by ionization potential
335		ATSC2i	ATSC (2, ‘i’)	2D	centered moreau-broto autocorrelation of lag 2 weighted by ionization potential
336		ATSC3i	ATSC (3, ‘i’)	2D	centered moreau-broto autocorrelation of lag 3 weighted by ionization potential

#	module	name	constructor	dim	description
337		ATSC4i	ATSC (4, ‘i’)	2D	centered moreau-broto autocorrelation of lag 4 weighted by ionization potential
338		ATSC5i	ATSC (5, ‘i’)	2D	centered moreau-broto autocorrelation of lag 5 weighted by ionization potential
339		ATSC6i	ATSC (6, ‘i’)	2D	centered moreau-broto autocorrelation of lag 6 weighted by ionization potential
340		ATSC7i	ATSC (7, ‘i’)	2D	centered moreau-broto autocorrelation of lag 7 weighted by ionization potential
341		ATSC8i	ATSC (8, ‘i’)	2D	centered moreau-broto autocorrelation of lag 8 weighted by ionization potential
342		AATSC0c	AATSC (0, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by gasteiger charge
343		AATSC1c	AATSC (1, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by gasteiger charge

#	module	name	constructor	dim	description
344		AATSC2c	AATSC (2, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by gasteiger charge
345		AATSC3c	AATSC (3, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by gasteiger charge
346		AATSC4c	AATSC (4, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by gasteiger charge
347		AATSC5c	AATSC (5, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by gasteiger charge
348		AATSC6c	AATSC (6, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by gasteiger charge
349		AATSC7c	AATSC (7, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by gasteiger charge

#	module	name	constructor	dim	description
350		AATSC8c	AATSC (8, ‘c’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by gasteiger charge
351		AATSC0dv	AATSC (0, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by valence electrons
352		AATSC1dv	AATSC (1, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by valence electrons
353		AATSC2dv	AATSC (2, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by valence electrons
354		AATSC3dv	AATSC (3, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by valence electrons
355		AATSC4dv	AATSC (4, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by valence electrons

#	module	name	constructor	dim	description
356		AATSC5dv	AATSC (5, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by valence electrons
357		AATSC6dv	AATSC (6, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by valence electrons
358		AATSC7dv	AATSC (7, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by valence electrons
359		AATSC8dv	AATSC (8, ‘dv’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by valence electrons
360		AATSC0d	AATSC (0, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by sigma electrons
361		AATSC1d	AATSC (1, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by sigma electrons

#	module	name	constructor	dim	description
362		AATSC2d	AATSC (2, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by sigma electrons
363		AATSC3d	AATSC (3, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by sigma electrons
364		AATSC4d	AATSC (4, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by sigma electrons
365		AATSC5d	AATSC (5, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by sigma electrons
366		AATSC6d	AATSC (6, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by sigma electrons
367		AATSC7d	AATSC (7, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by sigma electrons

#	module	name	constructor	dim	description
368		AATSC8d	AATSC (8, ‘d’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by sigma electrons
369		AATSC0s	AATSC (0, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by intrinsic state
370		AATSC1s	AATSC (1, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by intrinsic state
371		AATSC2s	AATSC (2, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by intrinsic state
372		AATSC3s	AATSC (3, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by intrinsic state
373		AATSC4s	AATSC (4, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by intrinsic state
374		AATSC5s	AATSC (5, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by intrinsic state

#	module	name	constructor	dim	description
375		AATSC6s	AATSC (6, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by intrinsic state
376		AATSC7s	AATSC (7, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by intrinsic state
377		AATSC8s	AATSC (8, ‘s’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by intrinsic state
378		AATSC0Z	AATSC (0, ‘Z’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by atomic number
379		AATSC1Z	AATSC (1, ‘Z’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by atomic number
380		AATSC2Z	AATSC (2, ‘Z’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by atomic number
381		AATSC3Z	AATSC (3, ‘Z’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by atomic number

#	module	name	constructor	dim	description
382		AATSC4Z	AATSC (4, 'Z')	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by atomic number
383		AATSC5Z	AATSC (5, 'Z')	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by atomic number
384		AATSC6Z	AATSC (6, 'Z')	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by atomic number
385		AATSC7Z	AATSC (7, 'Z')	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by atomic number
386		AATSC8Z	AATSC (8, 'Z')	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by atomic number
387		AATSC0m	AATSC (0, 'm')	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by mass
388		AATSC1m	AATSC (1, 'm')	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by mass

#	module	name	constructor	dim	description
389		AATSC2m	AATSC (2, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by mass
390		AATSC3m	AATSC (3, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by mass
391		AATSC4m	AATSC (4, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by mass
392		AATSC5m	AATSC (5, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by mass
393		AATSC6m	AATSC (6, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by mass
394		AATSC7m	AATSC (7, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by mass
395		AATSC8m	AATSC (8, ‘m’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by mass

#	module	name	constructor	dim	description
396		AATSC0v	AATSC (0, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by vdw volume
397		AATSC1v	AATSC (1, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by vdw volume
398		AATSC2v	AATSC (2, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by vdw volume
399		AATSC3v	AATSC (3, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by vdw volume
400		AATSC4v	AATSC (4, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by vdw volume
401		AATSC5v	AATSC (5, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by vdw volume
402		AATSC6v	AATSC (6, 'v')	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by vdw volume

#	module	name	constructor	dim	description
403		AATSC7v	AATSC (7, ‘v’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by vdw volume
404		AATSC8v	AATSC (8, ‘v’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by vdw volume
405		AATSC0se	AATSC (0, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by sanderson EN
406		AATSC1se	AATSC (1, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by sanderson EN
407		AATSC2se	AATSC (2, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by sanderson EN
408		AATSC3se	AATSC (3, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by sanderson EN
409		AATSC4se	AATSC (4, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by sanderson EN

#	module	name	constructor	dim	description
410		AATSC5se	AATSC (5, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by sanderson EN
411		AATSC6se	AATSC (6, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by sanderson EN
412		AATSC7se	AATSC (7, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by sanderson EN
413		AATSC8se	AATSC (8, ‘se’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by sanderson EN
414		AATSC0pe	AATSC (0, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by pauling EN
415		AATSC1pe	AATSC (1, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by pauling EN
416		AATSC2pe	AATSC (2, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by pauling EN

#	module	name	constructor	dim	description
417		AATSC3pe	AATSC (3, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by pauling EN
418		AATSC4pe	AATSC (4, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by pauling EN
419		AATSC5pe	AATSC (5, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by pauling EN
420		AATSC6pe	AATSC (6, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by pauling EN
421		AATSC7pe	AATSC (7, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by pauling EN
422		AATSC8pe	AATSC (8, ‘pe’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by pauling EN
423		AATSC0are	AATSC (0, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by allred-rocow EN

#	module	name	constructor	dim	description
424		AATSC1are	AATSC (1, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by allred-rocow EN
425		AATSC2are	AATSC (2, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by allred-rocow EN
426		AATSC3are	AATSC (3, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by allred-rocow EN
427		AATSC4are	AATSC (4, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by allred-rocow EN
428		AATSC5are	AATSC (5, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by allred-rocow EN
429		AATSC6are	AATSC (6, ‘are’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by allred-rocow EN

#	module	name	constructor	dim	description
430		AATSC7are	AATSC (7, 'are')	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by allred-rocow EN
431		AATSC8are	AATSC (8, 'are')	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by allred-rocow EN
432		AATSC0p	AATSC (0, 'p')	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by polarizability
433		AATSC1p	AATSC (1, 'p')	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by polarizability
434		AATSC2p	AATSC (2, 'p')	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by polarizability
435		AATSC3p	AATSC (3, 'p')	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by polarizability
436		AATSC4p	AATSC (4, 'p')	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by polarizability

#	module	name	constructor	dim	description
437		AATSC5p	AATSC (5, ‘p’)	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by polarizability
438		AATSC6p	AATSC (6, ‘p’)	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by polarizability
439		AATSC7p	AATSC (7, ‘p’)	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by polarizability
440		AATSC8p	AATSC (8, ‘p’)	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by polarizability
441		AATSC0i	AATSC (0, ‘i’)	2D	averaged and centered moreau-broto autocorrelation of lag 0 weighted by ionization potential
442		AATSC1i	AATSC (1, ‘i’)	2D	averaged and centered moreau-broto autocorrelation of lag 1 weighted by ionization potential
443		AATSC2i	AATSC (2, ‘i’)	2D	averaged and centered moreau-broto autocorrelation of lag 2 weighted by ionization potential

#	module	name	constructor	dim	description
444		AATSC3i	AATSC (3, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 3 weighted by ionization potential
445		AATSC4i	AATSC (4, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 4 weighted by ionization potential
446		AATSC5i	AATSC (5, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 5 weighted by ionization potential
447		AATSC6i	AATSC (6, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 6 weighted by ionization potential
448		AATSC7i	AATSC (7, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 7 weighted by ionization potential
449		AATSC8i	AATSC (8, 'i')	2D	averaged and centered moreau-broto autocorrelation of lag 8 weighted by ionization potential
450		MATS1c	MATS (1, 'c')	2D	moran coefficient of lag 1 weighted by gasteiger charge

#	module	name	constructor	dim	description
451		MATS2c	MATS (2, ‘c’)	2D	moran coefficient of lag 2 weighted by gasteiger charge
452		MATS3c	MATS (3, ‘c’)	2D	moran coefficient of lag 3 weighted by gasteiger charge
453		MATS4c	MATS (4, ‘c’)	2D	moran coefficient of lag 4 weighted by gasteiger charge
454		MATS5c	MATS (5, ‘c’)	2D	moran coefficient of lag 5 weighted by gasteiger charge
455		MATS6c	MATS (6, ‘c’)	2D	moran coefficient of lag 6 weighted by gasteiger charge
456		MATS7c	MATS (7, ‘c’)	2D	moran coefficient of lag 7 weighted by gasteiger charge
457		MATS8c	MATS (8, ‘c’)	2D	moran coefficient of lag 8 weighted by gasteiger charge
458		MATS1dv	MATS (1, ‘dv’)	2D	moran coefficient of lag 1 weighted by valence electrons
459		MATS2dv	MATS (2, ‘dv’)	2D	moran coefficient of lag 2 weighted by valence electrons
460		MATS3dv	MATS (3, ‘dv’)	2D	moran coefficient of lag 3 weighted by valence electrons

#	module	name	constructor	dim	description
461		MATS4dv	MATS (4, ‘dv’)	2D	moran coefficient of lag 4 weighted by valence electrons
462		MATS5dv	MATS (5, ‘dv’)	2D	moran coefficient of lag 5 weighted by valence electrons
463		MATS6dv	MATS (6, ‘dv’)	2D	moran coefficient of lag 6 weighted by valence electrons
464		MATS7dv	MATS (7, ‘dv’)	2D	moran coefficient of lag 7 weighted by valence electrons
465		MATS8dv	MATS (8, ‘dv’)	2D	moran coefficient of lag 8 weighted by valence electrons
466		MATS1d	MATS (1, ‘d’)	2D	moran coefficient of lag 1 weighted by sigma electrons
467		MATS2d	MATS (2, ‘d’)	2D	moran coefficient of lag 2 weighted by sigma electrons
468		MATS3d	MATS (3, ‘d’)	2D	moran coefficient of lag 3 weighted by sigma electrons
469		MATS4d	MATS (4, ‘d’)	2D	moran coefficient of lag 4 weighted by sigma electrons
470		MATS5d	MATS (5, ‘d’)	2D	moran coefficient of lag 5 weighted by sigma electrons

#	module	name	constructor	dim	description
471		MATS6d	MATS (6, ‘d’)	2D	moran coefficient of lag 6 weighted by sigma electrons
472		MATS7d	MATS (7, ‘d’)	2D	moran coefficient of lag 7 weighted by sigma electrons
473		MATS8d	MATS (8, ‘d’)	2D	moran coefficient of lag 8 weighted by sigma electrons
474		MATS1s	MATS (1, ‘s’)	2D	moran coefficient of lag 1 weighted by intrinsic state
475		MATS2s	MATS (2, ‘s’)	2D	moran coefficient of lag 2 weighted by intrinsic state
476		MATS3s	MATS (3, ‘s’)	2D	moran coefficient of lag 3 weighted by intrinsic state
477		MATS4s	MATS (4, ‘s’)	2D	moran coefficient of lag 4 weighted by intrinsic state
478		MATS5s	MATS (5, ‘s’)	2D	moran coefficient of lag 5 weighted by intrinsic state
479		MATS6s	MATS (6, ‘s’)	2D	moran coefficient of lag 6 weighted by intrinsic state
480		MATS7s	MATS (7, ‘s’)	2D	moran coefficient of lag 7 weighted by intrinsic state

#	module	name	constructor	dim	description
481		MATS8s	MATS (8, ‘s’)	2D	moran coefficient of lag 8 weighted by intrinsic state
482		MATS1Z	MATS (1, ‘Z’)	2D	moran coefficient of lag 1 weighted by atomic number
483		MATS2Z	MATS (2, ‘Z’)	2D	moran coefficient of lag 2 weighted by atomic number
484		MATS3Z	MATS (3, ‘Z’)	2D	moran coefficient of lag 3 weighted by atomic number
485		MATS4Z	MATS (4, ‘Z’)	2D	moran coefficient of lag 4 weighted by atomic number
486		MATS5Z	MATS (5, ‘Z’)	2D	moran coefficient of lag 5 weighted by atomic number
487		MATS6Z	MATS (6, ‘Z’)	2D	moran coefficient of lag 6 weighted by atomic number
488		MATS7Z	MATS (7, ‘Z’)	2D	moran coefficient of lag 7 weighted by atomic number
489		MATS8Z	MATS (8, ‘Z’)	2D	moran coefficient of lag 8 weighted by atomic number
490		MATS1m	MATS (1, ‘m’)	2D	moran coefficient of lag 1 weighted by mass
491		MATS2m	MATS (2, ‘m’)	2D	moran coefficient of lag 2 weighted by mass

#	module	name	constructor	dim	description
492		MATS3m	MATS (3, ‘m’)	2D	moran coefficient of lag 3 weighted by mass
493		MATS4m	MATS (4, ‘m’)	2D	moran coefficient of lag 4 weighted by mass
494		MATS5m	MATS (5, ‘m’)	2D	moran coefficient of lag 5 weighted by mass
495		MATS6m	MATS (6, ‘m’)	2D	moran coefficient of lag 6 weighted by mass
496		MATS7m	MATS (7, ‘m’)	2D	moran coefficient of lag 7 weighted by mass
497		MATS8m	MATS (8, ‘m’)	2D	moran coefficient of lag 8 weighted by mass
498		MATS1v	MATS (1, ‘v’)	2D	moran coefficient of lag 1 weighted by vdw volume
499		MATS2v	MATS (2, ‘v’)	2D	moran coefficient of lag 2 weighted by vdw volume
500		MATS3v	MATS (3, ‘v’)	2D	moran coefficient of lag 3 weighted by vdw volume
501		MATS4v	MATS (4, ‘v’)	2D	moran coefficient of lag 4 weighted by vdw volume
502		MATS5v	MATS (5, ‘v’)	2D	moran coefficient of lag 5 weighted by vdw volume
503		MATS6v	MATS (6, ‘v’)	2D	moran coefficient of lag 6 weighted by vdw volume
504		MATS7v	MATS (7, ‘v’)	2D	moran coefficient of lag 7 weighted by vdw volume

#	module	name	constructor	dim	description
505		MATS8v	MATS (8, ‘v’)	2D	moran coefficient of lag 8 weighted by vdw volume
506		MATS1se	MATS (1, ‘se’)	2D	moran coefficient of lag 1 weighted by sanderson EN
507		MATS2se	MATS (2, ‘se’)	2D	moran coefficient of lag 2 weighted by sanderson EN
508		MATS3se	MATS (3, ‘se’)	2D	moran coefficient of lag 3 weighted by sanderson EN
509		MATS4se	MATS (4, ‘se’)	2D	moran coefficient of lag 4 weighted by sanderson EN
510		MATS5se	MATS (5, ‘se’)	2D	moran coefficient of lag 5 weighted by sanderson EN
511		MATS6se	MATS (6, ‘se’)	2D	moran coefficient of lag 6 weighted by sanderson EN
512		MATS7se	MATS (7, ‘se’)	2D	moran coefficient of lag 7 weighted by sanderson EN
513		MATS8se	MATS (8, ‘se’)	2D	moran coefficient of lag 8 weighted by sanderson EN
514		MATS1pe	MATS (1, ‘pe’)	2D	moran coefficient of lag 1 weighted by pauling EN
515		MATS2pe	MATS (2, ‘pe’)	2D	moran coefficient of lag 2 weighted by pauling EN

#	module	name	constructor	dim	description
516		MATS3pe	MATS (3, ‘pe’)	2D	moran coefficient of lag 3 weighted by pauling EN
517		MATS4pe	MATS (4, ‘pe’)	2D	moran coefficient of lag 4 weighted by pauling EN
518		MATS5pe	MATS (5, ‘pe’)	2D	moran coefficient of lag 5 weighted by pauling EN
519		MATS6pe	MATS (6, ‘pe’)	2D	moran coefficient of lag 6 weighted by pauling EN
520		MATS7pe	MATS (7, ‘pe’)	2D	moran coefficient of lag 7 weighted by pauling EN
521		MATS8pe	MATS (8, ‘pe’)	2D	moran coefficient of lag 8 weighted by pauling EN
522		MATS1are	MATS (1, ‘are’)	2D	moran coefficient of lag 1 weighted by allred-rocow EN
523		MATS2are	MATS (2, ‘are’)	2D	moran coefficient of lag 2 weighted by allred-rocow EN
524		MATS3are	MATS (3, ‘are’)	2D	moran coefficient of lag 3 weighted by allred-rocow EN
525		MATS4are	MATS (4, ‘are’)	2D	moran coefficient of lag 4 weighted by allred-rocow EN
526		MATS5are	MATS (5, ‘are’)	2D	moran coefficient of lag 5 weighted by allred-rocow EN

#	module	name	constructor	dim	description
527		MATS6are	MATS (6, ‘are’)	2D	moran coefficient of lag 6 weighted by allred-rocow EN
528		MATS7are	MATS (7, ‘are’)	2D	moran coefficient of lag 7 weighted by allred-rocow EN
529		MATS8are	MATS (8, ‘are’)	2D	moran coefficient of lag 8 weighted by allred-rocow EN
530		MATS1p	MATS (1, ‘p’)	2D	moran coefficient of lag 1 weighted by polarizability
531		MATS2p	MATS (2, ‘p’)	2D	moran coefficient of lag 2 weighted by polarizability
532		MATS3p	MATS (3, ‘p’)	2D	moran coefficient of lag 3 weighted by polarizability
533		MATS4p	MATS (4, ‘p’)	2D	moran coefficient of lag 4 weighted by polarizability
534		MATS5p	MATS (5, ‘p’)	2D	moran coefficient of lag 5 weighted by polarizability
535		MATS6p	MATS (6, ‘p’)	2D	moran coefficient of lag 6 weighted by polarizability
536		MATS7p	MATS (7, ‘p’)	2D	moran coefficient of lag 7 weighted by polarizability

#	module	name	constructor	dim	description
537		MATS8p	MATS (8, ‘p’)	2D	moran coefficient of lag 8 weighted by polarizability
538		MATS1i	MATS (1, ‘i’)	2D	moran coefficient of lag 1 weighted by ionization potential
539		MATS2i	MATS (2, ‘i’)	2D	moran coefficient of lag 2 weighted by ionization potential
540		MATS3i	MATS (3, ‘i’)	2D	moran coefficient of lag 3 weighted by ionization potential
541		MATS4i	MATS (4, ‘i’)	2D	moran coefficient of lag 4 weighted by ionization potential
542		MATS5i	MATS (5, ‘i’)	2D	moran coefficient of lag 5 weighted by ionization potential
543		MATS6i	MATS (6, ‘i’)	2D	moran coefficient of lag 6 weighted by ionization potential
544		MATS7i	MATS (7, ‘i’)	2D	moran coefficient of lag 7 weighted by ionization potential
545		MATS8i	MATS (8, ‘i’)	2D	moran coefficient of lag 8 weighted by ionization potential
546		GATS1c	GATS (1, ‘c’)	2D	geary coefficient of lag 1 weighted by gasteiger charge

#	module	name	constructor	dim	description
547		GATS2c	GATS (2, ‘c’)	2D	geary coefficient of lag 2 weighted by gasteiger charge
548		GATS3c	GATS (3, ‘c’)	2D	geary coefficient of lag 3 weighted by gasteiger charge
549		GATS4c	GATS (4, ‘c’)	2D	geary coefficient of lag 4 weighted by gasteiger charge
550		GATS5c	GATS (5, ‘c’)	2D	geary coefficient of lag 5 weighted by gasteiger charge
551		GATS6c	GATS (6, ‘c’)	2D	geary coefficient of lag 6 weighted by gasteiger charge
552		GATS7c	GATS (7, ‘c’)	2D	geary coefficient of lag 7 weighted by gasteiger charge
553		GATS8c	GATS (8, ‘c’)	2D	geary coefficient of lag 8 weighted by gasteiger charge
554		GATS1dv	GATS (1, ‘dv’)	2D	geary coefficient of lag 1 weighted by valence electrons
555		GATS2dv	GATS (2, ‘dv’)	2D	geary coefficient of lag 2 weighted by valence electrons
556		GATS3dv	GATS (3, ‘dv’)	2D	geary coefficient of lag 3 weighted by valence electrons

#	module	name	constructor	dim	description
557		GATS4dv	GATS (4, ‘dv’)	2D	geary coefficient of lag 4 weighted by valence electrons
558		GATS5dv	GATS (5, ‘dv’)	2D	geary coefficient of lag 5 weighted by valence electrons
559		GATS6dv	GATS (6, ‘dv’)	2D	geary coefficient of lag 6 weighted by valence electrons
560		GATS7dv	GATS (7, ‘dv’)	2D	geary coefficient of lag 7 weighted by valence electrons
561		GATS8dv	GATS (8, ‘dv’)	2D	geary coefficient of lag 8 weighted by valence electrons
562		GATS1d	GATS (1, ‘d’)	2D	geary coefficient of lag 1 weighted by sigma electrons
563		GATS2d	GATS (2, ‘d’)	2D	geary coefficient of lag 2 weighted by sigma electrons
564		GATS3d	GATS (3, ‘d’)	2D	geary coefficient of lag 3 weighted by sigma electrons
565		GATS4d	GATS (4, ‘d’)	2D	geary coefficient of lag 4 weighted by sigma electrons
566		GATS5d	GATS (5, ‘d’)	2D	geary coefficient of lag 5 weighted by sigma electrons

#	module	name	constructor	dim	description
567		GATS6d	GATS (6, ‘d’)	2D	geary coefficient of lag 6 weighted by sigma electrons
568		GATS7d	GATS (7, ‘d’)	2D	geary coefficient of lag 7 weighted by sigma electrons
569		GATS8d	GATS (8, ‘d’)	2D	geary coefficient of lag 8 weighted by sigma electrons
570		GATS1s	GATS (1, ‘s’)	2D	geary coefficient of lag 1 weighted by intrinsic state
571		GATS2s	GATS (2, ‘s’)	2D	geary coefficient of lag 2 weighted by intrinsic state
572		GATS3s	GATS (3, ‘s’)	2D	geary coefficient of lag 3 weighted by intrinsic state
573		GATS4s	GATS (4, ‘s’)	2D	geary coefficient of lag 4 weighted by intrinsic state
574		GATS5s	GATS (5, ‘s’)	2D	geary coefficient of lag 5 weighted by intrinsic state
575		GATS6s	GATS (6, ‘s’)	2D	geary coefficient of lag 6 weighted by intrinsic state
576		GATS7s	GATS (7, ‘s’)	2D	geary coefficient of lag 7 weighted by intrinsic state

#	module	name	constructor	dim	description
577		GATS8s	GATS (8, ‘s’)	2D	geary coefficient of lag 8 weighted by intrinsic state
578		GATS1Z	GATS (1, ‘Z’)	2D	geary coefficient of lag 1 weighted by atomic number
579		GATS2Z	GATS (2, ‘Z’)	2D	geary coefficient of lag 2 weighted by atomic number
580		GATS3Z	GATS (3, ‘Z’)	2D	geary coefficient of lag 3 weighted by atomic number
581		GATS4Z	GATS (4, ‘Z’)	2D	geary coefficient of lag 4 weighted by atomic number
582		GATS5Z	GATS (5, ‘Z’)	2D	geary coefficient of lag 5 weighted by atomic number
583		GATS6Z	GATS (6, ‘Z’)	2D	geary coefficient of lag 6 weighted by atomic number
584		GATS7Z	GATS (7, ‘Z’)	2D	geary coefficient of lag 7 weighted by atomic number
585		GATS8Z	GATS (8, ‘Z’)	2D	geary coefficient of lag 8 weighted by atomic number
586		GATS1m	GATS (1, ‘m’)	2D	geary coefficient of lag 1 weighted by mass
587		GATS2m	GATS (2, ‘m’)	2D	geary coefficient of lag 2 weighted by mass

#	module	name	constructor	dim	description
588		GATS3m	GATS (3, ‘m’)	2D	geary coefficient of lag 3 weighted by mass
589		GATS4m	GATS (4, ‘m’)	2D	geary coefficient of lag 4 weighted by mass
590		GATS5m	GATS (5, ‘m’)	2D	geary coefficient of lag 5 weighted by mass
591		GATS6m	GATS (6, ‘m’)	2D	geary coefficient of lag 6 weighted by mass
592		GATS7m	GATS (7, ‘m’)	2D	geary coefficient of lag 7 weighted by mass
593		GATS8m	GATS (8, ‘m’)	2D	geary coefficient of lag 8 weighted by mass
594		GATS1v	GATS (1, ‘v’)	2D	geary coefficient of lag 1 weighted by vdw volume
595		GATS2v	GATS (2, ‘v’)	2D	geary coefficient of lag 2 weighted by vdw volume
596		GATS3v	GATS (3, ‘v’)	2D	geary coefficient of lag 3 weighted by vdw volume
597		GATS4v	GATS (4, ‘v’)	2D	geary coefficient of lag 4 weighted by vdw volume
598		GATS5v	GATS (5, ‘v’)	2D	geary coefficient of lag 5 weighted by vdw volume
599		GATS6v	GATS (6, ‘v’)	2D	geary coefficient of lag 6 weighted by vdw volume
600		GATS7v	GATS (7, ‘v’)	2D	geary coefficient of lag 7 weighted by vdw volume

#	module	name	constructor	dim	description
601		GATS8v	GATS (8, ‘v’)	2D	geary coefficient of lag 8 weighted by vdw volume
602		GATS1se	GATS (1, ‘se’)	2D	geary coefficient of lag 1 weighted by sanderson EN
603		GATS2se	GATS (2, ‘se’)	2D	geary coefficient of lag 2 weighted by sanderson EN
604		GATS3se	GATS (3, ‘se’)	2D	geary coefficient of lag 3 weighted by sanderson EN
605		GATS4se	GATS (4, ‘se’)	2D	geary coefficient of lag 4 weighted by sanderson EN
606		GATS5se	GATS (5, ‘se’)	2D	geary coefficient of lag 5 weighted by sanderson EN
607		GATS6se	GATS (6, ‘se’)	2D	geary coefficient of lag 6 weighted by sanderson EN
608		GATS7se	GATS (7, ‘se’)	2D	geary coefficient of lag 7 weighted by sanderson EN
609		GATS8se	GATS (8, ‘se’)	2D	geary coefficient of lag 8 weighted by sanderson EN
610		GATS1pe	GATS (1, ‘pe’)	2D	geary coefficient of lag 1 weighted by pauling EN
611		GATS2pe	GATS (2, ‘pe’)	2D	geary coefficient of lag 2 weighted by pauling EN

#	module	name	constructor	dim	description
612		GATS3pe	GATS (3, ‘pe’)	2D	geary coefficient of lag 3 weighted by pauling EN
613		GATS4pe	GATS (4, ‘pe’)	2D	geary coefficient of lag 4 weighted by pauling EN
614		GATS5pe	GATS (5, ‘pe’)	2D	geary coefficient of lag 5 weighted by pauling EN
615		GATS6pe	GATS (6, ‘pe’)	2D	geary coefficient of lag 6 weighted by pauling EN
616		GATS7pe	GATS (7, ‘pe’)	2D	geary coefficient of lag 7 weighted by pauling EN
617		GATS8pe	GATS (8, ‘pe’)	2D	geary coefficient of lag 8 weighted by pauling EN
618		GATS1are	GATS (1, ‘are’)	2D	geary coefficient of lag 1 weighted by allred-rocow EN
619		GATS2are	GATS (2, ‘are’)	2D	geary coefficient of lag 2 weighted by allred-rocow EN
620		GATS3are	GATS (3, ‘are’)	2D	geary coefficient of lag 3 weighted by allred-rocow EN
621		GATS4are	GATS (4, ‘are’)	2D	geary coefficient of lag 4 weighted by allred-rocow EN
622		GATS5are	GATS (5, ‘are’)	2D	geary coefficient of lag 5 weighted by allred-rocow EN

#	module	name	constructor	dim	description
623		GATS6are	GATS (6, ‘are’)	2D	geary coefficient of lag 6 weighted by allred-rocow EN
624		GATS7are	GATS (7, ‘are’)	2D	geary coefficient of lag 7 weighted by allred-rocow EN
625		GATS8are	GATS (8, ‘are’)	2D	geary coefficient of lag 8 weighted by allred-rocow EN
626		GATS1p	GATS (1, ‘p’)	2D	geary coefficient of lag 1 weighted by polarizability
627		GATS2p	GATS (2, ‘p’)	2D	geary coefficient of lag 2 weighted by polarizability
628		GATS3p	GATS (3, ‘p’)	2D	geary coefficient of lag 3 weighted by polarizability
629		GATS4p	GATS (4, ‘p’)	2D	geary coefficient of lag 4 weighted by polarizability
630		GATS5p	GATS (5, ‘p’)	2D	geary coefficient of lag 5 weighted by polarizability
631		GATS6p	GATS (6, ‘p’)	2D	geary coefficient of lag 6 weighted by polarizability
632		GATS7p	GATS (7, ‘p’)	2D	geary coefficient of lag 7 weighted by polarizability

#	module	name	constructor	dim	description
633		GATS8p	GATS (8, ‘p’)	2D	geary coefficient of lag 8 weighted by polarizability
634		GATS1i	GATS (1, ‘i’)	2D	geary coefficient of lag 1 weighted by ionization potential
635		GATS2i	GATS (2, ‘i’)	2D	geary coefficient of lag 2 weighted by ionization potential
636		GATS3i	GATS (3, ‘i’)	2D	geary coefficient of lag 3 weighted by ionization potential
637		GATS4i	GATS (4, ‘i’)	2D	geary coefficient of lag 4 weighted by ionization potential
638		GATS5i	GATS (5, ‘i’)	2D	geary coefficient of lag 5 weighted by ionization potential
639		GATS6i	GATS (6, ‘i’)	2D	geary coefficient of lag 6 weighted by ionization potential
640		GATS7i	GATS (7, ‘i’)	2D	geary coefficient of lag 7 weighted by ionization potential
641		GATS8i	GATS (8, ‘i’)	2D	geary coefficient of lag 8 weighted by ionization potential
642	BCUT	BCUTc-1h	BCUT (‘c’, 0)	2D	first heighest eigenvalue of Burden matrix weighted by gasteiger charge

#	module	name	constructor	dim	description
643		BCUTc-1l	BCUT ('c', -1)	2D	first lowest eigenvalue of Burden matrix weighted by gasteiger charge
644		BCUTdv-1h	BCUT ('dv', 0)	2D	first heighest eigenvalue of Burden matrix weighted by valence electrons
645		BCUTdv-1l	BCUT ('dv', -1)	2D	first lowest eigenvalue of Burden matrix weighted by valence electrons
646		BCUTd-1h	BCUT ('d', 0)	2D	first heighest eigenvalue of Burden matrix weighted by sigma electrons
647		BCUTd-1l	BCUT ('d', -1)	2D	first lowest eigenvalue of Burden matrix weighted by sigma electrons
648		BCUTs-1h	BCUT ('s', 0)	2D	first heighest eigenvalue of Burden matrix weighted by intrinsic state
649		BCUTs-1l	BCUT ('s', -1)	2D	first lowest eigenvalue of Burden matrix weighted by intrinsic state
650		BCUTZ-1h	BCUT ('Z', 0)	2D	first heighest eigenvalue of Burden matrix weighted by atomic number
651		BCUTZ-1l	BCUT ('Z', -1)	2D	first lowest eigenvalue of Burden matrix weighted by atomic number

#	module	name	constructor	dim	description
652		BCUTm-1h	BCUT ('m', 0)	2D	first heighest eigenvalue of Burden matrix weighted by mass
653		BCUTm-1l	BCUT ('m', -1)	2D	first lowest eigenvalue of Burden matrix weighted by mass
654		BCUTv-1h	BCUT ('v', 0)	2D	first heighest eigenvalue of Burden matrix weighted by vdw volume
655		BCUTv-1l	BCUT ('v', -1)	2D	first lowest eigenvalue of Burden matrix weighted by vdw volume
656		BCUTse-1h	BCUT ('se', 0)	2D	first heighest eigenvalue of Burden matrix weighted by sanderson EN
657		BCUTse-1l	BCUT ('se', -1)	2D	first lowest eigenvalue of Burden matrix weighted by sanderson EN
658		BCUTpe-1h	BCUT ('pe', 0)	2D	first heighest eigenvalue of Burden matrix weighted by pauling EN
659		BCUTpe-1l	BCUT ('pe', -1)	2D	first lowest eigenvalue of Burden matrix weighted by pauling EN
660		BCUTare-1h	BCUT ('are', 0)	2D	first heighest eigenvalue of Burden matrix weighted by allred-rocow EN
661		BCUTare-1l	BCUT ('are', -1)	2D	first lowest eigenvalue of Burden matrix weighted by allred-rocow EN

#	module	name	constructor	dim	description
662		BCUTp-1h	BCUT ('p', 0)	2D	first heighest eigenvalue of Burden matrix weighted by polarizability
663		BCUTp-1l	BCUT ('p', -1)	2D	first lowest eigenvalue of Burden matrix weighted by polarizability
664		BCUTi-1h	BCUT ('i', 0)	2D	first heighest eigenvalue of Burden matrix weighted by ionization potential
665		BCUTi-1l	BCUT ('i', -1)	2D	first lowest eigenvalue of Burden matrix weighted by ionization potential
666	BalabanJ	BalabanJ	BalabanJ ()	2D	Balaban's J index
667	BaryszMatrix	SpAbs_DzZ	BaryszMatrix ('Z', 'SpAbs')	2D	graph energy from Barysz matrix weighted by atomic number
668		SpMax_DzZ	BaryszMatrix ('Z', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by atomic number
669		SpDiam_DzZ	BaryszMatrix ('Z', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by atomic number
670		SpAD_DzZ	BaryszMatrix ('Z', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by atomic number
671		SpMAD_DzZ	BaryszMatrix ('Z', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by atomic number

#	module	name	constructor	dim	description
672		LogEE_DzZ	BaryszMatrix (‘Z’, ‘LogEE’)	2D	Estrada-like index from Barysz matrix weighted by atomic number
673		SM1_DzZ	BaryszMatrix (‘Z’, ‘SM1’)	2D	spectral moment from Barysz matrix weighted by atomic number
674		VE1_DzZ	BaryszMatrix (‘Z’, ‘VE1’)	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number
675		VE2_DzZ	BaryszMatrix (‘Z’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by atomic number
676		VE3_DzZ	BaryszMatrix (‘Z’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number
677		VR1_DzZ	BaryszMatrix (‘Z’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by atomic number
678		VR2_DzZ	BaryszMatrix (‘Z’, ‘VR2’)	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by atomic number

#	module	name	constructor	dim	description
679		VR3_DzZ	BaryszMatrix ('Z', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by atomic number
680		SpAbs_Dzm	BaryszMatrix ('m', 'SpAbs')	2D	graph energy from Barysz matrix weighted by mass
681		SpMax_Dzm	BaryszMatrix ('m', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by mass
682		SpDiam_Dzm	BaryszMatrix ('m', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by mass
683		SpAD_Dzm	BaryszMatrix ('m', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by mass
684		SpMAD_Dzm	BaryszMatrix ('m', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by mass
685		LogEE_Dzm	BaryszMatrix ('m', 'LogEE')	2D	Estrada-like index from Barysz matrix weighted by mass
686		SM1_Dzm	BaryszMatrix ('m', 'SM1')	2D	spectral moment from Barysz matrix weighted by mass
687		VE1_Dzm	BaryszMatrix ('m', 'VE1')	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by mass

#	module	name	constructor	dim	description
688		VE2_Dzm	BaryszMatrix ('m', 'VE2')	2D	average coefficient of the last eigenvector from Barysz matrix weighted by mass
689		VE3_Dzm	BaryszMatrix ('m', 'VE3')	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by mass
690		VR1_Dzm	BaryszMatrix ('m', 'VR1')	2D	Randic-like eigenvector-based index from Barysz matrix weighted by mass
691		VR2_Dzm	BaryszMatrix ('m', 'VR2')	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by mass
692		VR3_Dzm	BaryszMatrix ('m', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by mass
693		SpAbs_Dzv	BaryszMatrix ('v', 'SpAbs')	2D	graph energy from Barysz matrix weighted by vdw volume
694		SpMax_Dzv	BaryszMatrix ('v', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by vdw volume

#	module	name	constructor	dim	description
695		SpDiam_Dzv	BaryszMatrix ('v', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by vdw volume
696		SpAD_Dzv	BaryszMatrix ('v', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by vdw volume
697		SpMAD_Dzv	BaryszMatrix ('v', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by vdw volume
698		LogEE_Dzv	BaryszMatrix ('v', 'LogEE')	2D	Estrada-like index from Barysz matrix weighted by vdw volume
699		SM1_Dzv	BaryszMatrix ('v', 'SM1')	2D	spectral moment from Barysz matrix weighted by vdw volume
700		VE1_Dzv	BaryszMatrix ('v', 'VE1')	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by vdw volume
701		VE2_Dzv	BaryszMatrix ('v', 'VE2')	2D	average coefficient of the last eigenvector from Barysz matrix weighted by vdw volume
702		VE3_Dzv	BaryszMatrix ('v', 'VE3')	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by vdw volume

#	module	name	constructor	dim	description
703		VR1_Dzv	BaryszMatrix ('v', 'VR1')	2D	Randic-like eigenvector-based index from Barysz matrix weighted by vdw volume
704		VR2_Dzv	BaryszMatrix ('v', 'VR2')	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by vdw volume
705		VR3_Dzv	BaryszMatrix ('v', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by vdw volume
706		SpAbs_Dzse	BaryszMatrix ('se', 'SpAbs')	2D	graph energy from Barysz matrix weighted by sanderson EN
707		SpMax_Dzse	BaryszMatrix ('se', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by sanderson EN
708		SpDiam_Dzse	BaryszMatrix ('se', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by sanderson EN
709		SpAD_Dzse	BaryszMatrix ('se', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by sanderson EN
710		SpMAD_Dzse	BaryszMatrix ('se', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by sanderson EN

#	module	name	constructor	dim	description
711		LogEE_Dzse	BaryszMatrix (‘se’, ‘LogEE’)	2D	Estrada-like index from Barysz matrix weighted by sanderson EN
712		SM1_Dzse	BaryszMatrix (‘se’, ‘SM1’)	2D	spectral moment from Barysz matrix weighted by sanderson EN
713		VE1_Dzse	BaryszMatrix (‘se’, ‘VE1’)	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by sanderson EN
714		VE2_Dzse	BaryszMatrix (‘se’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by sanderson EN
715		VE3_Dzse	BaryszMatrix (‘se’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by sanderson EN
716		VR1_Dzse	BaryszMatrix (‘se’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by sanderson EN
717		VR2_Dzse	BaryszMatrix (‘se’, ‘VR2’)	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by sanderson EN

#	module	name	constructor	dim	description
718		VR3_Dzse	BaryszMatrix ('se', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by sanderson EN
719		SpAbs_Dzpe	BaryszMatrix ('pe', 'SpAbs')	2D	graph energy from Barysz matrix weighted by pauling EN
720		SpMax_Dzpe	BaryszMatrix ('pe', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by pauling EN
721		SpDiam_Dzpe	BaryszMatrix ('pe', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by pauling EN
722		SpAD_Dzpe	BaryszMatrix ('pe', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by pauling EN
723		SpMAD_Dzpe	BaryszMatrix ('pe', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by pauling EN
724		LogEE_Dzpe	BaryszMatrix ('pe', 'LogEE')	2D	Estrada-like index from Barysz matrix weighted by pauling EN
725		SM1_Dzpe	BaryszMatrix ('pe', 'SM1')	2D	spectral moment from Barysz matrix weighted by pauling EN
726		VE1_Dzpe	BaryszMatrix ('pe', 'VE1')	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by pauling EN

#	module	name	constructor	dim	description
727		VE2_Dzpe	BaryszMatrix (‘pe’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by pauling EN
728		VE3_Dzpe	BaryszMatrix (‘pe’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by pauling EN
729		VR1_Dzpe	BaryszMatrix (‘pe’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by pauling EN
730		VR2_Dzpe	BaryszMatrix (‘pe’, ‘VR2’)	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by pauling EN
731		VR3_Dzpe	BaryszMatrix (‘pe’, ‘VR3’)	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by pauling EN
732		SpAbs_Dzare	BaryszMatrix (‘are’, ‘SpAbs’)	2D	graph energy from Barysz matrix weighted by allred-rocow EN
733		SpMax_Dzare	BaryszMatrix (‘are’, ‘SpMax’)	2D	leading eigenvalue from Barysz matrix weighted by allred-rocow EN

#	module	name	constructor	dim	description
734		SpDiam_Dzare	BaryszMatrix (‘are’, ‘SpDiam’)	2D	spectral diamiter from Barysz matrix weighted by allred-rocow EN
735		SpAD_Dzare	BaryszMatrix (‘are’, ‘SpAD’)	2D	spectral absolute diviation from Barysz matrix weighted by allred-rocow EN
736		SpMAD_Dzare	BaryszMatrix (‘are’, ‘SpMAD’)	2D	spectral mean absolute diviation from Barysz matrix weighted by allred-rocow EN
737		LogEE_Dzare	BaryszMatrix (‘are’, ‘LogEE’)	2D	Estrada-like index from Barysz matrix weighted by allred-rocow EN
738		SM1_Dzare	BaryszMatrix (‘are’, ‘SM1’)	2D	spectral moment from Barysz matrix weighted by allred-rocow EN
739		VE1_Dzare	BaryszMatrix (‘are’, ‘VE1’)	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by allred-rocow EN
740		VE2_Dzare	BaryszMatrix (‘are’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by allred-rocow EN

#	module	name	constructor	dim	description
741		VE3_Dzare	BaryszMatrix (‘are’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by allred-rocow EN
742		VR1_Dzare	BaryszMatrix (‘are’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by allred-rocow EN
743		VR2_Dzare	BaryszMatrix (‘are’, ‘VR2’)	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by allred-rocow EN
744		VR3_Dzare	BaryszMatrix (‘are’, ‘VR3’)	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by allred-rocow EN
745		SpAbs_Dzp	BaryszMatrix (‘p’, ‘SpAbs’)	2D	graph energy from Barysz matrix weighted by polarizability
746		SpMax_Dzp	BaryszMatrix (‘p’, ‘SpMax’)	2D	leading eigenvalue from Barysz matrix weighted by polarizability
747		SpDiam_Dzp	BaryszMatrix (‘p’, ‘SpDiam’)	2D	spectral diamiter from Barysz matrix weighted by polarizability

#	module	name	constructor	dim	description
748		SpAD_Dzp	BaryszMatrix (‘p’, ‘SpAD’)	2D	spectral absolute diviation from Barysz matrix weighted by polarizability
749		SpMAD_Dzp	BaryszMatrix (‘p’, ‘SpMAD’)	2D	spectral mean absolute diviation from Barysz matrix weighted by polarizability
750		LogEE_Dzp	BaryszMatrix (‘p’, ‘LogEE’)	2D	Estrada-like index from Barysz matrix weighted by polarizability
751		SM1_Dzp	BaryszMatrix (‘p’, ‘SM1’)	2D	spectral moment from Barysz matrix weighted by polarizability
752		VE1_Dzp	BaryszMatrix (‘p’, ‘VE1’)	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability
753		VE2_Dzp	BaryszMatrix (‘p’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by polarizability
754		VE3_Dzp	BaryszMatrix (‘p’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability
755		VR1_Dzp	BaryszMatrix (‘p’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by polarizability

#	module	name	constructor	dim	description
756		VR2_Dzp	BaryszMatrix ('p', 'VR2')	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by polarizability
757		VR3_Dzp	BaryszMatrix ('p', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by polarizability
758		SpAbs_Dzi	BaryszMatrix ('i', 'SpAbs')	2D	graph energy from Barysz matrix weighted by ionization potential
759		SpMax_Dzi	BaryszMatrix ('i', 'SpMax')	2D	leading eigenvalue from Barysz matrix weighted by ionization potential
760		SpDiam_Dzi	BaryszMatrix ('i', 'SpDiam')	2D	spectral diamiter from Barysz matrix weighted by ionization potential
761		SpAD_Dzi	BaryszMatrix ('i', 'SpAD')	2D	spectral absolute diviation from Barysz matrix weighted by ionization potential
762		SpMAD_Dzi	BaryszMatrix ('i', 'SpMAD')	2D	spectral mean absolute diviation from Barysz matrix weighted by ionization potential

#	module	name	constructor	dim	description
763		LogEE_Dzi	BaryszMatrix (‘i’, ‘LogEE’)	2D	Estrada-like index from Barysz matrix weighted by ionization potential
764		SM1_Dzi	BaryszMatrix (‘i’, ‘SM1’)	2D	spectral moment from Barysz matrix weighted by ionization potential
765		VE1_Dzi	BaryszMatrix (‘i’, ‘VE1’)	2D	coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential
766		VE2_Dzi	BaryszMatrix (‘i’, ‘VE2’)	2D	average coefficient of the last eigenvector from Barysz matrix weighted by ionization potential
767		VE3_Dzi	BaryszMatrix (‘i’, ‘VE3’)	2D	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential
768		VR1_Dzi	BaryszMatrix (‘i’, ‘VR1’)	2D	Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential

#	module	name	constructor	dim	description
769		VR2_Dzi	BaryszMatrix ('i', 'VR2')	2D	normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
770		VR3_Dzi	BaryszMatrix ('i', 'VR3')	2D	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
771	BertzCT	BertzCT	BertzCT ()	2D	Bertz CT
772	BondCount	nBonds	BondCount ('any', False)	2D	number of all bonds in non-kekulized structure
773		nBondsO	BondCount ('heavy', False)	2D	number of bonds connecting to heavy atom in non-kekulized structure
774		nBondsS	BondCount ('single', False)	2D	number of single bonds in non-kekulized structure
775		nBondsD	BondCount ('double', False)	2D	number of double bonds in non-kekulized structure
776		nBondsT	BondCount ('triple', False)	2D	number of triple bonds in non-kekulized structure
777		nBondsA	BondCount ('aromatic', False)	2D	number of aromatic bonds in non-kekulized structure
778		nBondsM	BondCount ('multiple', False)	2D	number of multiple bonds in non-kekulized structure

#	module	name	constructor	dim	description
779		nBondsKS	BondCount ('single', True)	2D	number of single bonds in kekulized structure
780		nBondsKD	BondCount ('double', True)	2D	number of double bonds in kekulized structure
781	CPSA	PNSA1	PNSA (1)	3D	partial negative surface area (version 1)
782		PNSA2	PNSA (2)	3D	partial negative surface area (version 2)
783		PNSA3	PNSA (3)	3D	partial negative surface area (version 3)
784		PNSA4	PNSA (4)	3D	partial negative surface area (version 4)
785		PNSA5	PNSA (5)	3D	partial negative surface area (version 5)
786		PPSA1	PPSA (1)	3D	partial positive surface area (version 1)
787		PPSA2	PPSA (2)	3D	partial positive surface area (version 2)
788		PPSA3	PPSA (3)	3D	partial positive surface area (version 3)
789		PPSA4	PPSA (4)	3D	partial positive surface area (version 4)
790		PPSA5	PPSA (5)	3D	partial positive surface area (version 5)
791		DPSA1	DPSA (1)	3D	difference in charged partial surface area (version 1)
792		DPSA2	DPSA (2)	3D	difference in charged partial surface area (version 2)
793		DPSA3	DPSA (3)	3D	difference in charged partial surface area (version 3)

#	module	name	constructor	dim	description
794		DPSA4	DPSA (4)	3D	difference in charged partial surface area (version 4)
795		DPSA5	DPSA (5)	3D	difference in charged partial surface area (version 5)
796		FNSA1	FNSA (1)	3D	fractional charged partial negative surface area (version 1)
797		FNSA2	FNSA (2)	3D	fractional charged partial negative surface area (version 2)
798		FNSA3	FNSA (3)	3D	fractional charged partial negative surface area (version 3)
799		FNSA4	FNSA (4)	3D	fractional charged partial negative surface area (version 4)
800		FNSA5	FNSA (5)	3D	fractional charged partial negative surface area (version 5)
801		FPSA1	FPSA (1)	3D	fractional charged partial positive surface area (version 1)
802		FPSA2	FPSA (2)	3D	fractional charged partial positive surface area (version 2)
803		FPSA3	FPSA (3)	3D	fractional charged partial positive surface area (version 3)
804		FPSA4	FPSA (4)	3D	fractional charged partial positive surface area (version 4)

#	module	name	constructor	dim	description
805		FPSA5	FPSA (5)	3D	fractional charged partial positive surface area (version 5)
806		WNSA1	WNSA (1)	3D	surface weighted charged partial negative surface area (version 1)
807		WNSA2	WNSA (2)	3D	surface weighted charged partial negative surface area (version 2)
808		WNSA3	WNSA (3)	3D	surface weighted charged partial negative surface area (version 3)
809		WNSA4	WNSA (4)	3D	surface weighted charged partial negative surface area (version 4)
810		WNSA5	WNSA (5)	3D	surface weighted charged partial negative surface area (version 5)
811		WPSA1	WPSA (1)	3D	surface weighted charged partial positive surface area (version 1)
812		WPSA2	WPSA (2)	3D	surface weighted charged partial positive surface area (version 2)
813		WPSA3	WPSA (3)	3D	surface weighted charged partial positive surface area (version 3)

#	module	name	constructor	dim	description
814		WPSA4	WPSA (4)	3D	surface weighted charged partial positive surface area (version 4)
815		WPSA5	WPSA (5)	3D	surface weighted charged partial positive surface area (version 5)
816		RNCG	RNCG ()	2D	relative negative charge
817		RPCG	RPCG ()	2D	relative positive charge
818		RNCS	RNCS ()	3D	relative negative charge surface area
819		RPCS	RPCS ()	3D	relative positive charge surface area
820		TASA	TASA ()	3D	total hydrophobic surface area
821		TPSA	TPSA ()	3D	total polar surface area
822		RASA	RASA ()	3D	relative hydrophobic surface area
823		RPSA	RPSA ()	3D	relative polar surface area
824	CarbonTypes	C1SP1	CarbonTypes (1, 1)	2D	SP carbon bound to 1 other carbon
825		C2SP1	CarbonTypes (2, 1)	2D	SP carbon bound to 2 other carbons
826		C1SP2	CarbonTypes (1, 2)	2D	SP2 carbon bound to 1 other carbon
827		C2SP2	CarbonTypes (2, 2)	2D	SP2 carbon bound to 2 other carbons
828		C3SP2	CarbonTypes (3, 2)	2D	SP2 carbon bound to 3 other carbons

#	module	name	constructor	dim	description
829		C1SP3	CarbonTypes (1, 3)	2D	SP3 carbon bound to 1 other carbon
830		C2SP3	CarbonTypes (2, 3)	2D	SP3 carbon bound to 2 other carbons
831		C3SP3	CarbonTypes (3, 3)	2D	SP3 carbon bound to 3 other carbons
832		C4SP3	CarbonTypes (4, 3)	2D	SP3 carbon bound to 4 other carbons
833		HybRatio	HybridizationRatio ()	2D	hybridization ratio
834		FCSP3	FractionCSP3 ()	2D	the fraction of C atoms that are SP3 hybridized
835	Chi	Xch-3d	Chi ('chain', 3, 'd', False)	2D	3-ordered Chi chain weighted by sigma electrons
836		Xch-4d	Chi ('chain', 4, 'd', False)	2D	4-ordered Chi chain weighted by sigma electrons
837		Xch-5d	Chi ('chain', 5, 'd', False)	2D	5-ordered Chi chain weighted by sigma electrons
838		Xch-6d	Chi ('chain', 6, 'd', False)	2D	6-ordered Chi chain weighted by sigma electrons
839		Xch-7d	Chi ('chain', 7, 'd', False)	2D	7-ordered Chi chain weighted by sigma electrons
840		Xch-3dv	Chi ('chain', 3, 'dv', False)	2D	3-ordered Chi chain weighted by valence electrons
841		Xch-4dv	Chi ('chain', 4, 'dv', False)	2D	4-ordered Chi chain weighted by valence electrons
842		Xch-5dv	Chi ('chain', 5, 'dv', False)	2D	5-ordered Chi chain weighted by valence electrons

#	module	name	constructor	dim	description
843		Xch-6dv	Chi ('chain', 6, 'dv', False)	2D	6-ordered Chi chain weighted by valence electrons
844		Xch-7dv	Chi ('chain', 7, 'dv', False)	2D	7-ordered Chi chain weighted by valence electrons
845		Xc-3d	Chi ('cluster', 3, 'd', False)	2D	3-ordered Chi cluster weighted by sigma electrons
846		Xc-4d	Chi ('cluster', 4, 'd', False)	2D	4-ordered Chi cluster weighted by sigma electrons
847		Xc-5d	Chi ('cluster', 5, 'd', False)	2D	5-ordered Chi cluster weighted by sigma electrons
848		Xc-6d	Chi ('cluster', 6, 'd', False)	2D	6-ordered Chi cluster weighted by sigma electrons
849		Xc-3dv	Chi ('cluster', 3, 'dv', False)	2D	3-ordered Chi cluster weighted by valence electrons
850		Xc-4dv	Chi ('cluster', 4, 'dv', False)	2D	4-ordered Chi cluster weighted by valence electrons
851		Xc-5dv	Chi ('cluster', 5, 'dv', False)	2D	5-ordered Chi cluster weighted by valence electrons
852		Xc-6dv	Chi ('cluster', 6, 'dv', False)	2D	6-ordered Chi cluster weighted by valence electrons
853		Xpc-4d	Chi ('path_cluster', 4, 'd', False)	2D	4-ordered Chi path-cluster weighted by sigma electrons

#	module	name	constructor	dim	description
854		Xpc-5d	Chi ('path_cluster', 5, 'd', False)	2D	5-ordered Chi path-cluster weighted by sigma electrons
855		Xpc-6d	Chi ('path_cluster', 6, 'd', False)	2D	6-ordered Chi path-cluster weighted by sigma electrons
856		Xpc-4dv	Chi ('path_cluster', 4, 'dv', False)	2D	4-ordered Chi path-cluster weighted by valence electrons
857		Xpc-5dv	Chi ('path_cluster', 5, 'dv', False)	2D	5-ordered Chi path-cluster weighted by valence electrons
858		Xpc-6dv	Chi ('path_cluster', 6, 'dv', False)	2D	6-ordered Chi path-cluster weighted by valence electrons
859		Xp-0d	Chi ('path', 0, 'd', False)	2D	0-ordered Chi path weighted by sigma electrons
860		Xp-1d	Chi ('path', 1, 'd', False)	2D	1-ordered Chi path weighted by sigma electrons
861		Xp-2d	Chi ('path', 2, 'd', False)	2D	2-ordered Chi path weighted by sigma electrons
862		Xp-3d	Chi ('path', 3, 'd', False)	2D	3-ordered Chi path weighted by sigma electrons
863		Xp-4d	Chi ('path', 4, 'd', False)	2D	4-ordered Chi path weighted by sigma electrons
864		Xp-5d	Chi ('path', 5, 'd', False)	2D	5-ordered Chi path weighted by sigma electrons

#	module	name	constructor	dim	description
865		Xp-6d	Chi (‘path’, 6, ‘d’, False)	2D	6-ordered Chi path weighted by sigma electrons
866		Xp-7d	Chi (‘path’, 7, ‘d’, False)	2D	7-ordered Chi path weighted by sigma electrons
867		AXp-0d	Chi (‘path’, 0, ‘d’, True)	2D	0-ordered averaged Chi path weighted by sigma electrons
868		AXp-1d	Chi (‘path’, 1, ‘d’, True)	2D	1-ordered averaged Chi path weighted by sigma electrons
869		AXp-2d	Chi (‘path’, 2, ‘d’, True)	2D	2-ordered averaged Chi path weighted by sigma electrons
870		AXp-3d	Chi (‘path’, 3, ‘d’, True)	2D	3-ordered averaged Chi path weighted by sigma electrons
871		AXp-4d	Chi (‘path’, 4, ‘d’, True)	2D	4-ordered averaged Chi path weighted by sigma electrons
872		AXp-5d	Chi (‘path’, 5, ‘d’, True)	2D	5-ordered averaged Chi path weighted by sigma electrons
873		AXp-6d	Chi (‘path’, 6, ‘d’, True)	2D	6-ordered averaged Chi path weighted by sigma electrons
874		AXp-7d	Chi (‘path’, 7, ‘d’, True)	2D	7-ordered averaged Chi path weighted by sigma electrons
875		Xp-0dv	Chi (‘path’, 0, ‘dv’, False)	2D	0-ordered Chi path weighted by valence electrons

#	module	name	constructor	dim	description
876		Xp-1dv	Chi (‘path’, 1, ‘dv’, False)	2D	1-ordered Chi path weighted by valence electrons
877		Xp-2dv	Chi (‘path’, 2, ‘dv’, False)	2D	2-ordered Chi path weighted by valence electrons
878		Xp-3dv	Chi (‘path’, 3, ‘dv’, False)	2D	3-ordered Chi path weighted by valence electrons
879		Xp-4dv	Chi (‘path’, 4, ‘dv’, False)	2D	4-ordered Chi path weighted by valence electrons
880		Xp-5dv	Chi (‘path’, 5, ‘dv’, False)	2D	5-ordered Chi path weighted by valence electrons
881		Xp-6dv	Chi (‘path’, 6, ‘dv’, False)	2D	6-ordered Chi path weighted by valence electrons
882		Xp-7dv	Chi (‘path’, 7, ‘dv’, False)	2D	7-ordered Chi path weighted by valence electrons
883		AXp-0dv	Chi (‘path’, 0, ‘dv’, True)	2D	0-ordered averaged Chi path weighted by valence electrons
884		AXp-1dv	Chi (‘path’, 1, ‘dv’, True)	2D	1-ordered averaged Chi path weighted by valence electrons
885		AXp-2dv	Chi (‘path’, 2, ‘dv’, True)	2D	2-ordered averaged Chi path weighted by valence electrons
886		AXp-3dv	Chi (‘path’, 3, ‘dv’, True)	2D	3-ordered averaged Chi path weighted by valence electrons

#	module	name	constructor	dim	description
887		AXp-4dv	Chi ('path', 4, 'dv', True)	2D	4-ordered averaged Chi path weighted by valence electrons
888		AXp-5dv	Chi ('path', 5, 'dv', True)	2D	5-ordered averaged Chi path weighted by valence electrons
889		AXp-6dv	Chi ('path', 6, 'dv', True)	2D	6-ordered averaged Chi path weighted by valence electrons
890		AXp-7dv	Chi ('path', 7, 'dv', True)	2D	7-ordered averaged Chi path weighted by valence electrons
891	Constitutional	SZ	ConstitutionalSum ('Z')	2D	sum of constitutional weighted by atomic number
892		Sm	ConstitutionalSum ('m')	2D	sum of constitutional weighted by mass
893		Sv	ConstitutionalSum ('v')	2D	sum of constitutional weighted by vdw volume
894		Sse	ConstitutionalSum ('se')	2D	sum of constitutional weighted by sanderson EN
895		Spe	ConstitutionalSum ('pe')	2D	sum of constitutional weighted by pauling EN
896		Sare	ConstitutionalSum ('are')	2D	sum of constitutional weighted by allred-rocow EN
897		Sp	ConstitutionalSum ('p')	2D	sum of constitutional weighted by polarizability

#	module	name	constructor	dim	description
898		Si	ConstitutionalSum ('i')	2D	sum of constitutional weighted by ionization potential
899		MZ	ConstitutionalMean ('Z')	2D	mean of constitutional weighted by atomic number
900		Mm	ConstitutionalMean ('m')	2D	mean of constitutional weighted by mass
901		Mv	ConstitutionalMean ('v')	2D	mean of constitutional weighted by vdw volume
902		Mse	ConstitutionalMean ('se')	2D	mean of constitutional weighted by sanderson EN
903		Mpe	ConstitutionalMean ('pe')	2D	mean of constitutional weighted by pauling EN
904		Mare	ConstitutionalMean ('are')	2D	mean of constitutional weighted by allred-rocow EN
905		Mp	ConstitutionalMean ('p')	2D	mean of constitutional weighted by polarizability
906		Mi	ConstitutionalMean ('i')	2D	mean of constitutional weighted by ionization potential
907	DetourMatrix	SpAbs_Dt	DetourMatrix ('SpAbs')	2D	graph energy from detourn matrix
908		SpMax_Dt	DetourMatrix ('SpMax')	2D	leading eigenvalue from detourn matrix
909		SpDiam_Dt	DetourMatrix ('SpDiam')	2D	spectral diamiter from detourn matrix

#	module	name	constructor	dim	description
910		SpAD_Dt	DetourMatrix ('SpAD')	2D	spectral absolute diviation from detourn matrix
911		SpMAD_Dt	DetourMatrix ('SpMAD')	2D	spectral mean absolute diviation from detourn matrix
912		LogEE_Dt	DetourMatrix ('LogEE')	2D	Estrada-like index from detourn matrix
913		SM1_Dt	DetourMatrix ('SM1')	2D	spectral moment from detourn matrix
914		VE1_Dt	DetourMatrix ('VE1')	2D	coefficient sum of the last eigenvector from detourn matrix
915		VE2_Dt	DetourMatrix ('VE2')	2D	average coefficient of the last eigenvector from detourn matrix
916		VE3_Dt	DetourMatrix ('VE3')	2D	logarithmic coefficient sum of the last eigenvector from detourn matrix
917		VR1_Dt	DetourMatrix ('VR1')	2D	Randic-like eigenvector-based index from detourn matrix
918		VR2_Dt	DetourMatrix ('VR2')	2D	normalized Randic-like eigenvector-based index from detourn matrix
919		VR3_Dt	DetourMatrix ('VR3')	2D	logarithmic Randic-like eigenvector-based index from detourn matrix
920		DetourIndex	DetourIndex ()	2D	detour index
921	DistanceMatrix	SpAbs_D	DistanceMatrix ('SpAbs')	2D	graph energy from distance matrix

#	module	name	constructor	dim	description
922		SpMax_D	DistanceMatrix ('SpMax')	2D	leading eigenvalue from distance matrix
923		SpDiam_D	DistanceMatrix ('SpDiam')	2D	spectral diamiter from distance matrix
924		SpAD_D	DistanceMatrix ('SpAD')	2D	spectral absolute diviation from distance matrix
925		SpMAD_D	DistanceMatrix ('SpMAD')	2D	spectral mean absolute diviation from distance matrix
926		LogEE_D	DistanceMatrix ('LogEE')	2D	Estrada-like index from distance matrix
927		VE1_D	DistanceMatrix ('VE1')	2D	coefficient sum of the last eigenvector from distance matrix
928		VE2_D	DistanceMatrix ('VE2')	2D	average coefficient of the last eigenvector from distance matrix
929		VE3_D	DistanceMatrix ('VE3')	2D	logarithmic coefficient sum of the last eigenvector from distance matrix
930		VR1_D	DistanceMatrix ('VR1')	2D	Randic-like eigenvector-based index from distance matrix
931		VR2_D	DistanceMatrix ('VR2')	2D	normalized Randic-like eigenvector-based index from distance matrix
932		VR3_D	DistanceMatrix ('VR3')	2D	logarithmic Randic-like eigenvector-based index from distance matrix

#	module	name	constructor	dim	description
933	EState	NsLi	AtomTypeEState (‘count’, ‘sLi’)	2D	number of sLi
934		NssBe	AtomTypeEState (‘count’, ‘ssBe’)	2D	number of ssBe
935		NssssBe	AtomTypeEState (‘count’, ‘ssssBe’)	2D	number of ssssBe
936		NssBH	AtomTypeEState (‘count’, ‘ssBH’)	2D	number of ssBH
937		NsssB	AtomTypeEState (‘count’, ‘sssB’)	2D	number of sssB
938		NssssB	AtomTypeEState (‘count’, ‘ssssB’)	2D	number of ssssB
939		NsCH3	AtomTypeEState (‘count’, ‘sCH3’)	2D	number of sCH3
940		NdCH2	AtomTypeEState (‘count’, ‘dCH2’)	2D	number of dCH2
941		NssCH2	AtomTypeEState (‘count’, ‘ssCH2’)	2D	number of ssCH2
942		NtCH	AtomTypeEState (‘count’, ‘tCH’)	2D	number of tCH
943		NdsCH	AtomTypeEState (‘count’, ‘dsCH’)	2D	number of dsCH
944		NaaCH	AtomTypeEState (‘count’, ‘aaCH’)	2D	number of aaCH
945		NsssCH	AtomTypeEState (‘count’, ‘sssCH’)	2D	number of sssCH
946		NddC	AtomTypeEState (‘count’, ‘ddC’)	2D	number of ddC
947		NtsC	AtomTypeEState (‘count’, ‘tsC’)	2D	number of tsC
948		NdssC	AtomTypeEState (‘count’, ‘dssC’)	2D	number of dssC
949		NaasC	AtomTypeEState (‘count’, ‘aasC’)	2D	number of aasC
950		NaaaC	AtomTypeEState (‘count’, ‘aaaC’)	2D	number of aaaC
951		NssssC	AtomTypeEState (‘count’, ‘ssssC’)	2D	number of ssssC
952		NsNH3	AtomTypeEState (‘count’, ‘sNH3’)	2D	number of sNH3
953		NsNH2	AtomTypeEState (‘count’, ‘sNH2’)	2D	number of sNH2
954		NssNH2	AtomTypeEState (‘count’, ‘ssNH2’)	2D	number of ssNH2
955		NdNH	AtomTypeEState (‘count’, ‘dNH’)	2D	number of dNH
956		NssNH	AtomTypeEState (‘count’, ‘ssNH’)	2D	number of ssNH

#	module	name	constructor	dim	description
957		NaaNH	AtomTypeEState (‘count’, ‘aaNH’)	2D	number of aaNH
958		NtN	AtomTypeEState (‘count’, ‘tN’)	2D	number of tN
959		NsssNH	AtomTypeEState (‘count’, ‘sssNH’)	2D	number of sssNH
960		NdsN	AtomTypeEState (‘count’, ‘dsN’)	2D	number of dsN
961		NaaN	AtomTypeEState (‘count’, ‘aaN’)	2D	number of aaN
962		NsssN	AtomTypeEState (‘count’, ‘sssN’)	2D	number of sssN
963		NddsN	AtomTypeEState (‘count’, ‘ddsN’)	2D	number of ddsN
964		NaasN	AtomTypeEState (‘count’, ‘aasN’)	2D	number of aasN
965		NssssN	AtomTypeEState (‘count’, ‘ssssN’)	2D	number of ssssN
966		NsOH	AtomTypeEState (‘count’, ‘sOH’)	2D	number of sOH
967		NdO	AtomTypeEState (‘count’, ‘dO’)	2D	number of dO
968		NssO	AtomTypeEState (‘count’, ‘ssO’)	2D	number of ssO
969		NaaO	AtomTypeEState (‘count’, ‘aaO’)	2D	number of aaO
970		NsF	AtomTypeEState (‘count’, ‘sF’)	2D	number of sF
971		NsSiH3	AtomTypeEState (‘count’, ‘sSiH3’)	2D	number of sSiH3
972		NssSiH2	AtomTypeEState (‘count’, ‘ssSiH2’)	2D	number of ssSiH2
973		NsssSiH	AtomTypeEState (‘count’, ‘sssSiH’)	2D	number of sssSiH
974		NssssSi	AtomTypeEState (‘count’, ‘ssssSi’)	2D	number of ssssSi
975		NsPH2	AtomTypeEState (‘count’, ‘sPH2’)	2D	number of sPH2
976		NssPH	AtomTypeEState (‘count’, ‘ssPH’)	2D	number of ssPH
977		NsssP	AtomTypeEState (‘count’, ‘sssP’)	2D	number of sssP
978		NdsssP	AtomTypeEState (‘count’, ‘dsssP’)	2D	number of dsssP
979		NssssssP	AtomTypeEState (‘count’, ‘ssssssP’)	2D	number of ssssssP
980		NsSH	AtomTypeEState (‘count’, ‘sSH’)	2D	number of sSH

#	module	name	constructor	dim	description
981		NdS	AtomTypeEState (‘count’, ‘dS’)	2D	number of dS
982		NssS	AtomTypeEState (‘count’, ‘ssS’)	2D	number of ssS
983		NaaS	AtomTypeEState (‘count’, ‘aaS’)	2D	number of aaS
984		NdssS	AtomTypeEState (‘count’, ‘dssS’)	2D	number of dssS
985		NddssS	AtomTypeEState (‘count’, ‘ddssS’)	2D	number of ddssS
986		NsCl	AtomTypeEState (‘count’, ‘sCl’)	2D	number of sCl
987		NsGeH3	AtomTypeEState (‘count’, ‘sGeH3’)	2D	number of sGeH3
988		NssGeH2	AtomTypeEState (‘count’, ‘ssGeH2’)	2D	number of ssGeH2
989		NsssGeH	AtomTypeEState (‘count’, ‘sssGeH’)	2D	number of sssGeH
990		NssssGe	AtomTypeEState (‘count’, ‘ssssGe’)	2D	number of ssssGe
991		NsAsH2	AtomTypeEState (‘count’, ‘sAsH2’)	2D	number of sAsH2
992		NssAsH	AtomTypeEState (‘count’, ‘ssAsH’)	2D	number of ssAsH
993		NsssAs	AtomTypeEState (‘count’, ‘sssAs’)	2D	number of sssAs
994		NsssdAs	AtomTypeEState (‘count’, ‘sssdAs’)	2D	number of sssdAs
995		NssssAs	AtomTypeEState (‘count’, ‘ssssAs’)	2D	number of ssssAs
996		NsSeH	AtomTypeEState (‘count’, ‘sSeH’)	2D	number of sSeH
997		NdSe	AtomTypeEState (‘count’, ‘dSe’)	2D	number of dSe
998		NssSe	AtomTypeEState (‘count’, ‘ssSe’)	2D	number of ssSe
999		NaaSe	AtomTypeEState (‘count’, ‘aaSe’)	2D	number of aaSe
1000		NdssSe	AtomTypeEState (‘count’, ‘dssSe’)	2D	number of dssSe
1001		NddssSe	AtomTypeEState (‘count’, ‘ddssSe’)	2D	number of ddssSe
1002		NsBr	AtomTypeEState (‘count’, ‘sBr’)	2D	number of sBr
1003		NsSnH3	AtomTypeEState (‘count’, ‘sSnH3’)	2D	number of sSnH3
1004		NssSnH2	AtomTypeEState (‘count’, ‘ssSnH2’)	2D	number of ssSnH2

#	module	name	constructor	dim	description
1005		NsssSnH	AtomTypeEState (‘count’, ‘sssSnH’)	2D	number of sssSnH
1006		NsssSn	AtomTypeEState (‘count’, ‘ssssSn’)	2D	number of ssssSn
1007		NsI	AtomTypeEState (‘count’, ‘sI’)	2D	number of sI
1008		NsPbH3	AtomTypeEState (‘count’, ‘sPbH3’)	2D	number of sPbH3
1009		NssPbH2	AtomTypeEState (‘count’, ‘ssPbH2’)	2D	number of ssPbH2
1010		NsssPbH	AtomTypeEState (‘count’, ‘sssPbH’)	2D	number of sssPbH
1011		NssssPb	AtomTypeEState (‘count’, ‘ssssPb’)	2D	number of ssssPb
1012		SsLi	AtomTypeEState (‘sum’, ‘sLi’)	2D	sum of sLi
1013		SssBe	AtomTypeEState (‘sum’, ‘ssBe’)	2D	sum of ssBe
1014		SssssBe	AtomTypeEState (‘sum’, ‘ssssBe’)	2D	sum of ssssBe
1015		SssBH	AtomTypeEState (‘sum’, ‘ssBH’)	2D	sum of ssBH
1016		SsssB	AtomTypeEState (‘sum’, ‘sssB’)	2D	sum of sssB
1017		SssssB	AtomTypeEState (‘sum’, ‘ssssB’)	2D	sum of ssssB
1018		SsCH3	AtomTypeEState (‘sum’, ‘sCH3’)	2D	sum of sCH3
1019		SdCH2	AtomTypeEState (‘sum’, ‘dCH2’)	2D	sum of dCH2
1020		SssCH2	AtomTypeEState (‘sum’, ‘ssCH2’)	2D	sum of ssCH2
1021		StCH	AtomTypeEState (‘sum’, ‘tCH’)	2D	sum of tCH
1022		SdsCH	AtomTypeEState (‘sum’, ‘dsCH’)	2D	sum of dsCH
1023		SaaCH	AtomTypeEState (‘sum’, ‘aaCH’)	2D	sum of aaCH
1024		SsssCH	AtomTypeEState (‘sum’, ‘sssCH’)	2D	sum of sssCH
1025		SddC	AtomTypeEState (‘sum’, ‘ddC’)	2D	sum of ddC
1026		StsC	AtomTypeEState (‘sum’, ‘tsC’)	2D	sum of tsC
1027		SdssC	AtomTypeEState (‘sum’, ‘dssC’)	2D	sum of dssC
1028		SaasC	AtomTypeEState (‘sum’, ‘aasC’)	2D	sum of aasC
1029		SaaaC	AtomTypeEState (‘sum’, ‘aaaC’)	2D	sum of aaaC

#	module	name	constructor	dim	description
1030		SsssC	AtomTypeEState ('sum', 'ssssC')	2D	sum of ssssC
1031		SsNH3	AtomTypeEState ('sum', 'sNH3')	2D	sum of sNH3
1032		SsNH2	AtomTypeEState ('sum', 'sNH2')	2D	sum of sNH2
1033		SssNH2	AtomTypeEState ('sum', 'ssNH2')	2D	sum of ssNH2
1034		SdNH	AtomTypeEState ('sum', 'dNH')	2D	sum of dNH
1035		SssNH	AtomTypeEState ('sum', 'ssNH')	2D	sum of ssNH
1036		SaaNH	AtomTypeEState ('sum', 'aaNH')	2D	sum of aaNH
1037		StN	AtomTypeEState ('sum', 'tN')	2D	sum of tN
1038		SsssNH	AtomTypeEState ('sum', 'sssNH')	2D	sum of sssNH
1039		SdsN	AtomTypeEState ('sum', 'dsN')	2D	sum of dsN
1040		SaaN	AtomTypeEState ('sum', 'aaN')	2D	sum of aaN
1041		SsssN	AtomTypeEState ('sum', 'sssN')	2D	sum of sssN
1042		SddsN	AtomTypeEState ('sum', 'ddsN')	2D	sum of ddsN
1043		SaasN	AtomTypeEState ('sum', 'aasN')	2D	sum of aasN
1044		SssssN	AtomTypeEState ('sum', 'ssssN')	2D	sum of ssssN
1045		SsOH	AtomTypeEState ('sum', 'sOH')	2D	sum of sOH
1046		SdO	AtomTypeEState ('sum', 'dO')	2D	sum of dO
1047		SssO	AtomTypeEState ('sum', 'ssO')	2D	sum of ssO
1048		SaaO	AtomTypeEState ('sum', 'aaO')	2D	sum of aaO
1049		SsF	AtomTypeEState ('sum', 'sF')	2D	sum of sF
1050		SsSiH3	AtomTypeEState ('sum', 'sSiH3')	2D	sum of sSiH3
1051		SssSiH2	AtomTypeEState ('sum', 'ssSiH2')	2D	sum of ssSiH2
1052		SsssSiH	AtomTypeEState ('sum', 'sssSiH')	2D	sum of sssSiH
1053		SssssSi	AtomTypeEState ('sum', 'ssssSi')	2D	sum of ssssSi
1054		SsPH2	AtomTypeEState ('sum', 'sPH2')	2D	sum of sPH2

#	module	name	constructor	dim	description
1055		SssPH	AtomTypeEState ('sum', 'ssPH')	2D	sum of ssPH
1056		SsssP	AtomTypeEState ('sum', 'sssP')	2D	sum of sssP
1057		SdsssP	AtomTypeEState ('sum', 'dsssP')	2D	sum of dsssP
1058		SssssssP	AtomTypeEState ('sum', 'ssssssP')	2D	sum of ssssssP
1059		SsSH	AtomTypeEState ('sum', 'sSH')	2D	sum of sSH
1060		SdS	AtomTypeEState ('sum', 'dS')	2D	sum of dS
1061		SssS	AtomTypeEState ('sum', 'ssS')	2D	sum of ssS
1062		SaaS	AtomTypeEState ('sum', 'aaS')	2D	sum of aaS
1063		SdssS	AtomTypeEState ('sum', 'dssS')	2D	sum of dssS
1064		SddssS	AtomTypeEState ('sum', 'ddssS')	2D	sum of ddssS
1065		SsCl	AtomTypeEState ('sum', 'sCl')	2D	sum of sCl
1066		SsGeH3	AtomTypeEState ('sum', 'sGeH3')	2D	sum of sGeH3
1067		SssGeH2	AtomTypeEState ('sum', 'ssGeH2')	2D	sum of ssGeH2
1068		SsssGeH	AtomTypeEState ('sum', 'sssGeH')	2D	sum of sssGeH
1069		SssssGe	AtomTypeEState ('sum', 'ssssGe')	2D	sum of ssssGe
1070		SsAsH2	AtomTypeEState ('sum', 'sAsH2')	2D	sum of sAsH2
1071		SssAsH	AtomTypeEState ('sum', 'ssAsH')	2D	sum of ssAsH
1072		SsssAs	AtomTypeEState ('sum', 'sssAs')	2D	sum of sssAs
1073		SsssdAs	AtomTypeEState ('sum', 'sssdAs')	2D	sum of sssdAs
1074		SssssAs	AtomTypeEState ('sum', 'sssssAs')	2D	sum of sssssAs
1075		SsSeH	AtomTypeEState ('sum', 'sSeH')	2D	sum of sSeH
1076		SdSe	AtomTypeEState ('sum', 'dSe')	2D	sum of dSe
1077		SssSe	AtomTypeEState ('sum', 'ssSe')	2D	sum of ssSe
1078		SaaSe	AtomTypeEState ('sum', 'aaSe')	2D	sum of aaSe
1079		SdssSe	AtomTypeEState ('sum', 'dssSe')	2D	sum of dssSe

#	module	name	constructor	dim	description
1080		SddssSe	AtomTypeEState ('sum', 'ddssSe')	2D	sum of ddssSe
1081		SsBr	AtomTypeEState ('sum', 'sBr')	2D	sum of sBr
1082		SsSnH3	AtomTypeEState ('sum', 'sSnH3')	2D	sum of sSnH3
1083		SssSnH2	AtomTypeEState ('sum', 'ssSnH2')	2D	sum of ssSnH2
1084		SsssSnH	AtomTypeEState ('sum', 'sssSnH')	2D	sum of sssSnH
1085		SssssSn	AtomTypeEState ('sum', 'ssssSn')	2D	sum of ssssSn
1086		SsI	AtomTypeEState ('sum', 'sI')	2D	sum of sI
1087		SsPbH3	AtomTypeEState ('sum', 'sPbH3')	2D	sum of sPbH3
1088		SssPbH2	AtomTypeEState ('sum', 'ssPbH2')	2D	sum of ssPbH2
1089		SsssPbH	AtomTypeEState ('sum', 'sssPbH')	2D	sum of sssPbH
1090		SssssPb	AtomTypeEState ('sum', 'ssssPb')	2D	sum of ssssPb
1091		MAXsLi	AtomTypeEState ('max', 'sLi')	2D	max of sLi
1092		MAXssBe	AtomTypeEState ('max', 'ssBe')	2D	max of ssBe
1093		MAXssssBe	AtomTypeEState ('max', 'ssssBe')	2D	max of ssssBe
1094		MAXssBH	AtomTypeEState ('max', 'ssBH')	2D	max of ssBH
1095		MAXsssB	AtomTypeEState ('max', 'sssB')	2D	max of sssB
1096		MAXssssB	AtomTypeEState ('max', 'ssssB')	2D	max of ssssB
1097		MAXsCH3	AtomTypeEState ('max', 'sCH3')	2D	max of sCH3
1098		MAXdCH2	AtomTypeEState ('max', 'dCH2')	2D	max of dCH2
1099		MAXssCH2	AtomTypeEState ('max', 'ssCH2')	2D	max of ssCH2
1100		MAXtCH	AtomTypeEState ('max', 'tCH')	2D	max of tCH
1101		MAXdsCH	AtomTypeEState ('max', 'dsCH')	2D	max of dsCH
1102		MAXaaCH	AtomTypeEState ('max', 'aaCH')	2D	max of aaCH
1103		MAXsssCH	AtomTypeEState ('max', 'sssCH')	2D	max of sssCH
1104		MAXddC	AtomTypeEState ('max', 'ddC')	2D	max of ddC
1105		MAXtsC	AtomTypeEState ('max', 'tsC')	2D	max of tsC

#	module	name	constructor	dim	description
1106		MAXdssC	AtomTypeEState (‘max’, ‘dssC’)	2D	max of dssC
1107		MAXaasC	AtomTypeEState (‘max’, ‘aasC’)	2D	max of aasC
1108		MAXaaaC	AtomTypeEState (‘max’, ‘aaaC’)	2D	max of aaaC
1109		MAXssssC	AtomTypeEState (‘max’, ‘ssssC’)	2D	max of ssssC
1110		MAXsNH3	AtomTypeEState (‘max’, ‘sNH3’)	2D	max of sNH3
1111		MAXsNH2	AtomTypeEState (‘max’, ‘sNH2’)	2D	max of sNH2
1112		MAXssNH2	AtomTypeEState (‘max’, ‘ssNH2’)	2D	max of ssNH2
1113		MAXdNH	AtomTypeEState (‘max’, ‘dNH’)	2D	max of dNH
1114		MAXssNH	AtomTypeEState (‘max’, ‘ssNH’)	2D	max of ssNH
1115		MAXaaNH	AtomTypeEState (‘max’, ‘aaNH’)	2D	max of aaNH
1116		MAXtN	AtomTypeEState (‘max’, ‘tN’)	2D	max of tN
1117		MAXsssNH	AtomTypeEState (‘max’, ‘sssNH’)	2D	max of sssNH
1118		MAXdsN	AtomTypeEState (‘max’, ‘dsN’)	2D	max of dsN
1119		MAXaaN	AtomTypeEState (‘max’, ‘aaN’)	2D	max of aaN
1120		MAXsssN	AtomTypeEState (‘max’, ‘sssN’)	2D	max of sssN
1121		MAXddsN	AtomTypeEState (‘max’, ‘ddsN’)	2D	max of ddsN
1122		MAXaasN	AtomTypeEState (‘max’, ‘aasN’)	2D	max of aasN
1123		MAXssssN	AtomTypeEState (‘max’, ‘ssssN’)	2D	max of ssssN
1124		MAXsOH	AtomTypeEState (‘max’, ‘sOH’)	2D	max of sOH
1125		MAXdO	AtomTypeEState (‘max’, ‘dO’)	2D	max of dO
1126		MAXssO	AtomTypeEState (‘max’, ‘ssO’)	2D	max of ssO
1127		MAXaaO	AtomTypeEState (‘max’, ‘aaO’)	2D	max of aaO
1128		MAXsF	AtomTypeEState (‘max’, ‘sF’)	2D	max of sF
1129		MAXsSiH3	AtomTypeEState (‘max’, ‘sSiH3’)	2D	max of sSiH3
1130		MAXssSiH2	AtomTypeEState (‘max’, ‘ssSiH2’)	2D	max of ssSiH2

#	module	name	constructor	dim	description
1131		MAXsssSiH	AtomTypeEState (‘max’, ‘sssSiH’)	2D	max of sssSiH
1132		MAXssssSi	AtomTypeEState (‘max’, ‘ssssSi’)	2D	max of ssssSi
1133		MAXsPH2	AtomTypeEState (‘max’, ‘sPH2’)	2D	max of sPH2
1134		MAXssPH	AtomTypeEState (‘max’, ‘ssPH’)	2D	max of ssPH
1135		MAXsssP	AtomTypeEState (‘max’, ‘sssP’)	2D	max of sssP
1136		MAXdsssP	AtomTypeEState (‘max’, ‘dsssP’)	2D	max of dsssP
1137		MAXssssssP	AtomTypeEState (‘max’, ‘ssssssP’)	2D	max of ssssssP
1138		MAXsSH	AtomTypeEState (‘max’, ‘sSH’)	2D	max of sSH
1139		MAXdS	AtomTypeEState (‘max’, ‘dS’)	2D	max of dS
1140		MAXssS	AtomTypeEState (‘max’, ‘ssS’)	2D	max of ssS
1141		MAXaaS	AtomTypeEState (‘max’, ‘aaS’)	2D	max of aaS
1142		MAXdssS	AtomTypeEState (‘max’, ‘dssS’)	2D	max of dssS
1143		MAXddssS	AtomTypeEState (‘max’, ‘ddssS’)	2D	max of ddssS
1144		MAXsCl	AtomTypeEState (‘max’, ‘sCl’)	2D	max of sCl
1145		MAXsGeH3	AtomTypeEState (‘max’, ‘sGeH3’)	2D	max of sGeH3
1146		MAXssGeH2	AtomTypeEState (‘max’, ‘ssGeH2’)	2D	max of ssGeH2
1147		MAXsssGeH	AtomTypeEState (‘max’, ‘sssGeH’)	2D	max of sssGeH
1148		MAXssssGe	AtomTypeEState (‘max’, ‘ssssGe’)	2D	max of ssssGe
1149		MAXsAsH2	AtomTypeEState (‘max’, ‘sAsH2’)	2D	max of sAsH2
1150		MAXssAsH	AtomTypeEState (‘max’, ‘ssAsH’)	2D	max of ssAsH
1151		MAXsssAs	AtomTypeEState (‘max’, ‘sssAs’)	2D	max of sssAs
1152		MAXsssdAs	AtomTypeEState (‘max’, ‘sssdAs’)	2D	max of sssdAs
1153		MAXssssAs	AtomTypeEState (‘max’, ‘ssssAs’)	2D	max of ssssAs
1154		MAXsSeH	AtomTypeEState (‘max’, ‘sSeH’)	2D	max of sSeH
1155		MAXdSe	AtomTypeEState (‘max’, ‘dSe’)	2D	max of dSe

#	module	name	constructor	dim	description
1156		MAXssSe	AtomTypeEState ('max', 'ssSe')	2D	max of ssSe
1157		MAXaaSe	AtomTypeEState ('max', 'aaSe')	2D	max of aaSe
1158		MAXdssSe	AtomTypeEState ('max', 'dssSe')	2D	max of dssSe
1159		MAXddssSe	AtomTypeEState ('max', 'ddssSe')	2D	max of ddssSe
1160		MAXsBr	AtomTypeEState ('max', 'sBr')	2D	max of sBr
1161		MAXsSnH3	AtomTypeEState ('max', 'sSnH3')	2D	max of sSnH3
1162		MAXssSnH2	AtomTypeEState ('max', 'ssSnH2')	2D	max of ssSnH2
1163		MAXsssSnH	AtomTypeEState ('max', 'sssSnH')	2D	max of sssSnH
1164		MAXssssSn	AtomTypeEState ('max', 'ssssSn')	2D	max of ssssSn
1165		MAXsI	AtomTypeEState ('max', 'sI')	2D	max of sI
1166		MAXsPbH3	AtomTypeEState ('max', 'sPbH3')	2D	max of sPbH3
1167		MAXssPbH2	AtomTypeEState ('max', 'ssPbH2')	2D	max of ssPbH2
1168		MAXsssPbH	AtomTypeEState ('max', 'sssPbH')	2D	max of sssPbH
1169		MAXssssPb	AtomTypeEState ('max', 'ssssPb')	2D	max of ssssPb
1170		MINsLi	AtomTypeEState ('min', 'sLi')	2D	min of sLi
1171		MINssBe	AtomTypeEState ('min', 'ssBe')	2D	min of ssBe
1172		MINssssBe	AtomTypeEState ('min', 'ssssBe')	2D	min of ssssBe
1173		MINssBH	AtomTypeEState ('min', 'ssBH')	2D	min of ssBH
1174		MINsssB	AtomTypeEState ('min', 'sssB')	2D	min of sssB
1175		MINssssB	AtomTypeEState ('min', 'ssssB')	2D	min of ssssB
1176		MINsCH3	AtomTypeEState ('min', 'sCH3')	2D	min of sCH3
1177		MINdCH2	AtomTypeEState ('min', 'dCH2')	2D	min of dCH2
1178		MINssCH2	AtomTypeEState ('min', 'ssCH2')	2D	min of ssCH2
1179		MINtCH	AtomTypeEState ('min', 'tCH')	2D	min of tCH
1180		MINdsCH	AtomTypeEState ('min', 'dsCH')	2D	min of dsCH
1181		MINaaCH	AtomTypeEState ('min', 'aaCH')	2D	min of aaCH

#	module	name	constructor	dim	description
1182		MINsssCH	AtomTypeEState ('min', 'sssCH')	2D	min of sssCH
1183		MINddC	AtomTypeEState ('min', 'ddC')	2D	min of ddC
1184		MINtsC	AtomTypeEState ('min', 'tsC')	2D	min of tsC
1185		MINdssC	AtomTypeEState ('min', 'dssC')	2D	min of dssC
1186		MINaasC	AtomTypeEState ('min', 'aasC')	2D	min of aasC
1187		MINaaaC	AtomTypeEState ('min', 'aaaC')	2D	min of aaaC
1188		MINssssC	AtomTypeEState ('min', 'ssssC')	2D	min of ssssC
1189		MINsNH3	AtomTypeEState ('min', 'sNH3')	2D	min of sNH3
1190		MINsNH2	AtomTypeEState ('min', 'sNH2')	2D	min of sNH2
1191		MINssNH2	AtomTypeEState ('min', 'ssNH2')	2D	min of ssNH2
1192		MINdNH	AtomTypeEState ('min', 'dNH')	2D	min of dNH
1193		MINssNH	AtomTypeEState ('min', 'ssNH')	2D	min of ssNH
1194		MINaaNH	AtomTypeEState ('min', 'aaNH')	2D	min of aaNH
1195		MINtN	AtomTypeEState ('min', 'tN')	2D	min of tN
1196		MINsssNH	AtomTypeEState ('min', 'sssNH')	2D	min of sssNH
1197		MINdsN	AtomTypeEState ('min', 'dsN')	2D	min of dsN
1198		MINaaN	AtomTypeEState ('min', 'aaN')	2D	min of aaN
1199		MINsssN	AtomTypeEState ('min', 'sssN')	2D	min of sssN
1200		MINddsN	AtomTypeEState ('min', 'ddsN')	2D	min of ddsN
1201		MINaasN	AtomTypeEState ('min', 'aasN')	2D	min of aasN
1202		MINssssN	AtomTypeEState ('min', 'ssssN')	2D	min of ssssN
1203		MINsOH	AtomTypeEState ('min', 'sOH')	2D	min of sOH
1204		MINdO	AtomTypeEState ('min', 'dO')	2D	min of dO
1205		MINssO	AtomTypeEState ('min', 'ssO')	2D	min of ssO
1206		MINaaO	AtomTypeEState ('min', 'aaO')	2D	min of aaO
1207		MINsF	AtomTypeEState ('min', 'sF')	2D	min of sF

#	module	name	constructor	dim	description
1208		MINsSiH3	AtomTypeEState (‘min’, ‘sSiH3’)	2D	min of sSiH3
1209		MINssSiH2	AtomTypeEState (‘min’, ‘ssSiH2’)	2D	min of ssSiH2
1210		MINsssSiH	AtomTypeEState (‘min’, ‘sssSiH’)	2D	min of sssSiH
1211		MINssssSi	AtomTypeEState (‘min’, ‘ssssSi’)	2D	min of ssssSi
1212		MINsPH2	AtomTypeEState (‘min’, ‘sPH2’)	2D	min of sPH2
1213		MINssPH	AtomTypeEState (‘min’, ‘ssPH’)	2D	min of ssPH
1214		MINsssP	AtomTypeEState (‘min’, ‘sssP’)	2D	min of sssP
1215		MINdsssP	AtomTypeEState (‘min’, ‘dsssP’)	2D	min of dsssP
1216		MINssssssP	AtomTypeEState (‘min’, ‘ssssssP’)	2D	min of ssssssP
1217		MINsSH	AtomTypeEState (‘min’, ‘sSH’)	2D	min of sSH
1218		MINdS	AtomTypeEState (‘min’, ‘dS’)	2D	min of dS
1219		MINssS	AtomTypeEState (‘min’, ‘ssS’)	2D	min of ssS
1220		MINaaS	AtomTypeEState (‘min’, ‘aaS’)	2D	min of aaS
1221		MINdssS	AtomTypeEState (‘min’, ‘dssS’)	2D	min of dssS
1222		MINddssS	AtomTypeEState (‘min’, ‘ddssS’)	2D	min of ddssS
1223		MINsCl	AtomTypeEState (‘min’, ‘sCl’)	2D	min of sCl
1224		MINsGeH3	AtomTypeEState (‘min’, ‘sGeH3’)	2D	min of sGeH3
1225		MINssGeH2	AtomTypeEState (‘min’, ‘ssGeH2’)	2D	min of ssGeH2
1226		MINsssGeH	AtomTypeEState (‘min’, ‘sssGeH’)	2D	min of sssGeH
1227		MINssssGe	AtomTypeEState (‘min’, ‘ssssGe’)	2D	min of ssssGe
1228		MINsAsH2	AtomTypeEState (‘min’, ‘sAsH2’)	2D	min of sAsH2
1229		MINssAsH	AtomTypeEState (‘min’, ‘ssAsH’)	2D	min of ssAsH
1230		MINsssAs	AtomTypeEState (‘min’, ‘sssAs’)	2D	min of sssAs
1231		MINsssdAs	AtomTypeEState (‘min’, ‘sssdAs’)	2D	min of sssdAs
1232		MINssssAs	AtomTypeEState (‘min’, ‘ssssAs’)	2D	min of ssssAs
1233		MINsSeH	AtomTypeEState (‘min’, ‘sSeH’)	2D	min of sSeH

#	module	name	constructor	dim	description
1234		MINdSe	AtomTypeEState ('min', 'dSe')	2D	min of dSe
1235		MINssSe	AtomTypeEState ('min', 'ssSe')	2D	min of ssSe
1236		MINaaSe	AtomTypeEState ('min', 'aaSe')	2D	min of aaSe
1237		MINdssSe	AtomTypeEState ('min', 'dssSe')	2D	min of dssSe
1238		MINddssSe	AtomTypeEState ('min', 'ddssSe')	2D	min of ddssSe
1239		MINsBr	AtomTypeEState ('min', 'sBr')	2D	min of sBr
1240		MINsSnH3	AtomTypeEState ('min', 'sSnH3')	2D	min of sSnH3
1241		MINssSnH2	AtomTypeEState ('min', 'ssSnH2')	2D	min of ssSnH2
1242		MINsssSnH	AtomTypeEState ('min', 'sssSnH')	2D	min of sssSnH
1243		MINssssSn	AtomTypeEState ('min', 'ssssSn')	2D	min of ssssSn
1244		MINsI	AtomTypeEState ('min', 'sI')	2D	min of sI
1245		MINsPbH3	AtomTypeEState ('min', 'sPbH3')	2D	min of sPbH3
1246		MINssPbH2	AtomTypeEState ('min', 'ssPbH2')	2D	min of ssPbH2
1247		MINsssPbH	AtomTypeEState ('min', 'sssPbH')	2D	min of sssPbH
1248		MINssssPb	AtomTypeEState ('min', 'ssssPb')	2D	min of ssssPb
1249	EccentricConnectivityIndex	ECIndex	EccentricConnectivityIndex ()	2D	eccentric connectivity index
1250	ExtendedTopochemicalAtom	ETA_alpha	EtaCoreCount (False, False)	2D	ETA core count
1251		AETA_alpha	EtaCoreCount (True, False)	2D	averaged ETA core count
1252		ETA_shape_p	EtaShapeIndex ('p')	2D	ETA shape index (type: p)
1253		ETA_shape_y	EtaShapeIndex ('y')	2D	ETA shape index (type: y)
1254		ETA_shape_x	EtaShapeIndex ('x')	2D	ETA shape index (type: x)
1255		ETA_beta	EtaVEMCount ('', False)	2D	valence electron mobile count
1256		AETA_beta	EtaVEMCount ('', True)	2D	averaged valence electron mobile count

#	module	name	constructor	dim	description
1257		ETA_beta_s	EtaVEMCount ('s', False)	2D	sigma contribution to valence electron mobile count
1258		AETA_beta_s	EtaVEMCount ('s', True)	2D	averaged sigma contribution to valence electron mobile count
1259		ETA_beta_ns	EtaVEMCount ('ns', False)	2D	nonsigma contribution to valence electron mobile count
1260		AETA_beta_ns	EtaVEMCount ('ns', True)	2D	averaged nonsigma contribution to valence electron mobile count
1261		ETA_beta_ns_d	EtaVEMCount ('ns_d', False)	2D	delta contribution to valence electron mobile count
1262		AETA_beta_ns_d	EtaVEMCount ('ns_d', True)	2D	averaged delta contribution to valence electron mobile count
1263		ETA_eta	EtaCompositeIndex (False, False, False)	2D	ETA composite index for reference graph
1264		AETA_eta	EtaCompositeIndex (False, False, True)	2D	averaged ETA composite index for reference graph
1265		ETA_eta_L	EtaCompositeIndex (False, True, False)	2D	local ETA composite index for reference graph
1266		AETA_eta_L	EtaCompositeIndex (False, True, True)	2D	averaged local ETA composite index for reference graph

#	module	name	constructor	dim	description
1267		ETA_eta_R	EtaCompositeIndex (True, False, False)	2D	ETA composite index for reference graph
1268		AETA_eta_R	EtaCompositeIndex (True, False, True)	2D	averaged ETA composite index for reference graph
1269		ETA_eta_RL	EtaCompositeIndex (True, True, False)	2D	local ETA composite index for reference graph
1270		AETA_eta_RL	EtaCompositeIndex (True, True, True)	2D	averaged local ETA composite index for reference graph
1271		ETA_eta_F	EtaFunctionalityIndex (False, False)	2D	ETA functionality index
1272		AETA_eta_F	EtaFunctionalityIndex (False, True)	2D	averaged ETA functionality index
1273		ETA_eta_FL	EtaFunctionalityIndex (True, False)	2D	local ETA functionality index
1274		AETA_eta_FL	EtaFunctionalityIndex (True, True)	2D	averaged local ETA functionality index
1275		ETA_eta_B	EtaBranchingIndex (False, False)	2D	ETA branching index
1276		AETA_eta_B	EtaBranchingIndex (False, True)	2D	averaged ETA branching index
1277		ETA_eta_BR	EtaBranchingIndex (True, False)	2D	ETA branching index (use ring count)
1278		AETA_eta_BR	EtaBranchingIndex (True, True)	2D	averaged ETA branching index (use ring count)
1279		ETA_dAlpha_A	EtaDeltaAlpha ('A')	2D	ETA delta alpha (type: A)
1280		ETA_dAlpha_B	EtaDeltaAlpha ('B')	2D	ETA delta alpha (type: B)
1281		ETA_epsilon_1	EtaEpsilon (1)	2D	ETA epsilon (type: 1)

#	module	name	constructor	dim	description
1282		ETA_epsilon_2	EtaEpsilon (2)	2D	ETA epsilon (type: 2)
1283		ETA_epsilon_3	EtaEpsilon (3)	2D	ETA epsilon (type: 3)
1284		ETA_epsilon_4	EtaEpsilon (4)	2D	ETA epsilon (type: 4)
1285		ETA_epsilon_5	EtaEpsilon (5)	2D	ETA epsilon (type: 5)
1286		ETA_dEpsilon_A	EtaDeltaEpsilon ('A')	2D	ETA delta epsilon (type: A)
1287		ETA_dEpsilon_B	EtaDeltaEpsilon ('B')	2D	ETA delta epsilon (type: B)
1288		ETA_dEpsilon_C	EtaDeltaEpsilon ('C')	2D	ETA delta epsilon (type: C)
1289		ETA_dEpsilon_D	EtaDeltaEpsilon ('D')	2D	ETA delta epsilon (type: D)
1290		ETA_dBeta	EtaDeltaBeta (False)	2D	ETA delta beta
1291		AETA_dBeta	EtaDeltaBeta (True)	2D	averaged ETA delta beta
1292		ETA_psi_1	EtaPsi ()	2D	ETA psi
1293		ETA_dPsi_A	EtaDeltaPsi ('A')	2D	ETA delta psi (type: A)
1294		ETA_dPsi_B	EtaDeltaPsi ('B')	2D	ETA delta psi (type: B)
1295	FragmentComplexity	fragCpx	FragmentComplexity ()	2D	fragment complexity
1296	Framework	fMF	Framework ()	2D	molecular framework ratio
1297	GeometricalIndex	GeomDiameter	Diameter3D ()	3D	geometric diameter
1298		GeomRadius	Radius3D ()	3D	geometric radius
1299		GeomShapeIndex	GeometricalShapeIndex ()	3D	geometrical shape index
1300		GeomPetitjeanIndex	PetitjeanIndex3D ()	3D	geometric Petitjean index
1301	GravitationalIndex	GRAV	GravitationalIndex (True, False)	3D	heavy atom gravitational index
1302		GRAVH	GravitationalIndex (False, False)	3D	gravitational index

#	module	name	constructor	dim	description
1303		GRAVp	GravitationalIndex (True, True)	3D	heavy atom pair gravitational index
1304		GRAVHp	GravitationalIndex (False, True)	3D	pair gravitational index
1305	HydrogenBond	nHBAcc	HBondAcceptor ()	2D	number of hydrogen bond acceptor
1306		nHBDon	HBondDonor ()	2D	number of hydrogen bond donor
1307	InformationContent	IC0	InformationContent (0)	2D	0-ordered neighborhood information content
1308		IC1	InformationContent (1)	2D	1-ordered neighborhood information content
1309		IC2	InformationContent (2)	2D	2-ordered neighborhood information content
1310		IC3	InformationContent (3)	2D	3-ordered neighborhood information content
1311		IC4	InformationContent (4)	2D	4-ordered neighborhood information content
1312		IC5	InformationContent (5)	2D	5-ordered neighborhood information content
1313		TIC0	TotalIC (0)	2D	0-ordered neighborhood total information content
1314		TIC1	TotalIC (1)	2D	1-ordered neighborhood total information content
1315		TIC2	TotalIC (2)	2D	2-ordered neighborhood total information content

#	module	name	constructor	dim	description
1316		TIC3	TotalIC (3)	2D	3-ordered neighborhood total information content
1317		TIC4	TotalIC (4)	2D	4-ordered neighborhood total information content
1318		TIC5	TotalIC (5)	2D	5-ordered neighborhood total information content
1319		SIC0	StructuralIC (0)	2D	0-ordered structural information content
1320		SIC1	StructuralIC (1)	2D	1-ordered structural information content
1321		SIC2	StructuralIC (2)	2D	2-ordered structural information content
1322		SIC3	StructuralIC (3)	2D	3-ordered structural information content
1323		SIC4	StructuralIC (4)	2D	4-ordered structural information content
1324		SIC5	StructuralIC (5)	2D	5-ordered structural information content
1325		BIC0	BondingIC (0)	2D	0-ordered bonding information content
1326		BIC1	BondingIC (1)	2D	1-ordered bonding information content
1327		BIC2	BondingIC (2)	2D	2-ordered bonding information content

#	module	name	constructor	dim	description
1328		BIC3	BondingIC (3)	2D	3-ordered bonding information content
1329		BIC4	BondingIC (4)	2D	4-ordered bonding information content
1330		BIC5	BondingIC (5)	2D	5-ordered bonding information content
1331		CIC0	ComplementaryIC (0)	2D	0-ordered complementary information content
1332		CIC1	ComplementaryIC (1)	2D	1-ordered complementary information content
1333		CIC2	ComplementaryIC (2)	2D	2-ordered complementary information content
1334		CIC3	ComplementaryIC (3)	2D	3-ordered complementary information content
1335		CIC4	ComplementaryIC (4)	2D	4-ordered complementary information content
1336		CIC5	ComplementaryIC (5)	2D	5-ordered complementary information content
1337		MIC0	ModifiedIC (0)	2D	0-ordered modified information content
1338		MIC1	ModifiedIC (1)	2D	1-ordered modified information content
1339		MIC2	ModifiedIC (2)	2D	2-ordered modified information content
1340		MIC3	ModifiedIC (3)	2D	3-ordered modified information content

#	module	name	constructor	dim	description
1341		MIC4	ModifiedIC (4)	2D	4-ordered modified information content
1342		MIC5	ModifiedIC (5)	2D	5-ordered modified information content
1343		ZMIC0	ZModifiedIC (0)	2D	0-ordered Z-modified information content
1344		ZMIC1	ZModifiedIC (1)	2D	1-ordered Z-modified information content
1345		ZMIC2	ZModifiedIC (2)	2D	2-ordered Z-modified information content
1346		ZMIC3	ZModifiedIC (3)	2D	3-ordered Z-modified information content
1347		ZMIC4	ZModifiedIC (4)	2D	4-ordered Z-modified information content
1348		ZMIC5	ZModifiedIC (5)	2D	5-ordered Z-modified information content
1349	KappaShapeIndex	Kier1	KappaShapeIndex1 ()	2D	kappa shape index 1
1350		Kier2	KappaShapeIndex2 ()	2D	kappa shape index 2
1351		Kier3	KappaShapeIndex3 ()	2D	kappa shape index 3
1352	Lipinski	Lipinski	Lipinski ()	2D	Lipinski rule of five
1353		GhoseFilter	GhoseFilter ()	2D	Ghose filter
1354	LogS	FilterItLogS	LogS ()	2D	Filter-it™ LogS
1355	McGowanVolume	VMcGowan	McGowanVolume ()	2D	McGowan volume
1356	MoRSE	Mor01	MoRSE (None, 1)	3D	3D-MoRSE (distance = 1)
1357		Mor02	MoRSE (None, 2)	3D	3D-MoRSE (distance = 2)
1358		Mor03	MoRSE (None, 3)	3D	3D-MoRSE (distance = 3)

#	module	name	constructor	dim	description
1359		Mor04	MoRSE (None, 4)	3D	3D-MoRSE (distance = 4)
1360		Mor05	MoRSE (None, 5)	3D	3D-MoRSE (distance = 5)
1361		Mor06	MoRSE (None, 6)	3D	3D-MoRSE (distance = 6)
1362		Mor07	MoRSE (None, 7)	3D	3D-MoRSE (distance = 7)
1363		Mor08	MoRSE (None, 8)	3D	3D-MoRSE (distance = 8)
1364		Mor09	MoRSE (None, 9)	3D	3D-MoRSE (distance = 9)
1365		Mor10	MoRSE (None, 10)	3D	3D-MoRSE (distance = 10)
1366		Mor11	MoRSE (None, 11)	3D	3D-MoRSE (distance = 11)
1367		Mor12	MoRSE (None, 12)	3D	3D-MoRSE (distance = 12)
1368		Mor13	MoRSE (None, 13)	3D	3D-MoRSE (distance = 13)
1369		Mor14	MoRSE (None, 14)	3D	3D-MoRSE (distance = 14)
1370		Mor15	MoRSE (None, 15)	3D	3D-MoRSE (distance = 15)
1371		Mor16	MoRSE (None, 16)	3D	3D-MoRSE (distance = 16)
1372		Mor17	MoRSE (None, 17)	3D	3D-MoRSE (distance = 17)
1373		Mor18	MoRSE (None, 18)	3D	3D-MoRSE (distance = 18)
1374		Mor19	MoRSE (None, 19)	3D	3D-MoRSE (distance = 19)
1375		Mor20	MoRSE (None, 20)	3D	3D-MoRSE (distance = 20)
1376		Mor21	MoRSE (None, 21)	3D	3D-MoRSE (distance = 21)
1377		Mor22	MoRSE (None, 22)	3D	3D-MoRSE (distance = 22)
1378		Mor23	MoRSE (None, 23)	3D	3D-MoRSE (distance = 23)
1379		Mor24	MoRSE (None, 24)	3D	3D-MoRSE (distance = 24)
1380		Mor25	MoRSE (None, 25)	3D	3D-MoRSE (distance = 25)
1381		Mor26	MoRSE (None, 26)	3D	3D-MoRSE (distance = 26)
1382		Mor27	MoRSE (None, 27)	3D	3D-MoRSE (distance = 27)

#	module	name	constructor	dim	description
1383		Mor28	MoRSE (None, 28)	3D	3D-MoRSE (distance = 28)
1384		Mor29	MoRSE (None, 29)	3D	3D-MoRSE (distance = 29)
1385		Mor30	MoRSE (None, 30)	3D	3D-MoRSE (distance = 30)
1386		Mor31	MoRSE (None, 31)	3D	3D-MoRSE (distance = 31)
1387		Mor32	MoRSE (None, 32)	3D	3D-MoRSE (distance = 32)
1388		Mor01m	MoRSE ('m', 1)	3D	3D-MoRSE weighted by mass (distance = 1)
1389		Mor02m	MoRSE ('m', 2)	3D	3D-MoRSE weighted by mass (distance = 2)
1390		Mor03m	MoRSE ('m', 3)	3D	3D-MoRSE weighted by mass (distance = 3)
1391		Mor04m	MoRSE ('m', 4)	3D	3D-MoRSE weighted by mass (distance = 4)
1392		Mor05m	MoRSE ('m', 5)	3D	3D-MoRSE weighted by mass (distance = 5)
1393		Mor06m	MoRSE ('m', 6)	3D	3D-MoRSE weighted by mass (distance = 6)
1394		Mor07m	MoRSE ('m', 7)	3D	3D-MoRSE weighted by mass (distance = 7)
1395		Mor08m	MoRSE ('m', 8)	3D	3D-MoRSE weighted by mass (distance = 8)
1396		Mor09m	MoRSE ('m', 9)	3D	3D-MoRSE weighted by mass (distance = 9)
1397		Mor10m	MoRSE ('m', 10)	3D	3D-MoRSE weighted by mass (distance = 10)

#	module	name	constructor	dim	description
1398		Mor11m	MoRSE ('m', 11)	3D	3D-MoRSE weighted by mass (distance = 11)
1399		Mor12m	MoRSE ('m', 12)	3D	3D-MoRSE weighted by mass (distance = 12)
1400		Mor13m	MoRSE ('m', 13)	3D	3D-MoRSE weighted by mass (distance = 13)
1401		Mor14m	MoRSE ('m', 14)	3D	3D-MoRSE weighted by mass (distance = 14)
1402		Mor15m	MoRSE ('m', 15)	3D	3D-MoRSE weighted by mass (distance = 15)
1403		Mor16m	MoRSE ('m', 16)	3D	3D-MoRSE weighted by mass (distance = 16)
1404		Mor17m	MoRSE ('m', 17)	3D	3D-MoRSE weighted by mass (distance = 17)
1405		Mor18m	MoRSE ('m', 18)	3D	3D-MoRSE weighted by mass (distance = 18)
1406		Mor19m	MoRSE ('m', 19)	3D	3D-MoRSE weighted by mass (distance = 19)
1407		Mor20m	MoRSE ('m', 20)	3D	3D-MoRSE weighted by mass (distance = 20)
1408		Mor21m	MoRSE ('m', 21)	3D	3D-MoRSE weighted by mass (distance = 21)
1409		Mor22m	MoRSE ('m', 22)	3D	3D-MoRSE weighted by mass (distance = 22)
1410		Mor23m	MoRSE ('m', 23)	3D	3D-MoRSE weighted by mass (distance = 23)

#	module	name	constructor	dim	description
1411		Mor24m	MoRSE ('m', 24)	3D	3D-MoRSE weighted by mass (distance = 24)
1412		Mor25m	MoRSE ('m', 25)	3D	3D-MoRSE weighted by mass (distance = 25)
1413		Mor26m	MoRSE ('m', 26)	3D	3D-MoRSE weighted by mass (distance = 26)
1414		Mor27m	MoRSE ('m', 27)	3D	3D-MoRSE weighted by mass (distance = 27)
1415		Mor28m	MoRSE ('m', 28)	3D	3D-MoRSE weighted by mass (distance = 28)
1416		Mor29m	MoRSE ('m', 29)	3D	3D-MoRSE weighted by mass (distance = 29)
1417		Mor30m	MoRSE ('m', 30)	3D	3D-MoRSE weighted by mass (distance = 30)
1418		Mor31m	MoRSE ('m', 31)	3D	3D-MoRSE weighted by mass (distance = 31)
1419		Mor32m	MoRSE ('m', 32)	3D	3D-MoRSE weighted by mass (distance = 32)
1420		Mor01v	MoRSE ('v', 1)	3D	3D-MoRSE weighted by vdw volume (distance = 1)
1421		Mor02v	MoRSE ('v', 2)	3D	3D-MoRSE weighted by vdw volume (distance = 2)
1422		Mor03v	MoRSE ('v', 3)	3D	3D-MoRSE weighted by vdw volume (distance = 3)
1423		Mor04v	MoRSE ('v', 4)	3D	3D-MoRSE weighted by vdw volume (distance = 4)

#	module	name	constructor	dim	description
1424		Mor05v	MoRSE ('v', 5)	3D	3D-MoRSE weighted by vdw volume (distance = 5)
1425		Mor06v	MoRSE ('v', 6)	3D	3D-MoRSE weighted by vdw volume (distance = 6)
1426		Mor07v	MoRSE ('v', 7)	3D	3D-MoRSE weighted by vdw volume (distance = 7)
1427		Mor08v	MoRSE ('v', 8)	3D	3D-MoRSE weighted by vdw volume (distance = 8)
1428		Mor09v	MoRSE ('v', 9)	3D	3D-MoRSE weighted by vdw volume (distance = 9)
1429		Mor10v	MoRSE ('v', 10)	3D	3D-MoRSE weighted by vdw volume (distance = 10)
1430		Mor11v	MoRSE ('v', 11)	3D	3D-MoRSE weighted by vdw volume (distance = 11)
1431		Mor12v	MoRSE ('v', 12)	3D	3D-MoRSE weighted by vdw volume (distance = 12)
1432		Mor13v	MoRSE ('v', 13)	3D	3D-MoRSE weighted by vdw volume (distance = 13)
1433		Mor14v	MoRSE ('v', 14)	3D	3D-MoRSE weighted by vdw volume (distance = 14)
1434		Mor15v	MoRSE ('v', 15)	3D	3D-MoRSE weighted by vdw volume (distance = 15)
1435		Mor16v	MoRSE ('v', 16)	3D	3D-MoRSE weighted by vdw volume (distance = 16)
1436		Mor17v	MoRSE ('v', 17)	3D	3D-MoRSE weighted by vdw volume (distance = 17)

#	module	name	constructor	dim	description
1437		Mor18v	MoRSE ('v', 18)	3D	3D-MoRSE weighted by vdw volume (distance = 18)
1438		Mor19v	MoRSE ('v', 19)	3D	3D-MoRSE weighted by vdw volume (distance = 19)
1439		Mor20v	MoRSE ('v', 20)	3D	3D-MoRSE weighted by vdw volume (distance = 20)
1440		Mor21v	MoRSE ('v', 21)	3D	3D-MoRSE weighted by vdw volume (distance = 21)
1441		Mor22v	MoRSE ('v', 22)	3D	3D-MoRSE weighted by vdw volume (distance = 22)
1442		Mor23v	MoRSE ('v', 23)	3D	3D-MoRSE weighted by vdw volume (distance = 23)
1443		Mor24v	MoRSE ('v', 24)	3D	3D-MoRSE weighted by vdw volume (distance = 24)
1444		Mor25v	MoRSE ('v', 25)	3D	3D-MoRSE weighted by vdw volume (distance = 25)
1445		Mor26v	MoRSE ('v', 26)	3D	3D-MoRSE weighted by vdw volume (distance = 26)
1446		Mor27v	MoRSE ('v', 27)	3D	3D-MoRSE weighted by vdw volume (distance = 27)
1447		Mor28v	MoRSE ('v', 28)	3D	3D-MoRSE weighted by vdw volume (distance = 28)
1448		Mor29v	MoRSE ('v', 29)	3D	3D-MoRSE weighted by vdw volume (distance = 29)
1449		Mor30v	MoRSE ('v', 30)	3D	3D-MoRSE weighted by vdw volume (distance = 30)

#	module	name	constructor	dim	description
1450		Mor31v	MoRSE ('v', 31)	3D	3D-MoRSE weighted by vdw volume (distance = 31)
1451		Mor32v	MoRSE ('v', 32)	3D	3D-MoRSE weighted by vdw volume (distance = 32)
1452		Mor01se	MoRSE ('se', 1)	3D	3D-MoRSE weighted by sanderson EN (distance = 1)
1453		Mor02se	MoRSE ('se', 2)	3D	3D-MoRSE weighted by sanderson EN (distance = 2)
1454		Mor03se	MoRSE ('se', 3)	3D	3D-MoRSE weighted by sanderson EN (distance = 3)
1455		Mor04se	MoRSE ('se', 4)	3D	3D-MoRSE weighted by sanderson EN (distance = 4)
1456		Mor05se	MoRSE ('se', 5)	3D	3D-MoRSE weighted by sanderson EN (distance = 5)
1457		Mor06se	MoRSE ('se', 6)	3D	3D-MoRSE weighted by sanderson EN (distance = 6)
1458		Mor07se	MoRSE ('se', 7)	3D	3D-MoRSE weighted by sanderson EN (distance = 7)
1459		Mor08se	MoRSE ('se', 8)	3D	3D-MoRSE weighted by sanderson EN (distance = 8)
1460		Mor09se	MoRSE ('se', 9)	3D	3D-MoRSE weighted by sanderson EN (distance = 9)
1461		Mor10se	MoRSE ('se', 10)	3D	3D-MoRSE weighted by sanderson EN (distance = 10)
1462		Mor11se	MoRSE ('se', 11)	3D	3D-MoRSE weighted by sanderson EN (distance = 11)

#	module	name	constructor	dim	description
1463		Mor12se	MoRSE ('se', 12)	3D	3D-MoRSE weighted by sanderson EN (distance = 12)
1464		Mor13se	MoRSE ('se', 13)	3D	3D-MoRSE weighted by sanderson EN (distance = 13)
1465		Mor14se	MoRSE ('se', 14)	3D	3D-MoRSE weighted by sanderson EN (distance = 14)
1466		Mor15se	MoRSE ('se', 15)	3D	3D-MoRSE weighted by sanderson EN (distance = 15)
1467		Mor16se	MoRSE ('se', 16)	3D	3D-MoRSE weighted by sanderson EN (distance = 16)
1468		Mor17se	MoRSE ('se', 17)	3D	3D-MoRSE weighted by sanderson EN (distance = 17)
1469		Mor18se	MoRSE ('se', 18)	3D	3D-MoRSE weighted by sanderson EN (distance = 18)
1470		Mor19se	MoRSE ('se', 19)	3D	3D-MoRSE weighted by sanderson EN (distance = 19)
1471		Mor20se	MoRSE ('se', 20)	3D	3D-MoRSE weighted by sanderson EN (distance = 20)
1472		Mor21se	MoRSE ('se', 21)	3D	3D-MoRSE weighted by sanderson EN (distance = 21)
1473		Mor22se	MoRSE ('se', 22)	3D	3D-MoRSE weighted by sanderson EN (distance = 22)
1474		Mor23se	MoRSE ('se', 23)	3D	3D-MoRSE weighted by sanderson EN (distance = 23)
1475		Mor24se	MoRSE ('se', 24)	3D	3D-MoRSE weighted by sanderson EN (distance = 24)

#	module	name	constructor	dim	description
1476		Mor25se	MoRSE ('se', 25)	3D	3D-MoRSE weighted by sanderson EN (distance = 25)
1477		Mor26se	MoRSE ('se', 26)	3D	3D-MoRSE weighted by sanderson EN (distance = 26)
1478		Mor27se	MoRSE ('se', 27)	3D	3D-MoRSE weighted by sanderson EN (distance = 27)
1479		Mor28se	MoRSE ('se', 28)	3D	3D-MoRSE weighted by sanderson EN (distance = 28)
1480		Mor29se	MoRSE ('se', 29)	3D	3D-MoRSE weighted by sanderson EN (distance = 29)
1481		Mor30se	MoRSE ('se', 30)	3D	3D-MoRSE weighted by sanderson EN (distance = 30)
1482		Mor31se	MoRSE ('se', 31)	3D	3D-MoRSE weighted by sanderson EN (distance = 31)
1483		Mor32se	MoRSE ('se', 32)	3D	3D-MoRSE weighted by sanderson EN (distance = 32)
1484		Mor01p	MoRSE ('p', 1)	3D	3D-MoRSE weighted by polarizability (distance = 1)
1485		Mor02p	MoRSE ('p', 2)	3D	3D-MoRSE weighted by polarizability (distance = 2)
1486		Mor03p	MoRSE ('p', 3)	3D	3D-MoRSE weighted by polarizability (distance = 3)
1487		Mor04p	MoRSE ('p', 4)	3D	3D-MoRSE weighted by polarizability (distance = 4)
1488		Mor05p	MoRSE ('p', 5)	3D	3D-MoRSE weighted by polarizability (distance = 5)

#	module	name	constructor	dim	description
1489		Mor06p	MoRSE ('p', 6)	3D	3D-MoRSE weighted by polarizability (distance = 6)
1490		Mor07p	MoRSE ('p', 7)	3D	3D-MoRSE weighted by polarizability (distance = 7)
1491		Mor08p	MoRSE ('p', 8)	3D	3D-MoRSE weighted by polarizability (distance = 8)
1492		Mor09p	MoRSE ('p', 9)	3D	3D-MoRSE weighted by polarizability (distance = 9)
1493		Mor10p	MoRSE ('p', 10)	3D	3D-MoRSE weighted by polarizability (distance = 10)
1494		Mor11p	MoRSE ('p', 11)	3D	3D-MoRSE weighted by polarizability (distance = 11)
1495		Mor12p	MoRSE ('p', 12)	3D	3D-MoRSE weighted by polarizability (distance = 12)
1496		Mor13p	MoRSE ('p', 13)	3D	3D-MoRSE weighted by polarizability (distance = 13)
1497		Mor14p	MoRSE ('p', 14)	3D	3D-MoRSE weighted by polarizability (distance = 14)
1498		Mor15p	MoRSE ('p', 15)	3D	3D-MoRSE weighted by polarizability (distance = 15)
1499		Mor16p	MoRSE ('p', 16)	3D	3D-MoRSE weighted by polarizability (distance = 16)
1500		Mor17p	MoRSE ('p', 17)	3D	3D-MoRSE weighted by polarizability (distance = 17)
1501		Mor18p	MoRSE ('p', 18)	3D	3D-MoRSE weighted by polarizability (distance = 18)

#	module	name	constructor	dim	description
1502		Mor19p	MoRSE ('p', 19)	3D	3D-MoRSE weighted by polarizability (distance = 19)
1503		Mor20p	MoRSE ('p', 20)	3D	3D-MoRSE weighted by polarizability (distance = 20)
1504		Mor21p	MoRSE ('p', 21)	3D	3D-MoRSE weighted by polarizability (distance = 21)
1505		Mor22p	MoRSE ('p', 22)	3D	3D-MoRSE weighted by polarizability (distance = 22)
1506		Mor23p	MoRSE ('p', 23)	3D	3D-MoRSE weighted by polarizability (distance = 23)
1507		Mor24p	MoRSE ('p', 24)	3D	3D-MoRSE weighted by polarizability (distance = 24)
1508		Mor25p	MoRSE ('p', 25)	3D	3D-MoRSE weighted by polarizability (distance = 25)
1509		Mor26p	MoRSE ('p', 26)	3D	3D-MoRSE weighted by polarizability (distance = 26)
1510		Mor27p	MoRSE ('p', 27)	3D	3D-MoRSE weighted by polarizability (distance = 27)
1511		Mor28p	MoRSE ('p', 28)	3D	3D-MoRSE weighted by polarizability (distance = 28)
1512		Mor29p	MoRSE ('p', 29)	3D	3D-MoRSE weighted by polarizability (distance = 29)
1513		Mor30p	MoRSE ('p', 30)	3D	3D-MoRSE weighted by polarizability (distance = 30)
1514		Mor31p	MoRSE ('p', 31)	3D	3D-MoRSE weighted by polarizability (distance = 31)

#	module	name	constructor	dim	description
1515		Mor32p	MoRSE ('p', 32)	3D	3D-MoRSE weighted by polarizability (distance = 32)
1516	MoeType	LabuteASA	LabuteASA ()	2D	Labute's Approximate Surface Area
1517		PEOE_VSA1	PEOE_VSA (1)	2D	MOE Charge VSA Descriptor 1 (-inf < x < -0.30)
1518		PEOE_VSA2	PEOE_VSA (2)	2D	MOE Charge VSA Descriptor 2 (-0.30 <= x < -0.25)
1519		PEOE_VSA3	PEOE_VSA (3)	2D	MOE Charge VSA Descriptor 3 (-0.25 <= x < -0.20)
1520		PEOE_VSA4	PEOE_VSA (4)	2D	MOE Charge VSA Descriptor 4 (-0.20 <= x < -0.15)
1521		PEOE_VSA5	PEOE_VSA (5)	2D	MOE Charge VSA Descriptor 5 (-0.15 <= x < -0.10)
1522		PEOE_VSA6	PEOE_VSA (6)	2D	MOE Charge VSA Descriptor 6 (-0.10 <= x < -0.05)
1523		PEOE_VSA7	PEOE_VSA (7)	2D	MOE Charge VSA Descriptor 7 (-0.05 <= x < 0.00)
1524		PEOE_VSA8	PEOE_VSA (8)	2D	MOE Charge VSA Descriptor 8 (0.00 <= x < 0.05)
1525		PEOE_VSA9	PEOE_VSA (9)	2D	MOE Charge VSA Descriptor 9 (0.05 <= x < 0.10)
1526		PEOE_VSA10	PEOE_VSA (10)	2D	MOE Charge VSA Descriptor 10 (0.10 <= x < 0.15)
1527		PEOE_VSA11	PEOE_VSA (11)	2D	MOE Charge VSA Descriptor 11 (0.15 <= x < 0.20)

#	module	name	constructor	dim	description
1528		PEOE_VSA12	PEOE_VSA (12)	2D	MOE Charge VSA Descriptor 12 (0.20 <= x < 0.25)
1529		PEOE_VSA13	PEOE_VSA (13)	2D	MOE Charge VSA Descriptor 13 (0.25 <= x < 0.30)
1530		SMR_VSA1	SMR_VSA (1)	2D	MOE MR VSA Descriptor 1 (-inf < x < 1.29)
1531		SMR_VSA2	SMR_VSA (2)	2D	MOE MR VSA Descriptor 2 (1.29 <= x < 1.82)
1532		SMR_VSA3	SMR_VSA (3)	2D	MOE MR VSA Descriptor 3 (1.82 <= x < 2.24)
1533		SMR_VSA4	SMR_VSA (4)	2D	MOE MR VSA Descriptor 4 (2.24 <= x < 2.45)
1534		SMR_VSA5	SMR_VSA (5)	2D	MOE MR VSA Descriptor 5 (2.45 <= x < 2.75)
1535		SMR_VSA6	SMR_VSA (6)	2D	MOE MR VSA Descriptor 6 (2.75 <= x < 3.05)
1536		SMR_VSA7	SMR_VSA (7)	2D	MOE MR VSA Descriptor 7 (3.05 <= x < 3.63)
1537		SMR_VSA8	SMR_VSA (8)	2D	MOE MR VSA Descriptor 8 (3.63 <= x < 3.80)
1538		SMR_VSA9	SMR_VSA (9)	2D	MOE MR VSA Descriptor 9 (3.80 <= x < 4.00)
1539		SlogP_VSA1	SlogP_VSA (1)	2D	MOE logP VSA Descriptor 1 (-inf < x < -0.40)
1540		SlogP_VSA2	SlogP_VSA (2)	2D	MOE logP VSA Descriptor 2 (-0.40 <= x < -0.20)

#	module	name	constructor	dim	description
1541		SlogP_VSA3	SlogP_VSA (3)	2D	MOE logP VSA Descriptor 3 (-0.20 <= x < 0.00)
1542		SlogP_VSA4	SlogP_VSA (4)	2D	MOE logP VSA Descriptor 4 (0.00 <= x < 0.10)
1543		SlogP_VSA5	SlogP_VSA (5)	2D	MOE logP VSA Descriptor 5 (0.10 <= x < 0.15)
1544		SlogP_VSA6	SlogP_VSA (6)	2D	MOE logP VSA Descriptor 6 (0.15 <= x < 0.20)
1545		SlogP_VSA7	SlogP_VSA (7)	2D	MOE logP VSA Descriptor 7 (0.20 <= x < 0.25)
1546		SlogP_VSA8	SlogP_VSA (8)	2D	MOE logP VSA Descriptor 8 (0.25 <= x < 0.30)
1547		SlogP_VSA9	SlogP_VSA (9)	2D	MOE logP VSA Descriptor 9 (0.30 <= x < 0.40)
1548		SlogP_VSA10	SlogP_VSA (10)	2D	MOE logP VSA Descriptor 10 (0.40 <= x < 0.50)
1549		SlogP_VSA11	SlogP_VSA (11)	2D	MOE logP VSA Descriptor 11 (0.50 <= x < 0.60)
1550		EState_VSA1	EState_VSA (1)	2D	EState VSA Descriptor 1 (-inf < x < -0.39)
1551		EState_VSA2	EState_VSA (2)	2D	EState VSA Descriptor 2 (-0.39 <= x < 0.29)
1552		EState_VSA3	EState_VSA (3)	2D	EState VSA Descriptor 3 (0.29 <= x < 0.72)
1553		EState_VSA4	EState_VSA (4)	2D	EState VSA Descriptor 4 (0.72 <= x < 1.17)

#	module	name	constructor	dim	description
1554		EState_VSA5	EState_VSA (5)	2D	EState VSA Descriptor 5 (1.17 <= x < 1.54)
1555		EState_VSA6	EState_VSA (6)	2D	EState VSA Descriptor 6 (1.54 <= x < 1.81)
1556		EState_VSA7	EState_VSA (7)	2D	EState VSA Descriptor 7 (1.81 <= x < 2.05)
1557		EState_VSA8	EState_VSA (8)	2D	EState VSA Descriptor 8 (2.05 <= x < 4.69)
1558		EState_VSA9	EState_VSA (9)	2D	EState VSA Descriptor 9 (4.69 <= x < 9.17)
1559		EState_VSA10	EState_VSA (10)	2D	EState VSA Descriptor 10 (9.17 <= x < 15.00)
1560		VSA_EState1	VSA_EState (1)	2D	VSA EState Descriptor 1 (-inf < x < 4.78)
1561		VSA_EState2	VSA_EState (2)	2D	VSA EState Descriptor 2 (4.78 <= x < 5.00)
1562		VSA_EState3	VSA_EState (3)	2D	VSA EState Descriptor 3 (5.00 <= x < 5.41)
1563		VSA_EState4	VSA_EState (4)	2D	VSA EState Descriptor 4 (5.41 <= x < 5.74)
1564		VSA_EState5	VSA_EState (5)	2D	VSA EState Descriptor 5 (5.74 <= x < 6.00)
1565		VSA_EState6	VSA_EState (6)	2D	VSA EState Descriptor 6 (6.00 <= x < 6.07)
1566		VSA_EState7	VSA_EState (7)	2D	VSA EState Descriptor 7 (6.07 <= x < 6.45)

#	module	name	constructor	dim	description
1567		VSA_EState8	VSA_EState (8)	2D	VSA EState Descriptor 8 (6.45 <= x < 7.00)
1568		VSA_EState9	VSA_EState (9)	2D	VSA EState Descriptor 9 (7.00 <= x < 11.00)
1569	MolecularDistanceEdge	MDEC-11	MolecularDistanceEdge (1, 1, 'C')	2D	molecular distance edge between primary C and primary C
1570		MDEC-12	MolecularDistanceEdge (1, 2, 'C')	2D	molecular distance edge between primary C and secondary C
1571		MDEC-13	MolecularDistanceEdge (1, 3, 'C')	2D	molecular distance edge between primary C and tertiary C
1572		MDEC-14	MolecularDistanceEdge (1, 4, 'C')	2D	molecular distance edge between primary C and quaternary C
1573		MDEC-22	MolecularDistanceEdge (2, 2, 'C')	2D	molecular distance edge between secondary C and secondary C
1574		MDEC-23	MolecularDistanceEdge (2, 3, 'C')	2D	molecular distance edge between secondary C and tertiary C
1575		MDEC-24	MolecularDistanceEdge (2, 4, 'C')	2D	molecular distance edge between secondary C and quaternary C
1576		MDEC-33	MolecularDistanceEdge (3, 3, 'C')	2D	molecular distance edge between tertiary C and tertiary C

#	module	name	constructor	dim	description
1577		MDEC-34	MolecularDistanceEdge (3, 4, 'C')	2D	molecular distance edge between tertiary C and quaternary C
1578		MDEC-44	MolecularDistanceEdge (4, 4, 'C')	2D	molecular distance edge between quaternary C and quaternary C
1579		MDEO-11	MolecularDistanceEdge (1, 1, 'O')	2D	molecular distance edge between primary O and primary O
1580		MDEO-12	MolecularDistanceEdge (1, 2, 'O')	2D	molecular distance edge between primary O and secondary O
1581		MDEO-22	MolecularDistanceEdge (2, 2, 'O')	2D	molecular distance edge between secondary O and secondary O
1582		MDEN-11	MolecularDistanceEdge (1, 1, 'N')	2D	molecular distance edge between primary N and primary N
1583		MDEN-12	MolecularDistanceEdge (1, 2, 'N')	2D	molecular distance edge between primary N and secondary N
1584		MDEN-13	MolecularDistanceEdge (1, 3, 'N')	2D	molecular distance edge between primary N and tertiary N
1585		MDEN-22	MolecularDistanceEdge (2, 2, 'N')	2D	molecular distance edge between secondary N and secondary N
1586		MDEN-23	MolecularDistanceEdge (2, 3, 'N')	2D	molecular distance edge between secondary N and tertiary N

#	module	name	constructor	dim	description
1587		MDEN-33	MolecularDistanceEdge (3, 3, 'N')	2D	molecular distance edge between tertiary N and tertiary N
1588	MoleculariId	MID	MoleculariId ('any', False, 1e-10)	2D	molecular ID
1589		AMID	MoleculariId ('any', True, 1e-10)	2D	averaged molecular ID
1590		MID_h	MoleculariId ('hetero', False, 1e-10)	2D	molecular ID on h atoms
1591		AMID_h	MoleculariId ('hetero', True, 1e-10)	2D	averaged molecular ID on h atoms
1592		MID_C	MoleculariId ('C', False, 1e-10)	2D	molecular ID on C atoms
1593		AMID_C	MoleculariId ('C', True, 1e-10)	2D	averaged molecular ID on C atoms
1594		MID_N	MoleculariId ('N', False, 1e-10)	2D	molecular ID on N atoms
1595		AMID_N	MoleculariId ('N', True, 1e-10)	2D	averaged molecular ID on N atoms
1596		MID_O	MoleculariId ('O', False, 1e-10)	2D	molecular ID on O atoms
1597		AMID_O	MoleculariId ('O', True, 1e-10)	2D	averaged molecular ID on O atoms
1598		MID_X	MoleculariId ('X', False, 1e-10)	2D	molecular ID on halogen atoms
1599		AMID_X	MoleculariId ('X', True, 1e-10)	2D	averaged molecular ID on halogen atoms
1600	MomentOfInertia	MOMI-X	MomentOfInertia ('X')	3D	moment of inertia (axis = X)
1601		MOMI-Y	MomentOfInertia ('Y')	3D	moment of inertia (axis = Y)
1602		MOMI-Z	MomentOfInertia ('Z')	3D	moment of inertia (axis = Z)
1603	PBF	PBF	PBF ()	3D	PBF
1604	PathCount	MPC2	PathCount (2, False, False, False)	2D	2-ordered path count
1605		MPC3	PathCount (3, False, False, False)	2D	3-ordered path count

#	module	name	constructor	dim	description
1606		MPC4	PathCount (4, False, False, False)	2D	4-ordered path count
1607		MPC5	PathCount (5, False, False, False)	2D	5-ordered path count
1608		MPC6	PathCount (6, False, False, False)	2D	6-ordered path count
1609		MPC7	PathCount (7, False, False, False)	2D	7-ordered path count
1610		MPC8	PathCount (8, False, False, False)	2D	8-ordered path count
1611		MPC9	PathCount (9, False, False, False)	2D	9-ordered path count
1612		MPC10	PathCount (10, False, False, False)	2D	10-ordered path count
1613		TMPC10	PathCount (10, False, True, False)	2D	10-ordered total path count
1614		piPC1	PathCount (1, True, False, True)	2D	1-ordered pi-path count (log scale)
1615		piPC2	PathCount (2, True, False, True)	2D	2-ordered pi-path count (log scale)
1616		piPC3	PathCount (3, True, False, True)	2D	3-ordered pi-path count (log scale)
1617		piPC4	PathCount (4, True, False, True)	2D	4-ordered pi-path count (log scale)
1618		piPC5	PathCount (5, True, False, True)	2D	5-ordered pi-path count (log scale)
1619		piPC6	PathCount (6, True, False, True)	2D	6-ordered pi-path count (log scale)
1620		piPC7	PathCount (7, True, False, True)	2D	7-ordered pi-path count (log scale)
1621		piPC8	PathCount (8, True, False, True)	2D	8-ordered pi-path count (log scale)
1622		piPC9	PathCount (9, True, False, True)	2D	9-ordered pi-path count (log scale)
1623		piPC10	PathCount (10, True, False, True)	2D	10-ordered pi-path count (log scale)

#	module	name	constructor	dim	description
1624		TpiPC10	PathCount (10, True, True, True)	2D	10-ordered total pi-path count (log scale)
1625	Polarizability	apol	APol (False)	2D	atomic polarizability
1626		bpol	BPol (False)	2D	bond polarizability
1627	RingCount	nRing	RingCount (None, False, False, None, None)	2D	ring count
1628		n3Ring	RingCount (3, False, False, None, None)	2D	3-membered ring count
1629		n4Ring	RingCount (4, False, False, None, None)	2D	4-membered ring count
1630		n5Ring	RingCount (5, False, False, None, None)	2D	5-membered ring count
1631		n6Ring	RingCount (6, False, False, None, None)	2D	6-membered ring count
1632		n7Ring	RingCount (7, False, False, None, None)	2D	7-membered ring count
1633		n8Ring	RingCount (8, False, False, None, None)	2D	8-membered ring count
1634		n9Ring	RingCount (9, False, False, None, None)	2D	9-membered ring count
1635		n10Ring	RingCount (10, False, False, None, None)	2D	10-membered ring count
1636		n11Ring	RingCount (11, False, False, None, None)	2D	11-membered ring count
1637		n12Ring	RingCount (12, False, False, None, None)	2D	12-membered ring count
1638		nG12Ring	RingCount (12, True, False, None, None)	2D	12-or-greater-membered ring count
1639		nHRing	RingCount (None, False, False, None, True)	2D	hetero ring count
1640		n3HRing	RingCount (3, False, False, None, True)	2D	3-membered hetero ring count
1641		n4HRing	RingCount (4, False, False, None, True)	2D	4-membered hetero ring count
1642		n5HRing	RingCount (5, False, False, None, True)	2D	5-membered hetero ring count
1643		n6HRing	RingCount (6, False, False, None, True)	2D	6-membered hetero ring count

#	module	name	constructor	dim	description
1644		n7HRing	RingCount (7, False, False, None, True)	2D	7-membered hetero ring count
1645		n8HRing	RingCount (8, False, False, None, True)	2D	8-membered hetero ring count
1646		n9HRing	RingCount (9, False, False, None, True)	2D	9-membered hetero ring count
1647		n10HRing	RingCount (10, False, False, None, True)	2D	10-membered hetero ring count
1648		n11HRing	RingCount (11, False, False, None, True)	2D	11-membered hetero ring count
1649		n12HRing	RingCount (12, False, False, None, True)	2D	12-membered hetero ring count
1650		nG12HRing	RingCount (12, True, False, None, True)	2D	12-or-greater-membered hetero ring count
1651		naRing	RingCount (None, False, False, True, None)	2D	aromatic ring count
1652		n3aRing	RingCount (3, False, False, True, None)	2D	3-membered aromatic ring count
1653		n4aRing	RingCount (4, False, False, True, None)	2D	4-membered aromatic ring count
1654		n5aRing	RingCount (5, False, False, True, None)	2D	5-membered aromatic ring count
1655		n6aRing	RingCount (6, False, False, True, None)	2D	6-membered aromatic ring count
1656		n7aRing	RingCount (7, False, False, True, None)	2D	7-membered aromatic ring count
1657		n8aRing	RingCount (8, False, False, True, None)	2D	8-membered aromatic ring count
1658		n9aRing	RingCount (9, False, False, True, None)	2D	9-membered aromatic ring count
1659		n10aRing	RingCount (10, False, False, True, None)	2D	10-membered aromatic ring count
1660		n11aRing	RingCount (11, False, False, True, None)	2D	11-membered aromatic ring count

#	module	name	constructor	dim	description
1661		n12aRing	RingCount (12, False, False, True, None)	2D	12-membered aromatic ring count
1662		nG12aRing	RingCount (12, True, False, True, None)	2D	12-or-greater-membered aromatic ring count
1663		naHRing	RingCount (None, False, False, True, True)	2D	aromatic hetero ring count
1664		n3aHRing	RingCount (3, False, False, True, True)	2D	3-membered aromatic hetero ring count
1665		n4aHRing	RingCount (4, False, False, True, True)	2D	4-membered aromatic hetero ring count
1666		n5aHRing	RingCount (5, False, False, True, True)	2D	5-membered aromatic hetero ring count
1667		n6aHRing	RingCount (6, False, False, True, True)	2D	6-membered aromatic hetero ring count
1668		n7aHRing	RingCount (7, False, False, True, True)	2D	7-membered aromatic hetero ring count
1669		n8aHRing	RingCount (8, False, False, True, True)	2D	8-membered aromatic hetero ring count
1670		n9aHRing	RingCount (9, False, False, True, True)	2D	9-membered aromatic hetero ring count
1671		n10aHRing	RingCount (10, False, False, True, True)	2D	10-membered aromatic hetero ring count
1672		n11aHRing	RingCount (11, False, False, True, True)	2D	11-membered aromatic hetero ring count
1673		n12aHRing	RingCount (12, False, False, True, True)	2D	12-membered aromatic hetero ring count

#	module	name	constructor	dim	description
1674		nG12aHRing	RingCount (12, True, False, True, True)	2D	12-or-greater-membered aromatic hetero ring count
1675		nARing	RingCount (None, False, False, False, None)	2D	aliphatic ring count
1676		n3ARing	RingCount (3, False, False, False, None)	2D	3-membered aliphatic ring count
1677		n4ARing	RingCount (4, False, False, False, None)	2D	4-membered aliphatic ring count
1678		n5ARing	RingCount (5, False, False, False, None)	2D	5-membered aliphatic ring count
1679		n6ARing	RingCount (6, False, False, False, None)	2D	6-membered aliphatic ring count
1680		n7ARing	RingCount (7, False, False, False, None)	2D	7-membered aliphatic ring count
1681		n8ARing	RingCount (8, False, False, False, None)	2D	8-membered aliphatic ring count
1682		n9ARing	RingCount (9, False, False, False, None)	2D	9-membered aliphatic ring count
1683		n10ARing	RingCount (10, False, False, False, None)	2D	10-membered aliphatic ring count
1684		n11ARing	RingCount (11, False, False, False, None)	2D	11-membered aliphatic ring count
1685		n12ARing	RingCount (12, False, False, False, None)	2D	12-membered aliphatic ring count
1686		nG12ARing	RingCount (12, True, False, False, None)	2D	12-or-greater-membered aliphatic ring count
1687		nAHRing	RingCount (None, False, False, False, True)	2D	aliphatic hetero ring count
1688		n3AHRing	RingCount (3, False, False, False, True)	2D	3-membered aliphatic hetero ring count
1689		n4AHRing	RingCount (4, False, False, False, True)	2D	4-membered aliphatic hetero ring count

#	module	name	constructor	dim	description
1690		n5AHRing	RingCount (5, False, False, False, True)	2D	5-membered aliphatic hetero ring count
1691		n6AHRing	RingCount (6, False, False, False, True)	2D	6-membered aliphatic hetero ring count
1692		n7AHRing	RingCount (7, False, False, False, True)	2D	7-membered aliphatic hetero ring count
1693		n8AHRing	RingCount (8, False, False, False, True)	2D	8-membered aliphatic hetero ring count
1694		n9AHRing	RingCount (9, False, False, False, True)	2D	9-membered aliphatic hetero ring count
1695		n10AHRing	RingCount (10, False, False, False, True)	2D	10-membered aliphatic hetero ring count
1696		n11AHRing	RingCount (11, False, False, False, True)	2D	11-membered aliphatic hetero ring count
1697		n12AHRing	RingCount (12, False, False, False, True)	2D	12-membered aliphatic hetero ring count
1698		nG12AHRing	RingCount (12, True, False, False, True)	2D	12-or-greater-membered aliphatic hetero ring count
1699		nFRing	RingCount (None, False, True, None, None)	2D	fused ring count
1700		n4FRing	RingCount (4, False, True, None, None)	2D	4-membered fused ring count
1701		n5FRing	RingCount (5, False, True, None, None)	2D	5-membered fused ring count
1702		n6FRing	RingCount (6, False, True, None, None)	2D	6-membered fused ring count
1703		n7FRing	RingCount (7, False, True, None, None)	2D	7-membered fused ring count
1704		n8FRing	RingCount (8, False, True, None, None)	2D	8-membered fused ring count
1705		n9FRing	RingCount (9, False, True, None, None)	2D	9-membered fused ring count
1706		n10FRing	RingCount (10, False, True, None, None)	2D	10-membered fused ring count

#	module	name	constructor	dim	description
1707		n11FRing	RingCount (11, False, True, None, None)	2D	11-membered fused ring count
1708		n12FRing	RingCount (12, False, True, None, None)	2D	12-membered fused ring count
1709		nG12FRing	RingCount (12, True, True, None, None)	2D	12-or-greater-membered fused ring count
1710		nFHRing	RingCount (None, False, True, None, True)	2D	fused hetero ring count
1711		n4FHRing	RingCount (4, False, True, None, True)	2D	4-membered fused hetero ring count
1712		n5FHRing	RingCount (5, False, True, None, True)	2D	5-membered fused hetero ring count
1713		n6FHRing	RingCount (6, False, True, None, True)	2D	6-membered fused hetero ring count
1714		n7FHRing	RingCount (7, False, True, None, True)	2D	7-membered fused hetero ring count
1715		n8FHRing	RingCount (8, False, True, None, True)	2D	8-membered fused hetero ring count
1716		n9FHRing	RingCount (9, False, True, None, True)	2D	9-membered fused hetero ring count
1717		n10FHRing	RingCount (10, False, True, None, True)	2D	10-membered fused hetero ring count
1718		n11FHRing	RingCount (11, False, True, None, True)	2D	11-membered fused hetero ring count
1719		n12FHRing	RingCount (12, False, True, None, True)	2D	12-membered fused hetero ring count
1720		nG12FHRing	RingCount (12, True, True, None, True)	2D	12-or-greater-membered fused hetero ring count
1721		nFaRing	RingCount (None, False, True, True, None)	2D	aromatic fused ring count
1722		n4FaRing	RingCount (4, False, True, True, None)	2D	4-membered aromatic fused ring count
1723		n5FaRing	RingCount (5, False, True, True, None)	2D	5-membered aromatic fused ring count

#	module	name	constructor	dim	description
1724		n6FaRing	RingCount (6, False, True, True, None)	2D	6-membered aromatic fused ring count
1725		n7FaRing	RingCount (7, False, True, True, None)	2D	7-membered aromatic fused ring count
1726		n8FaRing	RingCount (8, False, True, True, None)	2D	8-membered aromatic fused ring count
1727		n9FaRing	RingCount (9, False, True, True, None)	2D	9-membered aromatic fused ring count
1728		n10FaRing	RingCount (10, False, True, True, None)	2D	10-membered aromatic fused ring count
1729		n11FaRing	RingCount (11, False, True, True, None)	2D	11-membered aromatic fused ring count
1730		n12FaRing	RingCount (12, False, True, True, None)	2D	12-membered aromatic fused ring count
1731		nG12FaRing	RingCount (12, True, True, True, None)	2D	12-or-greater-membered aromatic fused ring count
1732		nFaHRing	RingCount (None, False, True, True, True)	2D	aromatic fused hetero ring count
1733		n4FaHRing	RingCount (4, False, True, True, True)	2D	4-membered aromatic fused hetero ring count
1734		n5FaHRing	RingCount (5, False, True, True, True)	2D	5-membered aromatic fused hetero ring count
1735		n6FaHRing	RingCount (6, False, True, True, True)	2D	6-membered aromatic fused hetero ring count
1736		n7FaHRing	RingCount (7, False, True, True, True)	2D	7-membered aromatic fused hetero ring count
1737		n8FaHRing	RingCount (8, False, True, True, True)	2D	8-membered aromatic fused hetero ring count

#	module	name	constructor	dim	description
1738		n9FaHRing	RingCount (9, False, True, True, True)	2D	9-membered aromatic fused hetero ring count
1739		n10FaHRing	RingCount (10, False, True, True, True)	2D	10-membered aromatic fused hetero ring count
1740		n11FaHRing	RingCount (11, False, True, True, True)	2D	11-membered aromatic fused hetero ring count
1741		n12FaHRing	RingCount (12, False, True, True, True)	2D	12-membered aromatic fused hetero ring count
1742		nG12FaHRing	RingCount (12, True, True, True, True)	2D	12-or-greater-membered aromatic fused hetero ring count
1743		nFARing	RingCount (None, False, True, False, None)	2D	aliphatic fused ring count
1744		n4FARing	RingCount (4, False, True, False, None)	2D	4-membered aliphatic fused ring count
1745		n5FARing	RingCount (5, False, True, False, None)	2D	5-membered aliphatic fused ring count
1746		n6FARing	RingCount (6, False, True, False, None)	2D	6-membered aliphatic fused ring count
1747		n7FARing	RingCount (7, False, True, False, None)	2D	7-membered aliphatic fused ring count
1748		n8FARing	RingCount (8, False, True, False, None)	2D	8-membered aliphatic fused ring count
1749		n9FARing	RingCount (9, False, True, False, None)	2D	9-membered aliphatic fused ring count
1750		n10FARing	RingCount (10, False, True, False, None)	2D	10-membered aliphatic fused ring count
1751		n11FARing	RingCount (11, False, True, False, None)	2D	11-membered aliphatic fused ring count
1752		n12FARing	RingCount (12, False, True, False, None)	2D	12-membered aliphatic fused ring count

#	module	name	constructor	dim	description
1753		nG12FARing	RingCount (12, True, True, False, None)	2D	12-or-greater-membered aliphatic fused ring count
1754		nFAHRing	RingCount (None, False, True, False, True)	2D	aliphatic fused hetero ring count
1755		n4FAHRing	RingCount (4, False, True, False, True)	2D	4-membered aliphatic fused hetero ring count
1756		n5FAHRing	RingCount (5, False, True, False, True)	2D	5-membered aliphatic fused hetero ring count
1757		n6FAHRing	RingCount (6, False, True, False, True)	2D	6-membered aliphatic fused hetero ring count
1758		n7FAHRing	RingCount (7, False, True, False, True)	2D	7-membered aliphatic fused hetero ring count
1759		n8FAHRing	RingCount (8, False, True, False, True)	2D	8-membered aliphatic fused hetero ring count
1760		n9FAHRing	RingCount (9, False, True, False, True)	2D	9-membered aliphatic fused hetero ring count
1761		n10FAHRing	RingCount (10, False, True, False, True)	2D	10-membered aliphatic fused hetero ring count
1762		n11FAHRing	RingCount (11, False, True, False, True)	2D	11-membered aliphatic fused hetero ring count
1763		n12FAHRing	RingCount (12, False, True, False, True)	2D	12-membered aliphatic fused hetero ring count
1764		nG12FAHRing	RingCount (12, True, True, False, True)	2D	12-or-greater-membered aliphatic fused hetero ring count
1765	RotatableBond	nRot	RotatableBondsCount ()	2D	rotatable bonds count
1766		RotRatio	RotatableBondsRatio ()	2D	rotatable bonds ratio

#	module	name	constructor	dim	description
1767	SLogP	SLogP	SLogP ()	2D	Wildman-Crippen LogP
1768		SMR	SMR ()	2D	Wildman-Crippen MR
1769	TopoPSA	TopoPSA(NO)	TopoPSA (True)	2D	topological polar surface area (use only nitrogen and oxygen)
1770		TopoPSA	TopoPSA (False)	2D	topological polar surface area
1771	TopologicalCharge	GGI1	TopologicalCharge ('raw', 1)	2D	1-ordered raw topological charge
1772		GGI2	TopologicalCharge ('raw', 2)	2D	2-ordered raw topological charge
1773		GGI3	TopologicalCharge ('raw', 3)	2D	3-ordered raw topological charge
1774		GGI4	TopologicalCharge ('raw', 4)	2D	4-ordered raw topological charge
1775		GGI5	TopologicalCharge ('raw', 5)	2D	5-ordered raw topological charge
1776		GGI6	TopologicalCharge ('raw', 6)	2D	6-ordered raw topological charge
1777		GGI7	TopologicalCharge ('raw', 7)	2D	7-ordered raw topological charge
1778		GGI8	TopologicalCharge ('raw', 8)	2D	8-ordered raw topological charge
1779		GGI9	TopologicalCharge ('raw', 9)	2D	9-ordered raw topological charge
1780		GGI10	TopologicalCharge ('raw', 10)	2D	10-ordered raw topological charge
1781		JGI1	TopologicalCharge ('mean', 1)	2D	1-ordered mean topological charge
1782		JGI2	TopologicalCharge ('mean', 2)	2D	2-ordered mean topological charge

#	module	name	constructor	dim	description
1783		JGI3	TopologicalCharge ('mean', 3)	2D	3-ordered mean topological charge
1784		JGI4	TopologicalCharge ('mean', 4)	2D	4-ordered mean topological charge
1785		JGI5	TopologicalCharge ('mean', 5)	2D	5-ordered mean topological charge
1786		JGI6	TopologicalCharge ('mean', 6)	2D	6-ordered mean topological charge
1787		JGI7	TopologicalCharge ('mean', 7)	2D	7-ordered mean topological charge
1788		JGI8	TopologicalCharge ('mean', 8)	2D	8-ordered mean topological charge
1789		JGI9	TopologicalCharge ('mean', 9)	2D	9-ordered mean topological charge
1790		JGI10	TopologicalCharge ('mean', 10)	2D	10-ordered mean topological charge
1791		JGT10	TopologicalCharge ('global', 10)	2D	10-ordered global topological charge
1792	TopologicalIndex	Diameter	Diameter ()	2D	topological diameter
1793		Radius	Radius ()	2D	topological radius
1794		TopoShapeIndex	TopologicalShapeIndex ()	2D	topological shape index
1795		PetitjeanIndex	PetitjeanIndex ()	2D	Petitjean index
1796	VdwVolumeABC	Vabc	VdwVolumeABC ()	2D	ABC van der waals volume
1797	VertexAdjacencyInformation	VAdjMat	VertexAdjacencyInformation ()	2D	vertex adjacency information
1798	WalkCount	MWC01	WalkCount (1, False, False)	2D	walk count (leg-1)

#	module	name	constructor	dim	description
1799		MWC02	WalkCount (2, False, False)	2D	walk count (leg-2)
1800		MWC03	WalkCount (3, False, False)	2D	walk count (leg-3)
1801		MWC04	WalkCount (4, False, False)	2D	walk count (leg-4)
1802		MWC05	WalkCount (5, False, False)	2D	walk count (leg-5)
1803		MWC06	WalkCount (6, False, False)	2D	walk count (leg-6)
1804		MWC07	WalkCount (7, False, False)	2D	walk count (leg-7)
1805		MWC08	WalkCount (8, False, False)	2D	walk count (leg-8)
1806		MWC09	WalkCount (9, False, False)	2D	walk count (leg-9)
1807		MWC10	WalkCount (10, False, False)	2D	walk count (leg-10)
1808		TMWC10	WalkCount (10, True, False)	2D	total walk count (leg-10)
1809		SRW02	WalkCount (2, False, True)	2D	walk count (leg-2, only self returning walk)
1810		SRW03	WalkCount (3, False, True)	2D	walk count (leg-3, only self returning walk)
1811		SRW04	WalkCount (4, False, True)	2D	walk count (leg-4, only self returning walk)
1812		SRW05	WalkCount (5, False, True)	2D	walk count (leg-5, only self returning walk)
1813		SRW06	WalkCount (6, False, True)	2D	walk count (leg-6, only self returning walk)
1814		SRW07	WalkCount (7, False, True)	2D	walk count (leg-7, only self returning walk)
1815		SRW08	WalkCount (8, False, True)	2D	walk count (leg-8, only self returning walk)

#	module	name	constructor	dim	description
1816		SRW09	WalkCount (9, False, True)	2D	walk count (leg-9, only self returning walk)
1817		SRW10	WalkCount (10, False, True)	2D	walk count (leg-10, only self returning walk)
1818		TSRW10	WalkCount (10, True, True)	2D	total walk count (leg-10, only self returning walk)
1819	Weight	MW	Weight (True, False)	2D	exact molecular weight
1820		AMW	Weight (True, True)	2D	averaged exact molecular weight
1821	WienerIndex	WPath	WienerIndex (False)	2D	Wiener index
1822		WPol	WienerIndex (True)	2D	Wiener polarity index
1823	ZagrebIndex	Zagreb1	ZagrebIndex (1, 1)	2D	Zagreb index (version 1)
1824		Zagreb2	ZagrebIndex (2, 1)	2D	Zagreb index (version 2)
1825		mZagreb1	ZagrebIndex (1, -1)	2D	modified Zagreb index (version 1)
1826		mZagreb2	ZagrebIndex (2, -1)	2D	modified Zagreb index (version 2)