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A MP2 study of Highly Strained $C_{12}H_{12}$ Hydrocarbons derived from Trivalent Graphs.

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ABSTRACT

The electronic structure and reactivity indices of the family of strained hydrogenated hydrocarbons having twelve vertices, eight faces and eighteen edges formed by carbon atoms was analyzed. This family is composed by fourteen members, having all the formula $(CH)_{12}$. Geometries were fully optimized with an all-electron RHF calculation, followed by a Møller-Plesset correlation energy correction truncated at second-order with a 6-311g(d,p) basis set. Steric energy and local atomic reactivity indices were also calculated and discussed.

Keywords: hydrocarbons, $C_{12}H_{12}$, MP2, steric energy, strained hydrocarbons.

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INTRODUCTION

During the last quarter of century the realm of pure carbon compounds become enriched by fullerenes, nanotubes of several kinds, nanocones, graphene, etc. Less attention has been paid to the possible existence of carbon compounds with high strain energy that could exist in extreme conditions such as very high pressures or in some stellar objects (the pulsar PSR 1257+12, the millisecond pulsar PSR J1719-1438 and/or the extrasolar planet 55 Cancri e for example). As the number of different carbon compounds with high strain energy is extremely large, we need a rational approach for their study. The experimental and theoretical study of strained hydrocarbons is very active [1-52]. Being our interest the study of possible amorphous carbon components, it is then natural to begin to study compounds in which each carbon atom in the structure is bonded to three other carbon atoms. This gives us the possibility to study the stability of purely sp^3 -bonded systems able to form more complex structures by joining two or more single structures. To classify the different structures we shall use the geometric concept of polyhedron. In geometry, a polyhedron is simply a 3D solid which consists of a collection of polygons, usually joined at their edges. It is a special case of the more general polytope which can be defined on arbitrary dimensions. The graph obtained by collapsing a polyhedron into the plane is called the skeleton of the polyhedron. The graphs corresponding to polyhedra skeletons are called Schlegel graphs. These graphs have been employed in chemistry [53]. There is a formula, called the Descartes-Euler Polyhedral formula, which relates the number of vertices (V), faces (F) and edges (E) of a polyhedron:

$$F+V-E=2 \quad (1)$$

Here we focused our interest in the set of polyhedra with twelve vertices, eight faces and eighteen edges. They have all the formulas $(CH)_{12}$ for the hydrogenated form. Calling F_n the number of faces with N sides it can be shown that only fourteen polyhedra can be obtained [54]. They are listed in Table 1. Fig. 1 shows the corresponding Schlegel graphs.

Table 1: Possible polyhedra with 12 vertices, 8 faces and 18 edges.

Polyhedron	Symmetry	F_3	F_4	F_5	F_6	F_7
1	C_{2v}	2	4	0	0	2
2	C_1	3	1	2	1	1
3	C_1	2	3	1	1	1
4	C_s	2	2	3	0	1
5	I_h	4	0	0	4	0
6	C_s	3	1	1	3	0
7	C_{2v}	2	2	2	2	0
8	C_2	2	2	2	2	0
9	C_s	1	4	1	2	0
10	D_{6h}	0	6	0	2	0
11	C_{2v}	2	1	4	1	0
12	C_s	1	3	3	1	0
13	D_{3d}	2	0	6	0	0
14	D_{2d}	0	4	4	0	0

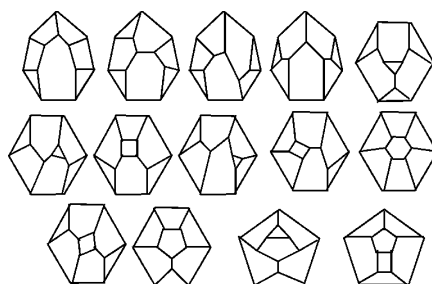


Figure 1: Schlegel graphs for the set of polyhedra with twelve vertices, eight faces and eighteen edges.

We can see that, if each point of the polyhedra corresponds to a carbon atom, then all atoms are bonded to three carbon atoms having only a free valence for hydrogenation. Fig. 2 shows the non hydrogenated equivalent molecules.

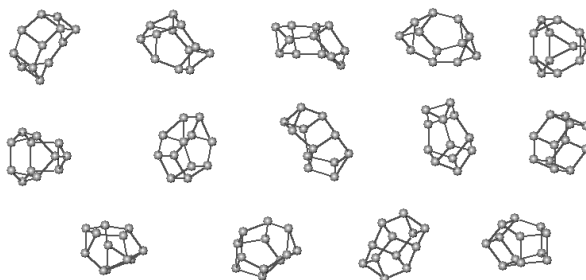


Figure 2: Non hydrogenated forms of the $C_{12}H_{12}$ set.

In this paper we present the results of an all-electron MP2 quantum-chemical study of the structure and reactivity of this set. As far as we know none of these molecules have been synthesized.

METHODS AND CALCULATIONS

All geometries were fully optimized with an all-electron Restricted Hartree-Fock calculation followed by a Møller-Plesset correlation energy correction truncated at second-order (MP2) with a 6-311g(d,p) basis set. The Gaussian 03 suite of programs was employed [55]. With the final geometries, a single-point calculation was carried out to get all the necessary extra information. The local atomic reactivity indices were calculated with the D-cent-QSAR software [56]. A property called “steric energy”, defined as the energy due to the position of the atoms in space in surplus of what would be estimated for an ideal constitutional isomer with ideal bond distances, angles, and dihedral angles, was calculated with Chem3D Ultra [57]. The steric energy has not a quantum-chemical origin, being historically directly rooted to Baeyer's Strain Theory [58].

RESULTS AND DISCUSSION

Table 2 shows the symmetry, the total and relative energies, the dipole moment and the steric energy.

Table 2: Symmetry, total and relative energies, dipole moment and steric energy.

Mol.	Symmetry	E (MP2) (au)	E_{REL} (Kcal/mol)	Dipole moment (D)	Steric energy (Kcal/mol)
1	C_{2v}	-463.18091425	119.56	0.06	155.92
2	C_1	-463.28039657	57.13	0.23	112.94
3	C_1	-463.25924559	70.41	0.07	135.81
4	C_5	-463.30134180	43.99	0.06	114.60
5	I_h	-463.31199845	37.30	0.00	70.78
6	C_5	-463.30500030	41.69	0.08	133.78
7	C_{2v}	-463.30634546	40.85	0.03	104.18
8	C_2	-463.30694659	40.47	0.01	105.00
9	C_5	-463.27805982	58.60	0.13	140.26
10	D_{6h}	-463.21133112	100.47	0.00	175.39
11	C_{2v}	-463.34660050	15.59	0.02	100.01
12	C_5	-463.30815354	39.72	0.11	118.92
13	D_{3d}	-463.37144484	0.00	0.00	67.25
14	D_{2d}	-463.31767986	33.74	0.00	133.49

We can see that the most stable system is molecule 13 followed by molecule 11. Molecules 10 and 11 are more than 100 Kcal/mol above molecule 13. If, steric energy can be considered as a semi-quantitative measure of the “distortion” of these molecular systems, then molecules 13 and 5 are the closest ones to an “ideal” situation. Figure 3 shows that there is no a linear relationship between E_{REL} and the steric energy.

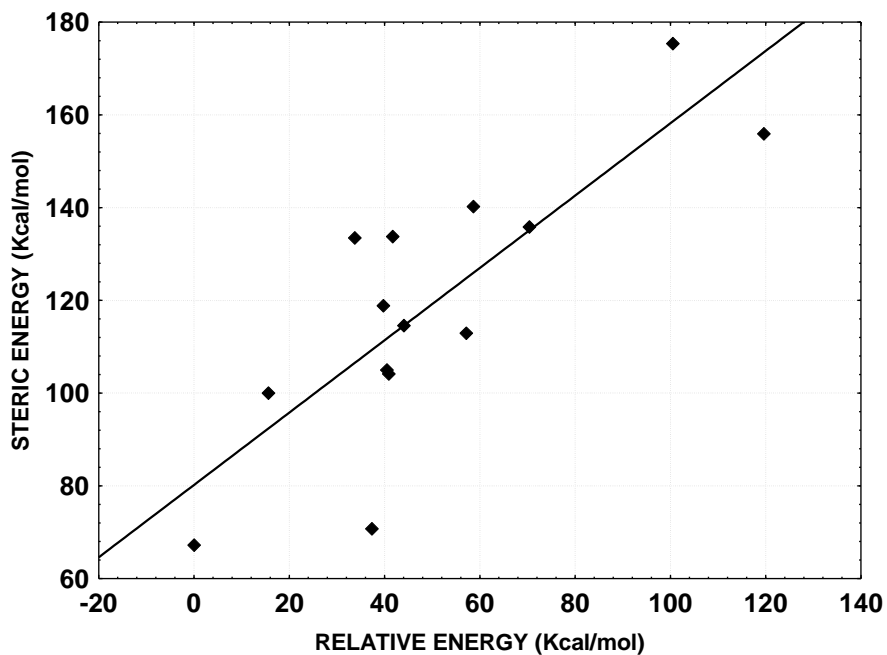


Figure 3: Plot of E_{REL} vs. steric energy.

Díaz showed that there exists the following operation allowing transforming one member of the $(CH)_{12}$ family into another:

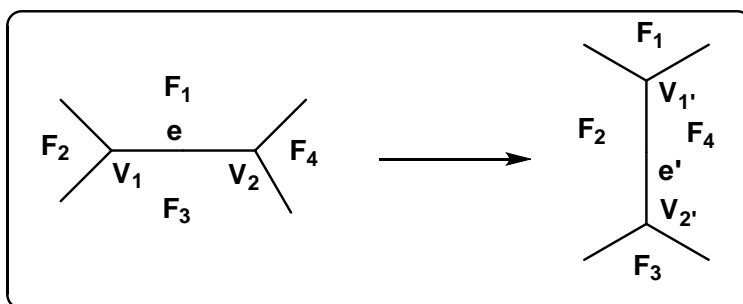


Figure 4: Operation to transform one molecule into another (F= face, e= edge, V= vertex).

Employing this operation we obtain the following relationships between the molecules:

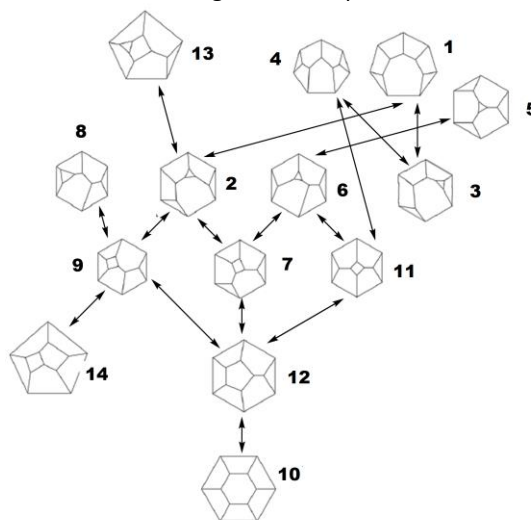


Figure 5: Possible transformations between the molecules accordingly to the operation shown in Fig. 4.

We can see that, if we start with molecule 13, we can produce only molecule 2. The aforementioned operation could serve as a starting point for a quantum-chemical analysis of the transformation mechanisms. Local atomic reactivity indices were successfully introduced in the study of formal quantitative structure-activity relationships [59, 60]. Tables 3 to 16 display, for each molecule, the local atomic chemical potential (μ , in eV), the local atomic hardness (η , in eV), the maximal amount of electronic charge that an atom may accept (Q^{\max}) and the local atomic electrophilic index (ω , in eV) (for the corresponding formulae, see [59]). Each Table is below the corresponding molecule.

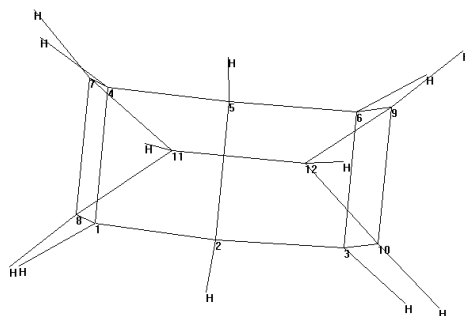


Figure 6: Molecule 1.

Table 3: Local atomic reactivity indices of molecule 1.

Atom	μ	η	Q^{\max}	ω
1	-2.2002	13.668	0.161	0.1771
2	-2.2002	13.668	0.161	0.1771
3	-2.2002	13.668	0.161	0.1771
4	-2.2002	13.668	0.161	0.1771
5	-2.2002	13.668	0.161	0.1771
6	-2.2002	13.668	0.161	0.1771
7	-2.2002	13.668	0.161	0.1771
8	-2.2002	13.668	0.161	0.1771
9	-2.2002	13.668	0.161	0.1771
10	-2.2002	13.668	0.161	0.1771
11	-1.5475	14.9733	0.1034	0.08
12	-1.5475	14.9733	0.1034	0.08

We can see that atoms 11 and 12 are hardest that the other carbon atoms and are less prone to receive extra charge. The hardness values are between 13.7 and 15 eV. All atoms show a very low electrophilicity.

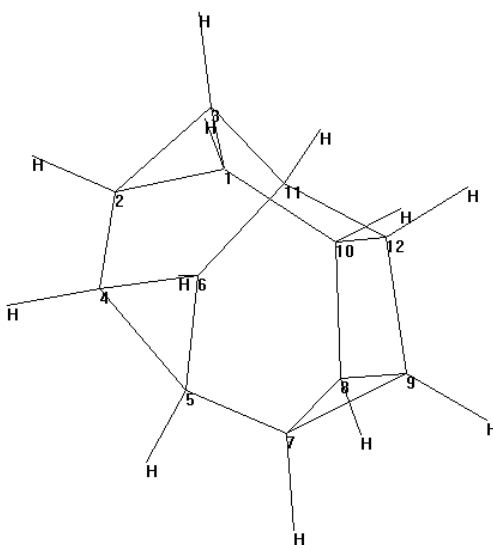


Figure 7: Molecule 2.

Table 4: Local atomic reactivity indices of molecule 2.

Atom	μ	η	Q^{\max}	ω
1	-1.9097	14.809	0.129	0.1231
2	-1.3051	16.0182	0.0815	0.0532
3	-2.16	14.3083	0.151	0.163
4	-1.3051	16.0182	0.0815	0.0532
5	-1.6611	15.3061	0.1085	0.0901
6	-1.7958	15.0367	0.1194	0.1072
7	-1.6611	15.3061	0.1085	0.0901
8	-1.9097	14.809	0.129	0.1231
9	-2.16	14.3083	0.151	0.163
10	-1.7052	15.218	0.1121	0.0955
11	-1.6611	15.3061	0.1085	0.0901
12	-1.9097	14.809	0.129	0.1231

Here we can observe that there is a variety of the amount of extra charge that a carbon atom may receive: from 0.08 to 0.13. In relation to molecule 1, the carbon atoms here have a higher hardness.

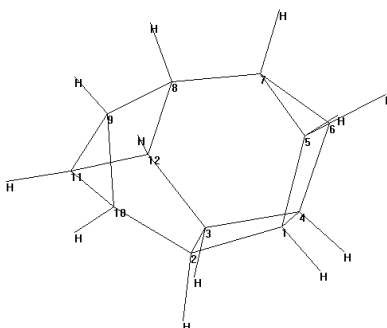


Figure 8: Molecule 3.

Table 5: Local atomic reactivity indices of molecule 3.

Atom	μ	η	Q^{\max}	ω
1	-1.7764	14.6745	0.1211	0.1075
2	-2.1113	14.0046	0.1508	0.1592
3	-1.7764	14.6745	0.1211	0.1075
4	-1.8164	14.5945	0.1245	0.113
5	-0.9721	16.283	0.0597	0.029
6	-2.1113	14.0046	0.1508	0.1592
7	-1.8164	14.5945	0.1245	0.113
8	-1.7764	14.6745	0.1211	0.1075
9	-1.8164	14.5945	0.1245	0.113
10	-0.9721	16.283	0.0597	0.029
11	-2.1711	13.8851	0.1564	0.1697
12	-1.8164	14.5945	0.1245	0.113

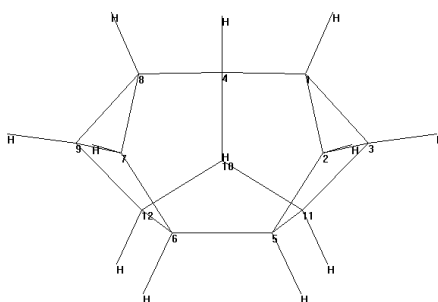


Figure 9: Molecule 4.

Table 6: Local atomic reactivity indices of molecule 4.

Atom	μ	η	Q^{\max}	ω
1	-1.8018	15.4694	0.1165	0.1049
2	-2.3656	14.3417	0.1649	0.1951
3	-2.3381	14.3967	0.1624	0.1899
4	-1.8399	15.3932	0.1195	0.11
5	-2.3381	14.3967	0.1624	0.1899
6	-2.3381	14.3967	0.1624	0.1899
7	-2.3656	14.3417	0.1649	0.1951
8	-1.8018	15.4694	0.1165	0.1049
9	-2.3381	14.3967	0.1624	0.1899
10	-1.8901	15.2928	0.1236	0.1168
11	-1.994	15.0849	0.1322	0.1318
12	-1.994	15.0849	0.1322	0.1318

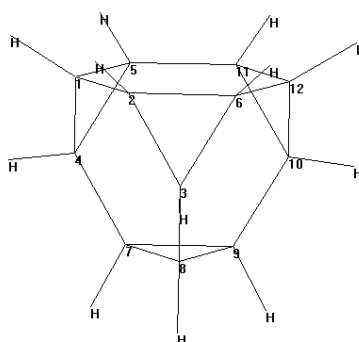


Figure 10: Molecule 5.

Table 7: Local atomic reactivity indices of molecule 5.

Atom	μ	η	Q^{\max}	ω
1	-1.5353	15.1676	0.1012	0.0777
2	-1.5353	15.1676	0.1012	0.0777
3	-1.5353	15.1676	0.1012	0.0777
4	-1.5353	15.1676	0.1012	0.0777
5	-1.5353	15.1676	0.1012	0.0777
6	-1.5353	15.1676	0.1012	0.0777
7	-1.5353	15.1676	0.1012	0.0777
8	-1.5353	15.1676	0.1012	0.0777
9	-1.5353	15.1676	0.1012	0.0777
10	-1.5353	15.1676	0.1012	0.0777
11	-1.5353	15.1676	0.1012	0.0777
12	-1.5353	15.1676	0.1012	0.0777

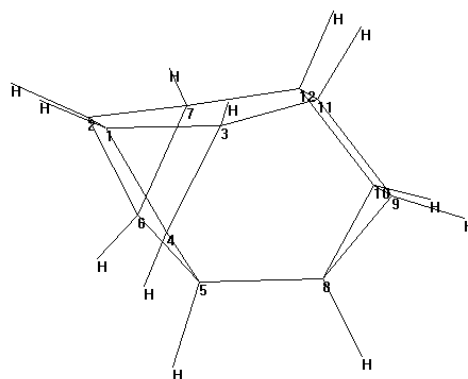


Figure 11: Molecule 6.

Table 8: Local atomic reactivity indices of molecule 6.

Atom	μ	η	Q^{\max}	ω
1	-1.2261	16.5636	0.074	0.0454
2	-1.2261	16.5636	0.074	0.0454
3	-1.9696	15.0767	0.1306	0.1286
4	-1.9696	15.0767	0.1306	0.1286
5	-1.7806	15.4547	0.1152	0.1026
6	-1.9696	15.0767	0.1306	0.1286
7	-1.9696	15.0767	0.1306	0.1286
8	-1.7806	15.4547	0.1152	0.1026
9	-2.278	14.4598	0.1575	0.1794
10	-2.278	14.4598	0.1575	0.1794
11	-1.6485	15.7189	0.1049	0.0864
12	-1.6485	15.7189	0.1049	0.0864

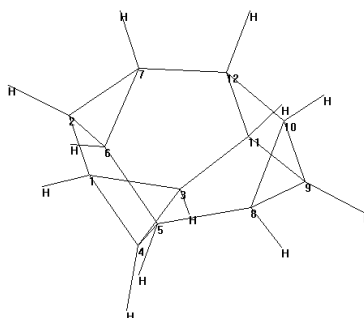


Figure 12: Molecule 7.

Table 9. Local atomic reactivity indices of molecule 7.

Atom	μ	η	s	Q^{\max}	ω
1	-2.087	15.1956	0.0658	0.1373	0.1433
2	-2.087	15.1956	0.0658	0.1373	0.1433
3	-1.8003	15.769	0.0634	0.1142	0.1028
4	-2.087	15.1956	0.0658	0.1373	0.1433
5	-1.8003	15.769	0.0634	0.1142	0.1028
6	-2.087	15.1956	0.0658	0.1373	0.1433
7	-1.961	15.4476	0.0647	0.1269	0.1245
8	-1.961	15.4476	0.0647	0.1269	0.1245
9	-2.373	14.6237	0.0684	0.1623	0.1925
10	-2.373	14.6237	0.0684	0.1623	0.1925
11	-1.961	15.4476	0.0647	0.1269	0.1245
12	-1.961	15.4476	0.0647	0.1269	0.1245

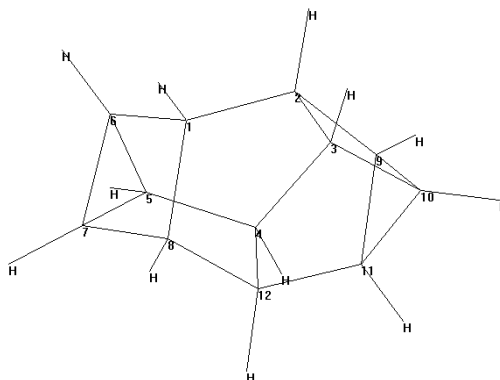


Figure 13: Molecule 8.

Table 10: Local atomic reactivity indices of molecule 8.

Atom	μ	η	Q^{\max}	ω
1	-1.0997	16.9861	0.0647	0.0356
2	-1.0997	16.9861	0.0647	0.0356
3	-2.3195	14.5466	0.1595	0.1849
4	-1.936	15.3137	0.1264	0.1224
5	-1.0997	16.9861	0.0647	0.0356
6	-1.0997	16.9861	0.0647	0.0356
7	-1.2857	16.6142	0.0774	0.0498
8	-2.3195	14.5466	0.1595	0.1849
9	-1.0997	16.9861	0.0647	0.0356
10	-1.2857	16.6142	0.0774	0.0498
11	-1.0997	16.9861	0.0647	0.0356
12	-1.936	15.3137	0.1264	0.1224

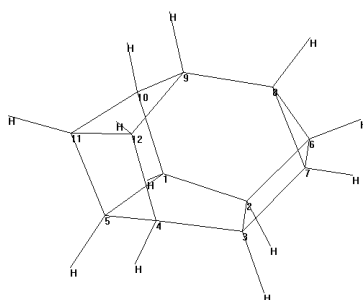


Figure 14: Molecule 9.

Table 11: Local atomic reactivity indices of molecule 9.

Atom	μ	η	Q^{\max}	ω
1	-1.921	15.1548	0.1268	0.1217
2	-1.2549	16.4871	0.0761	0.0478
3	-1.2549	16.4871	0.0761	0.0478
4	-1.921	15.1548	0.1268	0.1217
5	-2.326	14.3447	0.1622	0.1886
6	-1.2549	16.4871	0.0761	0.0478
7	-1.2549	16.4871	0.0761	0.0478
8	-2.0121	14.9725	0.1344	0.1352
9	-2.326	14.3447	0.1622	0.1886
10	-2.0121	14.9725	0.1344	0.1352
11	-2.326	14.3447	0.1622	0.1886
12	-2.0121	14.9725	0.1344	0.1352

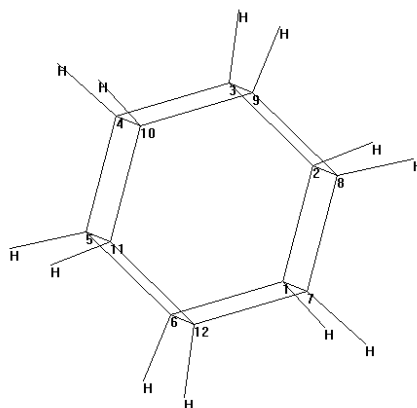


Figure 15: Molecule 10.

Table 12: Local atomic reactivity indices of molecule 10.

Atom	μ	η	Q^{\max}	ω
1	-2.5105	14.0182	0.1791	0.2248
2	-2.5105	14.0182	0.1791	0.2248
3	-2.5105	14.0182	0.1791	0.2248
4	-2.5105	14.0182	0.1791	0.2248
5	-2.5105	14.0182	0.1791	0.2248
6	-2.5105	14.0182	0.1791	0.2248
7	-2.5105	14.0182	0.1791	0.2248
8	-2.5105	14.0182	0.1791	0.2248
9	-2.5105	14.0182	0.1791	0.2248
10	-2.5105	14.0182	0.1791	0.2248
11	-2.5105	14.0182	0.1791	0.2248
12	-2.5105	14.0182	0.1791	0.2248

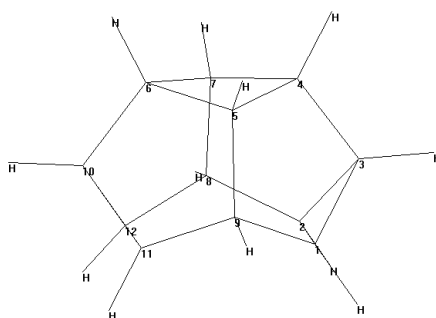


Figure 16: Molecule 11.

Table 13: Local atomic reactivity indices of molecule 11.

Atom	μ	η	Q^{\max}	ω
1	-1.4479	16.5412	0.0875	0.0634
2	-1.4479	16.5412	0.0875	0.0634
3	-2.4089	14.6193	0.1648	0.1985
4	-2.4089	14.6193	0.1648	0.1985
5	-1.9996	15.4378	0.1295	0.1295
6	-2.4089	14.6193	0.1648	0.1985
7	-1.9996	15.4378	0.1295	0.1295
8	-1.9007	15.6356	0.1216	0.1155
9	-1.9007	15.6356	0.1216	0.1155
10	-2.4089	14.6193	0.1648	0.1985
11	-1.4479	16.5412	0.0875	0.0634
12	-1.4479	16.5412	0.0875	0.0634

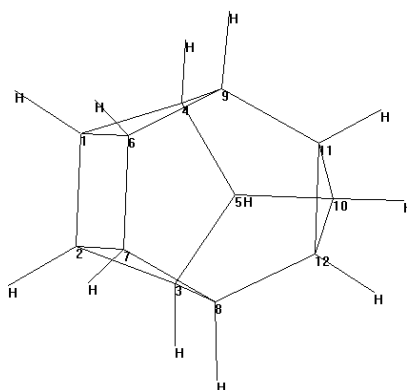


Figure 17: Molecule 12.

Table 14: Local atomic reactivity indices of molecule 12.

Atom	μ	η	Q^{\max}	ω
1	-2.4754	14.6707	0.1687	0.2088
2	-2.4754	14.6707	0.1687	0.2088
3	-2.1452	15.3312	0.1399	0.1501
4	-2.1452	15.3312	0.1399	0.1501
5	-1.6075	16.4065	0.098	0.0788
6	-2.1452	15.3312	0.1399	0.1501
7	-2.1452	15.3312	0.1399	0.1501
8	-1.9649	15.6917	0.1252	0.123
9	-1.9649	15.6917	0.1252	0.123
10	-2.4754	14.6707	0.1687	0.2088
11	-1.9649	15.6917	0.1252	0.123
12	-1.9649	15.6917	0.1252	0.123

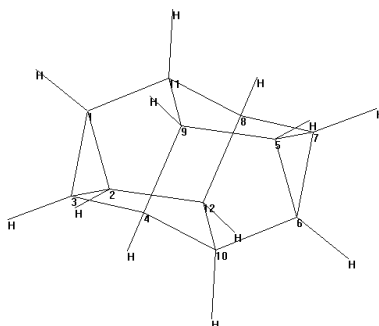


Figure 18: Molecule 13.

Table 15: Local atomic reactivity indices of molecule 13.

Atom	μ	η	Q^{\max}	ω
1	-1.8338	16.0727	0.1141	0.1046
2	-1.6584	16.4234	0.101	0.0837
3	-1.6584	16.4234	0.101	0.0837
4	-1.6584	16.4234	0.101	0.0837
5	-1.6584	16.4234	0.101	0.0837
6	-1.8338	16.0727	0.1141	0.1046
7	-1.6584	16.4234	0.101	0.0837
8	-1.6584	16.4234	0.101	0.0837
9	-2.0236	15.6931	0.1289	0.1305
10	-1.8338	16.0727	0.1141	0.1046
11	-1.8338	16.0727	0.1141	0.1046
12	-2.0236	15.6931	0.1289	0.1305

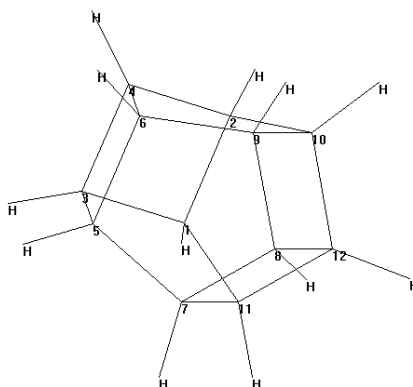


Figure 19: Molecule 14.

Table 16: Local atomic reactivity indices of molecule 14.

Atom	μ	η	Q^{\max}	ω
1	-2.7742	15.1382	0.1833	0.2542
2	-1.8332	17.0202	0.1077	0.0987
3	-2.7742	15.1382	0.1833	0.2542
4	-2.7742	15.1382	0.1833	0.2542
5	-1.8332	17.0202	0.1077	0.0987
6	-2.7742	15.1382	0.1833	0.2542
7	-2.7742	15.1382	0.1833	0.2542
8	-2.7742	15.1382	0.1833	0.2542
9	-1.8332	17.0202	0.1077	0.0987
10	-2.7742	15.1382	0.1833	0.2542
11	-1.8332	17.0202	0.1077	0.0987
12	-2.7742	15.1382	0.1833	0.2542

From Tables 3-16 we can observe that all carbon atoms have a high hardness, a low or very low electrophilicity and are prone to receive little extra charge. This is expected to happen in saturated hydrocarbons, strained or not. Nevertheless, we have doubts about the exact meaning of Q^{\max} . We commented in another paper that we expect that the units of this index be “electrons” but this index has not a unit [59]. Another important point to comment on is that the local atomic reactivity indices are calculated by assuming that, if the value of the Fukui index of any molecular orbital localized on a given atom is less than 0.1 small errors may appear in the case of small molecules.

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