Electronic Supplementary Information for

Quantitative structure-property relationships prediction of some physico–chemical properties of glycerol based solvents.

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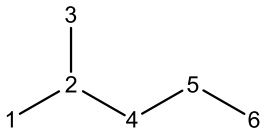
Content

Definition of the topological parameters

Topological indices are usually obtained from two-dimensional molecular structures (molecular graphs, G), mostly through the connectivity adjacency (A(G)) and topological distance matrices (D(G)), and the vertex degree vector (δ(G)):



A(G)

	1	2	3	4	5	6
1	0	1	0	0	0	0
2	1	0	1	1	0	0
3	0	1	0	0	0	0
4	0	1	0	0	1	0
5	0	0	0	1	0	1
6	0	0	0	0	1	0

δ(G)

	1	2	3	4	5	6
δ	1	3	1	2	2	1

D(G)

	1	2	3	4	5	6
1	0	1	2	2	3	4
2	1	0	1	1	2	3
3	2	1	0	2	3	4
4	2	1	2	0	1	2
5	3	2	2	1	0	1
6	4	3	3	2	1	0

Topological indices are calculated from different invariant features of the molecular graph, and contain information about molecular size, molecular shape, branching, molecular flexibility, etc. The exact definition of the indices used in this work are given below.

Balaban indices (JX, JY):15, 23

Balaban index is defined as:

$$J = \frac{M}{M - N + 2} \sum \frac{1}{\sqrt{s_i^a s_j^a}}$$

where M is the number of bonds, N is the number of atoms in the molecule, and s_i is calculated as the sum of terms from a modified topological distance matrix. In this modified distance matrix, each bond contributes with 1/b to the total connectivity, with b=1 for single bonds, b=2 for double bonds, b=3 for triple bonds, and b=1.5 for aromatic bonds:

$$s_i = \sum_{i=1}^{N} d_{ij}$$

Corrections for heteroatoms have been introduced through contributions for the modification of the electronegativity (X) and the atomic radii (Y):

$$X = 0{,}4196 - 0{,}0078i + 0{,}1567G_i$$
$$Y = 1{,}1191 - 0{,}0160i + 0{,}0537G_i$$

where i is the atomic number and G_i is the group number in the Periodic Table of the elements. From these corrections, the s_i^a values are defined as:

$s_i^a = X \cdot s_i$ (for JX index)
$s_i^a = Y \cdot s_i$ (for JY index)

Wiener index (W):16, 24

The Wiener index is defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule. It is easily computed from the topological distance matrix:

$$W = \frac{1}{2} \sum_i \sum_j d_{ij}$$

This index is a measure of the centrality of the graph, and hence it is related with the molecular compactness.

Zagreb index:17

It is defined as the sum of squares of the difference between the number of electrons participating in covalent bonds and the number of hydrogen atoms bonded to the same atom. This is equivalent to the sum of the squares of the vertices degrees, δ_i:

$$Zagreb = \sum_i \delta_i^2 = \sum_i (\sigma_i - h_i)^2$$

Randic and Kier & Hall connectivity indices (χ):18

χ indices were first proposed by Randic25 from the vertices degrees, as:

$\square = \sum_B \frac{1}{\delta_i \cdot \delta_j}$, extended to all bonds in the molecule (B).

Kier and Hall extended the definition by including the number of edges of a given sub-graph (h), and different kinds of sub-graphs (r):

$$^n\square_r(G) = \sum_{i=1}^{\sigma_n} \left(\prod_{j=1}^{h+1} \sqrt{\frac{1}{\delta_i}} \right)$$

where σ_n is the number of sub-graph of length h and δ is the vertex degree.
There are four kinds of sub-graphs, known as *path* (linear chains), *cluster* (branched chains), *path/cluster*, and *chain* (cycles), each one emphasizing a particular aspect of the molecular connectivity. The n superindex refers to the number of bonds considered to calculate the topological index. Thus, n=0 refers to individual atoms, n=1 refers to directly connected atoms, n=2 refers to three atoms connected through two consecutive bonds, and so on.

$$^nP_{(sub)} = \frac{1}{\sqrt{(\delta_i \times \delta_j \times \ldots \times \delta_n)}} = \prod_{i=1}^{n} \frac{1}{\sqrt{\delta_i}}$$, and hence

$$^n\chi_s \equiv Chi(n)(sub) = \sum {}^nP_{(sub)}$$

A further refinement*10d, 18* can be included to the χ indicesby considering the atom valences, thus allowing distinguishing the presence of heteroatoms in the structure. This is accomplished by calculating s "corrected" d value, using the atomic number and the number of valence electrons of the vertex atoms:

$$\delta^v = \frac{\left(Z^v - h\right)}{\left(Z - Z^v - 1\right)}$$

Where Z_v is the number of valence electrons, Z is the atomic number and h is the number of hydrogen atoms bonded to the vertex atom. The resulting "valence-corrected" indices are named as χ_v.

Kier & Hall count indices (SC):

SC is the count of sub-graphs of a given length present in the molecules. Thus, SC=0 is the number of atoms, SC=1, the number of chemical bonds, SC=2, the number of pair bonds, and so on. For longer sub-graphs, *path*, *cluster*, *path/cluster* and *chain* types can be also considered.

Kier shape indices (κ_n):

All the prededent topological indices are heavily influenced by the size of the molecular graph. Kier developed the κ indices to best discriminate between different shapes of the molecules. They are defined from sub-graphs of a given length, taking into account also the maximum and minimum connectivity of the molecule for the same length (a way to "normalize" the κ values, making them independent of the molecular size):

$$\kappa_n = K \cdot \frac{^mP_{\min} \cdot {}^mP_{\max}}{\left(^mP_i\right)^2}$$

Where m is the length chosen of the sub-graph, ^mP_i the number of sub-graphs of length m contained in the total graph, and $^mP_{max}$ and $^mP_{min}$ is the maximum and minimum number possible of sub-graphs of length m that can contain the total graph. Some examples are given below.

κ_1, K =2:

$$^1P_{\min} = N - 1$$

$$^1P_{\max} = \frac{N(N+1)}{2}$$

$$^1P_i = number\_of\_edges$$

κ_2, K =2:

$$^2P_{\min} = N - 2$$

$$^2P_{\max} = \frac{(N-1)(N-2)}{2}$$

$$^2P_i = number\_of\_adjacent\_edges$$

κ_3, K =4:

$$^3P_{\min} = N - 3$$

$$^3P_{\max} = \frac{(N-2)^2}{4}(N\_even)$$

$$^3P_{\max} = \frac{(N-1)(N-3)}{4}(N\_odd)$$

$$^3P_i = trios\_of\_adjacent\_edges$$

Similarly to the χ indices, a modification has been sugested for κ indices to account for the presence of heteroatoms in the molecular graph. *14, 26* In this modification, both the covalent radii and the hybridizations are considered. The $\square_n^\alpha$ indices are defined as the κ_n ones, but substituting N by N+α, where a is defined as:

$$\alpha = \sum_i \left(\frac{r_i}{r_{Csp^3}} - 1 \right)$$

Where r_i is the covalent radium of atom i and r_{Csp^3} is taken as 0.77 Å (the covalent radius of a carbon atom with sp^3 hybridization).

Molecular flexibility index (φ):14

The starting hypothesis to define f is that an infinitely long linear saturated hydrocarbon molecule (i.e. all-sp^3 C−C bonds) is infinitely flexible. Flexibility is reduced by the presence of a limited number of atoms, rings, branched chains, and the presence of atoms with covalent radii shorter than that of C_{sp^3}:

$$\varphi = \frac{\kappa_1^\alpha \kappa_2^\alpha}{N}$$

Table S1. Topological parameters of 62 glycerol based solvents.

Code	HBA	HBD	RB	φ	Bal^{JX}	Bal^{JY}	W	Z	κ_1^{am}	κ_2^{am}	κ_3^{am}	SC_p^0	SC_p^1	SC_p^2	SC_p^3	SC_c^3	${}^0\chi$	${}^1\chi$	${}^2\chi$	${}^3\chi_p$	${}^3\chi_{cl}$	${}^0\chi^{vm}$	${}^1\chi^{vm}$	${}^2\chi^{vm}$	${}^3\chi_p^{vm}$	${}^3\chi_{cl}^{vm}$
000	3	3	5	3.02	2.572	2.814	31	20	5.88	3.08	2.88	6	5	5	4	1	4.99	2.81	1.92	1.39	0.29	3.33	1.71	1.02	0.42	0.13
100	3	2	5	3.98	2.620	2.901	50	24	6.88	4.05	3.72	7	6	6	5	1	5.70	3.31	2.30	1.48	0.29	4.29	2.09	1.29	0.57	0.13
200	3	2	6	4.95	2.665	2.926	76	28	7.88	5.03	4.88	8	7	7	6	1	6.41	3.81	2.66	1.75	0.29	5.00	2.68	1.50	0.73	0.13
400	3	2	8	6.91	2.723	2.939	153	36	9.88	6.99	6.88	10	9	9	8	1	7.82	4.81	3.36	2.25	0.29	6.42	3.68	2.26	1.16	0.13
101	3	1	5	4.95	2.686	2.996	75	28	7.88	5.03	4.88	8	7	7	6	1	6.41	3.81	2.68	1.56	0.29	5.26	2.47	1.56	0.72	0.13
103i	3	1	6	5.58	2.915	3.193	143	38	9.88	5.65	6.88	10	9	10	8	2	7.98	4.66	3.87	2.02	0.70	6.83	3.45	2.49	0.98	0.37
104	3	1	8	7.89	2.788	3.033	202	40	10.88	7.98	7.78	11	10	10	9	1	8.53	5.31	3.74	2.33	0.29	7.38	4.06	2.54	1.31	0.13
104i	3	1	7	6.51	2.909	3.162	194	42	10.88	6.58	7.78	11	10	11	9	2	8.69	5.16	4.22	2.26	0.70	7.54	3.91	3.04	1.12	0.54
104t	3	1	6	4.65	3.173	3.444	180	46	10.88	4.70	7.78	11	10	13	9	5	8.91	4.96	4.99	2.17	1.85	7.76	3.76	3.53	1.07	1.24
403i	3	1	9	8.40	2.973	3.205	324	50	12.88	8.48	9.80	13	12	13	11	2	10.10	6.16	4.93	2.79	0.70	8.95	5.04	3.46	1.57	0.37
404	3	1	11	10.86	2.907	3.121	419	52	13.88	10.96	10.88	14	13	13	12	1	10.65	6.81	4.80	3.10	0.29	9.50	5.64	3.51	1.91	0.13
404t	3	1	9	7.15	3.152	3.380	388	58	13.88	7.21	10.88	14	13	16	12	5	11.03	6.46	6.05	2.94	1.85	9.88	5.35	4.51	1.66	1.24
404i	3	1	10	9.36	2.984	3.203	408	54	13.88	9.44	10.88	14	13	14	12	2	10.81	6.66	5.28	3.03	0.70	9.66	5.50	4.01	1.71	0.54
203i	3	1	7	6.51	2.950	3.214	192	42	10.88	6.58	7.78	11	10	11	9	2	8.69	5.16	4.22	2.29	0.70	7.54	4.04	2.70	1.14	0.37
204	3	1	9	8.88	2.845	3.082	262	44	11.88	8.97	8.88	12	11	11	10	1	9.23	5.81	4.10	2.60	0.29	8.08	4.64	2.74	1.47	0.13
204t	3	1	7	5.46	3.176	3.434	237	50	11.88	5.51	8.88	12	11	14	10	5	9.61	5.46	5.35	2.44	1.85	8.46	4.35	3.74	1.22	1.24
204i	3	1	8	7.45	2.950	3.193	253	46	11.88	7.53	8.88	12	11	12	10	2	9.40	5.66	4.57	2.53	0.70	8.25	4.50	3.25	1.28	0.54
3i03i	3	1	7	6.34	3.079	3.334	243	48	11.88	6.40	8.88	12	11	13	10	3	9.56	5.52	5.05	2.47	1.11	8.41	4.43	3.42	1.24	0.60
3i04t	3	1	7	5.53	3.273	3.522	296	56	12.88	5.58	9.80	13	12	16	11	6	10.48	5.81	6.18	2.62	2.26	9.33	4.75	4.46	1.33	1.48
3i04i	3	1	8	7.23	3.068	3.305	314	52	12.88	7.30	9.80	13	12	14	11	3	10.27	6.02	5.40	2.72	1.11	9.12	4.89	3.97	1.38	0.77
3i03F	6	1	7	6.06	3.115	3.499	378	60	13.67	6.21	10.67	14	13	17	12	6	11.19	6.31	6.53	2.86	2.26	8.17	4.25	3.17	1.20	0.54
403F	6	1	9	7.72	3.032	3.384	484	62	14.67	7.90	11.60	15	14	17	13	5	11.73	6.96	6.41	3.17	1.85	8.72	4.86	3.21	1.53	0.31
4t03F	6	1	7	5.55	3.267	3.639	450	68	14.67	5.67	11.60	15	14	20	13	9	12.11	6.60	7.66	3.01	3.41	9.10	4.57	4.21	1.29	1.42
4i03F	6	1	8	6.87	3.106	3.465	472	64	14.67	7.03	11.60	15	14	18	13	6	11.90	6.81	6.88	3.10	2.26	8.88	4.71	3.72	1.34	0.72
3F03F	9	1	7	6.05	3.136	3.615	557	72	15.46	6.26	12.46	16	15	21	14	9	12.82	7.10	8.01	3.25	3.41	7.94	4.07	2.91	1.15	0.49
5F05F	13	1	9	6.90	3.636	4.205	1283	108	21.18	7.17	6.88	22	21	33	32	17	17.82	9.60	11.16	7.06	4.70	10.45	5.33	4.09	2.02	0.84
7F07F	17	1	11	8.01	4.071	4.718	2399	144	26.90	8.33	6.20	28	27	45	50	25	22.82	12.10	14.41	10.13	6.20	12.96	6.58	5.24	2.82	1.17
111	3	0	5	5.93	2.907	3.263	102	32	8.88	6.01	4.39	9	8	8	8	1	7.11	4.35	2.85	1.97	0.20	6.22	2.85	1.77	1.04	0.12
113i	3	0	6	6.51	3.111	3.431	182	42	10.88	6.58	6.28	11	10	11	10	2	8.69	5.20	4.03	2.43	0.61	7.79	3.84	2.70	1.30	0.35
143i	3	0	9	9.36	3.331	3.612	369	54	13.88	9.44	9.26	14	13	14	13	2	10.81	6.70	5.12	3.07	0.61	9.92	5.42	3.68	1.82	0.35
114t	3	0	6	5.46	3.341	3.652	225	50	11.88	5.51	7.32	12	11	14	11	5	9.61	5.49	5.16	2.58	1.77	8.72	4.15	3.74	1.39	1.23
144t	3	0	9	8.02	3.513	3.789	436	62	14.88	8.08	10.17	15	14	17	14	5	11.73	6.99	6.25	3.22	1.77	10.84	5.74	4.73	1.91	1.23
114	3	0	8	8.88	2.974	3.260	250	44	11.88	8.97	7.32	12	11	11	11	1	9.23	5.85	3.91	2.74	0.20	8.34	4.44	2.74	1.63	0.12
144	3	0	11	11.8	3.246	3.505	470	56	14.88	11.95	10.17	15	14	14	14	1	11.36	7.35	5.00	3.38	0.20	10.46	6.03	3.73	2.15	0.12
114i	3	0	7	7.46	3.089	3.383	241	46	11.88	7.53	7.32	12	11	12	11	2	9.40	5.70	4.39	2.67	0.61	8.50	4.30	3.24	1.44	0.53
144i	3	0	10	10.3	3.330	3.595	458	58	14.88	10.40	10.17	15	14	15	14	2	11.52	7.20	5.48	3.31	0.61	10.62	5.89	4.23	1.96	0.53
123i	3	0	7	7.45	3.240	3.552	232	46	11.88	7.53	7.32	12	11	12	11	2	9.40	5.70	4.42	2.55	0.61	8.50	4.42	2.92	1.37	0.35
213i	3	0	7	7.45	3.158	3.465	237	46	11.88	7.53	7.32	12	11	12	11	2	9.40	5.70	4.39	2.70	0.61	8.50	4.42	2.90	1.46	0.35
124t	3	0	7	6.29	3.450	3.753	282	54	12.88	6.35	8.22	13	12	15	12	5	10.32	5.99	5.54	2.70	1.77	9.42	4.74	3.96	1.46	1.23
214t	3	0	7	6.29	3.366	3.665	288	54	12.88	6.35	8.22	13	12	15	12	5	10.32	5.99	5.52	2.85	1.77	9.42	4.74	3.94	1.54	1.23
124	3	0	9	9.87	3.114	3.395	310	48	12.88	9.96	8.22	13	12	12	12	1	9.94	6.35	4.29	2.86	0.20	9.05	5.03	2.96	1.70	0.12

214	3	0	9	9.87	3.045	3.322	316	48	12.88	9.96	8.22	13	12	12	12	1	9.94	6.35	4.27	3.01	0.20	9.05	5.03	2.95	1.79	0.12
124i	3	0	8	8.40	3.219	3.507	300	50	12.88	8.48	8.22	13	12	13	12	2	10.10	6.20	4.77	2.79	0.61	9.21	4.89	3.46	1.51	0.53
214i	3	0	8	8.40	3.146	3.430	306	50	12.88	8.48	8.22	13	12	13	12	2	10.10	6.20	4.74	2.94	0.61	9.21	4.89	3.45	1.60	0.53
223i	3	0	8	8.40	3.304	3.604	294	50	12.88	8.48	8.22	13	12	13	12	2	10.10	6.20	4.77	2.82	0.61	9.21	5.01	3.12	1.53	0.35
224t	3	0	8	7.15	3.498	3.792	352	58	13.88	7.21	9.26	14	13	16	13	5	11.03	6.49	5.90	2.97	1.77	10.13	5.33	4.16	1.61	1.23
224	3	0	10	10.86	3.197	3.471	383	52	13.88	10.96	9.26	14	13	13	13	1	10.65	6.85	4.65	3.13	0.20	9.75	5.62	3.17	1.86	0.12
224i	3	0	9	9.36	3.292	3.572	372	54	13.88	9.44	9.26	14	13	14	13	2	10.81	6.70	5.12	3.06	0.61	9.92	5.47	3.67	1.67	0.53
413i	3	0	9	9.36	3.175	3.445	384	54	13.88	9.44	9.26	14	13	14	13	2	10.81	6.70	5.10	3.20	0.61	9.92	5.42	3.67	1.90	0.35
423i	3	0	10	10.32	3.329	3.598	458	58	14.88	10.40	10.17	15	14	15	14	2	11.52	7.20	5.48	3.32	0.61	10.62	6.01	3.89	1.96	0.35
414t	3	0	9	8.02	3.349	3.616	454	62	14.88	8.08	10.17	15	14	17	14	5	11.73	6.99	6.22	3.35	1.77	10.84	5.74	4.71	1.98	1.23
424t	3	0	10	8.90	3.500	3.765	535	66	15.88	8.97	11.21	16	15	18	15	5	12.44	7.49	6.60	3.47	1.77	11.55	6.33	4.93	2.05	1.23
414	3	0	11	11.86	3.105	3.357	488	56	14.88	11.95	10.17	15	14	14	14	1	11.36	7.35	4.97	3.51	0.20	10.46	6.03	3.72	2.23	0.12
414i	3	0	10	10.32	3.182	3.439	476	58	14.88	10.40	10.17	15	14	15	14	2	11.52	7.20	5.45	3.44	0.61	10.62	5.89	4.22	2.03	0.53
424i	3	0	11	11.28	3.339	3.595	559	62	15.88	11.37	11.21	16	15	16	15	2	12.23	7.70	5.83	3.56	0.61	11.33	6.47	4.44	2.10	0.53
3i13F	6	0	7	6.87	3.304	3.723	444	64	14.67	7.03	9.96	15	14	18	14	6	11.90	6.85	6.70	3.27	2.17	9.14	4.64	3.37	1.52	0.53
4t13F	6	0	7	6.28	3.457	3.864	522	72	15.67	6.42	11.00	16	15	21	15	9	12.82	7.14	7.83	3.42	3.33	10.06	4.95	4.41	1.61	1.41
444	3	0	14	14.84	3.443	3.683	789	68	17.88	14.94	13.17	18	17	17	17	1	13.48	8.85	6.06	4.15	0.20	12.58	7.62	4.70	2.74	0.12
413F	6	0	9	8.60	3.223	3.610	559	66	15.67	8.78	11.00	16	15	18	15	5	12.44	7.49	6.58	3.58	1.77	9.68	5.24	3.42	1.85	0.30
3F13F	9	0	7	6.80	3.325	3.835	638	76	16.46	7.02	11.72	17	16	22	16	9	13.53	7.64	8.18	3.66	3.33	8.90	4.46	3.12	1.47	0.48
3F23F	9	0	8	7.57	3.476	3.980	736	80	17.46	7.80	12.76	18	17	23	17	9	14.23	8.14	8.56	3.78	3.33	9.61	5.04	3.34	1.54	0.48
3F43F	9	0	10	9.15	3.642	4.119	987	88	19.46	9.41	14.72	20	19	25	19	9	15.65	9.14	9.27	4.29	3.33	11.02	6.04	4.11	1.99	0.48

Table S2. DARC/PELCO parameters of 62 glycerol based solvents.

Code	A1	A2	B1	B2	FB2	A11	A21	FA21	B11	B21	FB21
000	0	0	0	0	0	0	0	0	0	0	0
100	0	1	0	0	0	0	0	0	0	0	0
200	0	1	0	1	0	0	0	0	0	0	0
400	0	1	0	1	0	0	1	0	0	1	0
101	0	2	0	0	0	0	0	0	0	0	0
103i	0	2	0	2	0	0	0	0	0	0	0
104	0	2	0	1	0	0	1	0	0	1	0
104i	0	2	0	1	0	0	2	0	0	0	0
104t	0	2	0	3	0	0	0	0	0	0	0
403i	0	2	0	3	0	0	1	0	0	1	0
404	0	2	0	2	0	0	2	0	0	2	0
404t	0	2	0	4	0	0	1	0	0	1	0
404i	0	2	0	2	0	0	3	0	0	1	0
203i	0	2	0	3	0	0	0	0	0	0	0
204	0	2	0	2	0	0	1	0	0	1	0
204t	0	2	0	4	0	0	0	0	0	0	0
204i	0	2	0	2	0	0	2	0	0	0	0
3i03i	0	2	0	4	0	0	0	0	0	0	0
3i04t	0	2	0	5	0	0	0	0	0	0	0
3i04i	0	2	0	3	0	0	2	0	0	0	0
3i03F	0	2	0	2	1	0	0	0	0	0	0
403F	0	2	0	1	1	0	1	0	0	1	0
4t03F	0	2	0	3	1	0	0	0	0	0	0
4i03F	0	2	0	1	1	0	2	0	0	0	0
3F03F	0	2	0	0	2	0	0	0	0	0	0
5F05F	0	2	0	0	2	0	0	2	0	0	0
7F07F	0	2	0	0	2	0	0	2	0	0	2
111	1	2	0	0	0	0	0	0	0	0	0
113i	1	2	0	2	0	0	0	0	0	0	0
143i	1	2	1	2	0	1	0	0	1	0	0
114t	1	2	0	3	0	0	0	0	0	0	0
144t	1	2	1	3	0	1	0	0	1	0	0
114	1	2	0	1	0	0	1	0	0	1	0
144	1	2	1	1	0	1	1	0	1	1	0
114i	1	2	0	1	0	0	2	0	0	0	0
144i	1	2	1	1	0	1	2	0	1	0	0
123i	1	2	1	2	0	0	0	0	0	0	0
213i	1	2	0	3	0	0	0	0	0	0	0
124t	1	2	1	3	0	0	0	0	0	0	0
214t	1	2	0	4	0	0	0	0	0	0	0
124	1	2	1	1	0	0	1	0	0	1	0
214	1	2	0	2	0	0	1	0	0	1	0
124i	1	2	1	1	0	0	2	0	0	0	0
214i	1	2	0	2	0	0	2	0	0	0	0
223i	1	2	1	3	0	0	0	0	0	0	0
224t	1	2	1	4	0	0	0	0	0	0	0
224	1	2	1	2	0	0	1	0	0	1	0
224i	1	2	1	2	0	0	2	0	0	0	0
413i	1	2	0	3	0	0	1	0	0	1	0
423i	1	2	1	3	0	0	1	0	0	1	0
414t	1	2	0	4	0	0	1	0	0	1	0
424t	1	2	1	4	0	0	1	0	0	1	0
414	1	2	0	2	0	0	2	0	0	2	0
414i	1	2	0	2	0	0	3	0	0	1	0
424i	1	2	1	2	0	0	3	0	0	1	0
3i13F	1	2	0	2	1	0	0	0	0	0	0
4t13F	1	2	0	3	1	0	0	0	0	0	0
444	1	2	1	2	0	1	2	0	1	2	0
413F	1	2	0	1	1	0	1	0	0	1	0
3F13F	1	2	0	0	2	0	0	0	0	0	0
3F23F	1	2	1	0	2	0	0	0	0	0	0
3F43F	1	2	1	0	2	1	0	0	1	0	0

Table S3. Pearson bivariate correlations between all the descriptors used in this work.

	A1	A2	B1	B2	BF2	C1	C2	CF2	D1	D2	DF2	HBA	HBD	RoB	MFx	BalJX	BalJY	W	Z	K1	K2	K3	SC0p	SC1p	SC2p	SC3p	SC3cl	Ji0	Ji1	Ji2	Ji3p	Ji3cl	Ji0v	Ji1v	Ji2v	Ji3pv	Ji3clv
A1	1																																				
A2	.281	1																																			
B1	.562	.158	1																																		
B2	.068	.298	.024	1																																	
BF2	-.088	.119	-.085	-.473	1																																
C1	.287	.081	.512	-.115	.014	1																															
C2	.083	.159	.069	-.049	-.304	.015	1																														
CF2	-.208	.045	-.117	-.277	.485	-.060	-.157	1																													
D1	.287	.081	.512	-.115	.014	**1.000**	.015	-.060	1																												
D2	.106	.086	.045	.069	-.247	.055	.521	-.127	.055	1																											
DF2	-.146	.032	-.082	-.194	.340	-.042	-.110	.701	-.042	-.089	1																										
HBA	-.148	.105	-.109	-.457	**.925**	-.014	-.285	.758	-.014	-.231	.629	1																									
HBD	**-.883**	-.700	-.496	-.197	.007	-.254	-.140	.133	-.254	-.121	.093	.059	1																								
RoB	.265	.331	.426	.053	.042	.435	.569	.191	.435	.709	.206	.122	-.360	1																							
MFx	.482	.398	.492	.009	-.131	.434	.615	-.028	.434	.722	.013	-.101	-.554	**.917**	1																						
BalJX	.464	.500	.456	.196	.462	.305	-.131	.469	.305	-.120	.434	.547	-.591	.444	.303	1																					
BalJY	.397	.457	.362	.034	.631	.243	-.223	.555	.243	-.202	.491	.704	-.520	.349	.199	**.975**	1																				
W	.037	.248	.117	-.245	.677	.181	-.011	.792	.181	.061	.771	**.855**	-.149	.531	.296	.744	**.807**	1																			
Z	.098	.396	.139	-.105	.750	.164	-.055	.703	.164	-.011	.618	**.855**	-.267	.492	.256	**.845**	**.901**	**.952**	1																		
K1	.222	.475	.258	-.064	.650	.260	.100	.605	.260	.154	.538	.741	-.398	.667	.471	**.857**	**.879**	**.924**	**.972**	1																	
K2	.480	.401	.490	-.007	-.105	.435	.609	-.012	.435	.718	.027	-.074	-.554	**.921**	**1.000**	.316	.216	.317	.278	.490	1																
K3	.194	.517	.292	.196	.396	.325	.284	-.198	.325	.319	-.158	.205	-.398	.598	.509	.474	.433	.317	.493	.603	.517	1															
SC0p	.204	.461	.241	-.087	.674	.249	.080	.621	.249	.135	.551	.765	-.378	.646	.446	**.852**	**.881**	**.933**	**.978**	**.999**	.466	.589	1														
SC1p	.204	.461	.241	-.087	.674	.249	.080	.621	.249	.135	.551	.765	-.378	.646	.446	**.852**	**.881**	**.933**	**.978**	**.999**	.466	.589	**1.000**	1													
SC2p	.037	.353	.080	-.114	.778	.114	-.130	.736	.114	-.093	.645	**.889**	-.200	.397	.145	.826	**.896**	**.945**	**.993**	**.938**	.167	.429	**.948**	**.948**	1												
SC3p	.085	.299	.117	-.186	.616	.129	-.032	**.846**	.129	.017	.783	**.828**	-.210	.494	.278	.777	**.831**	**.982**	**.943**	**.911**	.297	.231	**.918**	**.918**	**.940**	1											
SC3cl	-.150	.178	-.108	-.140	**.800**	-.046	-.357	.772	-.046	-.320	.668	**.920**	.025	.072	-.208	.692	**.800**	**.842**	**.886**	.751	-.186	.195	.771	.771	**.933**	**.846**	1										
Ji0	.159	.437	.198	-.093	.710	.213	.024	.660	.213	.070	.583	**.807**	-.333	.583	.366	**.854**	**.894**	**.946**	**.993**	**.993**	.387	.551	**.996**	**.996**	**.972**	**.934**	**.824**	1									
Ji1	.277	.486	.306	-.080	.601	.300	.168	.562	.300	.237	.504	**.686**	-.445	.737	.568	**.835**	**.845**	**.902**	**.939**	**.993**	.587	.623	**.990**	**.990**	**.893**	**.886**	.674	**.973**	1							
Ji2	.023	.378	.078	-.077	**.805**	.116	-.138	.667	.116	-.115	.572	**.877**	-.202	.375	.119	**.823**	**.893**	**.907**	**.985**	**.930**	.141	.508	**.939**	**.939**	**.992**	**.892**	**.927**	**.964**	**.881**	1						
Ji3p	.082	.288	.105	-.192	.608	.142	.016	**.844**	.142	.079	.756	**.816**	-.202	.544	.326	.757	**.808**	**.983**	**.940**	**.919**	.346	.255	**.926**	**.926**	**.931**	**.996**	**.820**	**.937**	**.901**	**.883**	1					
Ji3cl	-.148	.202	-.113	-.074	**.842**	-.047	-.399	.615	-.047	-.368	.509	**.878**	.011	-.002	-.278	.674	.783	.740	**.842**	.705	-.257	.322	.724	.724	**.892**	.726	**.970**	.778	.621	**.914**	.699	1				
Ji0v	.463	.631	.448	.301	.216	.359	.313	.283	.359	.332	.290	.289	-.654	**.803**	.700	**.842**	.751	.653	.736	**.854**	.707	.682	**.834**	**.834**	.666	.666	.392	.797	**.879**	.666	.681	.364	1			
Ji1v	.432	.559	.489	.268	.120	.405	.434	.197	.405	.493	.213	.182	-.595	**.912**	**.828**	.715	.608	.583	.636	.791	**.833**	.705	.768	.768	.550	.578	.235	.715	**.837**	.546	.607	.199	**.971**	1		
Ji2v	.265	.570	.301	.485	.171	.286	.253	.257	.286	.178	.264	.245	-.477	.632	.449	**.815**	.710	.571	.695	.764	.453	.656	.746	.746	.654	.586	.463	.729	.756	.673	.591	.472	**.922**	**.854**	1	
Ji3pv	.474	.494	.403	.112	.164	.401	.376	.357	.401	.527	.366	.286	-.595	**.902**	**.828**	.718	.639	.688	.684	**.823**	**.835**	.543	**.804**	**.804**	.604	.695	.307	.756	**.872**	.571	.725	.221	**.936**	**.953**	.774	1	
Ji3clv	-.037	.257	-.029	.586	.139	-.075	-.229	.189	-.075	-.363	.183	.187	-.098	-.109	-.333	.567	.515	.235	.402	.312	-.333	.219	.309	.309	.446	.278	.541	.351	.231	.484	.241	.614	.367	.197	.661	.107	1

Note that most topological parameters are heavily correlated to each other, which indicates that they recover essentially the same structural information. Also, there are two pairs of parameters fully dependent (r=1.000): **C1/D1, κ_2^{am}/φ.**

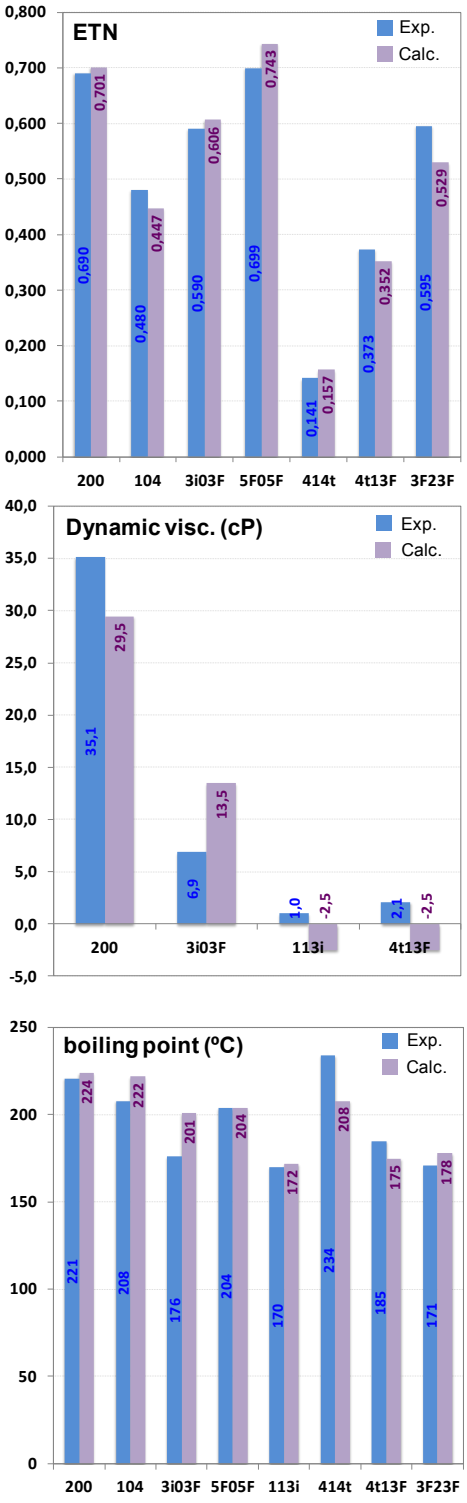


Figure S1. Predicted *vs.* experimental values of E_T^N, viscosity, and boiling point for the selected solvent test set using MLR analysis with topological parameters (equations 2–4 in the main text).

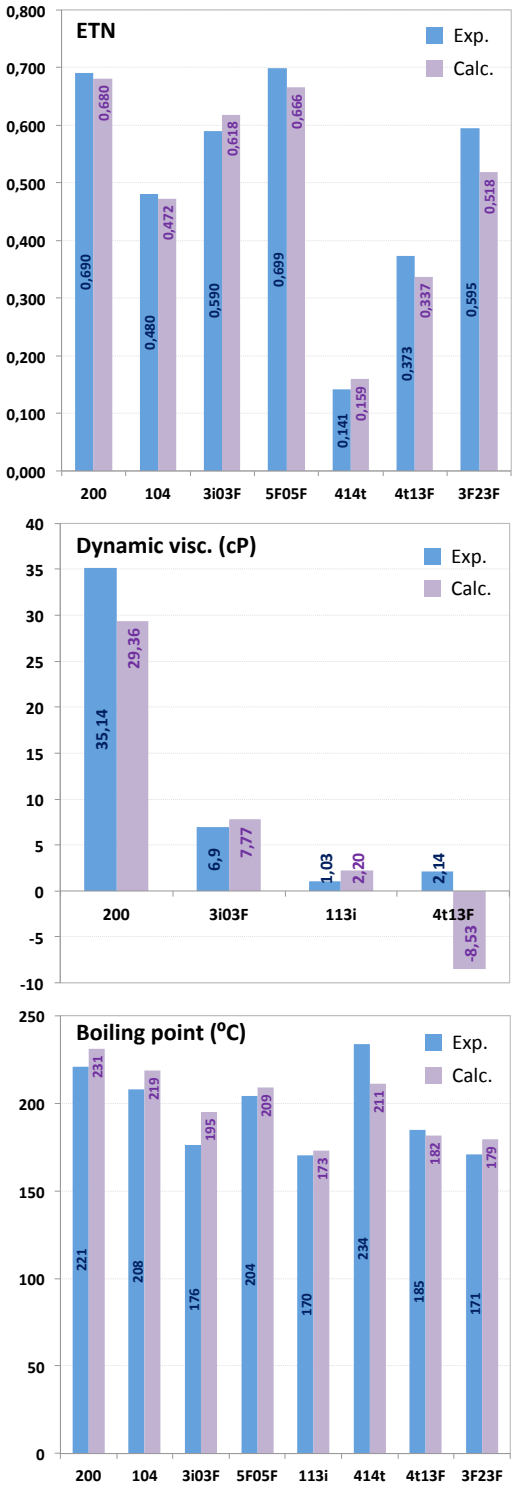


Figure S2. Predicted *vs.* experimental values of E_T^N, viscosity, and boiling point for the selected solvent test set using PLS analysis with topological parameters.

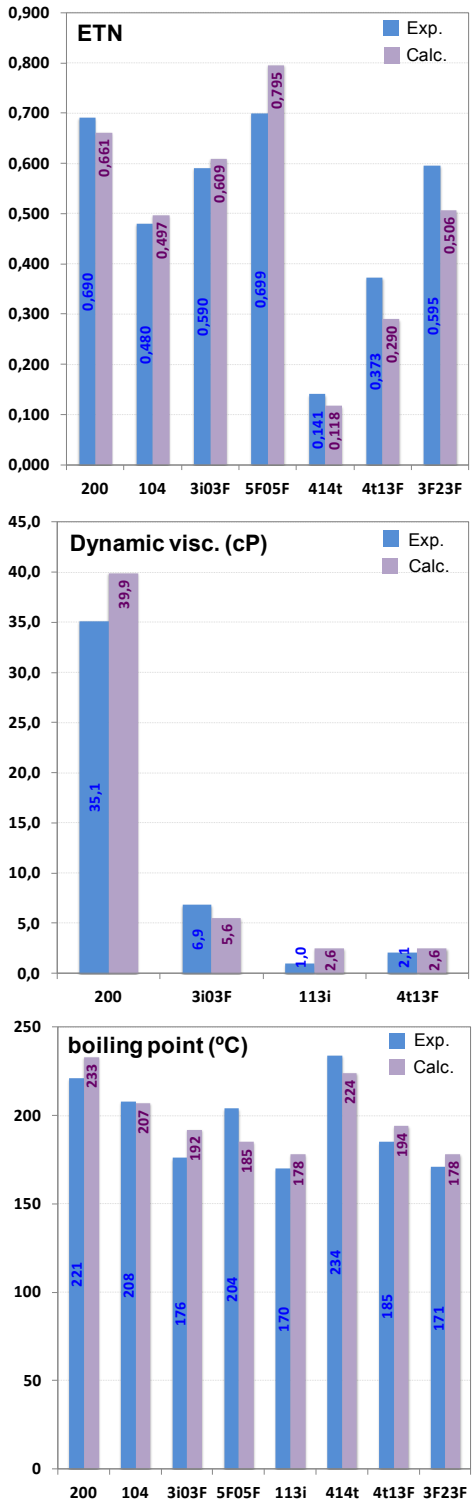


Figure S3. Predicted *vs.* experimental values of E_T^N, viscosity, and boiling point for the selected solvent test set using MLR analysis with DARC/PELCO descriptors (equations 5–7 in the text).

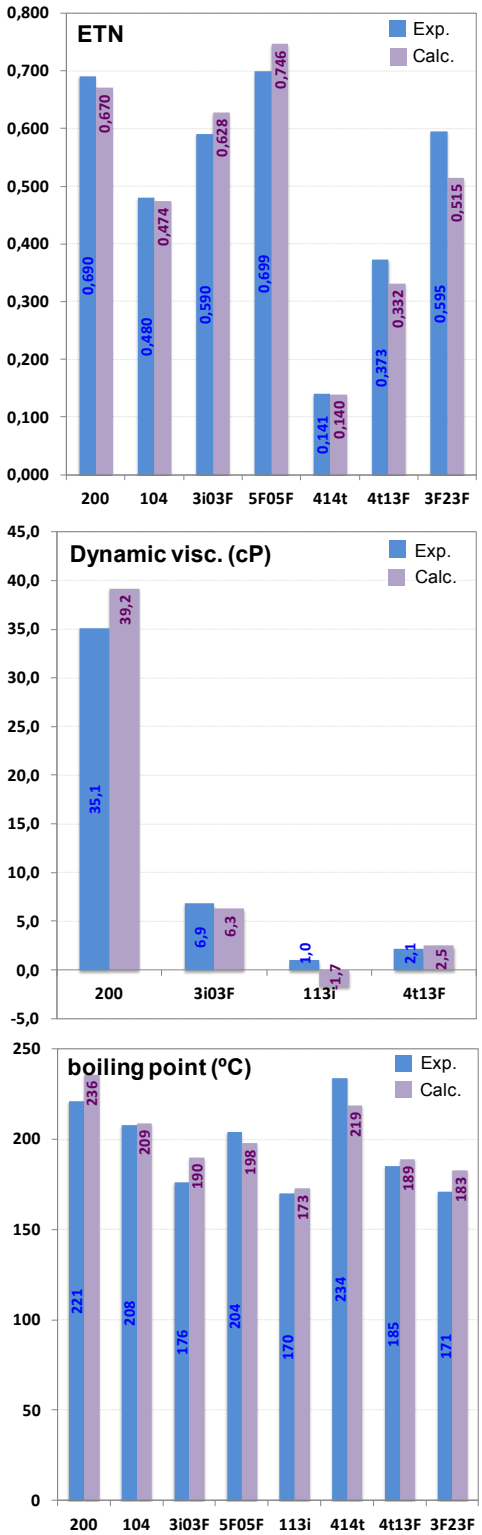


Figure S4. Predicted *vs.* experimental values of E_T^N, viscosity, and boiling point for the selected solvent test set using MLR analysis with mixed topological and DARC/PELCO descriptors (equations 8–10 in the text).

Table S4. Comparison between MLR and PLS model coefficients with DARC/PELCO descriptors for the three solvent properties studied.

Descriptor	E_T^N		Dynamic Viscosity (cP)		Boiling point (ºC)	
	MLR	**PLS**[a]	**MLR**	**PLS**[b]	**MLR**	**PLS**[c]
B0	0.851	0.796	70.79	71.800	278.2	279.3
A1	−0.278	−0.268	−3.52	−4.588	−6.1	−8.4
A2	−0.160	−0.116	−32.50	−34.448	−55.6	−55.7
B1	n.s.	−0.045	n.s.	0.083	n.s.	5.0
B2	−0.026	−0.034	n.s.	0.546	7.9	7.7
BF2	0.140	0.134	n.s.	2.606	7.0	6.7
C1	n.s.	0.003	n.s.	0.083	33.6	15.3
C2	−0.016	−0.018	n.s.	0.799	12.6	12. 5
CF2	−0.059	−0.055	6.90	2.816	12.0	9.5
D1	n.s.	0.003	n.s.	0.083	n.s.	15.3
D2	n.s.	−0.015	n.s.	0.799	19.1	18.9
DF2	n.s.	−0.033	n.s.	2.816	n.s.	3.0
N	46	46	17	17	62	62
R^2	0.972	0.968	0.981	0.991	0.933	0.935
σ	0.036	0.036	2.08	1.28	6.9	6.3

[a] 4 latent variables. [b] 5 latent variables. [c] 6 latent variables.

Given that **C1** and **D1** are linearly dependent (see Table S3), their behaviour differs in stepwise MLR and PLS analyses of the boiling point response. In the former case, the variable entering in the equation takes the full value (33.6), whereas in the "back-projection" of the PLS coefficients into the original variables, each coefficient takes half of the full value (15.3). Of course, the predictions within the solvent set used are therefore identical, given that all structures for which **C1**=1, have **D1**=1 too. Similar, but not the same behaviour is observed for other highly correlated parameters, such as **CF2** and **DF2**.

Table S5. Comparison between MLR and PLS model coefficients with mixed topological and DARC/PELCO descriptors for the three solvent properties studied.

Descriptor	E_T^N		Dynamic Viscosity (cP)		Boiling point (ºC)	
	MLR	PLS[a]	MLR	PLS[b]	MLR	PLS[c]
B0	0.523	0.865	67.55	156.41	292.6	171.2
A1	−0.099	−0.054	−5.27	6.333	n.s.	10.918
A2	n.s.	−0.005	−35.86	−27.740	−49.7	−26.743
B1	n.s.	−0.014	n.s.	5.713	n.s.	−3.438
B2	n.s.	−0.012	n.s.	−1.155	n.s.	2.847
BF2	0.177	0.007	n.s.	−0.224	n.s.	1.900
C1	n.s.	−0.004	n.s.	5.713	n.s.	4.677
C2	n.s.	0.024	n.s.	0.904	n.s.	5.368
CF2	n.s.	0.013	n.s.	−0.223	n.s.	−0.045
D1	n.s.	−0.004	n.s.	5.713	n.s.	4.677
D2	n.s.	0.014	n.s.	0.904	n.s.	4.454
DF2	n.s.	−0.006	n.s.	−0.223	n.s.	−3.253
HBA	n.s.	0.035	n.s.	−1.564	n.s.	−0.898
HBD	0.140	0.060	n.s.	21.407	n.s.	15.825
RB	n.s.	0.032	n.s.	−14.793	12.9	15.721
ϕ	n.s.	−0.014	n.s.	7.672	n.s.	−0.395
Bal^{JX}	n.s.	−0.013	n.s.	−30.362	n.s.	0.272
Bal^{JY}	n.s.	−0.014	n.s.	−18.803	−26.0	−0.564
W	n.s.	0.000	n.s.	−0.054	n.s.	−0.032
Z	n.s.	−0.002	n.s.	3.661	n.s.	1.387
κ_1	n.s.	−0.009	n.s.	−5.738	n.s.	0.526
κ_2	n.s.	−0.013	n.s.	8.699	n.s.	−0.765
κ_3	n.s.	0.022	n.s.	−5.679	n.s.	−8.078
SC^0_p	n.s.	−0.007	n.s.	−5.848	n.s.	0.463
SC^1_p	n.s.	−0.007	n.s.	−5.848	n.s.	0.463
SC^2_p	n.s.	0.006	n.s.	7.678	n.s.	0.231
SC^3_p	n.s.	−0.017	n.s.	−2.194	n.s.	−8.409
SC^3_{cl}	n.s.	0.012	n.s.	−3.522	n.s.	0.869
$^0\chi$	n.s.	−0.003	0.99	1.811	n.s.	0.144
$^1\chi$	n.s.	−0.007	n.s.	−3.813	n.s.	0.412
$^2\chi$	n.s.	0.008	n.s.	8.389	n.s.	−0.720
$^3\chi_p$	n.s.	0.003	n.s.	−1.152	n.s.	3.781
$^3\chi_{cl}$	n.s.	0.002	n.s.	−7.165	n.s.	2.006
$^0\chi^{vm}$	−0.026	−0.039	n.s.	3.486	−8.3	−3.314
$^1\chi^{vm}$	n.s.	−0.009	n.s.	−6.006	n.s.	2.333
$^2\chi^{vm}$	n.s.	−0.010	n.s.	12.129	20.4	3.026
$^3\chi_p^{vm}$	n.s.	−0.009	n.s.	5.831	n.s.	2.857
$^3\chi_{cl}^{vm}$	n.s.	−0.009	n.s.	−10.869	n.s.	1.690
N	46	46	17	17	62	62
R^2	0.968	0.968	0.989	0.999	0.932	0.935
σ	0.036	0.036	1.46	0.20	6.8	6.3

[a] 6 latent variables. [b] 13 latent variables. [c] 9 latent variables.

Table S6. Summary of MLR and PLS results with topological and DARC/PELCO descriptors for the three solvent properties studied.

Descriptor	E_T^N				Dynamic Viscosity (cP)				Boiling point (°C)			
	MLR	PLS	MLR	MLR	MLR	PLS	MLR	MLR	MLR	PLS	MLR	MLR
B0	0.206	1.000	0.851	0.523		30.97	70.79	67.55	111.1	−111.3	278.2	292.6
A1			−0.278	−0.099			−3.52	−5.27			−6.1	
A2			−0.160				−32.50	−35.86			−55.6	−49.7
B1												
B2			−0.026								7.9	
BF2			0.140	0.177							7.0	
C1											33.6	
C2			−0.016								12.6	
CF2			−0.059				6.90				12.0	
D1												
D2											19.1	
DF2												
HBA	0.073	0.014				0.238			−3.2	8.9		
HBD	0.194	0.137		0.140	14.50	9.387			24.7	46.7		
RB		0.010				0.713			11.8	6.4		12.9
ϕ		−0.010				−0.001				−2.4		
Bal^{JX}		−0.150				−3.210				31.1		
Bal^{JY}		−0.081				−2.638				35.4		−26.0
W		0.000				0.003				0.0		
Z		0.001				0.005				−0.2		
κ_1		0.003				−0.024				2.1		
κ_2		−0.009				0.004				−2.0		
κ_3		0.023				−1.118				−5.4		
$SC^0{}_p$		0.003				−0.013				2.3		
$SC^1{}_p$		0.003				−0.013				2.3		
$SC^2{}_p$		0.002				0.025				−1.7		
$SC^3{}_p$	−0.019	−0.001				0.136				−6.4		
$SC^3{}_{cl}$		0.004				0.105				−7.7		
$^0\chi$		0.004				0.000		0.99		1.1		
$^1\chi$		0.004				−0.034				10.8		
$^2\chi$		0.010				−0.106				−5.0		
$^3\chi_p$		−0.001				0.819				0.9		
$^3\chi_{cl}$		0.021				−0.188				2.6		
$^0\chi^{vm}$		−0.019		−0.026		−0.560				−11.2		−8.3
$^1\chi^{vm}$		−0.020				−0.344				−12.8		

$^{2}\chi^{vm}$ $^{3}\chi_{p}^{vm}$ $^{3}\chi_{cl}^{vm}$		−0.024 −0.080 −0.063				−1.185 0.445 −3.142				17.0 109.8 12.0		20.4
N	46	46	**46**	46	17	17	17	**17**	62	62	**62**	62
R^2	0.957	0.969	**0.972**	0.968	0.823	0.700	0.981	**0.989**	0.769	0.891	**0.933**	0.932
σ	0.044	0.036	**0.036**	0.036	7.51	7.29	2.08	**1.46**	12.2	8.1	**6,9**	6.8