

Supporting Information:

What is the Driving Force Behind Molecular Triangles and its guests? A Quantum Chemical Perspective about Host-Guest Interactions

Glaucio R. Nagurniak,^{*,†} Maurício J. Piotrowski,[‡] Álvaro Muñoz-Castro,[¶] João
B. S. Cascaldi,[§] Renato L. T. Parreira,[§] and Giovanni F. Caramori^{||}

[†]*Departamento de Química, Universidade Federal de Santa Catarina, Campus Blumenau,
89036-004, Blumenau, SC, Brazil;*

[‡]*Departamento de Física, Universidade Federal de Pelotas, Caixa postal 354, Capão do
Leão, RS, Brazil.*

[¶]*Lab. de Química Inorgánica y Materiales Moleculares, Universidad Autonoma de Chile,
Llano Subercaceaux 2801, San Miguel, Santiago, Chile.*

[§]*Núcleo de Pesquisas em Ciências Exatas e Tecnológicas, Universidade de Franca, Franca,
SP, Brazil.*

^{||}*Departamento de Química, Universidade Federal de Santa Catarina, Campus
Universitário Trindade, 88040-900 Florianópolis, SC, Brazil.*

E-mail: glaucio.grn@gmail.com

Tables

Table S1: Strain energy (in kcal·mol⁻¹) of XeC**1-4** and I⁻ C**1-4** structures

	XeC 1	I ⁻ C 1	XeC 2	I ⁻ C 2	XeC 3	I ⁻ C 3	XeC 4	I ⁻ C 4
ΔE_{tot}^{str}	1.22	3.87	10.22	10.74	8.53	9.19	7.80	9.86
ΔE_{HEX}^{str}	1.98	1.81	1.47	1.34	2.28	2.01	3.27	3.38
ΔE_{hex1}^{str}	0.86	1.21	1.35	1.34	0.27	0.15	1.12	0.21
ΔE_{hex2}^{str}	0.01	-0.13	-0.86	-0.93	1.23	1.14	0.41	1.49
ΔE_{hex3}^{str}	1.10	0.74	0.98	0.92	0.78	0.72	1.74	1.68
ΔE_{PMDI}^{str}	-0.75	2.06	-	-	0.69	1.29	1.62	2.62
ΔE_{pmdi1}^{str}	-0.06	0.57	-	-	0.69	1.29	1.12	1.37
ΔE_{pmdi2}^{str}	-0.03	0.91	-	-	-	-	0.50	1.25
ΔE_{pmdi3}^{str}	-0.66	0.58	-	-	-	-	-	-
ΔE_{NDI}^{str}	-	-	8.76	9.40	5.55	5.88	2.91	3.86
ΔE_{ndi1}^{str}	-	-	1.65	1.96	1.85	1.89	2.91	3.86
ΔE_{ndi2}^{str}	-	-	2.90	2.94	3.70	3.99	-	-
ΔE_{ndi3}^{str}	-	-	4.21	4.49	-	-	-	-

ΔE_{tot}^{str} is the sum of ΔE_{HEX}^{str} , ΔE_{PMDI}^{str} , and ΔE_{NDI}^{str} terms

Table S2: EDA-NOCV of guests \subset 1 using BP86-D3BJ/ZORA-TZ2P as level of theory.

	$I_3^- \subset 1$	$Br_3^- \subset 1$	$Cl_3^- \subset 1$	$F_3^- \subset 1$	$I^- \subset 1$	$Br^- \subset 1$	$Cl^- \subset 1$	$Xe \subset 1$	$Rb^+ \subset 1$
$^a \Delta E^{int}$	-50.20	-38.51	-35.66	-33.57	-43.01	-39.11	-41.66	-15.40	-21.60
$^a \Delta E^{Pauli}$	38.90	29.12	22.65	35.49	40.20	25.94	44.18	13.8	5.89
$^a \Delta E^{elst}$	-24.30	-20.61	-18.55	-32.90	-37.40	-27.75	-37.82	-5.89	7.46
$^b \%$	(27.27)	(30.48)	(31.81)	(47.64)	(44.95)	(42.66)	(44.06)	(20.17)	-
$^a \Delta E_{tot}^{orb}$	-24.38	-16.19	-16.12	-27.05	-27.18	-23.91	-37.98	-6.57	-20.07
$^b \%$	(27.36)	(23.95)	(27.65)	(39.17)	(32.67)	(36.76)	(44.25)	(22.50)	(57.44)
$^a \Delta E^{disp}$	-40.43	-30.81	-23.64	-9.11	-18.62	-13.39	-10.04	-16.74	-14.87
$^b \%$	(45.37)	(45.57)	(40.54)	(13.19)	(22.38)	(20.58)	(11.70)	(57.33)	(42.56)
$^c q_H$	-0.10	-0.09	-0.10	-0.11	-0.16	-0.16	-0.25	0.01	0.05
$^c q_G$	-0.90	-0.90	-0.90	-0.88	-0.84	-0.84	-0.75	-0.01	0.95

^a All values are reported in kcal·mol⁻¹;

^b Express the percentage of attractive energy, given by $\Delta E^{int} = \Delta E^{elst} + \Delta E^{orb} + \Delta E^{disp}$;

^c q_H and q_G denote the Hirshfeld charges of host and guest, respectively;

Table S3: EDA-NOCV of guests $\subset \mathbf{3}$ using BP86-D3BJ/ZORA-TZ2P as level of theory.

	$I_3^- \subset \mathbf{3}$	$Br_3^- \subset \mathbf{3}$	$Cl_3^- \subset \mathbf{3}$	$F_3^- \subset \mathbf{3}$	$I^- \subset \mathbf{3}$	$Br^- \subset \mathbf{3}$	$Cl^- \subset \mathbf{3}$	$Xe \subset \mathbf{3}$	$Rb^+ \subset \mathbf{3}$
${}^a \Delta E^{int}$	-53.47	-41.98	-38.92	-34.76	-44.24	-40.46	-42.45	-16.17	-24.53
${}^a \Delta E^{Pauli}$	41.01	33.66	25.57	35.54	52.65	28.02	21.28	13.73	8.61
${}^a \Delta E^{elst}$	-26.77	-24.37	-21.03	-31.84	-43.61	-28.29	-23.09	-6.09	4.17
${}^b \%$	(28.33)	(32.22)	(32.61)	(45.29)	(45.01)	(41.31)	(36.23)	(20.37)	-
${}^a \Delta E_{tot}^{orb}$	-25.00	-17.28	-16.97	-28.46	-33.04	-25.46	-29.38	-6.63	-22.78
${}^b \%$	(26.46)	(22.85)	(26.32)	(40.48)	(34.10)	(37.18)	(46.10)	(22.17)	(61.06)
${}^a \Delta E^{disp}$	-42.71	-33.98	-26.48	-10.01	-20.24	-14.73	-11.26	-17.18	-14.53
${}^b \%$	(45.21)	(44.93)	(41.07)	(14.24)	(20.89)	(21.51)	(17.67)	(57.46)	(38.94)
${}^c q_H$	-0.11	-0.11	-0.11	-0.11	-0.18	-0.16	-0.19	0.01	0.05
${}^c q_G$	-0.89	-0.89	-0.89	-0.89	-0.82	-0.84	-0.81	-0.01	0.95

^a All values are reported in kcal·mol⁻¹;

^b Express the percentage of attractive energy, given by $\Delta E^{int} = \Delta E^{elst} + \Delta E^{orb} + \Delta E^{disp}$;

^c q_H and q_G denote the Hirshfeld charges of host and guest, respectively;

Table S4: EDA-NOCV of guests \subset 4 using BP86-D3BJ/ZORA-TZ2P as level of theory.

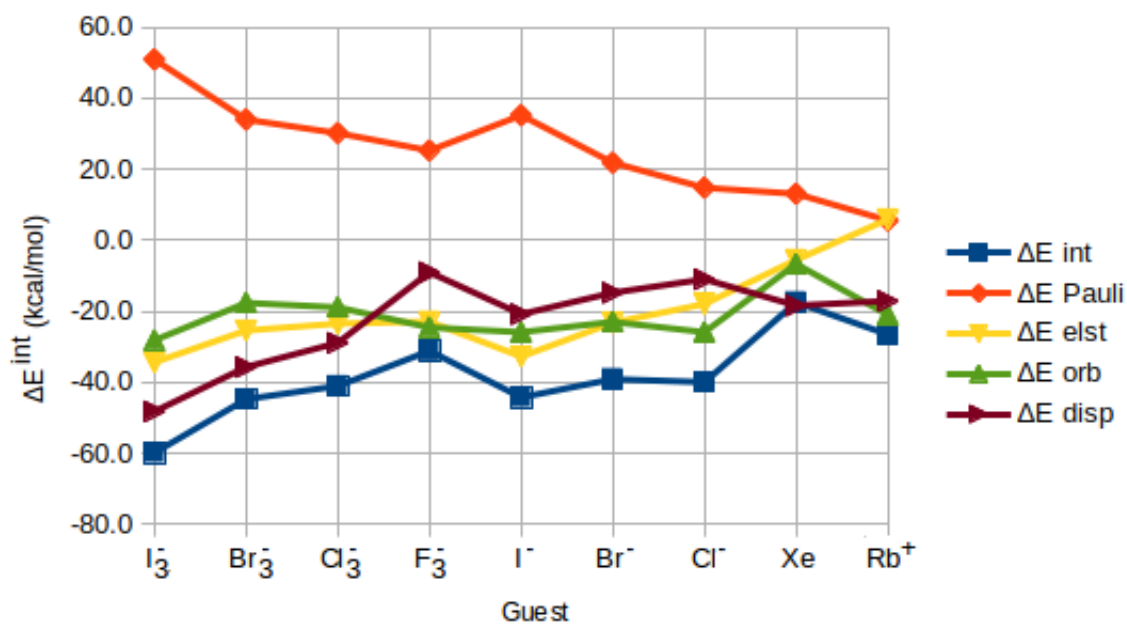
	$I_3^- \subset 4$	$Br_3^- \subset 4$	$Cl_3^- \subset 4$	$F_3^- \subset 4$	$I^- \subset 4$	$Br^- \subset 4$	$Cl^- \subset 4$	$Xe \subset 4$	$Rb^+ \subset 4$
$^a \Delta E^{int}$	-56.49	-40.70	-37.45	-30.31	-43.48	-40.59	-42.76	-17.02	-25.23
$^a \Delta E^{Pauli}$	48.10	30.70	22.20	17.09	38.96	36.80	27.10	13.90	6.06
$^a \Delta E^{elst}$	-31.96	-22.33	-18.60	-17.93	-35.25	-32.92	-26.20	-6.07	6.24
$^b \%$	(30.56)	(31.27)	(31.18)	(37.83)	(42.76)	(42.54)	(37.50)	(19.64)	-
$^a \Delta E_{tot}^{orb}$	-27.22	-16.59	-16.40	-21.23	-26.83	-29.81	-32.52	-6.78	-21.19
$^b \%$	(26.03)	(23.23)	(27.49)	(44.79)	(32.54)	(38.52)	(46.55)	(21.93)	(56.46)
$^a \Delta E^{disp}$	-45.40	-32.49	-24.65	-8.24	-20.36	-14.66	-11.14	-18.06	-16.34
$^b \%$	(43.41)	(45.50)	(41.32)	(17.38)	(24.70)	(18.94)	(15.95)	(58.43)	(43.54)
$^c q_H$	-0.13	-0.10	-0.10	-0.08	-0.14	-0.18	-0.21	0.01	0.05
$^c q_G$	-0.87	-0.89	-0.90	-0.91	-0.86	-0.82	-0.78	-0.01	0.95

^a All values are reported in kcal·mol⁻¹;

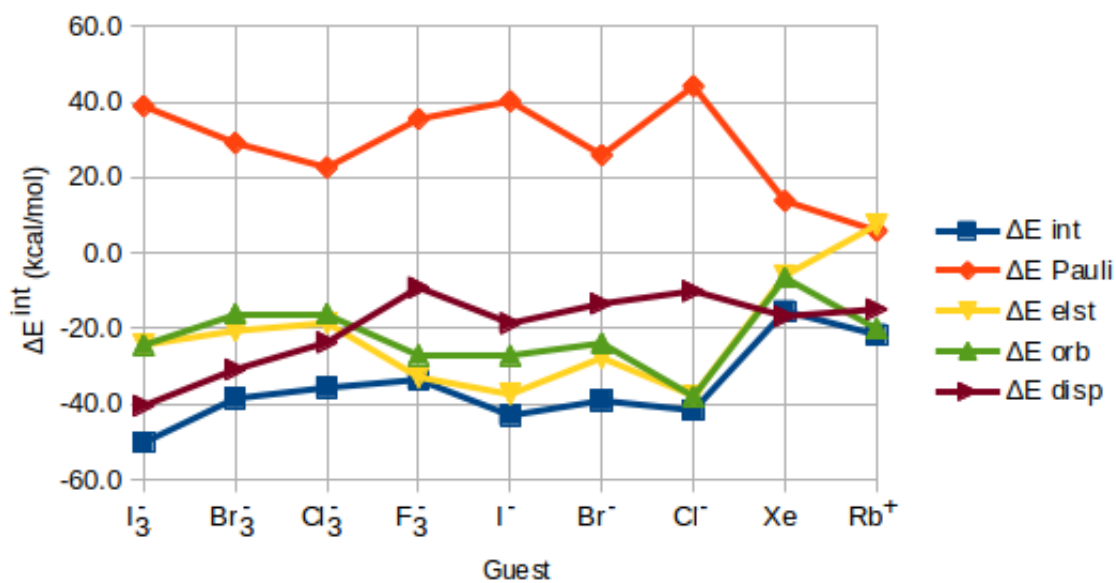
^b Express the percentage of attractive energy, given by $\Delta E^{int} = \Delta E^{elst} + \Delta E^{orb} + \Delta E^{disp}$;

^c q_H and q_G denote the Hirshfeld charges of host and guest, respectively;

Images

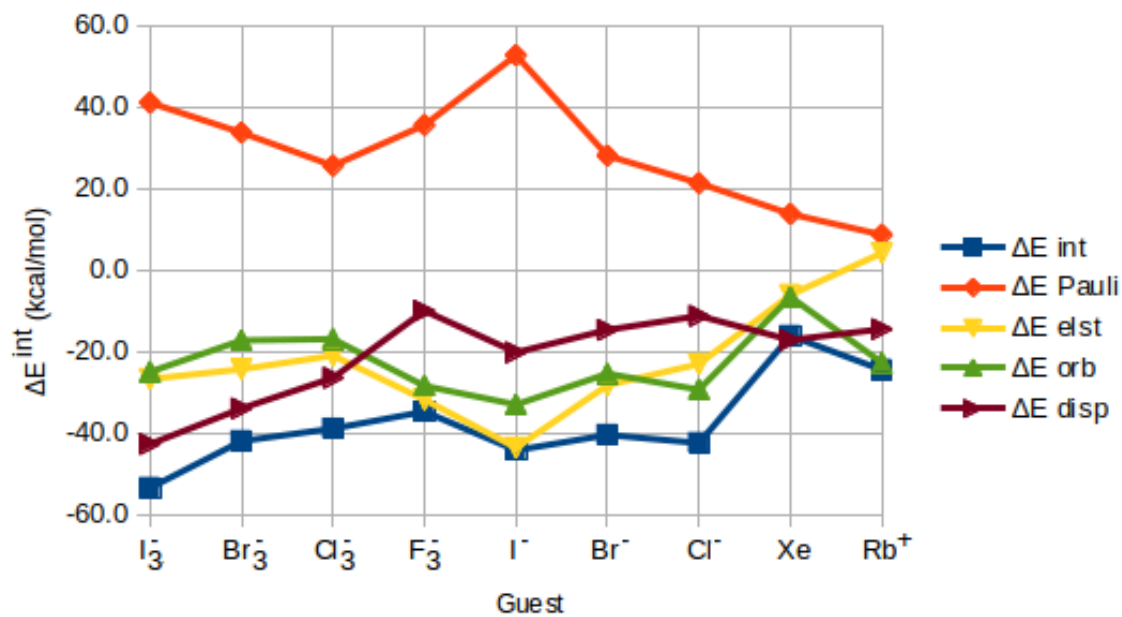


(a)

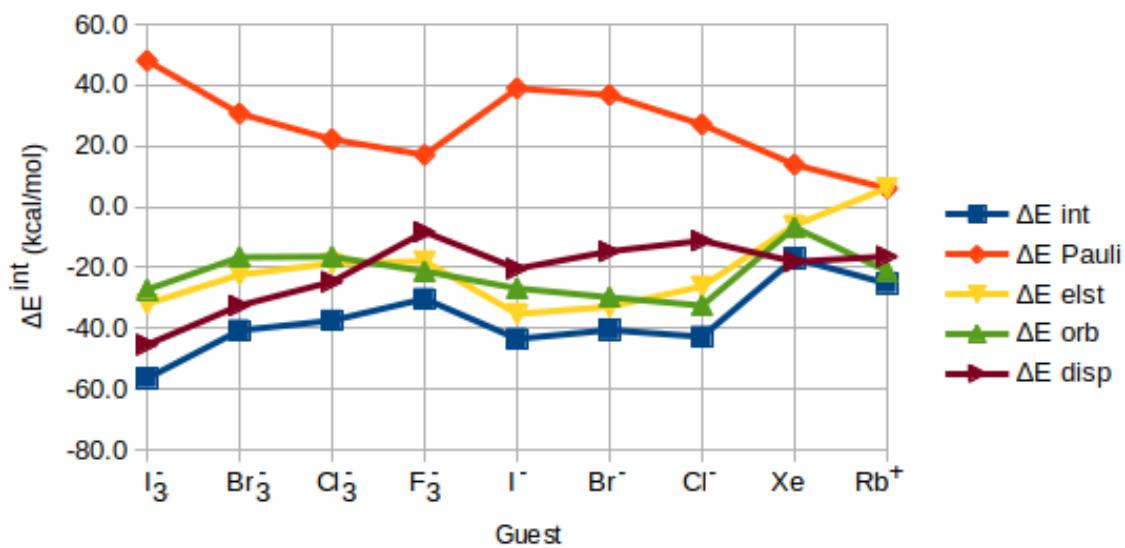


(b)

Figure S1: EDA-NOCV of 1-2 hosts, subfigure (a) and (b), respectively.



(a)



(b)

Figure S2: EDA-NOCV of **3-4** hosts, subfigure (a) and (b), respectively.

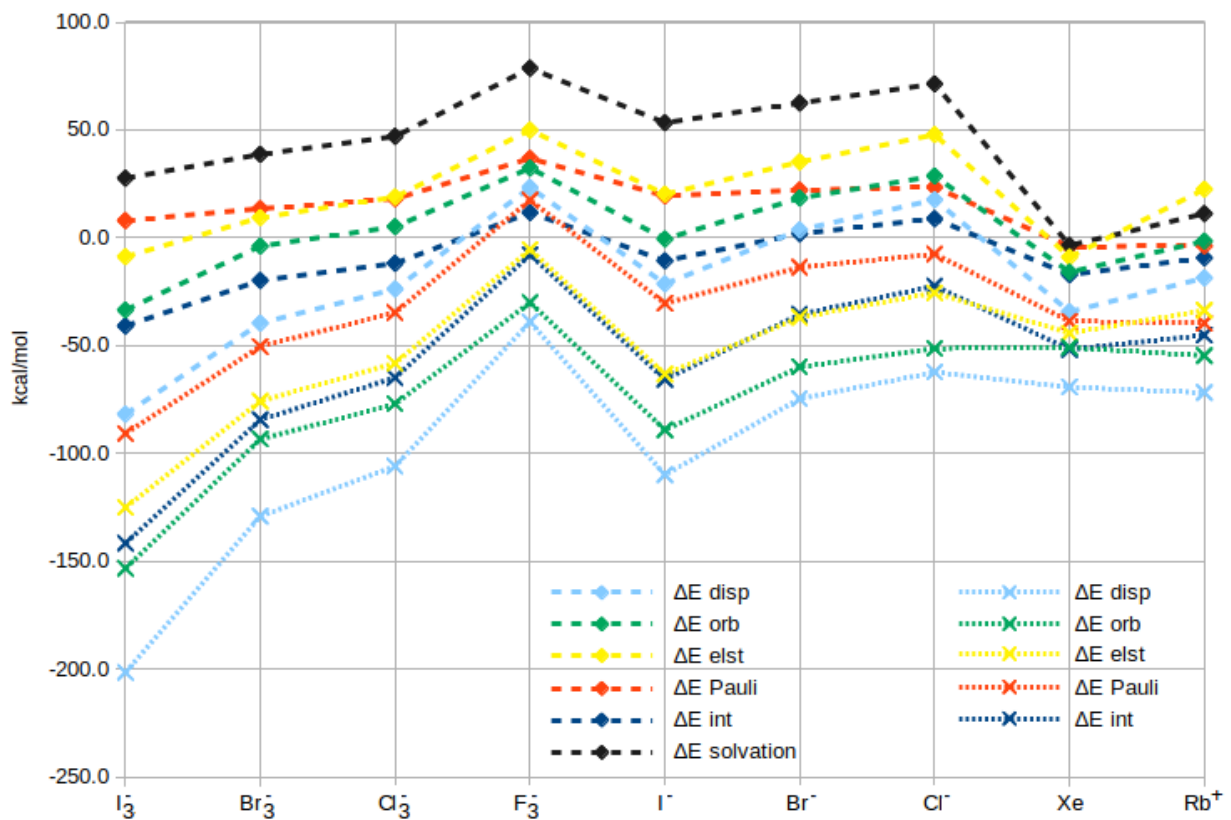


Figure S3: EDA-NOCV of **2** host with all guests of this study at vacuum (diamond-dashed lines) and at implicitly solvation model CH₂Cl₂ (cross-point lines).

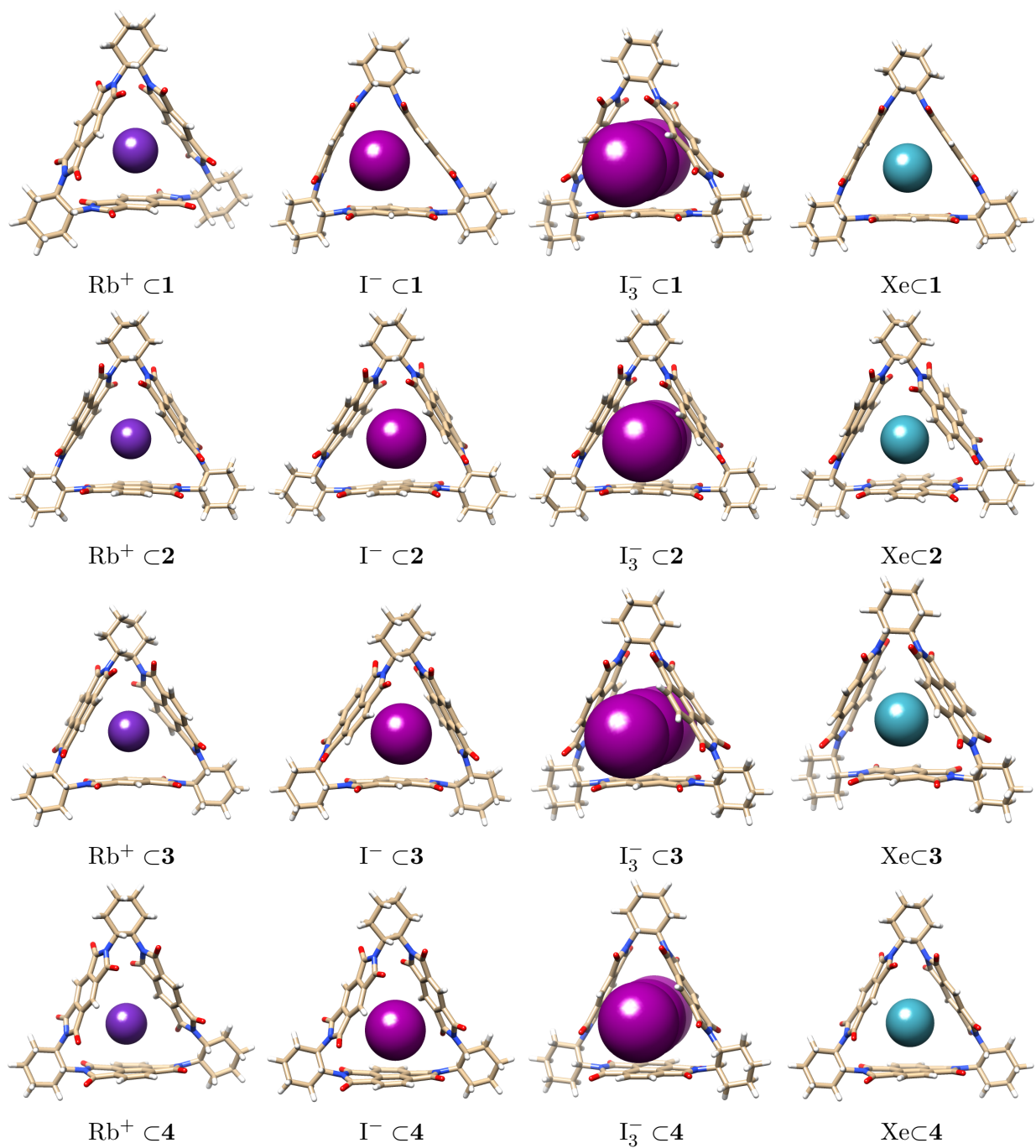


Figure S4: Molecular structures of guests $\subset 1-4$

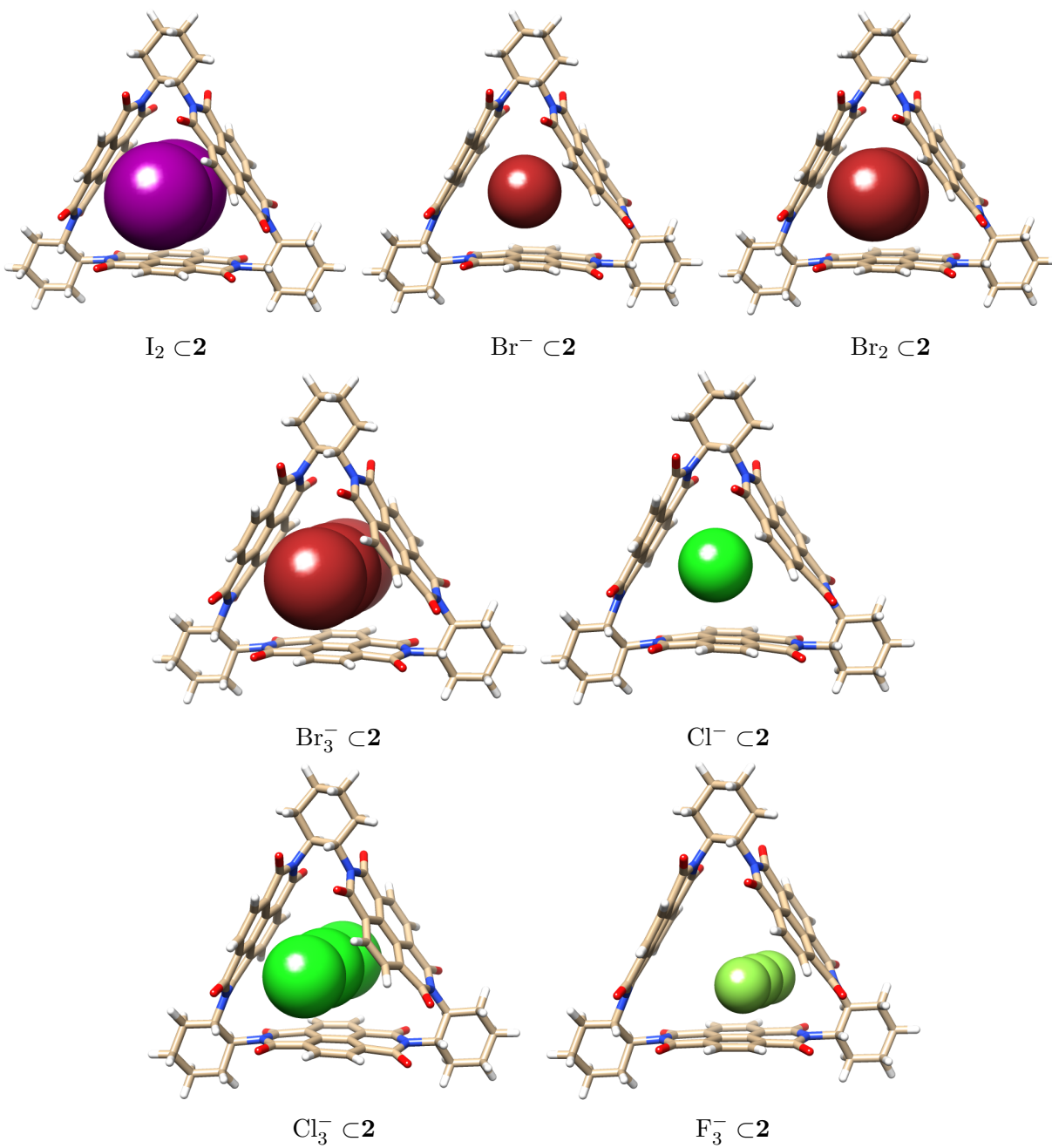


Figure S5: Molecular structures of halogens $\subset C_2$

Atomic Structures

1

C 3.912882000 14.048842000 -4.178050000
H 2.893671000 14.454384000 -4.263724000
C 4.724835000 16.097860000 -5.389244000
H 3.720206000 16.548865000 -5.363884000
C 4.945226000 15.263119000 -6.664365000
H 6.015472000 14.993492000 -6.720129000
H 4.735586000 15.884414000 -7.549000000
C 4.085938000 13.990765000 -6.698847000
H 4.368868000 13.366260000 -7.560842000
H 3.024568000 14.261535000 -6.846757000
C 4.200959000 13.167784000 -5.407185000
H 3.458755000 12.354357000 -5.412562000
H 5.197269000 12.707651000 -5.302476000
N 3.896478000 13.261970000 -2.946462000
H 5.933245000 14.832647000 -4.092597000
C 4.908016000 15.231523000 -4.132042000
H 5.459983000 16.916559000 -5.355286000
C 5.023528000 12.729622000 -2.291532000
O 6.190013000 12.928171000 -2.585893000
C 4.480752000 11.873981000 -1.187891000
C 5.176889000 11.098338000 -0.260278000
H 6.266707000 11.073546000 -0.223113000
C 4.373449000 10.359528000 0.610991000
C 4.775716000 9.442857000 1.722072000
C 2.968756000 10.395295000 0.556688000
C 2.431638000 9.498261000 1.631573000
C 2.272618000 11.173094000 -0.370115000
H 1.182709000 11.197463000 -0.407361000
C 3.076404000 11.912061000 -1.242341000
C 2.680701000 12.795748000 -2.383289000
N 3.563174000 8.996604000 2.305113000
O 5.892911000 9.118509000 2.074714000
O 1.267800000 9.241289000 1.888109000
O 1.566312000 13.063533000 -2.789822000
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C 4.144592000 12.345789000 4.996843000
C 4.325447000 10.857427000 4.961585000
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C 5.303473000 15.943899000 5.414664000
C 3.211438000 14.927121000 5.073907000
C 3.012264000 16.405322000 5.218853000

C 2.261031000 13.923352000 4.882554000
H 1.194103000 14.121236000 4.779850000
C 2.774527000 12.625963000 4.847903000
C 2.043730000 11.332231000 4.686501000
N 4.304506000 16.948168000 5.377135000
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H 5.722527000 18.408903000 5.508562000
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H 3.130281000 18.672158000 7.143721000
C 4.640335000 20.238607000 7.310411000
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H 4.358825000 20.527441000 8.335391000
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H 4.287256000 22.225061000 6.437176000
H 2.911395000 21.112648000 6.332795000
C 4.429391000 20.747526000 4.847019000
H 3.984514000 21.407840000 4.087043000
H 5.527407000 20.804881000 4.740781000
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C 5.302181000 16.980157000 -0.854076000
C 5.880599000 16.307534000 -2.060533000
C 3.562607000 16.494005000 -2.368064000
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H 2.678231000 4.973444000 4.485472000
C 2.322177000 6.700188000 5.770735000
H 2.444403000 6.137170000 6.709219000
H 1.238885000 6.713453000 5.552696000
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H 2.189882000 8.665161000 6.708272000
H 3.851808000 8.166734000 6.323276000
N 3.035951000 10.324360000 4.749959000
O 5.354045000 10.217651000 5.094560000

Rb⁺ c1

C 3.911389000 14.043605000 -4.206653000
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H 3.712370000 16.564047000 -5.349487000
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H 4.719035000 15.932982000 -7.542571000
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H 4.366406000 13.412140000 -7.593992000
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H 5.198319000 12.719347000 -5.350349000
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H 5.932259000 14.829606000 -4.115680000
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H 5.451869000 16.931962000 -5.340321000
C 5.021275000 12.693212000 -2.339349000
O 6.190839000 12.912711000 -2.601994000
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C 5.177123000 11.032817000 -0.319147000
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C 2.677267000 12.772326000 -2.419862000

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O 5.895666000 9.145987000 2.079542000
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C 5.090536000 13.361083000 5.207231000
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N 4.301526000 16.967236000 5.386329000
O 6.491162000 16.144978000 5.579226000
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H 3.990159000 21.432086000 4.097678000
H 5.531427000 20.829988000 4.755803000
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C 5.097743000 17.941639000 1.303390000
C 5.942204000 17.387986000 0.332440000
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C 3.904779000 17.033267000 -1.008269000

C 3.062613000 17.594647000 -0.044291000
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O 7.039423000 15.994921000 -2.268090000
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H 1.635892000 8.905970000 4.326152000
H 4.588409000 8.168488000 3.865015000
C 3.012593000 6.777721000 3.321587000
H 3.641062000 6.294528000 2.557205000
H 1.983219000 6.824536000 2.928684000
C 3.076848000 5.996442000 4.643494000
H 4.138210000 5.878715000 4.929202000
H 2.683217000 4.979087000 4.493097000
C 2.321307000 6.702341000 5.778565000
H 2.446526000 6.142654000 6.717658000
H 1.238059000 6.709804000 5.562210000
C 2.803421000 8.150963000 5.970822000
H 2.177403000 8.666355000 6.715756000
H 3.843090000 8.173946000 6.339329000
N 3.029601000 10.330306000 4.758355000
O 5.352941000 10.232896000 5.093828000
Rb 4.287736000 14.127689000 1.493306000

I⁻ c1

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H -2.471284000 1.574110000 13.882997000
Rb 1.898021000 5.703403000 12.101785000

I⁻ C3

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O 3.548195000 7.043360000 17.276279000
O -0.255521000 9.234339000 15.793703000
O -2.661142000 3.982002000 14.129398000
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O 3.698059000 8.031177000 7.763195000
O 1.332285000 11.218542000 13.609737000
O 5.684883000 3.240130000 8.433214000
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O -1.967054000 1.764128000 11.636937000
O 1.917409000 5.477383000 7.035556000
N -0.864144000 2.569196000 14.639839000
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H 5.816780000 7.871766000 6.544530000
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 H 3.931110000 6.065156000 6.553286000
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 I 2.512958000 5.191772000 12.392558000

$I_3^- \subset \mathbf{3}$

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O 3.714282000 8.033718000 7.707301000
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O 5.713769000 3.284155000 8.460517000
O 1.895510000 -0.200069000 13.268948000
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C 0.433521000 6.828564000 15.698232000
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XeC₃

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O 5.647518000 3.291680000 8.402453000
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H -2.527365000 1.607196000 13.863525000
Xe 2.240397000 5.436195000 12.429558000

4

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O 4.463510000 19.635182000 6.082218000
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C 1.856801000 9.396748000 3.748835000
H 2.798837000 8.857644000 3.559178000
C 0.873326000 9.100570000 2.603621000
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H -0.144260000 7.406678000 1.715916000
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Rb⁺ C4

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I⁻ C4

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$I_3 \subset 4$

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C 5.320421000 11.074497000 9.628163000
C 6.021603000 10.322683000 8.687692000
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