Electronic Supplementary Information (ESI) for the manuscript:
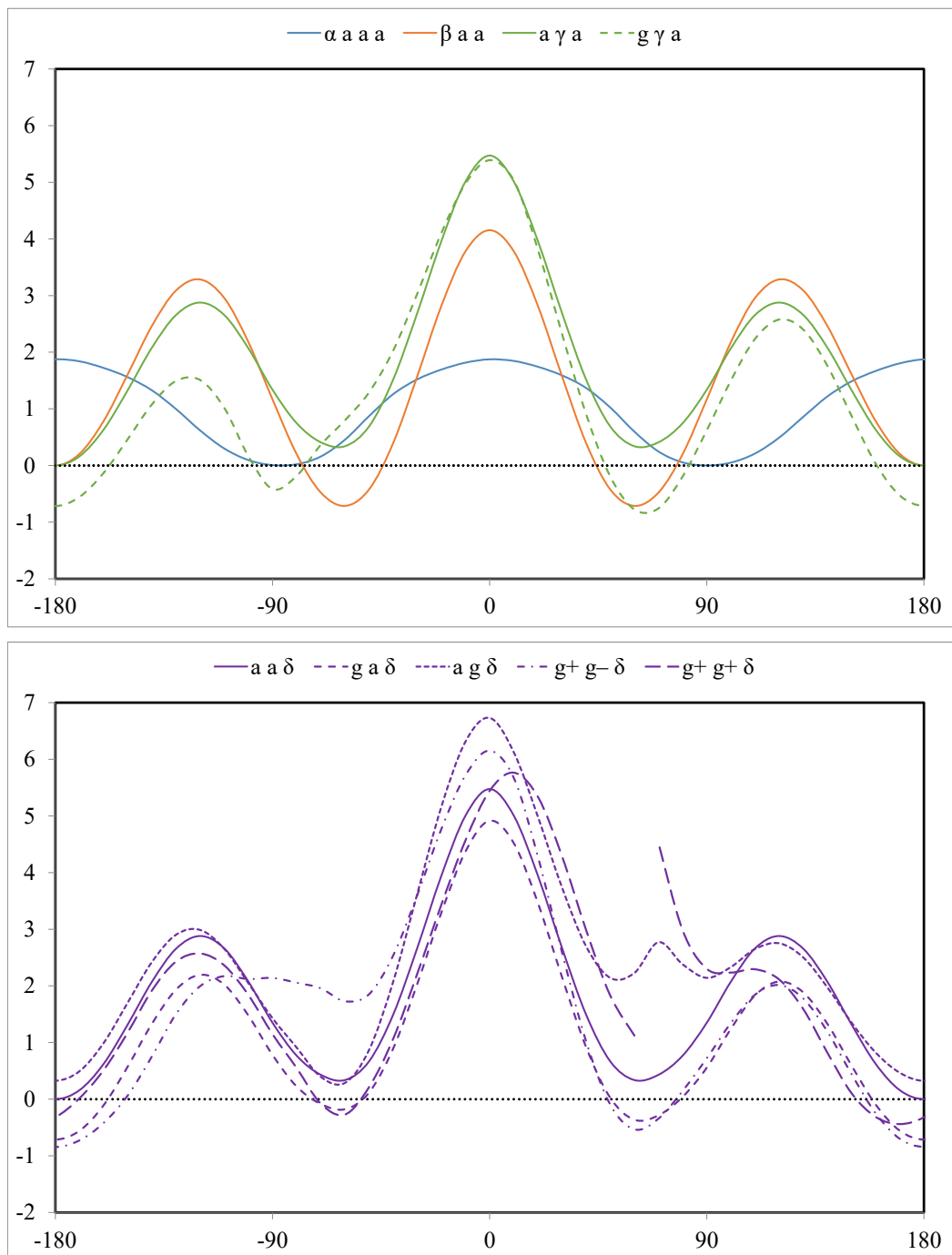
Exploring short intramolecular interactions in alkylaromatic substrates

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Content:

Figure S1. Potential energy curves for the rotation about dihedral angles α, β, γ, and δ, obtained from relaxed scansion of said angles in steps of 10° at MP2/6-311G(d,p) level. The ε angle was only considered in its anti configuration. Curves are labelled following the same criterion used in the main text, with the investigated torsion angle explicitly indicated with the corresponding Greek letter. Vertical axis shows energy in kcal/mol relative to all-anti aaa configuration, horizontal axis shows angles in degrees.

Table S1. Configuration of all dihedral angles of the side chain for the 15 conformers of compound **1**.[a]

	α	β	γ	δ	ε
aaa	88.2	180.0	180.0	180.0	180.0
aag	87.8	-179.1	-174.0	-62.1	-174.3
aga	88.9	-176.0	-62.8	-173.8	-179.0
ag^+g^+	89.1	-177.0	-58.0	-56.9	-174.3
ax^+g^-	86.3	176.6	-96.2	59.8	175.8
ag^+x^-	88.9	-176.8	-59.7	96.2	-177.0
gaa	74.9	60.3	177.6	179.3	-179.8
g^+ag^-	73.5	61.4	-176.2	-62.4	-173.8
g^+ag^+	73.9	60.3	173.4	62.1	173.4
g^+x^-a	76.7	55.8	-90.0	171.6	179.9
$g^+g^-g^-$	62.6	63.8	-74.5	-60.2	-178.9
$g^+g^-x^+$	45.4	75.1	-63.3	97.8	-166.1
g^+g^+a	68.4	55.7	62.3	176.0	178.7
$g^+x^+g^-$	70.2	60.5	91.5	-61.1	-173.0
$g^+g^+g^+$	66.1	57.0	58.9	57.4	174.4

[a] Angles in degrees
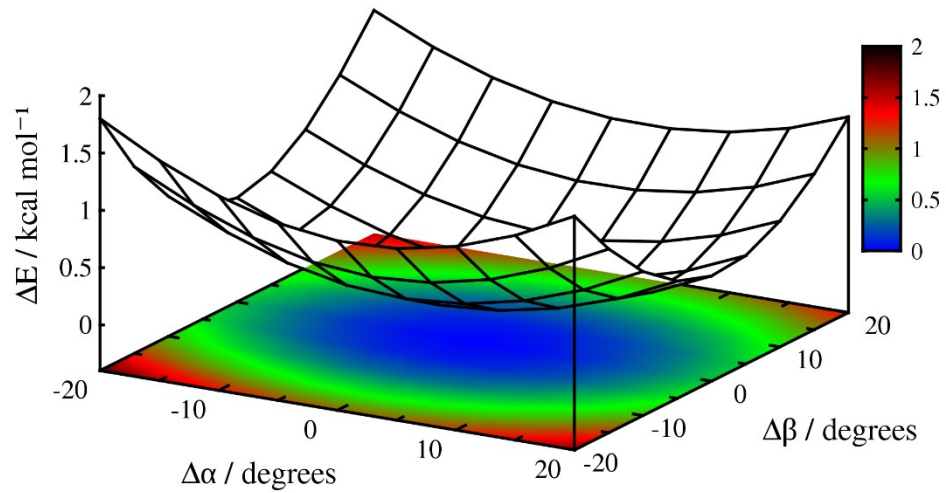
Figure S2. Potential energy surface associated with the deformation of α and β angles in conformer **1b**.
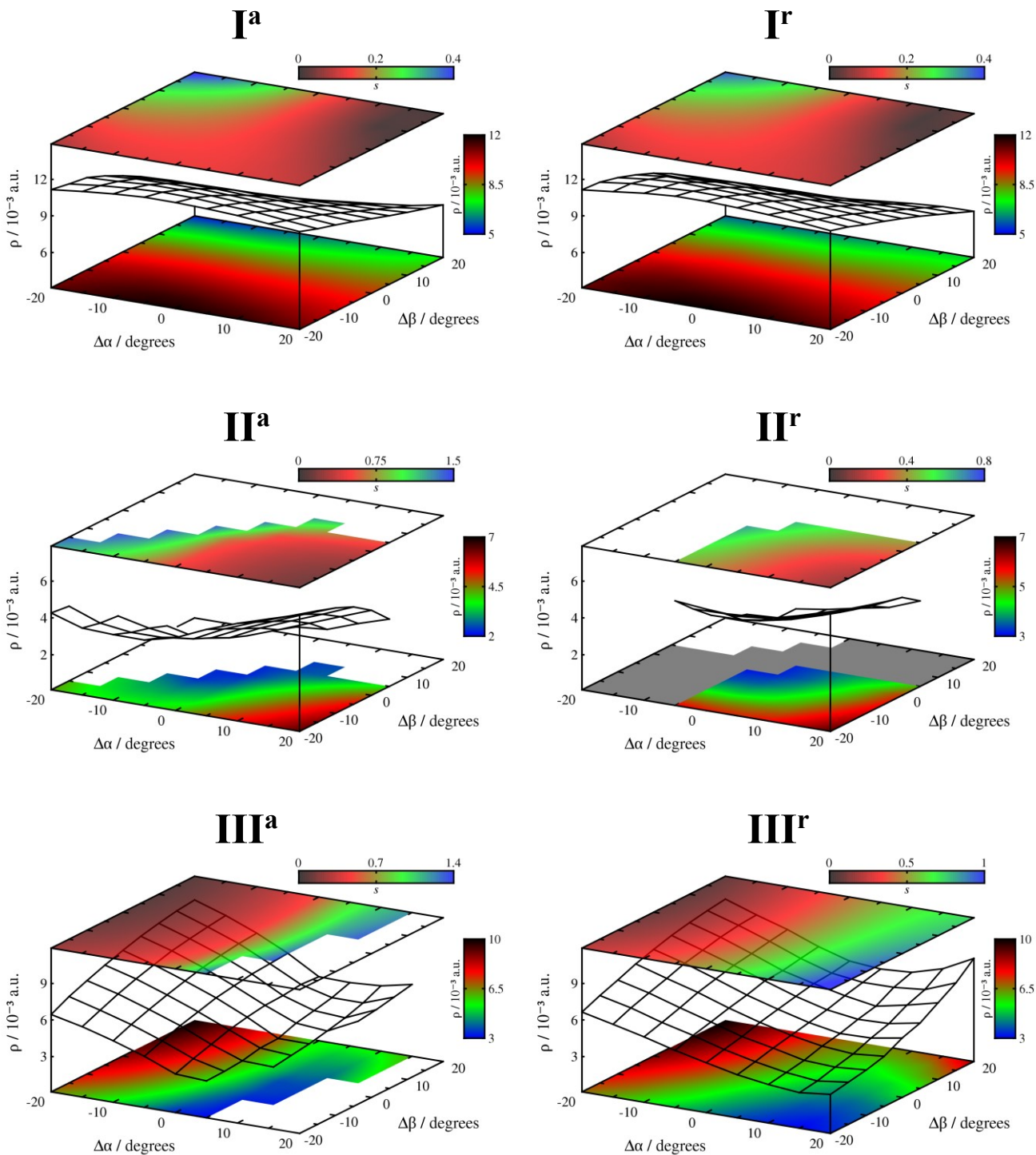
Figure S3. Values of $\rho(s_{min})$ and s_{min} obtained for conformer **1b** as a function of $\{\Delta\alpha,\Delta\beta\}$. The former is represented as both a three-dimensional surface and a heat map on the bottom of each graph, while the latter is reported on top as a semi-transparent heatmap. White regions indicate no minimum is obtained, grey regions indicate the trough only appears as a shoulder on another trough.

IV^a

IV^r

V^a

V^r
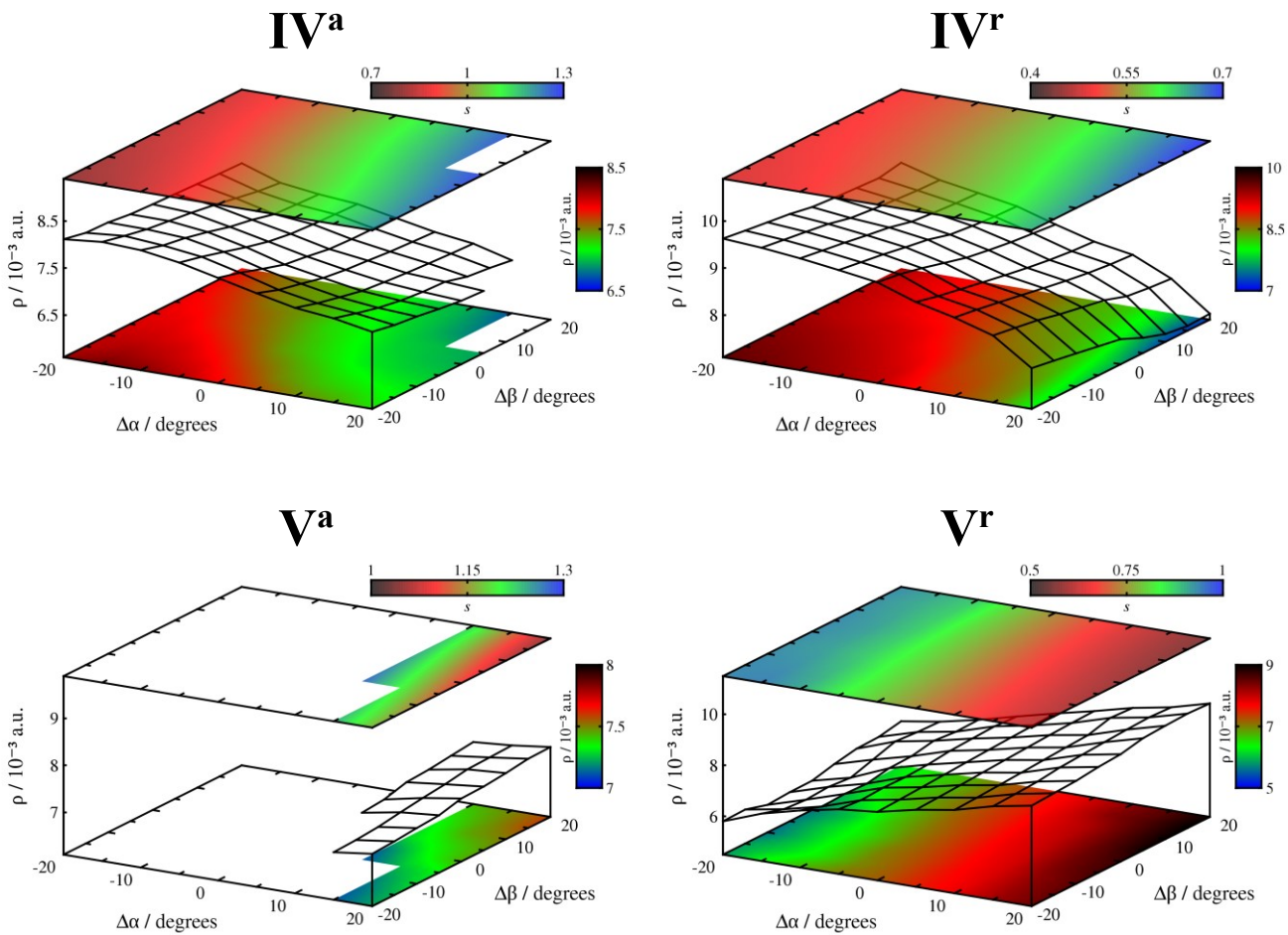
Figure S3. *Follows from previous page*

The complete basis set limit extrapolated energies discussed in the manuscript were obtained as follows:

$$E_{MP2/CBS}^{tot} = E_{HF/aQz}^{exch} + E_{MP2/aTQz}^{corr}$$

$$E_{CCSD(T)/CBS}^{tot} = E_{MP2/CBS}^{tot} + \delta_{[CCSD(T)-MP2]/aDz}$$

$$\delta_{[CCSD(T)-MP2]/aDz} = E_{CCSD(T)/aDz}^{corr} - E_{MP2/aDz}^{corr}$$

Helgaker's formula for aTQz extrapolation was employed (A. Halkier, T. Helgaker, P. Jørgensen, W. Klopper, H. Koch, J. Olsen and A. K. Wilson, *Chem. Phys. Lett.*, 1998, **286**, 243–252). As for the $\delta_{[CCSD(T)-MP2]/aDz}$ term, we were indeed forced to use a small aDz (aug-cc-pVDZ) basis set due to the size of the largest system studied. Such basis set, however, has in at least one instance been deemed as inappropriate for the treatment of noncovalent interactions, and for hydrogen-bonded complexes in particular (M. S. Marshall, L. A. Burns, C. D. Sherrill, *J. Chem. Phys.*, 2011, **135**, 194102). Because of this, we tested larger basis sets on smaller molecular systems in order to assess the reliability of our benchmark calculations. CCSD(T)/Tz (cc-pVTZ) and CCSD(T)/aTz (aug-cc-pVTZ) were thus performed on both conformational isomers of compounds **22** and **23**, namely 2-phenylethanol and 2-pheylethanethiol.

The results, collected below, convinced us of the soundness of our choice. Using either a $\delta_{[CCSD(T)-MP2]}$ term computed via aTz basis set, or performing a direct extrapolation of the basis set effect via Helgaker's formula at the CCSD(T) level, bears little effect on the final extrapolated relative energies, with an error over the reference data ($\delta_{[CCSD(T)-MP2]/aDz}$) always well within 0.1 kcal/mol.

Table S2. Results of the complete basis set extrapolation test performed.[a]

	ΔE (**22b** – **22a**)	error	ΔE (**23b** – **23a**)	error
CCSD(T)/aDz[b]	-1.487	-0.180	-0.875	-0.226
CCSD(T)/Tz[b]	-1.391	-0.084	-0.533	+0.116
CCSD(T)/aTz[b]	-1.388	-0.081	-0.721	-0.072
CCSD(T)/CBS(aDz)[c]	-1.307	reference	-0.649	reference
CCSD(T)/CBS(Tz)[c]	-1.249	+0.058	-0.588	+0.061
CCSD(T)/CBS(aTz)[c]	-1.273	+0.034	-0.590	+0.059
CCSD(T)/CBS[aDTz][d]	-1.376	+0.069	-0.713	-0.064

[a] All energies in kcal/mol

[b] Non-extrapolated energies

[c] CBS(X) refers to a basis set extrapolations using X basis set to compute the $\delta_{[CCSD(T)-MP2]}$ term

[d] direct CBS extrapolation at coupled-cluster level following Helgaker's formula, using aDz and aTz basis sets

A series of tests have been performed in order to evaluate the weight of the optimized geometries on the final extrapolated relative energies. Compounds **1** (limited to conformers **a** and **b**), **19** and **22** were chosen for these tests, as they represent respectively a prototypical all-Carbon alkylaromatic species, a heteroaromatic species with one stabilized and one destabilized gauche conformers, and the species featuring the most stabilized gauche conformer out of the set presented in the main text.

New geometry optimizations and zero-point correction calculations were carried out at MP2 level with a aDz basis set (aug-cc-pVDz), and at B3LYP level using Grimme's D3 and D3BJ dispersion corrections (the latter featuring Becke-Johnson damping function) with either aDz or aTz (aug-cc-pVTZ) basis sets (refer to the main text for the corresponding citations). CCSD(T)/CBS, MP2/CBS, and relative zero-point correction ($\Delta E_{zero-point}$) energies have been computed for each set of optimized geometries.

With reference to **Table S3** through **S5**, showing selected geometrical parameters from all re-optimized structures, MP2/aDz structures are generally in good agreement with reference MP2/6-311G(d,p) ones, while all dispersion-corrected B3LYP structures (with few exceptions) show the largest deformations.

Table S3. Values of the α angle in re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b
MP2/6-311G(d,p)	74.9	117.1	84.1	85.0
MP2/aDz	75.0	116.4	79.6	82.6
B3LYP-D3/aDz	77.0	115.9	92.4	84.4
B3LYP-D3/aTz	75.6	116.4	93.7	84.4
B3LYP-D3BJ/aDz	76.2	115.6	88.0	83.6
B3LYP-D3BJ/aTz	74.9	116.1	88.4	83.4

[a] All angles in degrees

Table S4. Values of the β angle in re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b
MP2/6-311G(d,p)	60.3	58.8	58.4	60.5
MP2/aDz	59.7	56.5	55.8	60.8
B3LYP-D3/aDz	64.2	61.6	62.9	63.0
B3LYP-D3/aTz	64.5	62.7	64.2	63.2
B3LYP-D3BJ/aDz	63.1	60.5	61.5	62.3
B3LYP-D3BJ/aTz	63.5	61.6	62.8	62.4

[a] All angles in degrees

Table S5. Distance between the electron accepting Hydrogen atom and the Carbon atom of the aromatic ring bearing the substituent in re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b
MP2/6-311G(d,p)	2.696	2.674	2.708	2.517
MP2/aDz	2.663	2.626	2.635	2.529
B3LYP-D3/aDz	2.775	2.734	2.803	2.652
B3LYP-D3/aTz	2.780	2.744	2.819	2.656
B3LYP-D3BJ/aDz	2.756	2.718	2.774	2.622
B3LYP-D3BJ/aTz	2.762	2.727	2.793	2.624

[a] All distances in Å

Owing to the shallowness of the potential energy minimum point shown for conformer **1b** in **Figure S2** along $\Delta\alpha$ and $\Delta\beta$ axes, however, such geometrical deformations do not translate in pronounced differences in complete basis set extrapolated energies compared to MP2/6-311G(d,p) optimized geometries. With reference to **Tables S6** and **S7**, only in one instance the error produced exceeds 0.1 kcal/mol, while mean unsigned errors (MUE) never exceed 0.07 kcal/mol overall. The best agreement with CCSD(T)/CBS extrapolated energies is obtained from B3LYP-D3/aTz structures (with a MUE equal to 0.009 kcal/mol), while B3LYP-D3BJ/aDz ones show the best agreement with reference MP2/CBS data (with a MUE equal to 0.016 kcal/mol). Similar results are obtained for relative zero-point correction energies (**Table S8**), with mean unsigned errors in the range of 0.050–0.062 kcal/mol for all five test sets. Noticeable is however the case of compound **1**, for which $\Delta E_{zero\text{-}point}$ is always underestimated by 0.09–0.14 kcal/mol compared to reference data.

Considering the results collected in **Table S3** through **S8**, MP2/6-311G(d,p) optimized geometries and zero-point corrections appear to be an adequate choice, not only for the present dataset but also feasibly affordable for larger molecular systems.

Table S6. CCSD(T)/CBS extrapolated energies (with the corresponding signed errors in parentheses) and mean unsigned errors (MUE) obtained from re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b	MUE
MP2/6-311G(d,p)	-0.049	-0.244	0.444	-1.307	reference
MP2/aDz	0.041 (+0.090)	-0.182 (+0.062)	0.538 (+0.094)	-1.328 (-0.021)	0.066
B3LYP-D3/aDz	-0.088 (-0.039)	-0.258 (-0.014)	0.417 (-0.027)	-1.321 (-0.014)	0.024
B3LYP-D3/aTz	-0.073 (-0.024)	-0.243 (+0.001)	0.442 (-0.002)	-1.318 (-0.011)	0.009
B3LYP-D3BJ/aDz	-0.098 (-0.049)	-0.264 (-0.020)	0.401 (-0.043)	-1.338 (-0.031)	0.036
B3LYP-D3BJ/aTz	-0.084 (-0.035)	-0.253 (-0.009)	0.425 (-0.019)	-1.335 (-0.028)	0.022

[a] Energies in kcal/mol

Table S7. MP2/CBS extrapolated energies (with the corresponding signed errors in parentheses) and mean unsigned errors (MUE) obtained from re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b	MUE
MP2/6-311G(d,p)	-0.400	-0.537	0.119	-1.543	reference
MP2/aDz	-0.344 (+0.056)	-0.504 (+0.033)	0.153 (+0.034)	-1.550 (-0.007)	0.032
B3LYP-D3/aDz	-0.376 (+0.024)	-0.502 (+0.035)	0.182 (+0.063)	-1.493 (+0.050)	0.043
B3LYP-D3/aTz	-0.346 (-0.054)	-0.475 (+0.062)	0.225 (+0.106)	-1.485 (+0.058)	0.070
B3LYP-D3BJ/aDz	-0.402 (-0.002)	-0.517 (+0.020)	0.138 (+0.019)	-1.520 (+0.023)	0.016
B3LYP-D3BJ/aTz	-0.368 (+0.032)	-0.494 (+0.043)	0.181 (+0.062)	-1.511 (+0.032)	0.042

[a] Energies in kcal/mol

Table S8. $\Delta E_{zero\text{-}point}$ energies (with the corresponding signed errors in parentheses) and mean unsigned errors (MUE) obtained from re-optimized structures of conformers **1b**, **19b**, **19c**, and **22b**.[a]

	1b	19b	19c	22b	MUE
MP2/6-311G(d,p)	0.198	0.130	0.104	0.155	reference
MP2/aDz	0.054 (-0.144)	0.103 (-0.027)	0.133 (+0.029)	0.204 (+0.049)	0.062
B3LYP-D3/aDz	0.093 (-0.105)	0.076 (-0.054)	0.107 (+0.003)	0.196 (+0.041)	0.051
B3LYP-D3/aTz	0.106 (-0.092)	0.041 (-0.089)	0.085 (-0.019)	0.186 (+0.031)	0.057
B3LYP-D3BJ/aDz	0.075 (-0.123)	0.113 (-0.017)	0.073 (-0.031)	0.185 (+0.030)	0.050
B3LYP-D3BJ/aTz	0.093 (-0.105)	0.067 (-0.063)	0.051 (-0.053)	0.166 (+0.011)	0.058

[a] Energies in kcal/mol

aaa (Isomer 1a)

```
C    0.006112   -0.102621    0.164686
C    0.002901   -0.049393    1.562173
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C    2.418759   -0.102621    0.164686
C    2.421971   -0.049393    1.562173
C    1.212436   -0.019311    2.264723
H    3.360903   -0.131144   -0.379500
H    3.365365   -0.032141    2.101361
H    1.212436    0.019500    3.350325
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C    1.212436   -0.123036   -2.058663
C    1.212435    1.309967   -2.610490
C    1.212436    1.363881   -4.138155
C    1.212436    2.791599   -4.684865
C    1.212436    2.854776   -6.212628
C    1.212436    4.288837   -6.743184
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H    0.329132   -0.654527   -2.434948
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H    2.092882    1.839302   -2.222489
H    2.093795    0.830027   -4.519486
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H    2.093068    3.324837   -4.301243
H    2.092407    2.320234   -6.592010
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aag

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C   -0.415188   -0.052875    0.993434
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C    1.972660    1.020830   -4.392028
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H    2.746815   -0.573414   -2.241059
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H    2.241233    1.864363   -2.420171
H    2.961746    0.549853   -4.468971
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H    2.345069    2.212310   -6.150594
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H    0.336050    3.341245   -4.139896
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aga

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C    2.137826    1.060852    0.216014
C    2.132589    0.822424    1.594008
C    1.399518   -0.248544    2.116619
H    2.712941    1.891493   -0.188946
H    2.697860    1.470875    2.258077
H    1.396110   -0.437483    3.186357
H    0.113431   -1.919252    1.651204
H    0.132751   -1.490684   -0.794229
C    1.377616    0.533023   -2.137013
C    0.227693    1.495149   -2.473893
C    0.067079    1.765515   -3.973002
C    1.274842    2.451507   -4.614112
C    1.032551    2.846278   -6.071618
C    2.252234    3.508174   -6.713257
H    2.333847    0.968000   -2.448444
H    1.243321   -0.397891   -2.703715
H   -0.702992    1.071726   -2.075106
H    0.392494    2.442940   -1.943730
H   -0.129827    0.817820   -4.493414
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H    1.527328    3.350621   -4.033847
H    2.150585    1.792051   -4.569010
H    0.754720    1.950713   -6.641674
H    0.173789    3.527549   -6.119273
H    2.057061    3.787755   -7.752803
H    2.532046    4.414098   -6.165822
H    3.111394    2.829716   -6.700749
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ag+g+

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C    0.844814   -0.646621   -0.121729
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C    1.884051    1.529729   -0.188840
C    1.836911    1.599375    1.207063
C    1.287757    0.543360    1.942513
H    2.317072    2.349687   -0.759140
H    2.226219    2.475223    1.719247
H    1.252467    0.593741    3.027067
H    0.372582   -1.409472    1.839597
H    0.464951   -1.525685   -0.638931
C    1.388412    0.367144   -2.377133
C    0.104079    0.992750   -2.941552
C    0.003865    0.920473   -4.469428
C    1.163116    1.591064   -5.215931
C    1.358363    3.065750   -4.860486
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H    2.567554    4.784169   -5.451409
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```

ax⁺g⁻

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C	0.967191	0.858988	1.935356
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H	-0.653467	0.325035	-5.002603
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ag⁺x⁻

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C	1.277174	0.790612	-0.745291
C	1.052727	1.924502	0.050430
C	0.865099	1.806304	1.431209
C	0.889241	0.544726	2.035642
H	1.038415	2.907382	-0.417106
H	0.699477	2.695594	2.033475
H	0.746513	0.450497	3.108391
H	1.135469	-1.576439	1.716341
H	1.471969	-1.355834	-0.733718
C	1.412194	0.918039	-2.241181
C	0.039813	0.848755	-2.927620
C	0.086251	0.892938	-4.459440
C	0.733889	2.166105	-5.034477
C	2.216003	2.012427	-5.389147
C	2.834695	3.318968	-5.886365
H	1.901558	1.868935	-2.480970
H	2.052649	0.114520	-2.627540
H	-0.460661	-0.073046	-2.603645
H	-0.574410	1.682250	-2.560697
H	0.625829	0.011279	-4.832282
H	-0.942377	0.803992	-4.828657
H	0.201248	2.473725	-5.943197
H	0.614997	2.991810	-4.318232
H	2.773749	1.648501	-4.519970
H	2.310035	1.240590	-6.163536
H	3.884217	3.186035	-6.165123
H	2.295344	3.692545	-6.763017
H	2.785739	4.089397	-5.109777

gaa (Isomer 1b)

C	0.016850	0.072941	0.092947
C	-0.016662	0.080005	1.490490
C	1.208934	-0.196098	-0.598584
C	2.369846	-0.455341	0.144846
C	2.342955	-0.448887	1.543929
C	1.149532	-0.177156	2.220532
H	3.299316	-0.668709	-0.379086
H	3.251652	-0.654036	2.103583
H	1.125836	-0.173503	3.306581
H	-0.949641	0.284488	2.008939
H	-0.893257	0.267432	-0.471661
C	1.237293	-0.148427	-2.106019
C	1.218024	1.296996	-2.632174
C	2.414248	2.121300	-2.158054
C	2.424061	3.539781	-2.727596
C	3.610508	4.373756	-2.243341
C	3.608428	5.791542	-2.815734
H	2.139490	-0.653370	-2.473581
H	0.374279	-0.693538	-2.508188
H	1.200971	1.279972	-3.730174
H	0.290671	1.785585	-2.304744
H	2.412130	2.171078	-1.062190
H	3.342760	1.608082	-2.447354
H	2.439843	3.492517	-3.825305
H	1.489362	4.045850	-2.448966
H	3.591472	4.416612	-1.147176
H	4.541684	3.864068	-2.521401
H	4.464725	6.370637	-2.457376
H	3.650441	5.766554	-3.909502
H	2.695723	6.322794	-2.526973

g⁺ag⁻

C	0.032041	-0.088981	-0.279917
C	-0.457124	-0.236701	1.021225
C	1.405063	-0.202236	-0.551765
C	2.278362	-0.464318	0.514146
C	1.795080	-0.612084	1.819137
C	0.425520	-0.494758	2.076467
H	3.344270	-0.557776	0.316458
H	2.486418	-0.816528	2.632321
H	0.047777	-0.610872	3.088344
H	-1.523624	-0.151466	1.211899
H	-0.658127	0.105097	-1.098981
C	1.917834	0.004776	-1.955274
C	1.897844	1.487721	-2.366410
C	2.788086	2.359463	-1.480381
C	2.714714	3.853392	-1.811025
C	3.189104	4.210716	-3.221084
C	3.239256	5.721846	-3.450812
H	2.944485	-0.375281	-2.031649
H	1.305917	-0.573960	-2.658400
H	2.215899	1.564876	-3.412905
H	0.865553	1.860714	-2.315394
H	2.500803	2.210468	-0.432721
H	3.829578	2.018104	-1.572485
H	1.680565	4.201255	-1.678885
H	3.324713	4.408665	-1.086013
H	4.186060	3.778963	-3.380397
H	2.526061	3.754406	-3.964500
H	3.566544	5.963254	-4.466497
H	2.250565	6.167087	-3.298807
H	3.932236	6.197087	-2.749027

g⁺ag⁺

C	0.205756	-0.069244	-0.719248
C	-0.611503	-0.012991	0.413482
C	1.598802	-0.198116	-0.598021
C	2.155090	-0.265690	0.687776
C	1.342384	-0.209238	1.825621
C	-0.043439	-0.078162	1.691093
H	3.232835	-0.369408	0.795342
H	1.790610	-0.265230	2.814050
H	-0.676409	-0.035793	2.572929
H	-1.688270	0.081132	0.300452
H	-0.239983	-0.024387	-1.711340
C	2.468287	-0.203394	-1.830825
C	2.593000	1.202793	-2.441969
C	3.217067	2.210069	-1.475184
C	3.499630	3.575671	-2.108699
C	2.246258	4.297839	-2.607626
C	2.546299	5.719212	-3.085328
H	3.468023	-0.576042	-1.574625
H	2.047105	-0.889096	-2.576590
H	3.205233	1.148237	-3.352986
H	1.595492	1.542573	-2.744957
H	2.555787	2.341799	-0.609515
H	4.156258	1.789845	-1.088803
H	4.001672	4.214885	-1.370167
H	4.202533	3.453041	-2.944734
H	1.791210	3.729836	-3.426789
H	1.507328	4.326892	-1.796079
H	1.644834	6.217672	-3.453968
H	2.958140	6.322598	-2.269911
H	3.281445	5.705623	-3.896713

g⁺x⁻a

C	0.129935	0.702394	-0.280718
C	0.127968	1.370249	0.946966
C	1.312887	0.151724	-0.799472
C	2.489446	0.256109	-0.042621
C	2.495119	0.926855	1.185639
C	1.315754	1.496013	1.678104
H	3.408233	-0.184848	-0.423760
H	3.416800	1.004371	1.756429
H	1.317784	2.018752	2.630491
H	-0.795629	1.794172	1.332267
H	-0.791771	0.617640	-0.853712
C	1.332298	-0.431717	-2.188108
C	1.372156	0.664278	-3.272803
C	2.552475	1.638772	-3.116174
C	2.246066	2.862918	-2.246341
C	3.485022	3.703154	-1.941401
C	3.160802	4.920837	-1.075529
H	2.214724	-1.073416	-2.303193
H	0.447930	-1.062548	-2.342662
H	1.420418	0.170940	-4.251437
H	0.431058	1.229468	-3.249273
H	3.412087	1.101471	-2.691704
H	2.869798	1.990234	-4.106364
H	1.499661	3.484946	-2.760672
H	1.795148	2.549179	-1.300351
H	4.217678	3.070255	-1.424048
H	3.952076	4.024308	-2.881680
H	4.057670	5.504905	-0.847552
H	2.448080	5.578446	-1.584062
H	2.709804	4.603065	-0.129594

g⁺g⁻g⁻

C	0.268619	1.431433	-0.639098
C	0.171486	2.031167	0.620048
C	1.190674	0.399419	-0.877033
C	1.983190	-0.047725	0.190437
C	1.890709	0.547253	1.453497
C	0.989345	1.594910	1.669604
H	2.694687	-0.853692	0.021835
H	2.519425	0.193184	2.266206
H	0.917622	2.061633	2.648028
H	-0.543877	2.832889	0.784243
H	-0.373939	1.771236	-1.449195
C	1.342983	-0.181832	-2.261818
C	1.833352	0.831912	-3.310849
C	3.242601	1.391069	-3.062415
C	3.387509	2.425302	-1.935544
C	2.554155	3.691717	-2.131763
C	2.762071	4.691321	-0.993359
H	2.048395	-1.021795	-2.224744
H	0.378517	-0.590029	-2.592053
H	1.833809	0.325661	-4.284874
H	1.110755	1.651923	-3.394654
H	3.920169	0.548431	-2.865199
H	3.593082	1.855410	-3.994444
H	3.131853	1.980527	-0.969609
H	4.446295	2.713492	-1.874869
H	2.816300	4.154229	-3.093013
H	1.491592	3.431389	-2.182726
H	2.174240	5.602018	-1.144841
H	2.459414	4.243690	-0.040771
H	3.816445	4.976785	-0.914363

g⁺g⁻x⁺

C	0.392724	1.042724	-0.332200
C	0.157452	1.609553	0.925079
C	1.665604	0.564776	-0.683583
C	2.686218	0.637949	0.277813
C	2.458045	1.200455	1.538179
C	1.189717	1.690267	1.866210
H	3.674994	0.255851	0.030222
H	3.267065	1.250510	2.262195
H	1.007621	2.130582	2.842557
H	-0.834825	1.977475	1.172731
H	-0.425345	0.975732	-1.045009
C	1.921552	-0.102242	-2.020674
C	1.331796	0.586441	-3.263297
C	2.047594	1.853304	-3.751725
C	2.040650	3.036375	-2.766426
C	3.325518	3.156108	-1.941802
C	3.164870	4.105319	-0.755997
H	3.004751	-0.217976	-2.158326
H	1.508677	-1.119318	-1.970255
H	1.348596	-0.145478	-4.081297
H	0.274125	0.819803	-3.089172
H	3.086688	1.601726	-4.007643
H	1.567011	2.152455	-4.691390
H	1.898225	3.975627	-3.316046
H	1.184697	2.944370	-2.087230
H	3.617747	2.168180	-1.574259
H	4.135389	3.498518	-2.599285
H	4.104053	4.229098	-0.207540
H	2.834468	5.094092	-1.092999
H	2.415799	3.710652	-0.062166

g⁺g⁺a

```
C   -0.240114    0.110246   -0.482698
C   -0.982397    0.546109    0.618557
C    1.153327    0.281334   -0.527987
C    1.784264    0.905558    0.558350
C    1.046725    1.344315    1.664127
C   -0.340685    1.173576    1.692882
H    2.864837    1.031009    0.545707
H    1.554194    1.823411    2.497197
H   -0.915702    1.513490    2.549548
H   -2.059149    0.400104    0.637627
H   -0.743538   -0.381739   -1.312833
C    1.931086   -0.150969   -1.746978
C    1.612568    0.730797   -2.969085
C    1.841831    2.225337   -2.727123
C    3.292560    2.588471   -2.409670
C    3.508831    4.095612   -2.268805
C    4.953610    4.453533   -1.919588
H    3.004168   -0.117012   -1.528449
H    1.689361   -1.193688   -1.988677
H    2.224926    0.400013   -3.818828
H    0.564291    0.572050   -3.251759
H    1.528876    2.779175   -3.622221
H    1.197373    2.563675   -1.905789
H    3.603879    2.103143   -1.476762
H    3.947732    2.198873   -3.202259
H    3.220528    4.588462   -3.205866
H    2.834190    4.477497   -1.492203
H    5.088734    5.535334   -1.827108
H    5.246125    3.993791   -0.969821
H    5.639042    4.091416   -2.692816
```

g⁺x⁺g⁻

```
C   -0.163002   -0.004336   -0.360991
C   -1.207453    0.328108    0.506370
C    1.090849    0.619010   -0.253351
C    1.270382    1.589775    0.743354
C    0.228027    1.928693    1.613837
C   -1.016156    1.302184    1.493382
H    2.239714    2.073630    0.844248
H    0.386647    2.682306    2.380623
H   -1.826740    1.562448    2.168133
H   -2.168987   -0.169466    0.411830
H   -0.314957   -0.767178   -1.122346
C    2.197417    0.275841   -1.220514
C    1.911428    0.809990   -2.638853
C    1.761902    2.337604   -2.737523
C    3.060305    3.093418   -3.044362
C    4.173605    2.938399   -2.006802
C    5.363048    3.854412   -2.298932
H    3.142710    0.677382   -0.843929
H    2.310096   -0.814779   -1.272495
H    2.708357    0.476378   -3.318039
H    0.986620    0.335353   -2.988496
H    1.044075    2.571116   -3.533194
H    1.322250    2.722273   -1.808433
H    3.441650    2.767886   -4.022630
H    2.826657    4.162296   -3.143622
H    3.770854    3.161561   -1.010264
H    4.518308    1.898493   -1.984877
H    6.163629    3.720253   -1.565394
H    5.774547    3.644917   -3.291797
H    5.055691    4.904955   -2.278259
```

g⁺g⁺g⁺

```
C   -0.125026    0.083524   -0.290511
C   -1.281551    0.494044    0.378453
C    1.091435    0.763677   -0.114205
C    1.118214    1.868441    0.749529
C   -0.036447    2.284816    1.422267
C   -1.242055    1.602971    1.231927
H    2.055839    2.396568    0.908854
H    0.005408    3.142401    2.088455
H   -2.139956    1.924169    1.752180
H   -2.212223   -0.047879    0.232675
H   -0.160682   -0.783613   -0.947179
C    2.321049    0.326578   -0.873716
C    2.173713    0.549407   -2.389228
C    1.867462    2.001964   -2.769571
C    2.919962    3.017748   -2.312451
C    4.331156    2.734270   -2.829436
C    5.315815    3.845454   -2.462522
H    3.195059    0.871217   -0.497752
H    2.508415   -0.738718   -0.687856
H    3.088312    0.211788   -2.891693
H    1.361892   -0.087956   -2.761436
H    1.768836    2.063482   -3.861658
H    0.894050    2.282115   -2.348711
H    2.613561    4.015285   -2.654745
H    2.940350    3.067577   -1.216749
H    4.692531    1.782713   -2.422127
H    4.295505    2.614708   -3.920352
H    6.323845    3.626664   -2.827324
H    4.998589    4.800831   -2.892804
H    5.368413    3.968676   -1.375644
```

Isomer 2a

```
C    -0.043413   -0.084885    0.214714
C    -0.020738   -0.057014    1.618729
C     1.192411   -0.035438    2.309627
C     2.419328   -0.051106    1.629769
C     2.389316   -0.090440    0.227862
C     1.181379   -0.112245   -0.472089
C     3.724358   -0.101140    2.381403
C     4.160270   -1.544845    2.669959
C     5.482300   -1.632309    3.432390
C     5.913473   -3.070975    3.718042
C     7.235247   -3.167352    4.480619
C     7.651920   -4.612130    4.758053
H     3.326451   -0.100471   -0.326010
H     1.183329   -0.140851   -1.559946
H    -0.960055   -0.042376    2.168025
H     1.185496   -0.002098    3.397715
H     4.507911    0.401963    1.800133
H     3.628110    0.442162    3.330350
H     3.369126   -2.045415    3.243923
H     4.246474   -2.085498    1.718026
H     6.268186   -1.126929    2.854134
H     5.389827   -1.086859    4.381779
H     5.126151   -3.575767    4.294564
H     6.003814   -3.615781    2.768256
H     8.018655   -2.661211    3.902536
H     7.141604   -2.621268    5.427777
H     8.598965   -4.659284    5.303873
H     6.891050   -5.125369    5.354935
H     7.773005   -5.165530    3.821199
N    -1.260702   -0.180553   -0.482638
H    -2.030810    0.245222    0.016930
H    -1.207110    0.207314   -1.415701
```

Isomer 2b

```
C     0.046879    0.082641    0.020194
C     0.007406    0.082674    1.424749
C     1.160676   -0.174094    2.167737
C     2.385562   -0.454728    1.542331
C     2.415767   -0.459907    0.140446
C     1.266908   -0.204673   -0.612347
C     3.606948   -0.786186    2.362394
C     3.545074   -2.212870    2.934255
C     3.454963   -3.285815    1.850055
C     3.442292   -4.706140    2.414871
C     3.335926   -5.782108    1.333820
C     3.319818   -7.198451    1.909605
H     3.352310   -0.672141   -0.371749
H     1.315309   -0.217257   -1.699441
H    -0.930546    0.298187    1.932813
H     1.107867   -0.155949    3.255069
H     4.505261   -0.687720    1.739547
H     3.706084   -0.068448    3.186557
H     4.435232   -2.393979    3.551967
H     2.672848   -2.295628    3.596340
H     2.548892   -3.124735    1.253098
H     4.307064   -3.176341    1.163520
H     4.355327   -4.874034    3.002907
H     2.597995   -4.808968    3.110600
H     2.423996   -5.609461    0.748761
H     4.179143   -5.674706    0.639773
H     3.243384   -7.952321    1.120318
H     4.234815   -7.394820    2.477957
H     2.469540   -7.329856    2.586692
N    -1.127200    0.267501   -0.730738
H    -1.807798    0.845865   -0.255139
H    -0.945992    0.645614   -1.651665
```

Isomer 3a

```
C    -0.067581   -0.189681    0.238320
C    -0.032590   -0.118266    1.636093
C     1.194901   -0.083394    2.298361
C     2.408630   -0.105419    1.592009
C     2.354767   -0.178107    0.193533
C     1.131451   -0.213941   -0.483518
C     3.727434   -0.135953    2.320636
C     4.155234   -1.570136    2.663454
C     5.489955   -1.636997    3.405500
C     5.913504   -3.066102    3.745375
C     7.247925   -3.141836    4.487987
C     7.656953   -4.577175    4.820251
H     3.280674   -0.193170   -0.378028
H     1.109917   -0.262553   -1.571046
H    -0.971530   -0.093099    2.180867
H     1.211647   -0.023486    3.384890
H     4.503870    0.333904    1.703437
H     3.653812    0.449068    3.246351
H     3.370492   -2.038359    3.272446
H     4.219809   -2.151895    1.734254
H     6.269597   -1.164477    2.792138
H     5.419210   -1.050289    4.331809
H     5.132385   -3.538064    4.357052
H     5.982062   -3.652174    2.818601
H     8.025112   -2.668466    3.874828
H     7.176010   -2.554601    5.412116
H     8.613194   -4.609532    5.350829
H     6.902608   -5.057014    5.452151
H     7.756473   -5.171577    3.906257
O    -1.297869   -0.222029   -0.359175
H    -1.159706   -0.265510   -1.309669
```

Isomer 3b

```
C     0.008477    0.141790    0.181961
C    -0.006233    0.123432    1.582357
C     1.165375   -0.158874    2.284441
C     2.374611   -0.420375    1.618060
C     2.371359   -0.394438    0.217417
C     1.203227   -0.113638   -0.500152
C     3.615892   -0.773330    2.398560
C     3.561720   -2.209896    2.945640
C     3.437210   -3.262702    1.845187
C     3.438440   -4.693031    2.384356
C     3.296411   -5.749064    1.287863
C     3.295947   -7.175547    1.838242
H     3.294705   -0.590722   -0.323470
H     1.221962   -0.095910   -1.588674
H    -0.939244    0.332239    2.097107
H     1.143824   -0.165189    3.372636
H     4.497560   -0.667383    1.753754
H     3.740217   -0.070953    3.232290
H     4.467567   -2.405746    3.535119
H     2.707957   -2.301168    3.630225
H     2.513996   -3.089914    1.278394
H     4.268721   -3.142066    1.135653
H     4.368808   -4.872957    2.940673
H     2.615873   -4.806921    3.103925
H     2.366757   -5.564969    0.734968
H     4.117627   -5.630070    0.569736
H     3.193382   -7.914848    1.038255
H     4.228078   -7.383212    2.373708
H     2.467248   -7.318197    2.539338
O    -1.169091    0.422122   -0.455118
H    -0.999582    0.407879   -1.401458
```

Isomer 4a

```
C    -0.002158   -0.115531    0.162511
C     0.014475   -0.058857    1.564071
C     1.221428   -0.034369    2.268750
C     2.451042   -0.052838    1.593673
C     2.434879   -0.112609    0.192166
C     1.227659   -0.137098   -0.512031
C     3.750669   -0.099644    2.354879
C     4.176267   -1.543607    2.657966
C     5.492421   -1.631361    3.430367
C     5.913516   -3.070031    3.730626
C     7.229404   -3.167084    4.503223
C     7.636205   -4.611754    4.795354
H     3.377927   -0.129745   -0.351459
H     1.239403   -0.179669   -1.599431
H    -0.927506   -0.039930    2.108768
H     1.211211    0.009959    3.356451
H     4.539862    0.394394    1.773831
H     3.649023    0.451816    3.298317
H     3.378579   -2.035235    3.230619
H     4.266507   -2.092472    1.711109
H     6.284891   -1.134968    2.853430
H     5.396044   -1.077673    4.374514
H     5.119481   -3.565789    4.305777
H     6.007592   -3.623037    2.785956
H     8.019516   -2.669943    3.926494
H     7.132073   -2.612738    5.445174
H     8.579131   -4.659374    5.348149
H     6.868480   -5.115963    5.391142
H     7.760892   -5.173487    3.863957
C    -1.304809   -0.098912   -0.599445
H    -1.614576    0.928195   -0.821943
H    -1.210267   -0.632381   -1.549612
H    -2.103926   -0.570682   -0.020498
```

Isomer 4b

```
C     0.009035    0.062136    0.092240
C    -0.004563    0.067091    1.495597
C     1.157577   -0.192053    2.226833
C     2.374924   -0.455141    1.579343
C     2.389077   -0.458222    0.177104
C     1.225472   -0.199468   -0.554483
C     3.608169   -0.788137    2.381019
C     3.556182   -2.219499    2.942459
C     3.453835   -3.285133    1.852043
C     3.457991   -4.709203    2.407529
C     3.338196   -5.778501    1.321287
C     3.340153   -7.198658    1.887783
H     3.321859   -0.661756   -0.345384
H     1.260770   -0.208583   -1.642186
H    -0.936360    0.270808    2.019720
H     1.123613   -0.181425    3.315029
H     4.498225   -0.681951    1.747990
H     3.712768   -0.076313    3.209378
H     4.455258   -2.402482    3.546216
H     2.693725   -2.309015    3.616299
H     2.537185   -3.125486    1.270931
H     4.293818   -3.166412    1.152339
H     4.382055   -4.876095    2.978263
H     2.626641   -4.820935    3.117324
H     2.414982   -5.607162    0.753733
H     4.168222   -5.661753    0.613031
H     3.253608   -7.947611    1.094915
H     4.266342   -7.393686    2.438120
H     2.503016   -7.339313    2.579219
C    -1.237142    0.381272   -0.696968
H    -1.316279    1.457916   -0.884299
H    -1.228759   -0.126329   -1.665786
H    -2.135125    0.069807   -0.155695
```

Isomer 5a

```
C     0.025953    -0.130525     0.179649
C     0.016143    -0.066436     1.577100
C     1.225682    -0.042230     2.274312
C     2.453709    -0.058996     1.595523
C     2.441434    -0.120748     0.193680
C     1.239414    -0.145459    -0.516360
C     3.752963    -0.101485     2.356302
C     4.178187    -1.546118     2.659209
C     5.494497    -1.631181     3.431546
C     5.916270    -3.069571     3.732207
C     7.232350    -3.164449     4.504778
C     7.640318    -4.608601     4.797590
H     3.385266    -0.134824    -0.347149
H     1.240982    -0.191865    -1.600653
H    -0.928216    -0.051714     2.111696
H     1.218436     0.005121     3.361151
H     4.540577     0.392947     1.774142
H     3.649647     0.450410     3.298876
H     3.381239    -2.038251     3.232448
H     4.269213    -2.095528     1.712749
H     6.286187    -1.134442     2.854032
H     5.397320    -1.077104     4.375262
H     5.122782    -3.565597     4.307779
H     6.010897    -3.622886     2.787836
H     8.021855    -2.666931     3.927604
H     7.134421    -2.609686     5.446383
H     8.583267    -4.654622     5.350297
H     6.873282    -5.113180     5.393872
H     7.765688    -5.170747     3.866585
C    -1.266643    -0.089372    -0.577529
F    -1.637489     1.177127    -0.845590
F    -1.178545    -0.730528    -1.756216
F    -2.271754    -0.654947     0.113745
```

Isomer 5b

```
C     0.032437     0.049746     0.106509
C    -0.004039     0.073639     1.505491
C     1.159990    -0.189388     2.229185
C     2.374116    -0.460177     1.577849
C     2.390328    -0.471743     0.175441
C     1.232548    -0.210628    -0.562015
C     3.606342    -0.792732     2.379987
C     3.550024    -2.224111     2.941910
C     3.449812    -3.291300     1.852654
C     3.463869    -4.714407     2.410627
C     3.344491    -5.785712     1.326332
C     3.358135    -7.204732     1.895332
H     3.322761    -0.679790    -0.344323
H     1.256005    -0.225515    -1.646880
H    -0.937178     0.281672     2.019294
H     1.130849    -0.172141     3.316701
H     4.496578    -0.687913     1.747635
H     3.709208    -0.079641     3.207123
H     4.448083    -2.405410     3.547001
H     2.687149    -2.312255     3.615398
H     2.530058    -3.139946     1.273936
H     4.286975    -3.169162     1.150221
H     4.391682    -4.874888     2.976869
H     2.636658    -4.829202     3.124636
H     2.417111    -5.621062     0.763654
H     4.170009    -5.665094     0.613507
H     3.271530    -7.955023     1.103910
H     4.288599    -7.393463     2.440536
H     2.525651    -7.349365     2.591459
C    -1.199958     0.394064    -0.673732
F    -1.301397     1.722985    -0.868251
F    -1.204317    -0.182597    -1.887957
F    -2.319431     0.003999    -0.039093
```

Isomer 6a

```
C     0.009950    -0.107312     0.171407
C     0.002498    -0.050766     1.575340
C     1.213416    -0.027353     2.268362
C     2.441630    -0.048171     1.588845
C     2.428954    -0.106400     0.186312
C     1.229382    -0.130552    -0.526175
C     3.740812    -0.093012     2.349027
C     4.162979    -1.539190     2.650454
C     5.479376    -1.627242     3.422332
C     5.898068    -3.066853     3.721469
C     7.214190    -3.164963     4.493572
C     7.619162    -4.610234     4.784914
H     3.372780    -0.120183    -0.354565
H     1.227401    -0.168577    -1.611469
H    -0.943846    -0.027381     2.107502
H     1.206967     0.020663     3.355192
H     4.528986     0.400435     1.766866
H     3.638624     0.458396     3.291963
H     3.365318    -2.030284     3.223611
H     4.252756    -2.088050     1.703544
H     6.271818    -1.131639     2.844923
H     5.383478    -1.073824     4.366536
H     5.103749    -3.561720     4.296868
H     5.991322    -3.619484     2.776576
H     8.004522    -2.668575     3.916576
H     7.117634    -2.610858     5.435694
H     8.562155    -4.658569     5.337286
H     6.851317    -5.113760     5.381019
H     7.743172    -5.171801     3.853392
C    -1.230160    -0.128670    -0.551583
N    -2.246855    -0.146968    -1.144259
```

Isomer 6b

```
C     0.023373     0.074033     0.093398
C    -0.015945     0.090200     1.498427
C     1.147923    -0.173273     2.220661
C     2.362459    -0.449648     1.571436
C     2.382477    -0.458109     0.168430
C     1.228927    -0.197876    -0.573951
C     3.592355    -0.783634     2.376077
C     3.532856    -2.215922     2.936009
C     3.434685    -3.281522     1.844984
C     3.448284    -4.705430     2.400988
C     3.330432    -5.775110     1.314918
C     3.344183    -7.194892     1.881961
H     3.315983    -0.667150    -0.349023
H     1.252981    -0.204417    -1.659658
H    -0.949920     0.308694     2.007666
H     1.117329    -0.155326     3.308138
H     4.484117    -0.678874     1.745963
H     3.693576    -0.071439     3.204177
H     4.429302    -2.398337     3.543034
H     2.668422    -2.304189     3.607508
H     2.515686    -3.130103     1.264942
H     4.273001    -3.158230     1.144125
H     4.375502    -4.866352     2.968006
H     2.620295    -4.821383     3.113873
H     2.403491    -5.610151     0.751600
H     4.156623    -5.653087     0.603120
H     3.258623    -7.943942     1.089306
H     4.274243    -7.384025     2.427677
H     2.511095    -7.340941     2.577038
C    -1.168364     0.343838    -0.660151
N    -2.145791     0.564143    -1.277653
```

Isomer 7a

```
C     0.033673    -0.106976     0.181797
C    -0.003309    -0.060148     1.574265
C     1.208554    -0.035718     2.267756
C     2.438172    -0.048800     1.590870
C     2.428755    -0.099559     0.188145
C     1.231579    -0.120369    -0.530534
C     3.735720    -0.093709     2.353598
C     4.161123    -1.539968     2.649895
C     5.476123    -1.627285     3.424142
C     5.898485    -3.066833     3.718336
C     7.213252    -3.164041     4.492856
C     7.622024    -4.609235     4.779214
H     3.373623    -0.109661    -0.350700
H     1.213346    -0.146398    -1.613613
H    -0.957737    -0.048618     2.087110
H     1.199417     0.008815     3.354569
H     4.524080     0.404198     1.775567
H     3.630398     0.453362     3.298671
H     3.363650    -2.035681     3.219364
H     4.254496    -2.084703     1.700924
H     6.268297    -1.126979     2.850423
H     5.376628    -1.077969     4.370373
H     5.104459    -3.566426     4.290045
H     5.995453    -3.615359     2.771425
H     8.003293    -2.662910     3.919573
H     7.112990    -2.614064     5.437008
H     8.563975    -4.656908     5.333418
H     6.854463    -5.117525     5.371631
H     7.749771    -5.166645     3.845702
N    -1.240584    -0.128199    -0.564762
O    -2.272882    -0.294375     0.081978
O    -1.185359     0.019703    -1.783995
```

Isomer 7b

```
C     0.042022     0.069019     0.110387
C    -0.023773     0.089686     1.503007
C     1.142673    -0.172766     2.223557
C     2.357379    -0.449243     1.575049
C     2.377985    -0.458494     0.172190
C     1.226264    -0.195444    -0.574093
C     3.586646    -0.783600     2.380257
C     3.528081    -2.216996     2.937347
C     3.433357    -3.280887     1.844356
C     3.448910    -4.705691     2.398009
C     3.334076    -5.773767     1.310041
C     3.350155    -7.194447     1.874756
H     3.310939    -0.670094    -0.344932
H     1.233769    -0.192459    -1.657649
H    -0.965484     0.304133     1.994232
H     1.111969    -0.152095     3.310847
H     4.479186    -0.676684     1.751670
H     3.686399    -0.073103     3.209929
H     4.423734    -2.399247     3.545576
H     2.662586    -2.307633     3.607211
H     2.514823    -3.130448     1.263346
H     4.272353    -3.154883     1.144785
H     4.375855    -4.865877     2.965670
H     2.620424    -4.824301     3.109875
H     2.407262    -5.609741     0.746229
H     4.160591    -5.648938     0.599110
H     3.266613    -7.942330     1.080783
H     4.280193    -7.382704     2.420807
H     2.516856    -7.343266     2.568993
N    -1.183583     0.347430    -0.665289
O    -2.245467     0.395940    -0.047461
O    -1.061923     0.510746    -1.877685
```

Isomer 8a

```
C     0.009369    -0.107729     0.149912
C     0.001660    -0.105533     1.548979
C     1.208085    -0.081109     2.255801
C     2.437355    -0.049445     1.579813
C     2.431917    -0.052951     0.176624
C     1.228624    -0.077347    -0.535570
C     3.735948    -0.089819     2.343829
C     4.196323    -1.531780     2.599953
C     5.514363    -1.613525     3.374643
H     3.378936    -0.023546    -0.358974
H     1.242370    -0.072396    -1.622181
H    -0.926572    -0.123732    -0.401203
H    -0.941622    -0.122559     2.088296
H     1.199260    -0.073632     3.344128
H     4.513396     0.443741     1.782459
H     3.617774     0.428133     3.304054
H     3.413838    -2.065270     3.156412
H     4.307440    -2.049643     1.637658
H     6.294164    -1.079755     2.818478
H     5.402305    -1.094766     4.334149
N     6.003530    -2.966987     3.649152
H     6.108147    -3.461020     2.767104
H     5.287626    -3.474784     4.161642
```

Isomer 8b

```
C     0.006342     0.073790     0.096177
C    -0.020233     0.090532     1.495442
C     1.146637    -0.167936     2.220537
C     2.357797    -0.440508     1.564448
C     2.371953    -0.450199     0.161874
C     1.206764    -0.194084    -0.569391
C     3.596593    -0.761140     2.364795
C     3.545799    -2.180140     2.955220
C     3.475148    -3.273037     1.885433
H     3.304651    -0.656605    -0.359114
H     1.236583    -0.204923    -1.655593
H    -0.898904     0.274739    -0.469604
H    -0.947412     0.305567     2.019924
H     1.123759    -0.146870     3.308636
H     4.482478    -0.668679     1.723809
H     3.708684    -0.032386     3.176635
H     4.436027    -2.349495     3.576382
H     2.671510    -2.269548     3.614002
H     2.581405    -3.127610     1.270472
H     4.337229    -3.173086     1.213906
N     3.453695    -4.647468     2.393570
H     4.261165    -4.787933     2.994857
H     2.642897    -4.758849     2.996232
```

Isomer 9a

```
C    0.001695   -0.094727    0.162439
C    0.003689   -0.074263    1.561467
C    1.214947   -0.057907    2.259868
C    2.439402   -0.052119    1.574596
C    2.424771   -0.073880    0.171905
C    1.216204   -0.090545   -0.531770
C    3.742040   -0.098918    2.332023
C    4.156037   -1.541515    2.650707
C    5.483175   -1.624569    3.394706
H    3.368263   -0.064360   -0.370587
H    1.222423   -0.100060   -1.618388
H   -0.938219   -0.104858   -0.381969
H   -0.935905   -0.071547    2.107336
H    1.213856   -0.037411    3.347990
H    4.529870    0.386741    1.742543
H    3.645887    0.464000    3.268915
H    3.381093   -2.025477    3.255789
H    4.229035   -2.107022    1.711380
H    6.276227   -1.160560    2.788991
H    5.417142   -1.071132    4.335684
O    5.822922   -2.956386    3.754275
H    5.847882   -3.454064    2.933698
```

Isomer 9b

```
C    0.016206    0.070460    0.092309
C   -0.017698    0.044604    1.491324
C    1.149047   -0.217441    2.215011
C    2.367093   -0.451518    1.557091
C    2.388924   -0.419283    0.155135
C    1.223660   -0.159001   -0.574634
C    3.608199   -0.775419    2.353452
C    3.557434   -2.193113    2.943979
C    3.446684   -3.271031    1.872874
H    3.327453   -0.594980   -0.366803
H    1.258993   -0.136779   -1.660476
H   -0.889382    0.273762   -0.472026
H   -0.950952    0.228050    2.016865
H    1.119580   -0.232090    3.302889
H    4.491359   -0.680308    1.709366
H    3.724038   -0.049657    3.167024
H    4.465599   -2.371727    3.536847
H    2.701918   -2.289934    3.621867
H    2.521095   -3.146758    1.307014
H    4.285773   -3.174508    1.166010
O    3.387974   -4.577823    2.428947
H    4.184219   -4.678201    2.955583
```

Isomer 10a

```
C    0.007482   -0.100235    0.165398
C    0.003697   -0.047588    1.563452
C    1.212370   -0.028160    2.266443
C    2.438828   -0.050817    1.585546
C    2.430490   -0.106025    0.183684
C    1.224591   -0.125631   -0.524050
C    3.738631   -0.097939    2.347509
C    4.153400   -1.545033    2.644190
C    5.468976   -1.614279    3.416206
C    5.891247   -3.026327    3.715965
H    3.376202   -0.121223   -0.354723
H    1.234714   -0.161417   -1.610003
H   -0.930279   -0.113099   -0.382579
H   -0.938015   -0.022531    2.104958
H    1.207230    0.017423    3.353815
H    4.528357    0.395373    1.766990
H    3.636823    0.452362    3.291347
H    3.360930   -2.034731    3.220134
H    4.249996   -2.091562    1.699998
H    6.278523   -1.149011    2.845720
H    5.384718   -1.091877    4.373960
F    7.051915   -3.058053    4.395978
F    4.973817   -3.672031    4.460114
F    6.067889   -3.741966    2.589454
```

Isomer 10b

```
C    0.020611    0.050249    0.085180
C   -0.016070    0.052261    1.484465
C    1.149904   -0.192417    2.215477
C    2.370203   -0.433224    1.563921
C    2.394804   -0.429885    0.161535
C    1.230182   -0.186628   -0.575331
C    3.607734   -0.747540    2.367822
C    3.554780   -2.162913    2.963988
C    3.423018   -3.227718    1.877930
H    3.335627   -0.609493   -0.355028
H    1.267417   -0.184771   -1.661282
H   -0.884340    0.240563   -0.484590
H   -0.950997    0.242625    2.004406
H    1.118703   -0.184338    3.303433
H    4.495785   -0.654471    1.730473
H    3.716508   -0.022035    3.182635
H    4.461795   -2.348647    3.549320
H    2.701618   -2.239096    3.646410
H    2.490045   -3.102604    1.321900
H    4.252117   -3.159363    1.166081
C    3.430460   -4.622956    2.435260
F    3.303439   -5.542554    1.461826
F    4.575669   -4.893385    3.091854
F    2.420144   -4.816401    3.304144
```

Isomer 11a

```
C     0.012462    -0.075011     0.167366
C     0.008902    -0.031371     1.565730
C     1.217530    -0.029663     2.269102
C     2.444386    -0.061575     1.589199
C     2.435290    -0.107509     0.186962
C     1.229659    -0.109409    -0.521535
C     3.743330    -0.126501     2.351326
C     4.146318    -1.578137     2.641291
C     5.458241    -1.667054     3.411907
C     5.864988    -3.091296     3.703046
H     3.381072    -0.130351    -0.351043
H     1.239975    -0.138796    -1.607745
H    -0.925185    -0.074353    -0.381051
H    -0.932731     0.000095     2.107172
H     1.212524     0.008275     3.356765
H     4.537180     0.364030     1.773677
H     3.645953     0.421002     3.297506
H     3.351132    -2.071434     3.210599
H     4.235686    -2.127979     1.698179
H     6.276417    -1.193049     2.856619
H     5.391735    -1.136496     4.369259
O     5.253742    -4.083597     3.382638
O     7.034670    -3.135309     4.388769
H     7.210992    -4.076213     4.527058
```

Isomer 11b

```
C     0.013203     0.028163     0.099290
C    -0.007089     0.049937     1.498736
C     1.165925    -0.191388     2.219665
C     2.377620    -0.449033     1.558301
C     2.385261    -0.465793     0.155674
C     1.213686    -0.226147    -0.571337
C     3.622555    -0.756418     2.353704
C     3.568372    -2.161014     2.974138
C     3.440753    -3.248270     1.914188
H     3.318812    -0.659583    -0.368870
H     1.238479    -0.240318    -1.657629
H    -0.897096     0.216166    -0.462806
H    -0.934730     0.253687     2.026765
H     1.147580    -0.168844     3.307681
H     4.503649    -0.676757     1.704579
H     3.743070    -0.016101     3.153738
H     4.469744    -2.339113     3.571132
H     2.718054    -2.230923     3.660402
H     2.530684    -3.109128     1.318759
H     4.276507    -3.215303     1.205443
C     3.383498    -4.631074     2.512521
O     3.276244    -4.892360     3.688359
O     3.453569    -5.585384     1.551038
H     3.385660    -6.425543     2.025433
```

Isomer 12a

```
C     1.190319    -0.122418    -0.464970
N     0.001944    -0.097780     0.162065
C     0.038362    -0.049018     1.504571
C     1.218212    -0.025277     2.252628
C     2.454060    -0.048675     1.594453
C     2.421416    -0.102129     0.195468
C     3.751713    -0.093053     2.355076
C     4.172374    -1.539687     2.655191
C     5.488056    -1.629458     3.428052
C     5.905918    -3.069489     3.726279
C     7.221341    -3.169159     4.499358
C     7.625438    -4.614890     4.789749
H     3.346043    -0.119279    -0.376818
H     1.151601    -0.158167    -1.552100
H    -0.928367    -0.025112     2.004056
H     1.173043     0.019669     3.338296
H     4.540102     0.400198     1.773075
H     3.647953     0.457235     3.298471
H     3.373941    -2.030681     3.227189
H     4.262583    -2.087479     1.707807
H     6.281310    -1.133741     2.851836
H     5.391786    -1.076886     4.372726
H     5.110856    -3.564509     4.300532
H     5.999614    -3.621315     2.780952
H     8.012429    -2.672632     3.923501
H     7.124347    -2.615868     5.441925
H     8.567978    -4.664352     5.342862
H     6.856782    -5.118570     5.384701
H     7.749833    -5.175651     3.857779
```

Isomer 12b

```
C     2.410177     0.020592     0.175925
C     1.173386     0.032244    -0.476465
N    -0.009769    -0.019011     0.157125
C     0.036780    -0.082159     1.499202
C     1.221742    -0.099675     2.238609
C     2.453703    -0.047050     1.573196
C     3.751587    -0.113547     2.334466
C     4.047112    -1.540996     2.827213
C     4.176223    -2.552684     1.689083
C     4.535296    -3.955675     2.178407
C     4.648426    -4.976145     1.045505
C     5.006616    -6.375648     1.546151
H     1.128049     0.086093    -1.562563
H     3.330139     0.067054    -0.401822
H    -0.925795    -0.117744     2.005779
H     1.182815    -0.146211     3.324607
H     4.573226     0.224717     1.691198
H     3.706931     0.567389     3.193192
H     3.245433    -1.860051     3.506369
H     4.976562    -1.530819     3.411449
H     3.234445    -2.596510     1.128002
H     4.946297    -2.206353     0.984749
H     5.486330    -3.918032     2.727380
H     3.773004    -4.293348     2.894040
H     3.696913    -5.009918     0.500359
H     5.407656    -4.633263     0.331264
H     5.082201    -7.089688     0.720787
H     5.966468    -6.363767     2.072636
H     4.245941    -6.742702     2.242705
```

Isomer 13a

```
N    1.245620   -0.050555   -0.516883
C    0.089397   -0.083693    0.166739
C    0.017001   -0.098637    1.563060
C    1.204661   -0.084847    2.295703
C    2.426054   -0.050507    1.610416
C    2.375230   -0.035792    0.208265
C    3.742042   -0.098272    2.337983
C    4.148715   -1.541584    2.669756
C    5.484281   -1.629963    3.407800
C    5.888083   -3.066876    3.738596
C    7.224240   -3.164765    4.475480
C    7.613845   -4.607403    4.799165
H    3.304583   -0.002312   -0.360794
H   -0.818007   -0.094306   -0.433296
H   -0.948801   -0.118530    2.059187
H    1.188992   -0.091000    3.383841
H    4.522126    0.364755    1.721081
H    3.674058    0.482851    3.266251
H    3.359729   -2.003585    3.278060
H    4.203427   -2.117319    1.736423
H    6.268184   -1.165511    2.794062
H    5.424189   -1.047010    4.337148
H    5.102817   -3.530709    4.351185
H    5.944723   -3.648894    2.808600
H    8.005494   -2.699717    3.861233
H    7.164366   -2.580962    5.402631
H    8.571697   -4.655647    5.325454
H    6.855484   -5.079425    5.432117
H    7.701183   -5.198725    3.882001
```

Isomer 13b

```
C    2.366469    0.034024    0.199092
N    1.234699    0.049652   -0.523803
C    0.080420   -0.018732    0.159723
C    0.011305   -0.098602    1.554405
C    1.200497   -0.115386    2.283908
C    2.421143   -0.048122    1.598507
C    3.734550   -0.108041    2.332233
C    4.047591   -1.531260    2.825018
C    4.159096   -2.545119    1.686991
C    4.531677   -3.946013    2.172155
C    4.628760   -4.967929    1.039059
C    5.000663   -6.365317    1.535618
H    3.294269    0.093771   -0.369917
H   -0.828412   -0.004718   -0.438170
H   -0.953221   -0.143888    2.051389
H    1.186401   -0.171760    3.370682
H    4.540202    0.229562    1.668506
H    3.708369    0.579415    3.186560
H    3.261347   -1.852381    3.521228
H    4.988401   -1.514990    3.390628
H    3.207625   -2.593017    1.142723
H    4.914456   -2.197394    0.967869
H    5.492074   -3.904040    2.704310
H    3.783433   -4.285434    2.901775
H    3.668220   -5.005853    0.510323
H    5.374062   -4.623420    0.311190
H    5.064604   -7.080409    0.710168
H    5.969454   -6.349127    2.045383
H    4.253575   -6.734109    2.245899
```

Isomer 13c

```
N    1.235336   -0.032199   -0.533352
C    0.076014   -0.007893    0.146834
C   -0.000704    0.003075    1.542293
C    1.184905   -0.020197    2.279724
C    2.408399   -0.051990    1.599257
C    2.361616   -0.053713    0.195972
C    3.729504   -0.127499    2.318154
C    4.287968   -1.561108    2.338087
C    3.372846   -2.552308    3.055998
C    3.963581   -3.960265    3.130621
C    3.044276   -4.961181    3.831078
C    3.644860   -6.365531    3.899753
H    3.292999   -0.065401   -0.370988
H   -0.829052    0.008953   -0.456552
H   -0.967905    0.030025    2.035370
H    1.166133   -0.009530    3.367488
H    4.450845    0.537725    1.828406
H    3.607288    0.228139    3.348817
H    4.447432   -1.897585    1.305234
H    5.270216   -1.553971    2.828598
H    3.175153   -2.188128    4.074604
H    2.403587   -2.595457    2.543802
H    4.176058   -4.315503    2.112920
H    4.926827   -3.923855    3.657900
H    2.830757   -4.600257    4.845167
H    2.084331   -4.994455    3.300786
H    2.971824   -7.065556    4.403575
H    3.842440   -6.750179    2.894018
H    4.592936   -6.353863    4.447143
```

Isomer 14a

```
C     2.360170    -0.033658     0.613680
C     1.451138    -0.110392    -0.430892
C     0.151753     0.135839     0.100568
C     0.313375     0.348261     1.464561
N     1.650779     0.242557     1.755020
C    -1.147565     0.104540    -0.647887
C    -1.567309    -1.319766    -1.037006
C    -2.886440    -1.367474    -1.807846
C    -3.301832    -2.786175    -2.197752
C    -4.621936    -2.842136    -2.967234
C    -5.022054    -4.267501    -3.349714
H     3.434215    -0.148025     0.634456
H    -0.414789     0.570469     2.232190
H     1.695800    -0.311204    -1.465700
H    -1.936813     0.554790    -0.031618
H    -1.070031     0.715406    -1.557103
H    -1.650410    -1.923636    -0.123896
H    -0.771397    -1.774086    -1.641359
H    -3.679491    -0.913885    -1.197100
H    -2.798561    -0.753830    -2.715186
H    -2.508588    -3.239197    -2.808268
H    -3.386550    -3.399477    -1.290090
H    -5.968334    -4.285776    -3.898672
H    -4.255092    -4.727191    -3.981471
H    -5.137018    -4.889057    -2.455770
H    -5.411464    -2.388279    -2.355035
H    -4.534028    -2.227537    -3.872023
H     2.055403     0.367060     2.669203
```

Isomer 14b

```
C     2.290569     0.016075     0.579184
C     1.383667    -0.155122    -0.456407
C     0.097687     0.234434     0.019245
C     0.264890     0.627531     1.341724
N     1.593060     0.490786     1.660955
C    -1.194618     0.180286    -0.741053
C    -1.634343    -1.261615    -1.043495
C    -1.867435    -2.087902     0.219973
C    -2.330851    -3.514676    -0.073204
C    -2.554850    -4.346752     1.189839
C    -3.013562    -5.773126     0.884873
H     3.356417    -0.153190     0.629117
H    -0.454758     0.991114     2.061971
H     1.622404    -0.511706    -1.449832
H    -1.980727     0.679348    -0.159037
H    -1.096922     0.734825    -1.682982
H    -2.555936    -1.242861    -1.641130
H    -0.864676    -1.749611    -1.655792
H    -0.940621    -2.117938     0.805887
H    -2.619088    -1.583898     0.844987
H    -3.262677    -3.484604    -0.654981
H    -1.582955    -4.013145    -0.705394
H    -3.168123    -6.350765     1.801242
H    -3.955661    -5.764696     0.327058
H    -2.268427    -6.296083     0.276589
H    -1.622774    -4.373115     1.768197
H    -3.300766    -3.845330     1.819534
H     1.998526     0.713656     2.555937
```

Isomer 14c

```
C     1.149633     0.075541    -0.606159
C    -0.091015     0.281352    -0.019656
C     0.047295     0.081287     1.383919
C     1.380840    -0.246123     1.608747
N     2.027068    -0.245803     0.398111
C    -1.033377     0.150648     2.424008
C    -1.663190    -1.220599     2.722866
C    -2.334573    -1.853149     1.505025
C    -2.991541    -3.197955     1.815871
C    -3.655081    -3.840067     0.597200
C    -4.305418    -5.186079     0.918546
H     1.471837     0.134950    -1.635532
H     1.907462    -0.464622     2.527454
H    -0.999715     0.553636    -0.540356
H    -0.626308     0.569179     3.352982
H    -1.818908     0.838319     2.085426
H    -0.880782    -1.895784     3.094317
H    -2.403636    -1.110670     3.527432
H    -3.094825    -1.161221     1.114150
H    -1.591611    -1.985781     0.709455
H    -2.233366    -3.884700     2.217359
H    -3.742778    -3.064133     2.606724
H    -4.774230    -5.627801     0.034035
H    -3.560442    -5.894070     1.296108
H    -5.076213    -5.068731     1.687250
H    -4.409930    -3.150900     0.197856
H    -2.902212    -3.970873    -0.190176
H     3.008956    -0.430826     0.267855
```

Isomer 15a

```
C    1.436999   -0.160745   -0.442219
C    0.134274    0.140856    0.078919
C    0.335669    0.419202    1.407564
O    1.651326    0.320111    1.738682
C    2.310918   -0.032372    0.604002
C   -1.172322    0.104194   -0.652953
C   -1.575698   -1.320490   -1.056628
C   -2.903463   -1.372246   -1.812034
C   -3.306329   -2.790538   -2.216168
C   -4.635576   -2.851039   -2.969380
C   -5.023473   -4.275631   -3.366813
H    3.379071   -0.150380    0.700675
H   -0.332215    0.700283    2.208061
H    1.691408   -0.425833   -1.459041
H   -1.957409    0.535310   -0.018937
H   -1.111654    0.730186   -1.552685
H   -1.640506   -1.938331   -0.151706
H   -0.783321   -1.756761   -1.678671
H   -3.693756   -0.936665   -1.185125
H   -2.833625   -0.745250   -2.711652
H   -2.515870   -3.225395   -2.843241
H   -3.372095   -3.417137   -1.316164
H   -5.976531   -4.297185   -3.903594
H   -4.259629   -4.717081   -4.015083
H   -5.119533   -4.911022   -2.480461
H   -5.422268   -2.415477   -2.340559
H   -4.566629   -2.222754   -3.866347
```

Isomer 15b

```
C    1.374130   -0.189771   -0.482595
C    0.085375    0.235110   -0.015385
C    0.294863    0.666435    1.270424
O    1.602878    0.546319    1.624569
C    2.248971    0.024330    0.549091
C   -1.215159    0.176961   -0.757601
C   -1.650017   -1.267106   -1.054941
C   -1.864142   -2.095698    0.210613
C   -2.339354   -3.519210   -0.079644
C   -2.543127   -4.354722    1.184526
C   -3.015264   -5.777236    0.882421
H    3.309945   -0.130699    0.670084
H   -0.362856    1.072334    2.024461
H    1.619907   -0.590235   -1.456374
H   -1.993889    0.672467   -0.163794
H   -1.128208    0.734353   -1.698483
H   -2.579090   -1.249172   -1.639852
H   -0.888745   -1.751740   -1.680314
H   -0.928528   -2.133890    0.781950
H   -2.602411   -1.590174    0.849785
H   -3.281830   -3.481877   -0.643380
H   -1.606075   -4.018683   -0.727933
H   -3.154792   -6.357387    1.799462
H   -3.968099   -5.761656    0.343374
H   -2.284883   -6.301742    0.257842
H   -1.600357   -4.388374    1.744735
H   -3.274050   -3.851865    1.830302
```

Isomer 15c

```
C   -0.133471    0.222793   -0.023155
C    0.021918    0.109282    1.398686
C    1.368894   -0.073005    1.596786
O    2.044634   -0.080327    0.416855
C    1.119990    0.101811   -0.562090
C   -1.045996    0.139130    2.452021
C   -1.655813   -1.246114    2.725044
C   -2.336347   -1.864172    1.504435
C   -3.003918   -3.204829    1.811239
C   -3.669733   -3.839061    0.589732
C   -4.334315   -5.178638    0.908518
H    1.503597    0.124979   -1.570294
H    1.971392   -0.196759    2.484383
H   -1.053404    0.383801   -0.567805
H   -0.625714    0.537029    3.383470
H   -1.841611    0.828524    2.143094
H   -0.862120   -1.918810    3.075570
H   -2.387505   -1.158271    3.539664
H   -3.092302   -1.164030    1.119944
H   -1.598348   -2.003246    0.705323
H   -2.251686   -3.897678    2.212985
H   -3.755454   -3.065875    2.600716
H   -4.803875   -5.615139    0.021963
H   -3.597689   -5.893955    1.288410
H   -5.106913   -5.053939    1.674165
H   -4.416493   -3.142175    0.188545
H   -2.915670   -3.977335   -0.195216
```

Isomer 16a

```
C    1.403103   -0.099489   -0.443372
C    0.118891    0.150233    0.121829
C    0.204252    0.356482    1.486900
S    1.815191    0.258469    2.062759
C    2.416919   -0.067657    0.491458
C   -1.168327    0.122359   -0.653994
C   -1.583835   -1.307371   -1.027564
C   -2.888506   -1.361329   -1.822183
C   -3.303411   -2.785253   -2.192991
C   -4.608632   -2.848222   -2.986922
C   -5.009321   -4.278529   -3.349707
H    3.477492   -0.213086    0.335124
H   -0.606730    0.570112    2.171696
H    1.574708   -0.283487   -1.499171
H   -1.965406    0.586430   -0.060031
H   -1.062057    0.719439   -1.569189
H   -1.687077   -1.895599   -0.106422
H   -0.779591   -1.775278   -1.610264
H   -3.689889   -0.892404   -1.234665
H   -2.779799   -0.765277   -2.738825
H   -2.501060   -3.253759   -2.779388
H   -3.409244   -3.380554   -1.275720
H   -5.944751   -4.301778   -3.916590
H   -4.233039   -4.754466   -3.957536
H   -5.145530   -4.882070   -2.446516
H   -5.407121   -2.378465   -2.398906
H   -4.499465   -2.251640   -3.901369
```

Isomer 16b

```
C    1.347593   -0.141840   -0.471710
C    0.068861    0.245259    0.024429
C    0.140941    0.624630    1.352491
S    1.732716    0.516515    1.977452
C    2.344063   -0.043372    0.477398
C   -1.202354    0.182288   -0.776079
C   -1.621179   -1.268340   -1.067247
C   -1.851098   -2.083974    0.204167
C   -2.326334   -3.509176   -0.076989
C   -2.537453   -4.333430    1.193350
C   -3.008086   -5.758541    0.901318
H    3.397894   -0.262262    0.367681
H   -0.671243    0.960669    1.984713
H    1.528767   -0.470618   -1.490088
H   -2.005987    0.685375   -0.223993
H   -1.072220    0.724875   -1.720872
H   -2.539461   -1.263977   -1.669514
H   -0.844245   -1.754385   -1.671866
H   -0.921706   -2.118319    0.785861
H   -2.594197   -1.570324    0.831330
H   -3.265654   -3.475888   -0.646198
H   -1.589812   -4.014717   -0.716862
H   -3.153140   -6.330352    1.822735
H   -3.957700   -5.747672    0.356503
H   -2.274076   -6.288700    0.285845
H   -1.597785   -4.361973    1.759023
H   -3.271909   -3.824677    1.830466
```

Isomer 16c

```
C   -0.132905    0.357183    0.020333
C    0.031336    0.084810    1.408143
C    1.317637   -0.347480    1.684398
S    2.297360   -0.415250    0.281826
C    1.014856    0.131813   -0.712921
C   -1.059232    0.182561    2.441092
C   -1.691659   -1.186616    2.741763
C   -2.311788   -1.844237    1.509770
C   -2.987477   -3.179201    1.822492
C   -3.593011   -3.849919    0.589166
C   -4.264008   -5.185148    0.912670
H    1.168272    0.261785   -1.775876
H    1.729256   -0.619406    2.648430
H   -1.060418    0.710664   -0.418474
H   -0.655296    0.609147    3.366979
H   -1.836187    0.869785    2.083611
H   -0.919990   -1.850073    3.154134
H   -2.461436   -1.066066    3.516024
H   -3.050485   -1.159152    1.068826
H   -1.535250   -2.000182    0.750847
H   -2.251710   -3.856820    2.277315
H   -3.775474   -3.023074    2.572260
H   -4.690095   -5.647890    0.017491
H   -3.541556   -5.885310    1.344507
H   -5.071512   -5.045728    1.638762
H   -4.324354   -3.168855    0.135838
H   -2.802828   -4.003353   -0.156417
```

Isomer 17a

```
C     0.095463   -0.151551    0.128337
C    -0.031920    0.158125    1.483371
C     1.123635    0.195019    2.266275
C     2.364655   -0.078104    1.674213
N     2.490941   -0.379602    0.365798
C     1.373132   -0.411212   -0.376514
C     3.637761   -0.107739    2.476475
C     4.108809   -1.549725    2.706379
C     5.433818   -1.631586    3.463341
C     5.900107   -3.069443    3.691920
C     7.232719   -3.162852    4.435674
C     7.683454   -4.606855    4.658445
H     1.510842   -0.652213   -1.428931
H    -0.769731   -0.191700   -0.525939
H    -1.004617    0.369358    1.918906
H     1.072634    0.433885    3.324997
H     4.411451    0.438599    1.924786
H     3.488491    0.393913    3.440559
H     3.334412   -2.095834    3.262566
H     4.206691   -2.037147    1.728792
H     6.203912   -1.085618    2.901484
H     5.332248   -1.125765    4.433600
H     5.131363   -3.612771    4.258550
H     5.990907   -3.576402    2.721587
H     7.997872   -2.620519    3.866152
H     7.139107   -2.651471    5.402055
H     8.638375   -4.651966    5.190527
H     6.941570   -5.156463    5.246835
H     7.803960   -5.125239    3.701726
```

Isomer 17b

```
C     1.284119   -0.347594   -0.390031
C     0.031857   -0.091058    0.176789
C    -0.032560    0.187943    1.542791
C     1.156826    0.196774    2.274620
C     2.368168   -0.070655    1.622270
N     2.433514   -0.341447    0.302845
C     3.681410   -0.112832    2.360283
C     4.267930   -1.532053    2.358742
C     3.362343   -2.547702    3.055004
C     3.966493   -3.951044    3.101551
C     3.053781   -4.978703    3.771177
C     3.669959   -6.377433    3.812646
H     1.373301   -0.566214   -1.452565
H    -0.861809   -0.110917   -0.439040
H    -0.983587    0.392523    2.026714
H     1.154372    0.407108    3.340516
H     4.381584    0.572513    1.868718
H     3.539921    0.232177    3.392075
H     4.425633   -1.835578    1.317349
H     5.248370   -1.520080    2.852354
H     3.154526   -2.207921    4.080189
H     2.395568   -2.590567    2.536538
H     4.190470   -4.278927    2.077226
H     4.925639   -3.916526    3.636525
H     2.827444   -4.643916    4.791490
H     2.098520   -5.010953    3.232255
H     3.000859   -7.097303    4.293473
H     3.881565   -6.735650    2.799982
H     4.612900   -6.367613    4.368925
```

Isomer 17c

```
C     1.315091   -0.044101   -0.443622
C     0.054780   -0.069773    0.158465
C    -0.013901   -0.086262    1.553656
C     1.180446   -0.078406    2.274317
C     2.403028   -0.053464    1.585181
N     2.473114   -0.035461    0.239200
C     3.708961   -0.100799    2.333558
C     4.030078   -1.524908    2.818879
C     4.125035   -2.538819    1.678926
C     4.529865   -3.932527    2.158846
C     4.599770   -4.960052    1.028820
C     5.010561   -6.349183    1.518041
H     1.407162   -0.026122   -1.527897
H    -0.843099   -0.073841   -0.451531
H    -0.972014   -0.100571    2.065810
H     1.176116   -0.086469    3.361318
H     4.497973    0.245119    1.658243
H     3.670416    0.578762    3.193979
H     3.256374   -1.849395    3.528424
H     4.979850   -1.508111    3.369729
H     3.160200   -2.601115    1.160669
H     4.850039   -2.180053    0.935990
H     5.507893   -3.876864    2.656767
H     3.812118   -4.277448    2.916352
H     3.620714   -5.015108    0.536617
H     5.311724   -4.608627    0.271562
H     5.053419   -7.068637    0.694855
H     5.997816   -6.315998    1.990230
H     4.296846   -6.724345    2.258770
```

Isomer 18a

```
N     1.352657    -0.086525     1.801971
C     2.233845    -0.254949     0.761699
C     1.566060     0.085458    -0.404743
C     0.246618     0.468641    -0.039345
C     0.134862     0.359646     1.341888
C    -1.025600     0.572919     2.259368
C    -1.615651    -0.738575     2.800444
C    -2.819404    -0.518356     3.716269
C    -3.405789    -1.822328     4.257512
C    -4.613374    -1.609984     5.171050
C    -5.188022    -2.923273     5.702933
H     3.247080    -0.588315     0.932466
H    -0.545419     0.793296    -0.700903
H     1.986153     0.060581    -1.400499
H    -0.734143     1.214206     3.103824
H    -1.800658     1.116397     1.706849
H    -0.838727    -1.290171     3.347292
H    -1.905535    -1.368342     1.949951
H    -2.524198     0.123510     4.558015
H    -3.597223     0.025968     3.163328
H    -3.698393    -2.463119     3.414562
H    -2.627080    -2.367036     4.809123
H    -6.050407    -2.749712     6.353351
H    -5.510381    -3.565908     4.877336
H    -4.433996    -3.469527     6.278855
H    -4.317607    -0.968690     6.010915
H    -5.388042    -1.064852     4.617310
H     1.571969    -0.243366     2.773754
```

Isomer 18b

```
N     1.479989     0.200961     1.776181
C     2.276266    -0.060613     0.687409
C     1.453688    -0.090503    -0.428476
C     0.127488     0.162420     0.017852
C     0.165673     0.346615     1.394973
C    -0.920057     0.582727     2.395327
C    -1.136347    -0.620457     3.330213
C    -1.496545    -1.898697     2.575199
C    -1.740935    -3.090886     3.500044
C    -2.093287    -4.373484     2.745968
C    -2.330102    -5.561167     3.679261
H     3.343438    -0.192727     0.790938
H    -0.768189     0.206841    -0.587310
H     1.776914    -0.273935    -1.443638
H    -0.704382     1.479694     2.992427
H    -1.846932     0.784694     1.846146
H    -1.931693    -0.381337     4.048680
H    -0.224373    -0.795895     3.917720
H    -2.397005    -1.715601     1.971796
H    -0.692881    -2.140486     1.868764
H    -0.842588    -3.265886     4.108528
H    -2.551961    -2.850101     4.201382
H    -2.581238    -6.467400     3.120102
H    -1.435249    -5.768302     4.275159
H    -3.152626    -5.351194     4.370734
H    -2.990104    -4.195108     2.139446
H    -1.282524    -4.608284     2.045164
H     1.812965     0.300339     2.722980
```

Isomer 18c

```
N     1.456292     0.143388     1.815584
C     2.276984    -0.116831     0.745794
C     1.492148    -0.066241    -0.397077
C     0.164574     0.230260     0.014262
C     0.162690     0.357735     1.399441
C    -0.956286     0.588293     2.365321
C    -1.707038    -0.705052     2.727431
C    -0.802493    -1.765558     3.353374
C    -1.560337    -3.022072     3.782098
C    -0.653867    -4.094944     4.386132
C    -1.422538    -5.346581     4.810716
H     3.333853    -0.296221     0.878655
H    -0.703304     0.347973    -0.621061
H     1.843238    -0.216386    -1.408521
H    -0.563068     1.046296     3.283929
H    -1.658721     1.309389     1.931981
H    -2.524195    -0.465845     3.421757
H    -2.163230    -1.113624     1.816957
H    -0.020148    -2.043504     2.636165
H    -0.294747    -1.336179     4.230579
H    -2.334578    -2.749721     4.512537
H    -2.083457    -3.439551     2.910937
H    -0.756152    -6.101084     5.239219
H    -2.180270    -5.098549     5.561032
H    -1.933828    -5.794541     3.952578
H     0.116228    -4.364439     3.652535
H    -0.128912    -3.672291     5.252365
H     1.749932     0.161757     2.780411
```

Isomer 19a

```
C    2.092629   -0.377587    0.819314
C    1.575545    0.056589   -0.371384
C    0.250741    0.512121   -0.079592
C    0.060673    0.325709    1.267216
O    1.184116   -0.219872    1.820581
C   -1.088356    0.550412    2.186196
C   -1.676269   -0.760237    2.728712
C   -2.839297   -0.531367    3.693330
C   -3.430741   -1.833950    4.232279
C   -4.588984   -1.615355    5.206175
C   -5.170750   -2.927341    5.733522
H    3.042561   -0.798088    1.110629
H   -0.472144    0.928338   -0.766458
H    2.079004    0.049337   -1.327067
H   -0.769508    1.180017    3.027236
H   -1.858764    1.104808    1.638096
H   -0.881701   -1.321381    3.235195
H   -2.012306   -1.374150    1.883221
H   -2.495867    0.085942    4.534828
H   -3.627254    0.040097    3.183489
H   -3.777643   -2.448429    3.390244
H   -2.639752   -2.407980    4.734006
H   -5.996822   -2.749432    6.428402
H   -5.547767   -3.541369    4.909268
H   -4.404217   -3.505523    6.259527
H   -4.238340   -1.002422    6.046026
H   -5.374853   -1.038358    4.702648
```

Isomer 19b

```
C    2.158309   -0.140559    0.709771
C    1.432942   -0.054093   -0.447997
C    0.093229    0.251466   -0.048314
C    0.102645    0.333050    1.321892
O    1.363266    0.092661    1.790072
C   -0.947305    0.576569    2.349402
C   -1.123809   -0.625024    3.291941
C   -1.501395   -1.907846    2.552558
C   -1.732677   -3.090738    3.492612
C   -2.085907   -4.383574    2.756775
C   -2.314547   -5.559729    3.706568
H    3.195626   -0.343411    0.926477
H   -0.770611    0.393988   -0.681655
H    1.810860   -0.192950   -1.450405
H   -0.696096    1.471187    2.933186
H   -1.888251    0.781201    1.825569
H   -1.897497   -0.387487    4.033371
H   -0.187596   -0.783764    3.840390
H   -2.410750   -1.730385    1.960649
H   -0.708602   -2.162409    1.837687
H   -0.828501   -3.253512    4.095265
H   -2.538950   -2.844397    4.197348
H   -2.564839   -6.474134    3.160479
H   -1.416421   -5.755567    4.301250
H   -3.134810   -5.343463    4.398738
H   -2.986400   -4.215523    2.152610
H   -1.278011   -4.625697    2.055031
```

Isomer 19c

```
C    2.176453   -0.151994    0.793621
C    1.481628   -0.085892   -0.384635
C    0.134623    0.234250   -0.026825
C    0.107025    0.341476    1.342684
O    1.354625    0.105374    1.847123
C   -0.983645    0.580866    2.329928
C   -1.724737   -0.710787    2.717827
C   -0.804618   -1.775369    3.314035
C   -1.561654   -3.018772    3.780486
C   -0.644822   -4.102597    4.348268
C   -1.412335   -5.339170    4.816772
H    3.208384   -0.347194    1.040719
H   -0.709140    0.374922   -0.687381
H    1.886200   -0.239907   -1.374399
H   -0.548304    1.038524    3.226065
H   -1.693731    1.299348    1.905352
H   -2.515110   -0.464337    3.439558
H   -2.217635   -1.117484    1.825406
H   -0.054417   -2.067735    2.569011
H   -0.252101   -1.344838    4.160745
H   -2.297795   -2.732116    4.544241
H   -2.130650   -3.432823    2.936522
H   -0.738403   -6.102133    5.217651
H   -2.129070   -5.074778    5.601048
H   -1.971549   -5.783580    3.987036
H    0.085657   -4.388579    3.581201
H   -0.072697   -3.682957    5.185284
```

Isomer 20a

```
C     2.388312   -0.261505    0.511397
C     1.483384    0.067788   -0.476491
C     0.208625    0.401816    0.053496
C     0.154091    0.325743    1.433584
S     1.681095   -0.162548    2.071784
C    -1.032897    0.548690    2.322592
C    -1.627742   -0.760945    2.860156
C    -2.865077   -0.537104    3.728748
C    -3.455143   -1.839002    4.270941
C    -4.694683   -1.625456    5.140240
C    -5.272529   -2.936484    5.674199
H     3.425981   -0.547115    0.401752
H    -0.648920    0.693433   -0.544374
H     1.732315    0.071718   -1.531701
H    -0.765820    1.199574    3.165237
H    -1.795346    1.080298    1.739769
H    -0.862813   -1.292074    3.441268
H    -1.882430   -1.406032    2.009523
H    -2.604434    0.120452    4.569541
H    -3.629724   -0.010303    3.141363
H    -3.712672   -2.496330    3.429217
H    -2.689192   -2.365570    4.856612
H    -6.157734   -2.762210    6.292997
H    -5.560542   -3.595812    4.849045
H    -4.532110   -3.464875    6.283402
H    -4.433661   -0.967739    5.978862
H    -5.456400   -1.097878    4.552481
```

Isomer 20b

```
C     2.390140   -0.106283    0.472444
C     1.387109   -0.092849   -0.474333
C     0.113409    0.170728    0.097609
C     0.158372    0.359757    1.466894
S     1.776264    0.203929    2.045411
C    -0.984670    0.594043    2.409180
C    -1.228411   -0.603372    3.342940
C    -1.492617   -1.900621    2.581011
C    -1.795528   -3.082670    3.501212
C    -2.038741   -4.387075    2.741666
C    -2.337768   -5.564157    3.670465
H     3.448936   -0.272774    0.325302
H    -0.814530    0.222230   -0.462817
H     1.565004   -0.264779   -1.529926
H    -0.813536    1.499809    3.004144
H    -1.883703    0.771161    1.805717
H    -2.083341   -0.380040    3.994708
H    -0.355481   -0.737541    3.995072
H    -2.337767   -1.748163    1.894278
H    -0.622802   -2.139108    1.956605
H    -0.956775   -3.221065    4.197449
H    -2.677587   -2.852202    4.114624
H    -2.508329   -6.486602    3.107457
H    -1.502276   -5.735983    4.356803
H    -3.230629   -5.364602    4.271870
H    -2.874684   -4.243624    2.045412
H    -1.156162   -4.612288    2.130071
```

Isomer 20c

```
C     2.440800    0.009844    0.536846
C     1.443524   -0.139721   -0.406641
C     0.150881    0.073360    0.139796
C     0.174083    0.387589    1.488161
S     1.793170    0.409030    2.073100
C    -1.000079    0.599607    2.400649
C    -1.735072   -0.716627    2.704742
C    -0.839423   -1.763960    3.364020
C    -1.597589   -3.030240    3.761539
C    -0.698061   -4.096535    4.387189
C    -1.465791   -5.357917    4.783572
H     3.510215   -0.081234    0.401600
H    -0.772928    0.007679   -0.426439
H     1.640549   -0.385685   -1.444110
H    -0.665658    1.052779    3.342114
H    -1.692434    1.311104    1.934474
H    -2.591938   -0.504073    3.358182
H    -2.135695   -1.123896    1.767617
H    -0.026601   -2.030040    2.677566
H    -0.367315   -1.327446    4.256096
H    -2.396687   -2.770605    4.469609
H    -2.089875   -3.448979    2.872852
H    -0.804197   -6.107710    5.227491
H    -2.247122   -5.121420    5.513154
H    -1.947871   -5.806976    3.909153
H     0.096103   -4.354132    3.675399
H    -0.202811   -3.672077    5.269611
```

Isomer 21a

```
C     2.421752     0.045878     1.500086
C     1.221791     0.071112     2.227171
C    -0.012219    -0.047453     1.579806
C    -0.062554    -0.182047     0.188248
C     1.126631    -0.206228    -0.548506
C     2.357447    -0.087083     0.104426
C     3.746953     0.241134     2.189275
C     4.112666     1.725277     2.278516
H     4.154774     2.133650     1.262651
H     1.258466     0.169094     3.310470
H    -0.931505    -0.033549     2.159154
H    -1.019631    -0.277355    -0.316690
H     1.095412    -0.316617    -1.629124
H     3.281777    -0.111488    -0.469371
H     3.705968    -0.180376     3.202113
H     4.545786    -0.277503     1.648767
H     3.301898     2.253889     2.805923
N     5.435134     1.880737     2.891568
H     5.682217     2.865715     2.914073
H     5.379299     1.586526     3.862769
```

Isomer 21b

```
C     2.397787     0.040838     1.515580
C     1.191806     0.044473     2.234777
C    -0.035160    -0.080240     1.573595
C    -0.073408    -0.202505     0.180599
C     1.122085    -0.206498    -0.546935
C     2.345810    -0.080130     0.117528
C     3.716870     0.238560     2.218581
C     4.118509     1.718545     2.237988
H     4.281827     2.052008     1.199708
H     1.223113     0.143372     3.317007
H    -0.959391    -0.080890     2.145325
H    -1.025284    -0.303680    -0.333033
H     1.100931    -0.308238    -1.628697
H     3.274404    -0.090854    -0.450214
H     3.647418    -0.113849     3.253151
H     4.498699    -0.339733     1.711818
H     5.070623     1.820700     2.770519
N     3.108000     2.495342     2.959631
H     2.256957     2.520316     2.404542
H     3.420255     3.458013     3.042637
```

Isomer 21a'

```
C     2.421106     0.019821     1.492198
C     1.223980     0.065150     2.223491
C    -0.013646    -0.035044     1.580365
C    -0.071183    -0.166136     0.188671
C     1.114738    -0.208168    -0.552358
C     2.349452    -0.107531     0.096280
C     3.748261     0.206166     2.179284
C     4.135541     1.694765     2.264137
H     4.165336     2.109059     1.250134
H     1.265709     0.161724     3.306736
H    -0.930448    -0.006687     2.163037
H    -1.031386    -0.246384    -0.312840
H     1.078043    -0.314843    -1.633151
H     3.270440    -0.145848    -0.482337
H     3.709391    -0.208356     3.194835
H     4.534117    -0.334047     1.635885
H     3.345838     2.233976     2.799254
N     5.412462     1.981491     2.916521
H     5.396747     1.598841     3.857829
H     6.152431     1.483669     2.429337
```

Isomer 21b'

```
C     2.389086     0.010049     1.537184
C     1.177865    -0.026961     2.245391
C    -0.045137    -0.133416     1.573144
C    -0.073551    -0.189159     0.176261
C     1.126990    -0.152643    -0.542538
C     2.345033    -0.044124     0.134375
C     3.702610     0.202686     2.248430
C     4.129100     1.685788     2.243178
H     4.263818     2.009669     1.204931
H     1.197693     0.004481     3.332642
H    -0.972490    -0.167594     2.138594
H    -1.021223    -0.274335    -0.347714
H     1.113357    -0.202470    -1.627953
H     3.276567    -0.019022    -0.427939
H     3.617268    -0.140162     3.287477
H     4.482297    -0.399863     1.765315
H     5.101555     1.782406     2.739067
N     3.196803     2.609927     2.883418
H     2.286439     2.522540     2.439828
H     3.061336     2.329281     3.850838
```

Isomer 22a

```
C     2.425715     0.033515     1.499711
C     1.233992     0.092564     2.228642
C     0.004115    -0.017213     1.570780
C    -0.025904    -0.199551     0.184135
C     1.169027    -0.257908    -0.539954
C     2.408954    -0.153752     0.108867
C     3.692969    -0.144794    -0.678458
C     4.069118     1.278304    -1.101906
H     3.254746     1.704523    -1.705496
O     5.312276     1.332318    -1.784833
H     3.381513     0.113862     2.013616
H     1.264947     0.229185     3.306164
H    -0.922677     0.026041     2.135660
H    -0.977334    -0.290546    -0.332783
H     1.142787    -0.406208    -1.617773
H     4.516245    -0.555401    -0.084306
H     3.587896    -0.768757    -1.575687
H     4.184885     1.902880    -0.212447
H     5.208725     0.791979    -2.571506
```

Isomer 22b

```
C     2.414057     0.030680     1.516584
C     1.212478     0.068691     2.233737
C    -0.008654    -0.040003     1.561151
C    -0.022058    -0.203807     0.171078
C     1.179880    -0.238027    -0.541613
C     2.413728    -0.135326     0.121543
C     3.703057    -0.089103    -0.657139
C     4.016370     1.345330    -1.102940
H     3.226671     1.690306    -1.786914
O     4.163639     2.224411    -0.002047
H     3.364249     0.101200     2.041151
H     1.230955     0.188918     3.313523
H    -0.941847    -0.014050     2.116399
H    -0.967242    -0.296179    -0.356931
H     1.165753    -0.368573    -1.621926
H     4.529823    -0.447376    -0.034590
H     3.635373    -0.733754    -1.541634
H     4.967836     1.370448    -1.640626
H     3.332109     2.180959     0.480145
```

Isomer 23a

```
C     2.395014     0.016669     1.538255
C     1.195161     0.058093     2.255030
C    -0.026924    -0.043744     1.581526
C    -0.041486    -0.199158     0.191176
C     1.161225    -0.239795    -0.520829
C     2.393147    -0.141447     0.143904
C     3.685826    -0.116508    -0.630958
C     4.035208     1.312031    -1.057855
H     3.231339     1.730541    -1.669161
S     5.622324     1.439817    -1.935407
H     3.344904     0.089832     2.064270
H     1.213515     0.172380     3.335432
H    -0.959969    -0.014156     2.136884
H    -0.987017    -0.284921    -0.337307
H     1.147479    -0.367717    -1.601587
H     4.503564    -0.517717    -0.022856
H     3.601101    -0.749622    -1.522376
H     4.137477     1.944447    -0.170851
H     5.280106     0.622017    -2.934864
```

Isomer 23b

```
C     2.416864    -0.063552     1.553299
C     1.206045    -0.028160     2.254422
C    -0.007359    -0.053703     1.559898
C    -0.004435    -0.128480     0.162007
C     1.207103    -0.163033    -0.533764
C     2.432313    -0.136994     0.152267
C     3.729073    -0.116273    -0.615616
C     4.004990     1.255778    -1.244100
H     3.185102     1.536033    -1.911172
S     4.281758     2.571801    -0.023571
H     3.360572    -0.045251     2.093168
H     1.211310     0.024545     3.339731
H    -0.947846    -0.027861     2.102772
H    -0.943520    -0.156752    -0.383887
H     1.205261    -0.229160    -1.620270
H     4.559634    -0.379376     0.047432
H     3.689505    -0.862191    -1.419959
H     4.923498     1.216800    -1.837717
H     3.106307     2.420572     0.594010
```

Representation of the *s* vs. sign(λ_2)ρ NCI plots for selected isomers of compounds **2-23**.

2b

3b

4b

5b

6b

7b

8b

9b

10b

S

sign(λ_2) × ρ / a.u.

sign(λ_2) × ρ / a.u.

sign(λ_2) × ρ / a.u.

11b

12a

12b

S

sign(λ_2) × ρ / a.u.

sign(λ_2) × ρ / a.u.

sign(λ_2) × ρ / a.u.

13a

13b

13c

14a

14b

14c
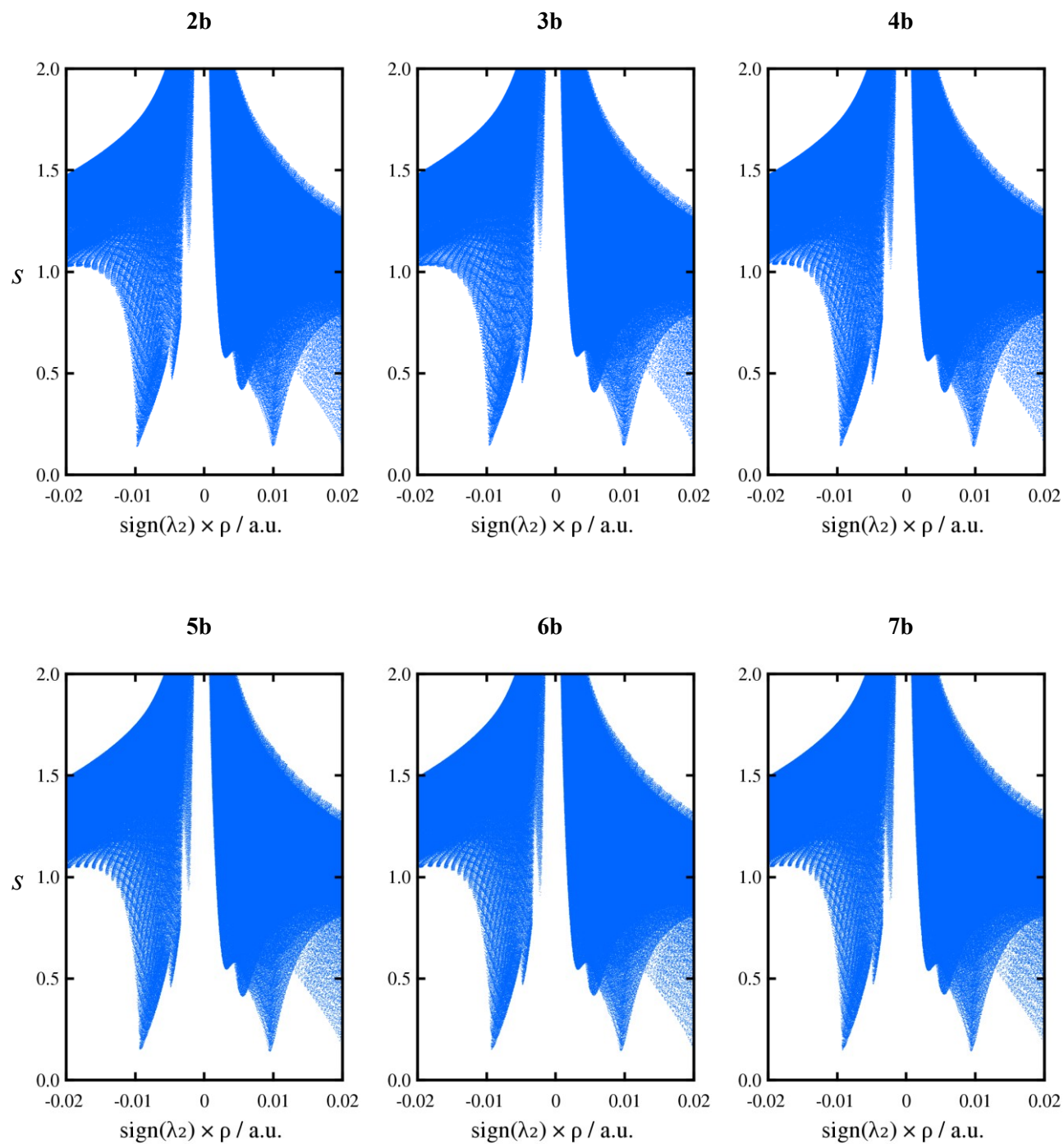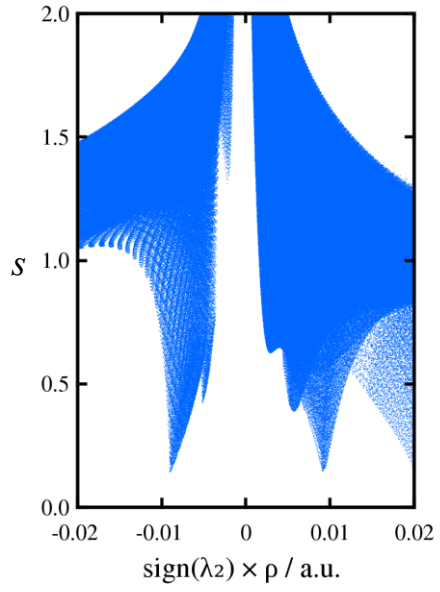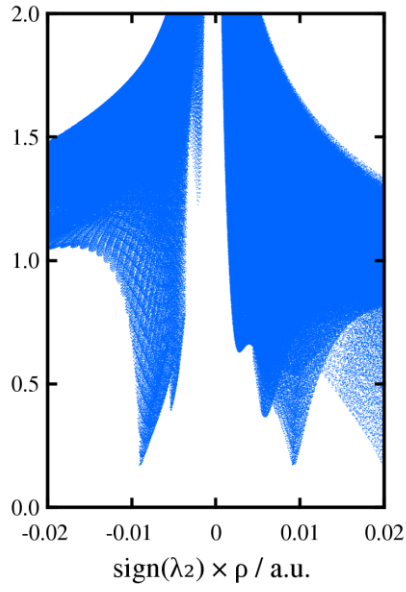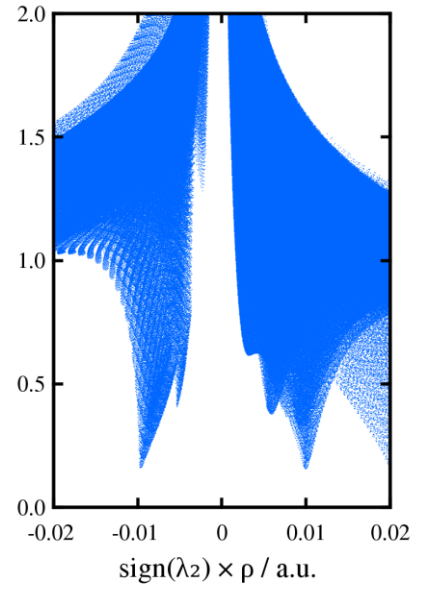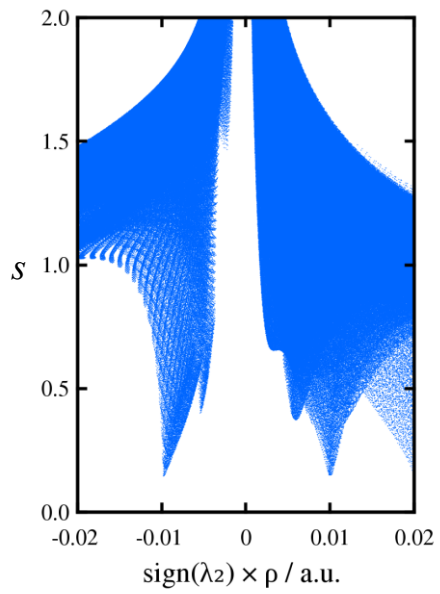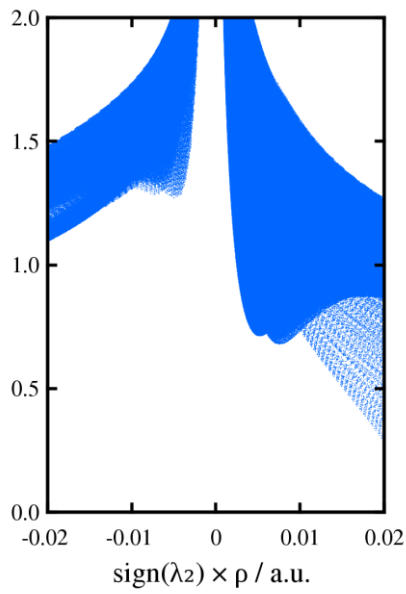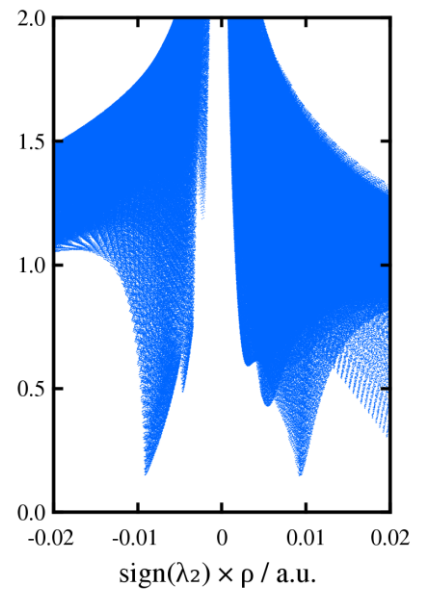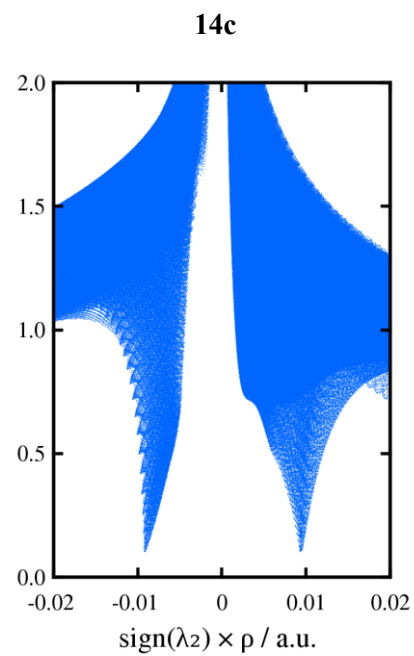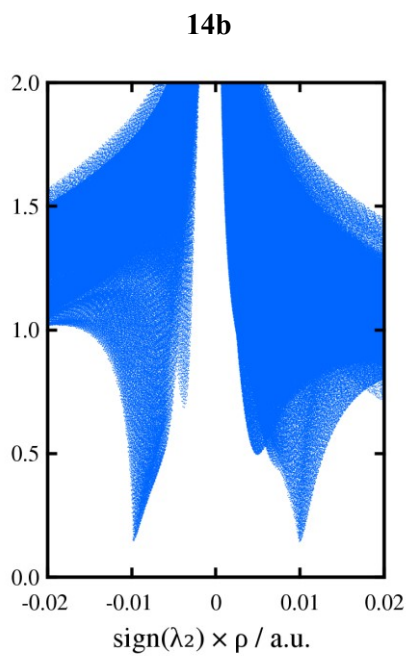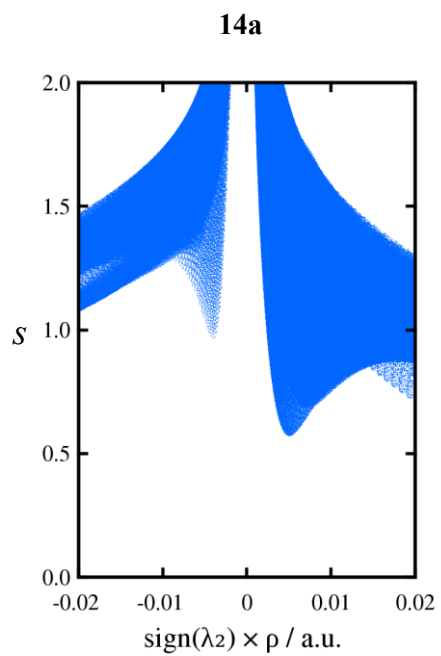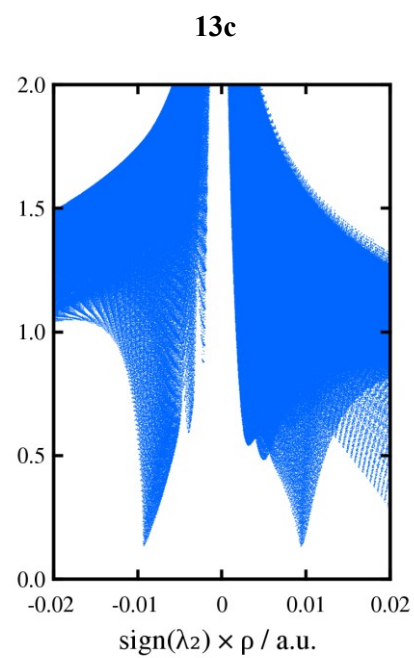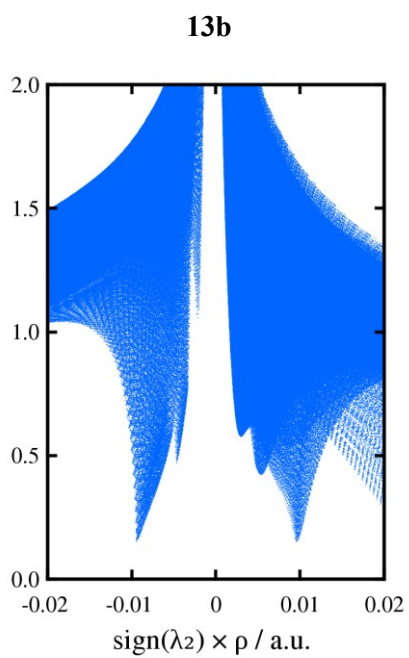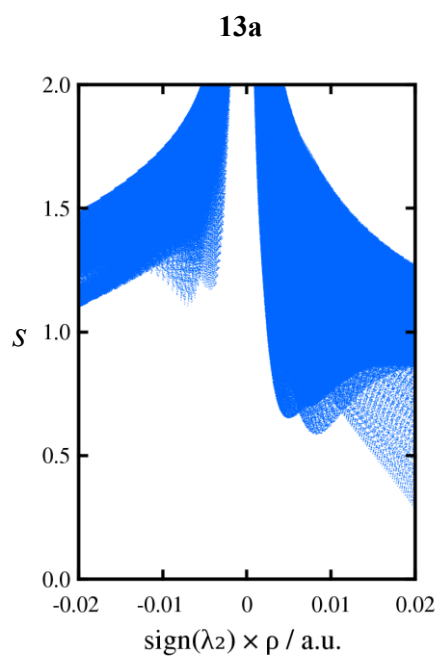
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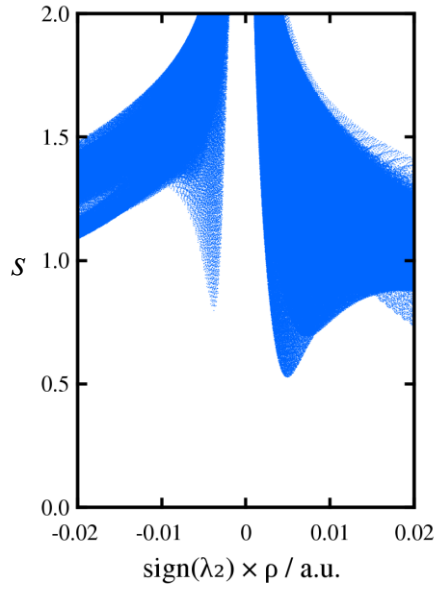
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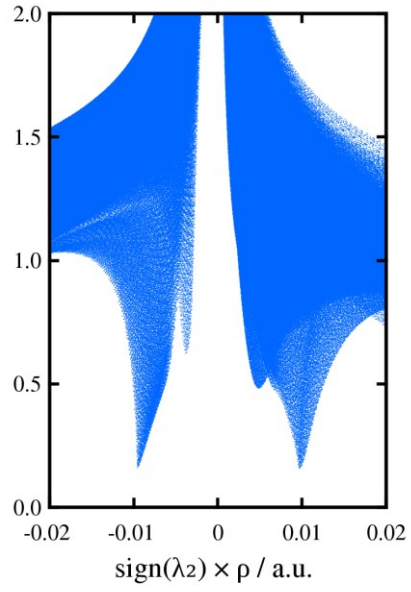
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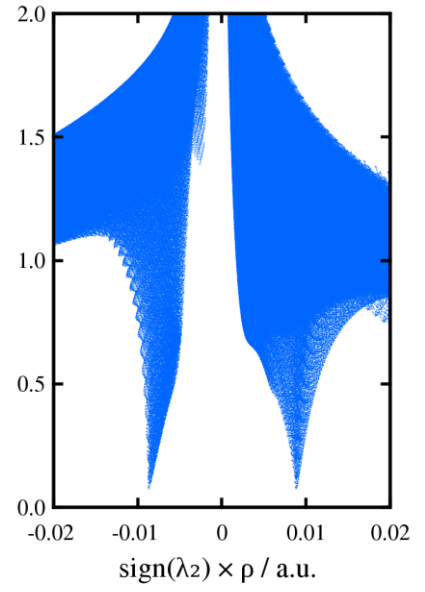
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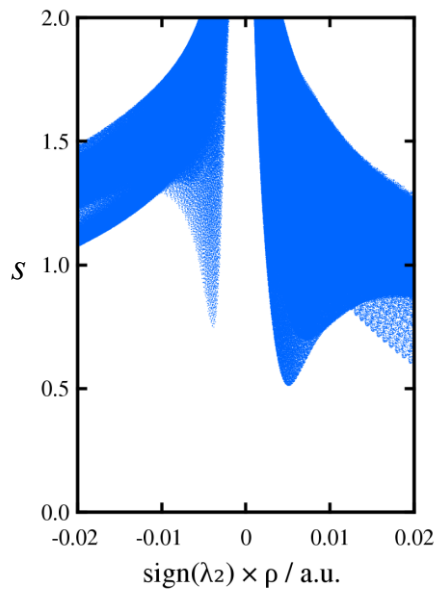
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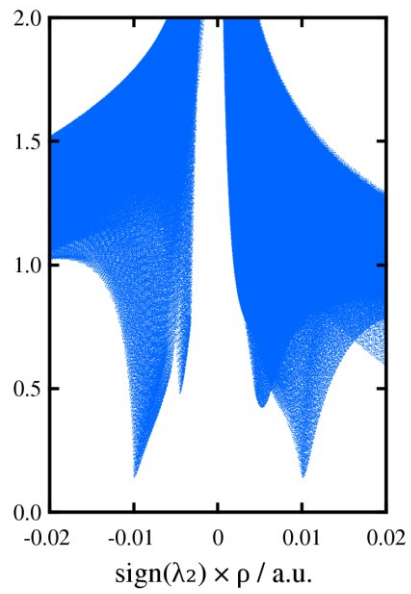
16c
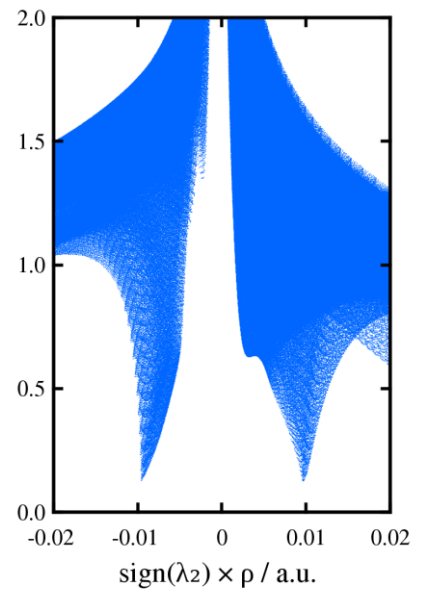
17a

17b

17c

18a

18b

18c

19a

19b

19c

20a

20b
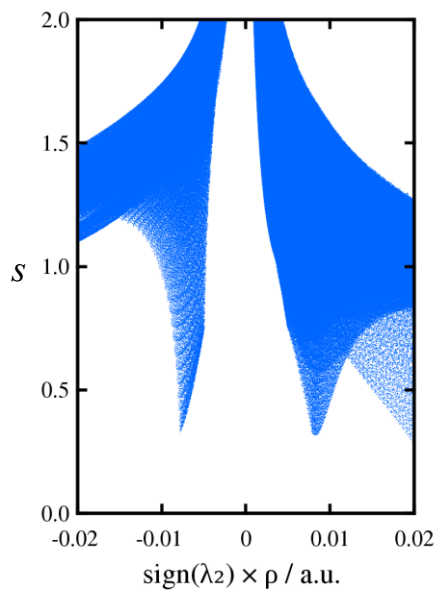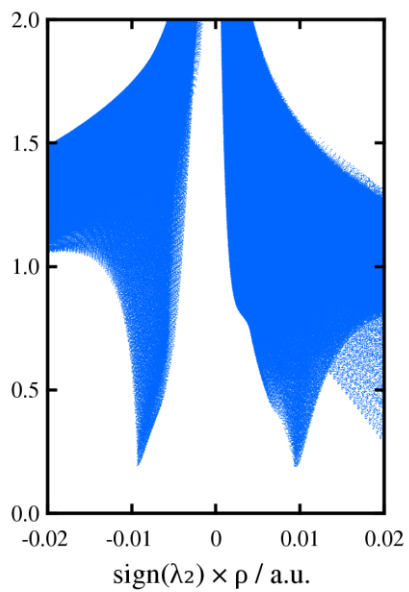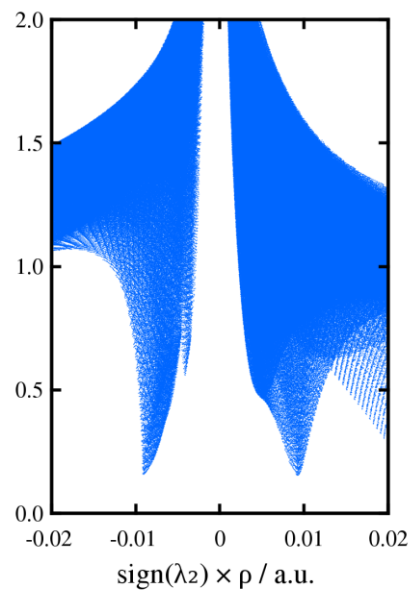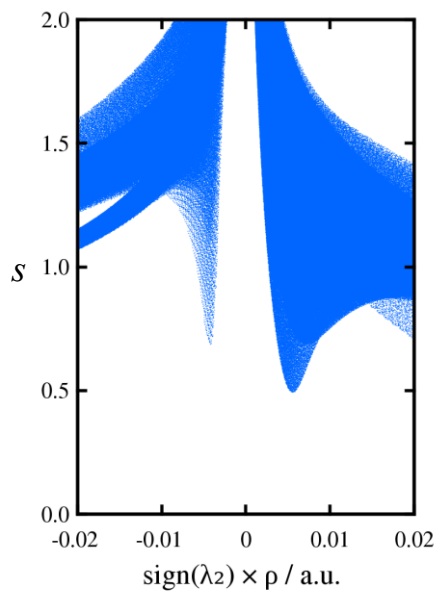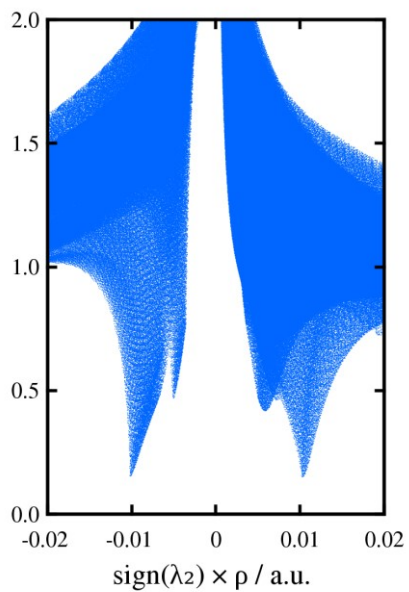
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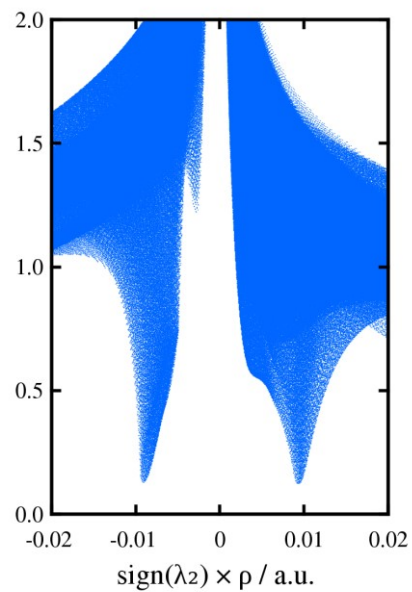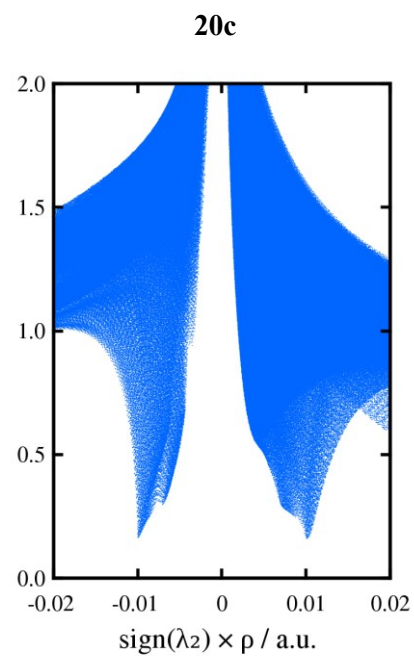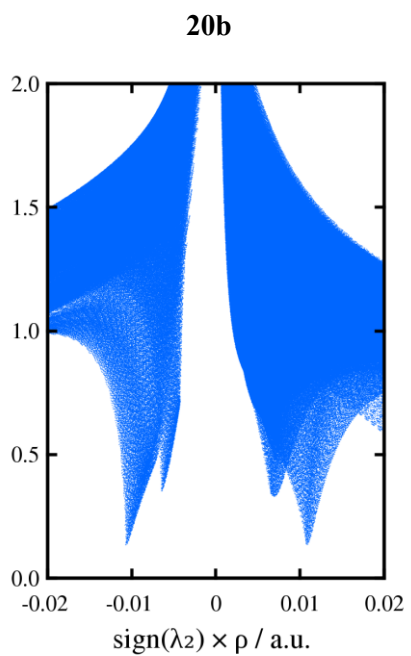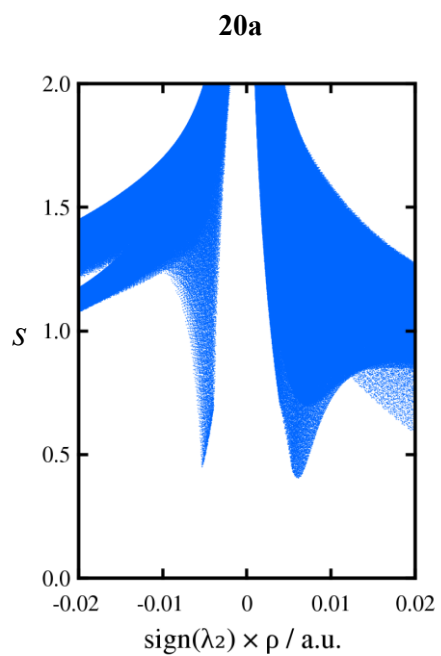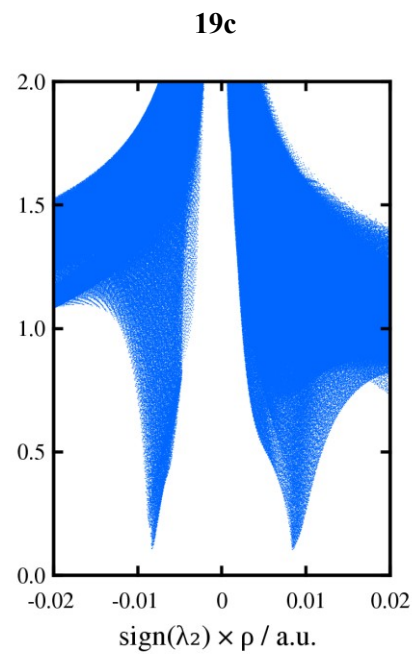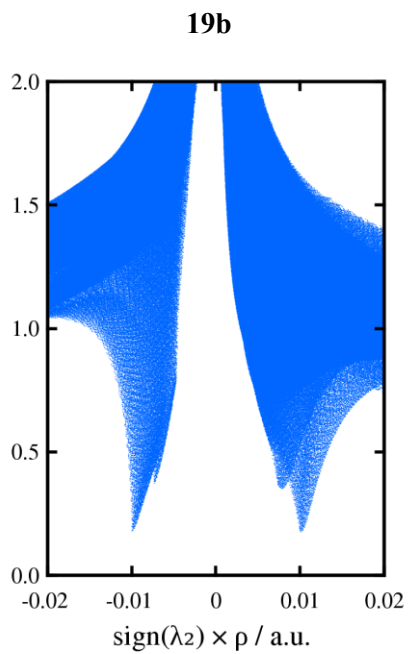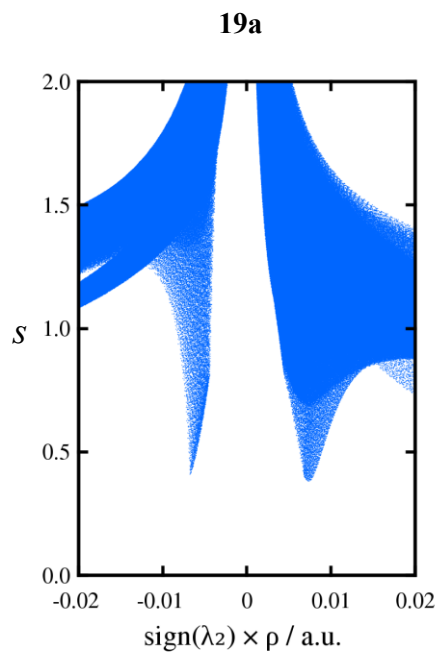
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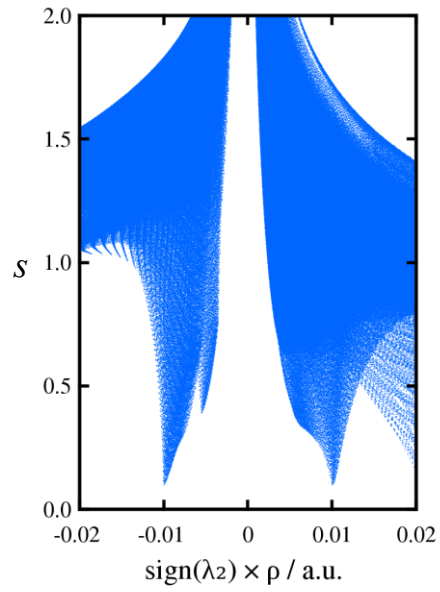
21b'
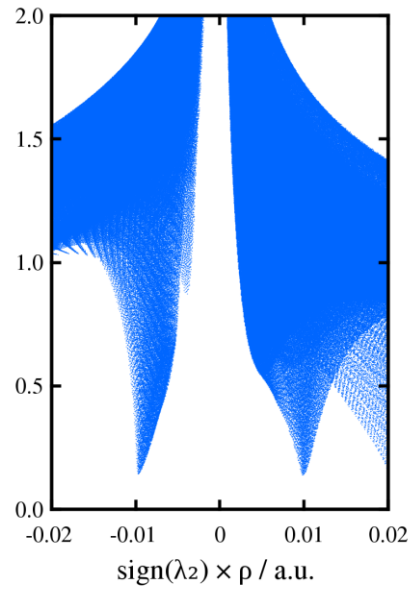
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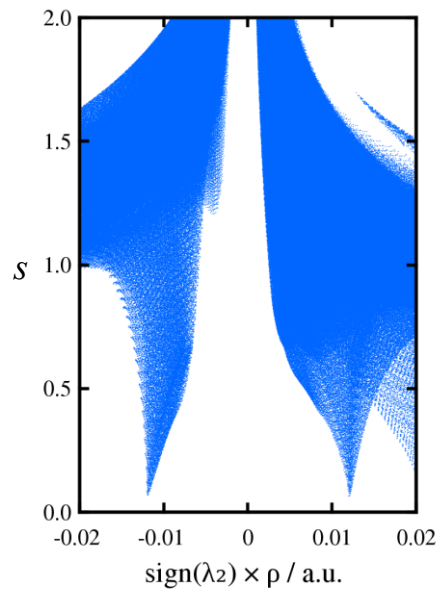
23b
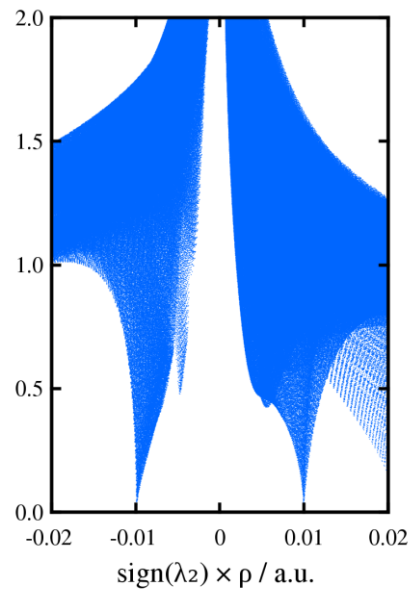
NCI analysis results obtained for selected conformational isomers of compounds **1-23**.
(Atomic units are used throughout)

1a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$	**1b**	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/	**I**[a]	0.00944	0.141	0.00174
I[r]	/	/	/	**I**[r]	0.00953	0.139	0.00174
II[a]	/	/	/	**II**[a]	0.00223	0.998	0.00180
II[r]	/	/	/	**II**[r]	0.00317	0.558	0.00161
III[a]	0.00453	1.266	0.00588	**III**[a]	0.00495	0.444	0.00232
III[r]	0.00527	0.703	0.00399	**III**[r]	0.00564	0.405	0.00252
IV[a]	0.00708	1.217	0.01023	**IV**[a]	0.00753	1.032	0.00943
IV[r]	0.00801	0.634	0.00629	**IV**[r]	0.00884	0.550	0.00622
V[a]	0.00708	1.217	0.01023	**V**[a]	/	/	/
V[r]	0.00801	0.634	0.00629	**V**[r]	0.00733	0.757	0.00667

2b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$	**3b**	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00974	0.13991	0.00180	**I**[a]	0.00969	0.14487	0.00185
I[r]	0.00985	0.14224	0.00186	**I**[r]	0.00987	0.14526	0.00190
II[a]	0.00227	1.09831	0.00203	**II**[a]	0.00225	1.10409	0.00201
II[r]	0.00315	0.57640	0.00164	**II**[r]	0.00316	0.58308	0.00167
III[a]	0.00470	0.47061	0.00229	**III**[a]	0.00482	0.45524	0.00229
III[r]	0.00547	0.42104	0.00251	**III**[r]	0.00558	0.40696	0.00249
IV[a]	0.00700	1.04147	0.00863	**IV**[a]	0.00714	1.03688	0.00881
IV[r]	0.00848	0.56142	0.00601	**IV**[r]	0.00842	0.55979	0.00593
V[a]	/	/	/	**V**[a]	/	/	/
V[r]	0.00725	0.77697	0.00674	**V**[r]	0.00720	0.77938	0.00670

4b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$	**5b**	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00951	0.14347	0.00179	**I**[a]	0.00930	0.15049	0.00182
I[r]	0.00980	0.14054	0.00182	**I**[r]	0.00952	0.14237	0.00178
II[a]	0.00230	1.01386	0.00191	**II**[a]	0.00230	0.93761	0.00176
II[r]	0.00316	0.56023	0.00161	**II**[r]	0.00323	0.54528	0.00161
III[a]	0.00490	0.44878	0.00231	**III**[a]	0.00487	0.45916	0.00234
III[r]	0.00560	0.40647	0.00250	**III**[r]	0.00550	0.41178	0.00247
IV[a]	0.00735	1.02845	0.00910	**IV**[a]	0.00736	1.03547	0.00917
IV[r]	0.00872	0.55669	0.00619	**IV**[r]	0.00877	0.55999	0.00627
V[a]	/	/	/	**V**[a]	/	/	/
V[r]	0.00723	0.76772	0.00664	**V**[r]	0.00729	0.76111	0.00666

6b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$	**7b**	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00927	0.15070	0.00181	**I**[a]	0.00923	0.14874	0.00178
I[r]	0.00945	0.14493	0.00179	**I**[r]	0.00935	0.14444	0.00176
II[a]	0.00224	0.91024	0.00165	**II**[a]	0.00233	0.89079	0.00171
II[r]	0.00322	0.54394	0.00160	**II**[r]	0.00324	0.53858	0.00160
III[a]	0.00477	0.47079	0.00234	**III**[a]	0.00475	0.47405	0.00234
III[r]	0.00554	0.41681	0.00253	**III**[r]	0.00553	0.42140	0.00255
IV[a]	0.00719	1.05352	0.00905	**IV**[a]	0.00714	1.05408	0.00896
IV[r]	0.00858	0.56254	0.00611	**IV**[r]	0.00853	0.56440	0.00609
V[a]	/	/	/	**V**[a]	/	/	/
V[r]	0.00732	0.76014	0.00668	**V**[r]	0.00731	0.75860	0.00666

8b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00903	0.14476	0.00168
I[r]	0.00909	0.14527	0.00170
II[a]	0.00221	1.31187	0.00234
II[r]	0.00296	0.62509	0.00165
III[a]	0.00513	0.42497	0.00232
III[r]	0.00568	0.38903	0.00244
IV[a]	0.00722	1.01203	0.00874
IV[r]	0.00901	0.54951	0.00637
V[a]	/	/	/
V[r]	0.00743	0.76468	0.00685

9b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00907	0.17099	0.00200
I[r]	0.00913	0.17172	0.00203
II[a]	0.00210	1.22498	0.00204
II[r]	0.00273	0.62904	0.00149
III[a]	0.00537	0.39171	0.00228
III[r]	0.00579	0.36557	0.00235
IV[a]	0.00743	0.98265	0.00881
IV[r]	0.00913	0.53773	0.00635
V[a]	/	/	/
V[r]	0.00740	0.79109	0.00706

10b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00970	0.15987	0.00205
I[r]	0.00998	0.15586	0.00207
II[a]	0.00232	1.28212	0.00244
II[r]	0.00323	0.61502	0.00182
III[a]	0.00534	0.40785	0.00236
III[r]	0.00591	0.37721	0.00250
IV[a]	0.00723	1.00306	0.00867
IV[r]	0.00904	0.54279	0.00632
V[a]	/	/	/
V[r]	0.00728	0.77765	0.00679

11b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00977	0.14662	0.00189
I[r]	0.00988	0.14924	0.00196
II[a]	0.00224	1.46731	0.00266
II[r]	0.00328	0.65410	0.00197
III[a]	0.00543	0.40195	0.00237
III[r]	0.00586	0.37358	0.00244
IV[a]	0.00715	1.00848	0.00859
IV[r]	0.00892	0.54245	0.00621
V[a]	/	/	/
V[r]	0.00728	0.78123	0.00682

12a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/
I[r]	/	/	/
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00492	1.27195	0.00658
III[r]	0.00521	0.71301	0.00398
IV[a]	0.00726	1.28497	0.01118
IV[r]	0.00755	0.67891	0.00622
V[a]	0.00726	1.28497	0.01118
V[r]	0.00755	0.67891	0.00622

12b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00913	0.15015	0.00177
I[r]	0.00925	0.14839	0.00178
II[a]	0.00235	1.18503	0.00229
II[r]	0.00313	0.59170	0.00168
III[a]	0.00469	0.48627	0.00236
III[r]	0.00539	0.42819	0.00250
IV[a]	0.00706	1.11323	0.00932
IV[r]	0.00839	0.59533	0.00628
V[a]	/	/	/
V[r]	0.00686	0.80428	0.00649

13a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/
I[r]	/	/	/
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00452	1.17261	0.00542
III[r]	0.00499	0.65200	0.00344
IV[a]	0.00701	1.10638	0.00918
IV[r]	0.00827	0.58598	0.00606
V[a]	/	/	/
V[r]	0.00730	0.73579	0.00644

13b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00947	0.15258	0.00189
I[r]	0.00953	0.15197	0.00190
II[a]	0.00217	1.05620	0.00183
II[r]	0.00299	0.57674	0.00154
III[a]	0.00469	0.47050	0.00228
III[r]	0.00543	0.42352	0.00250
IV[a]	0.00681	0.98428	0.00786
IV[r]	0.00870	0.53408	0.00591
V[a]	/	/	/
V[r]	0.00678	0.82848	0.00658

13c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00931	0.13566	0.00164
I[r]	0.00937	0.13257	0.00162
II[a]	0.00222	0.87657	0.00157
II[r]	0.00317	0.54103	0.00156
III[a]	0.00398	0.59393	0.00232
III[r]	0.00497	0.48318	0.00254
IV[a]	0.00674	1.15703	0.00912
IV[r]	0.00800	0.61680	0.00610
V[a]	/	/	/
V[r]	0.00737	0.71675	0.00636

14a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/
I[r]	/	/	/
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00390	0.96586	0.00366
III[r]	0.00512	0.57171	0.00312
IV[a]	/	/	/
IV[r]	0.00566	0.93681	0.00585
V[a]	/	/	/
V[r]	/	/	/

14b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00982	0.14802	0.00193
I[r]	0.00989	0.14452	0.00190
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00375	0.68658	0.00248
III[r]	0.00500	0.49579	0.00262
IV[a]	/	/	/
IV[r]	0.00550	0.91468	0.00549
V[a]	/	/	/
V[r]	/	/	/

14c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00922	0.10212	0.00122
I[r]	0.00927	0.10245	0.00123
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00557	1.29630	0.00791
III[r]	0.00567	0.71748	0.00448
IV[a]	/	/	/
IV[r]	0.00528	0.96105	0.00547
V[a]	/	/	/
V[r]	0.00605	1.10294	0.00752

15a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/
I[r]	/	/	/
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00382	0.79835	0.00295
III[r]	0.00494	0.52681	0.00274
IV[a]	/	/	/
IV[r]	0.00527	0.98109	0.00557
V[a]	/	/	/
V[r]	/	/	/

15b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00958	0.16026	0.00202
I[r]	0.00976	0.15858	0.00205
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00385	0.62360	0.00233
III[r]	0.00478	0.48309	0.00241
IV[a]	/	/	/
IV[r]	0.00540	0.97338	0.00571
V[a]	/	/	/
V[r]	/	/	/

15c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00875	0.07482	0.00083
I[r]	0.00878	0.07470	0.00084
II[a]	/	/	/
II[r]	/	/	/
III[a]	/	/	/
III[r]	0.00581	0.80573	0.00521
IV[a]	/	/	/
IV[r]	0.00511	1.07630	0.00586
V[a]	/	/	/
V[r]	0.00556	1.09347	0.00666

16a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	/	/	/
I[r]	/	/	/
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00378	0.74888	0.00273
III[r]	0.00501	0.51199	0.00272
IV[a]	/	/	/
IV[r]	0.00673	0.79992	0.00629
V[a]	/	/	/
V[r]	0.00550	1.03584	0.00623

16b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00993	0.14252	0.00188
I^r	0.01009	0.14090	0.00190
II^a	/	/	/
II^r	/	/	/
III^a	0.00451	0.47914	0.00221
III^r	0.00524	0.42331	0.00238
IV^a	/	/	/
IV^r	0.00682	0.77697	0.00622
V^a	/	/	/
V^r	0.00562	1.08472	0.00671

16c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00954	0.12941	0.00162
I^r	0.00967	0.12615	0.00161
II^a	0.00241	1.34969	0.00270
II^r	0.00322	0.62795	0.00185
III^a	0.00423	1.11756	0.00473
III^r	0.00540	0.61783	0.00362
IV^a	/	/	/
IV^r	0.00622	0.79100	0.00560
V^a	/	/	/
V^r	0.00594	0.99724	0.00664

17a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	/	/	/
I^r	/	/	/
II^a	/	/	/
II^r	/	/	/
III^a	0.00782	0.33046	0.00317
III^r	0.00837	0.31778	0.00334
IV^a	0.00753	1.07351	0.00981
IV^r	0.00864	0.56806	0.00623
V^a	/	/	/
V^r	0.01214	0.79123	0.01366

17b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00927	0.19298	0.00233
I^r	0.00958	0.19000	0.00239
II^a	/	/	/
II^r	/	/	/
III^a	0.00927	0.24327	0.00293
III^r	0.00955	0.23694	0.00297
IV^a	0.00733	0.99110	0.00873
IV^r	0.00889	0.54239	0.00618
V^a	/	/	/
V^r	0.01267	0.86466	0.01580

17c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00901	0.15794	0.00183
I^r	0.00921	0.15351	0.00183
II^a	/	/	/
II^r	/	/	/
III^a	0.00415	0.55913	0.00231
III^r	0.00518	0.46784	0.00260
IV^a	0.01101	1.10789	0.01678
IV^r	0.01288	0.62565	0.01169
V^a	/	/	/
V^r	0.00744	0.75178	0.00676

18a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	/	/	/
I^r	/	/	/
II^a	/	/	/
II^r	/	/	/
III^a	0.00416	0.68772	0.00285
III^r	0.00560	0.49297	0.00303
IV^a	/	/	/
IV^r	0.00523	0.94862	0.00532
V^a	/	/	/
V^r	0.00698	1.04715	0.00864

18b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.01018	0.15492	0.00211
I^r	0.01025	0.15012	0.00207
II^a	/	/	/
II^r	/	/	/
III^a	0.00502	0.46940	0.00250
III^r	0.00581	0.41731	0.00270
IV^a	/	/	/
IV^r	0.00532	0.93301	0.00537
V^a	/	/	/
V^r	/	/	/

18c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00904	0.12845	0.00150
I^r	0.00929	0.12402	0.00150
II^a	/	/	/
II^r	/	/	/
III^a	/	/	/
III^r	0.00565	0.78484	0.00488
IV^a	/	/	/
IV^r	0.00743	0.79157	0.00710
V^a	/	/	/
V^r	0.00493	1.15554	0.00600

19a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	/	/	/
I^r	/	/	/
II^a	/	/	/
II^r	/	/	/
III^a	0.00675	0.40996	0.00323
III^r	0.00738	0.38245	0.00340
IV^a	/	/	/
IV^r	0.00497	1.01542	0.00532
V^a	/	/	/
V^r	/	/	/

19b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00996	0.18044	0.00239
I^r	0.01012	0.17645	0.00239
II^a	/	/	/
II^r	/	/	/
III^a	0.00733	0.37342	0.00329
III^r	0.00794	0.35209	0.00345
IV^a	/	/	/
IV^r	0.00490	1.00226	0.00516
V^a	/	/	/
V^r	/	/	/

19c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00831	0.10815	0.00113
I^r	0.00837	0.10546	0.00111
II^a	/	/	/
II^r	/	/	/
III^a	/	/	/
III^r	0.00587	0.83580	0.00548
IV^a	/	/	/
IV^r	0.01136	0.82000	0.01295
V^a	/	/	/
V^r	0.00525	1.20757	0.00682

20a	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	/	/	/
I^r	/	/	/
II^a	/	/	/
II^r	/	/	/
III^a	0.00530	0.44940	0.00257
III^r	0.00617	0.40575	0.00284
IV^a	/	/	/
IV^r	0.00614	0.78155	0.00544
V^a	/	/	/
V^r	/	/	/

20b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.01072	0.13408	0.00196
I^r	0.01085	0.13692	0.00204
II^a	/	/	/
II^r	/	/	/
III^a	0.00641	0.35308	0.00260
III^r	0.00691	0.33047	0.00269
IV^a	0.00744	1.36914	0.01230
IV^r	0.00661	0.75812	0.00581
V^a	/	/	/
V^r	/	/	/

20c	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I^a	0.00992	0.16484	0.00217
I^r	0.01005	0.16118	0.00216
II^a	/	/	/
II^r	/	/	/
III^a	0.00352	0.94209	0.00312
III^r	0.00480	0.56630	0.00284
IV^a	/	/	/
IV^r	0.00935	0.80652	0.00982
V^a	/	/	/
V^r	0.00546	1.10242	0.00655

21b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00998	0.09970	0.00133
I[r]	0.01003	0.09880	0.00132
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00384	1.12184	0.00418
III[r]	0.00465	0.62453	0.00300
IV[a]	0.00699	1.16572	0.00964
IV[r]	0.00831	0.61291	0.00638
V[a]	/	/	/
V[r]	0.00795	0.66241	0.00650

21b'	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00969	0.14299	0.00183
I[r]	0.00992	0.13943	0.00184
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00387	0.87304	0.00328
III[r]	0.00508	0.54210	0.00293
IV[a]	0.00767	1.08532	0.01015
IV[r]	0.00850	0.57318	0.00615
V[a]	/	/	/
V[r]	0.00754	0.70182	0.00642

22b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.01188	0.06841	0.00115
I[r]	0.01203	0.06430	0.00110
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00420	1.20624	0.00506
III[r]	0.00494	0.65992	0.00344
IV[a]	0.00735	1.16807	0.01033
IV[r]	0.00850	0.61291	0.00658
V[a]	/	/	/
V[r]	0.00769	0.66594	0.00625

23b	$\rho(s_{min})$	s_{min}	$\nabla\rho(s_{min})$
I[a]	0.00990	0.02719	0.00036
I[r]	0.00996	0.02754	0.00037
II[a]	/	/	/
II[r]	/	/	/
III[a]	0.00477	0.47855	0.00238
III[r]	0.00561	0.42381	0.00261
IV[a]	0.00766	1.05176	0.00983
IV[r]	0.00896	0.56334	0.00649
V[a]	/	/	/
V[r]	0.00754	0.74430	0.00681

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