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DFT modeling of indoline spiropyrans with a cationic substituent in the gas phase

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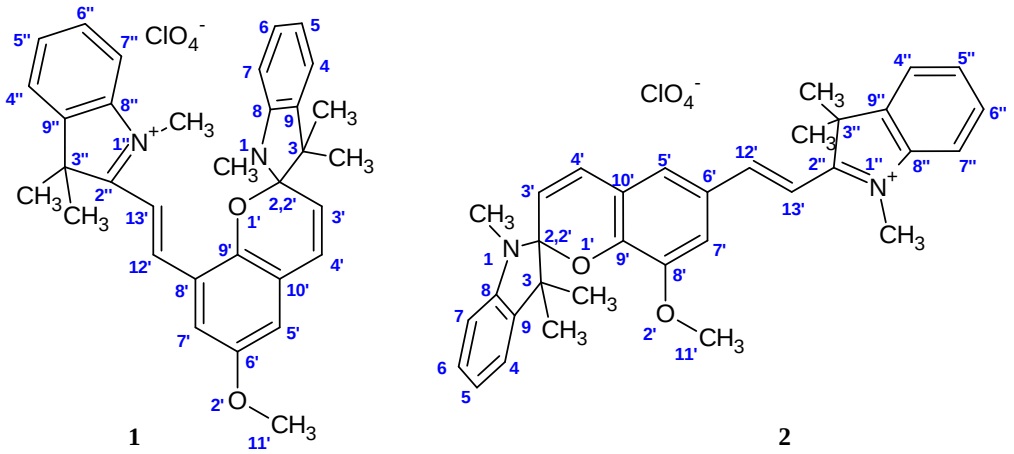
Table S8 The summary NBO results for 3-center 4-electron hyperbonds search in structures of compounds **1** and **2** with and without perchlorate anion calculated by B3LYP/6-311++G(d,p) method.



Scheme S1 Scheme of atoms labeling in compounds **1** and **2**.

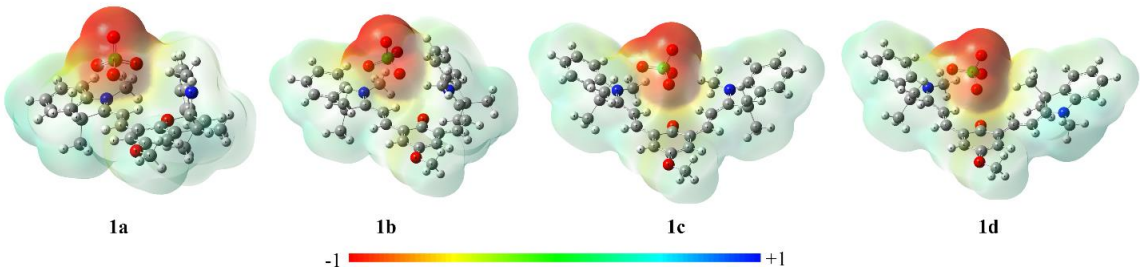


Figure S1 The quality ESP map changes between **1a-1d** structures (from the side view of molecules).

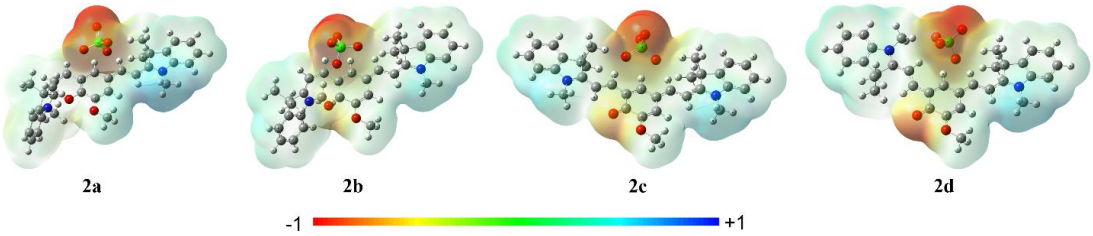


Figure S2 The quality ESP map changes between **2a-2d** structures (from the side view of molecules).

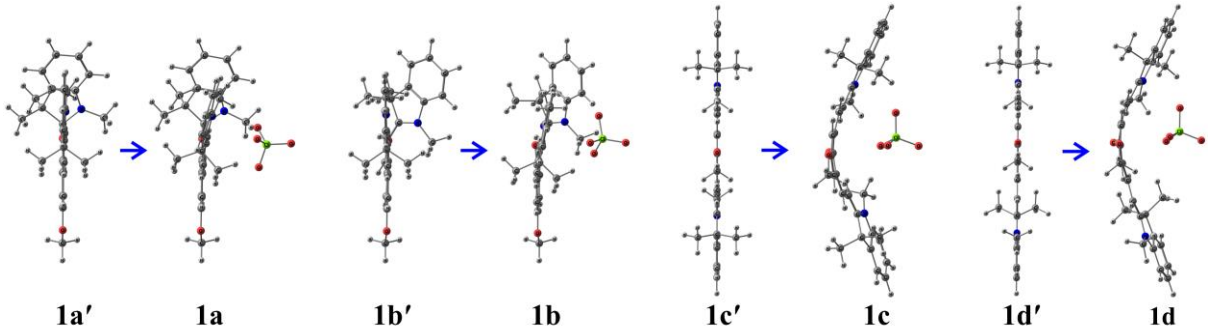


Figure S3 The quality geometry changes in the structures of the compound **1** upon going from structures without an anion to structures with an anion (for the structures **1a, 1a′, 1b, 1b′** - profile view of molecule, for the structures **1c, 1c′, 1d, 1d′** - bottom view of molecule).

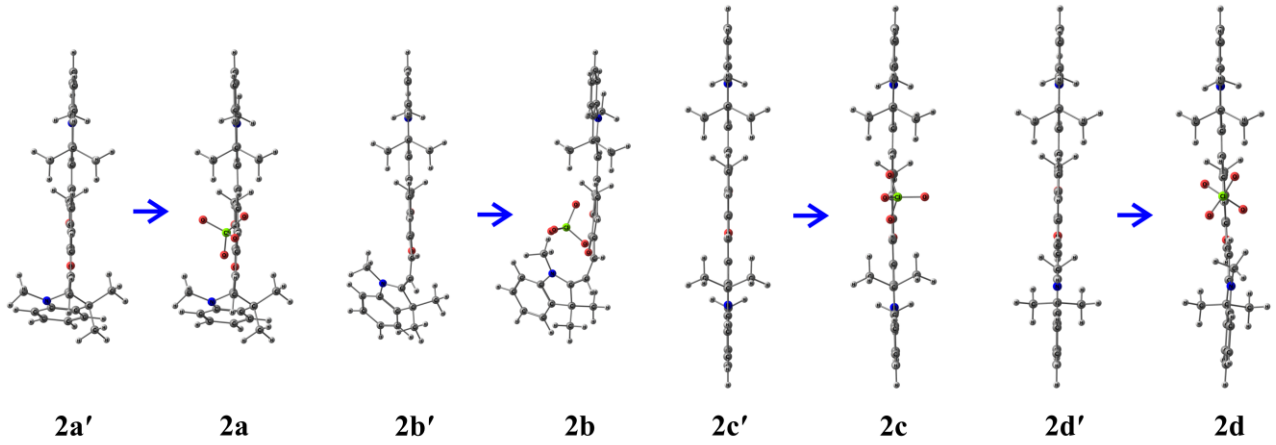


Figure S4 The quality geometry changes in the structures of the compound **2** upon going from structures without an anion to structures with an anion (for the structures **2a, 2a′, 2b, 2b′ -** profile view of molecule, for the structures **2c, 2c′, 2d, 2d′ -** bottom view of molecule).

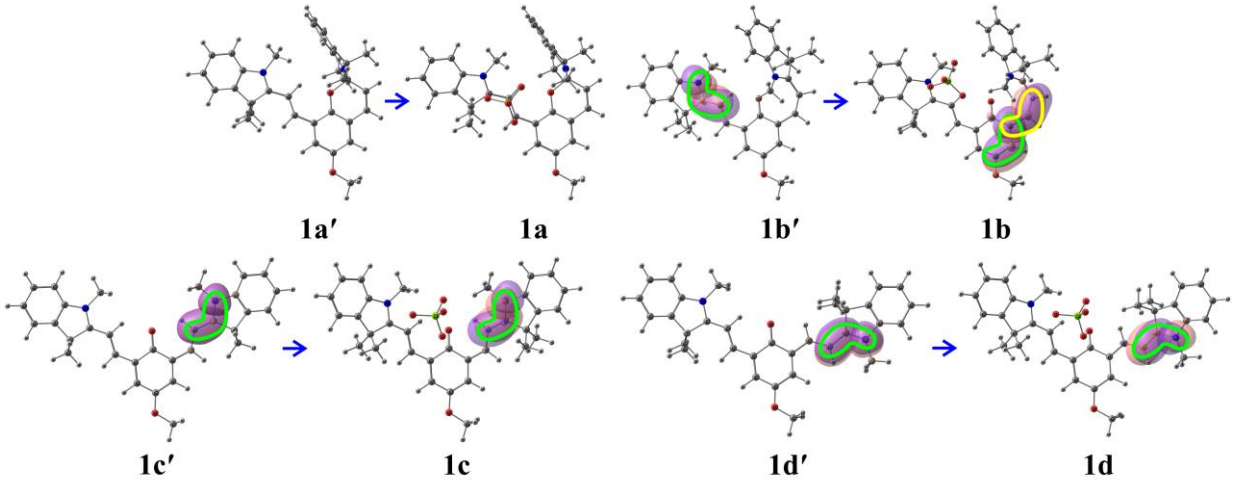


Figure S5 The quality effect of the perchlorate anion on 3c-4e hyperbonds in the isomeric structures of the compound **1** (from the side view of molecules). Green and yellow lines schematically outline the centers of considered hyperbonds.

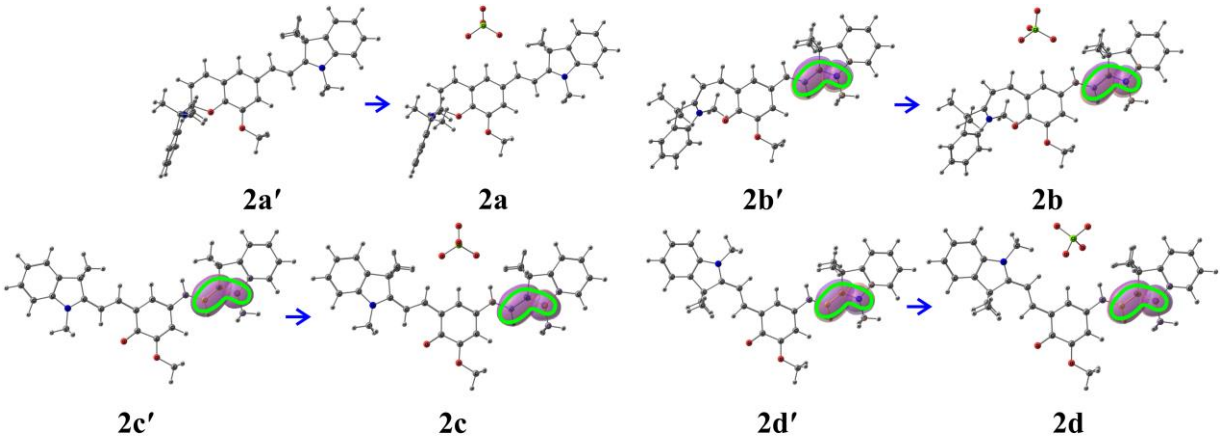
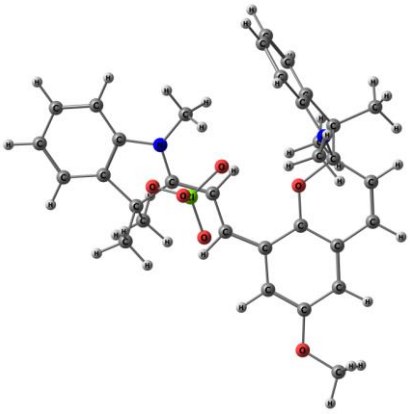
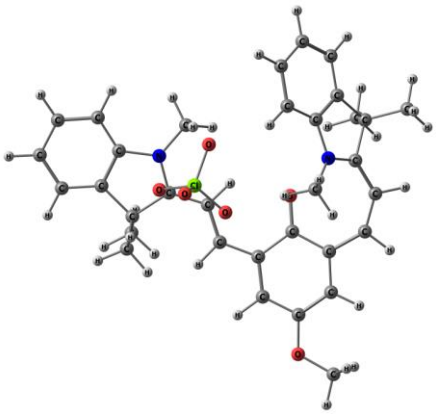
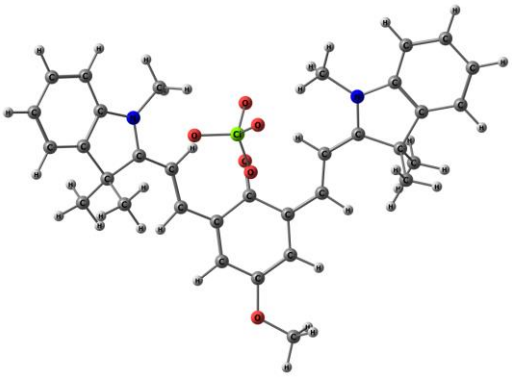
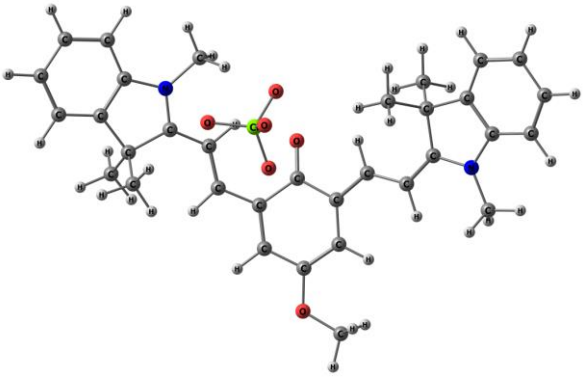
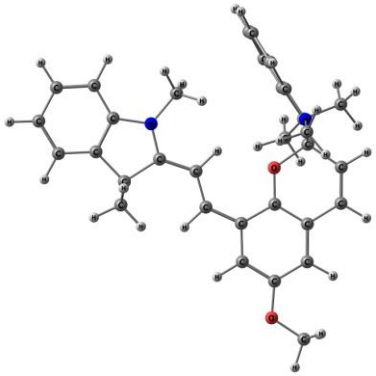
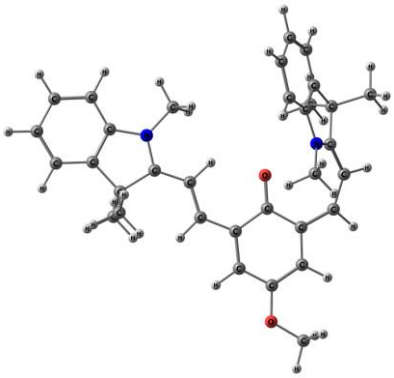
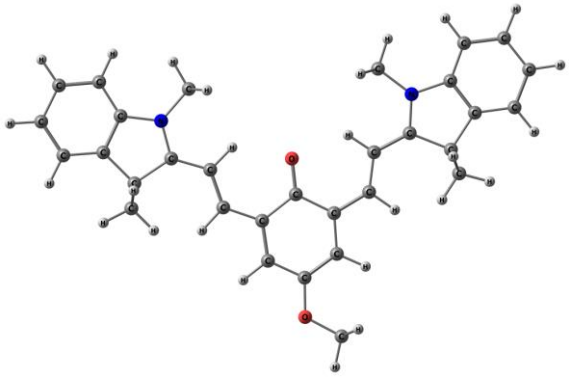
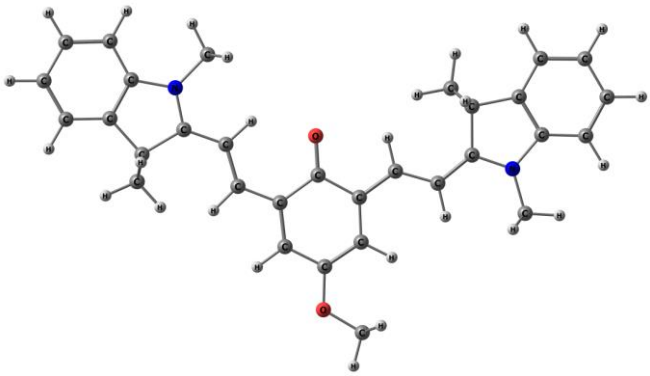
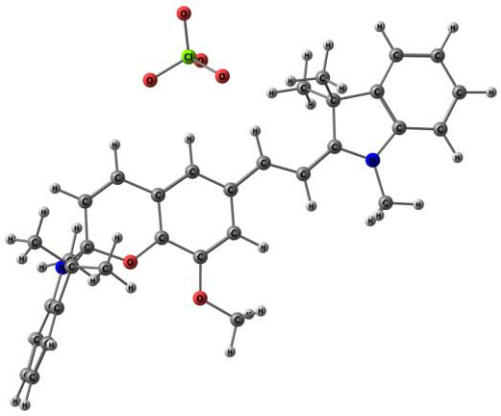
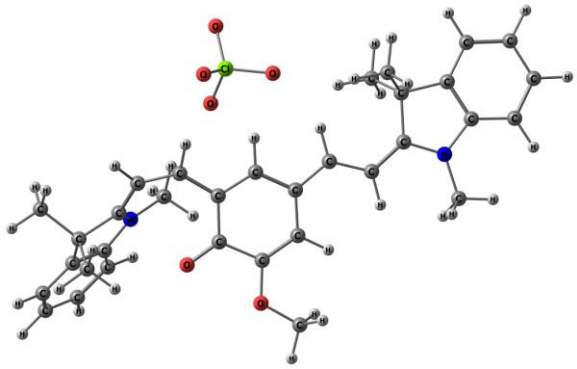
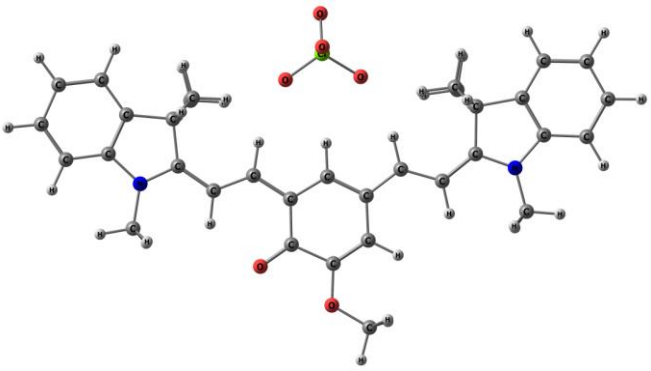
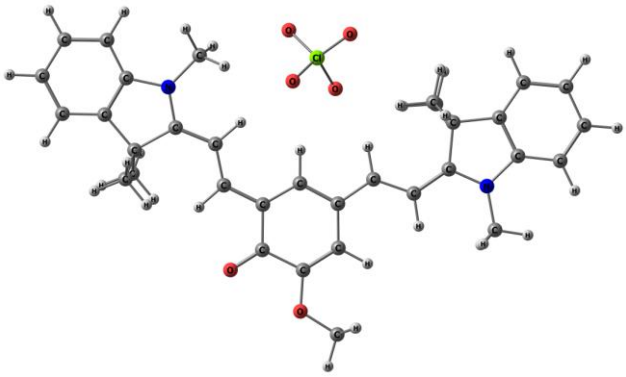


Figure S6 The quality effect of the perchlorate anion on 3c-4e hyperbonds in the isomeric structures of the compound **2** (from the side view of molecules). Green lines schematically outline the centers of considered hyperbonds.

Table S1 Graphical summary of the compounds **1** and **2** and the links to sections with calculation experiment details.

Compound 1			
Structure	**Calculation visualization (front view of molecule)**	**Geometry**	**Overview**
SP form **1a**		g.1a	o.1a
cis-isomer of *MC* form **1b**		g.1b	o.1b
TTC-TTC isomer of *MC* form **1c**		g.1c	o.1c
TTT-TTC isomer of *MC* form **1d**		g.1d	o.1d

SP form without perchlorate anion **1a′**		g.1a′	o.1a′
cis-isomer of *MC* form without perchlorate anion **1b′**		g.1b′	o.1b′
TTC-TTC isomer of *MC* form without perchlorate anion **1c′**		g.1c′	o.1c′
TTT-TTC isomer of *MC* form without perchlorate anion **1d′**		g.1d′	o.1d′

Compound 2			
Structure	**Calculation visualization (front view of molecule)**	**Geometry**	**Overview**
SP form **2a**		g.2a	o.2a
cis-isomer of *MC* form **2b**		g.2b	o.2b
TTC-TTC isomer of *MC* form **2c**		g.2c	o.2c
TTT-TTC isomer of *MC* form **2d**		g.2d	o.2d

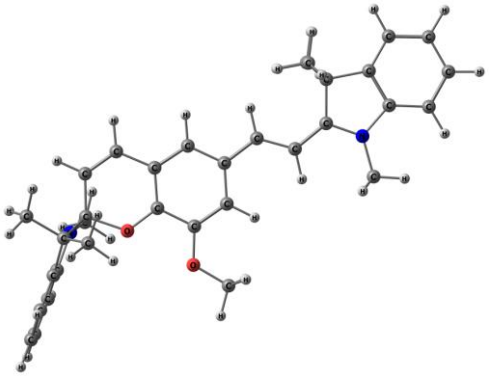
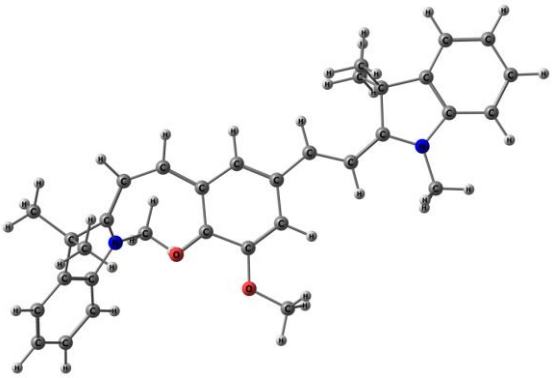
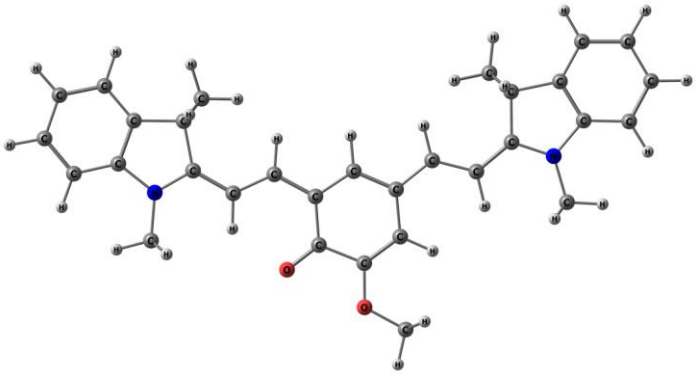
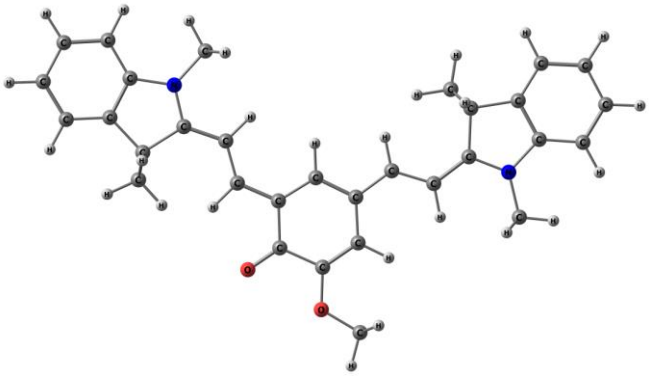
SP form without perchlorate anion **2a′**		g.2a′	o.2a′
cis-isomer of *MC* form without perchlorate anion **2b′**		g.2b′	o.2b′
TTC-TTC isomer of *MC* form without perchlorate anion **2c′**		g.2c′	o.2c′
TTT-TTC isomer of *MC* form without perchlorate anion **2d′**		g.2d′	o.2d′

Table S2 The optimized cartesian coordinates (Å) of the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method.

Compound 1					
Key	**Structure**	**Geometry**			
g.1a	**1a**	N	2.388156000	2.265181000	0.977778000
		C	2.573997000	2.679681000	-1.357570000
		C	0.498283000	4.311681000	-1.302264000
		H	0.516425000	4.524209000	-2.366524000
		C	-0.441048000	4.947378000	-0.475590000
		H	-1.149222000	5.649252000	-0.900613000
		C	-0.457902000	4.678636000	0.892336000
		H	-1.187132000	5.170687000	1.526845000
		C	0.442341000	3.775885000	1.468959000
		H	0.398571000	3.552525000	2.527199000
		C	1.373609000	3.160055000	0.634958000
		C	1.400060000	3.423566000	-0.742243000
		C	2.423089000	1.604937000	2.280966000
		H	1.534910000	0.990936000	2.456167000
		H	2.495019000	2.361255000	3.066506000
		H	3.316075000	0.982183000	2.337094000
		C	2.280157000	2.020496000	-2.710140000
		H	3.133741000	1.424568000	-3.046306000
		H	2.102200000	2.793106000	-3.463036000
		H	1.404775000	1.374258000	-2.666807000
		C	3.745631000	3.676428000	-1.522967000
		H	4.630085000	3.187859000	-1.941062000
		H	4.015351000	4.143720000	-0.573286000
		H	3.443249000	4.470268000	-2.209381000
		C	2.891341000	1.627168000	-0.209793000
		O	2.032072000	0.430384000	-0.491836000
		O	3.711899000	-4.841085000	-0.584000000
		C	4.330227000	1.230567000	-0.082143000
		H	5.024515000	2.039727000	0.100144000
		C	4.755757000	-0.034914000	-0.141034000
		H	5.811479000	-0.258965000	-0.024657000
		C	4.282451000	-2.471107000	-0.358835000
		H	5.341716000	-2.659640000	-0.238715000
		C	3.377543000	-3.516975000	-0.535452000
		C	2.028288000	-3.218483000	-0.676346000
		H	1.333860000	-4.041116000	-0.797795000
		C	1.538057000	-1.898461000	-0.640941000
		C	2.475606000	-0.842890000	-0.474698000
		C	3.838479000	-1.142921000	-0.332250000
		C	5.070474000	-5.203220000	-0.379357000
		H	5.719092000	-4.786173000	-1.158155000
		H	5.099623000	-6.290064000	-0.433445000
		H	5.425888000	-4.880937000	0.605571000
		C	0.108188000	-1.749555000	-0.776802000
		H	-0.391261000	-2.690167000	-0.968458000
		C	-0.666630000	-0.636525000	-0.649901000
		H	-0.199516000	0.299223000	-0.387674000
		N	-2.806219000	0.431961000	-0.493976000
		C	-2.084026000	-0.650816000	-0.771571000
		C	-3.007597000	-1.773490000	-1.265689000
		C	-5.623169000	-1.530644000	-1.543102000
		H	-5.781848000	-2.540977000	-1.903136000
		C	-6.707039000	-0.659766000	-1.393732000
		H	-7.705980000	-0.998283000	-1.642035000
		C	-6.516018000	0.639962000	-0.921969000
		H	-7.367396000	1.300303000	-0.807428000

		C	-5.243172000	1.104610000	-0.587463000
		H	-5.105464000	2.111974000	-0.217999000
		C	-4.183134000	0.220860000	-0.746002000
		C	-4.354483000	-1.078213000	-1.217486000
		C	-2.276052000	1.667249000	0.094298000
		H	-3.108245000	2.257343000	0.466105000
		H	-1.732845000	2.245302000	-0.655354000
		H	-1.628345000	1.412197000	0.933351000
		C	-3.013655000	-2.997016000	-0.311902000
		H	-2.084646000	-3.564233000	-0.372316000
		H	-3.831150000	-3.661407000	-0.601990000
		H	-3.151231000	-2.679637000	0.721528000
		C	-2.663126000	-2.185798000	-2.717051000
		H	-1.677157000	-2.648549000	-2.777215000
		H	-2.680325000	-1.325624000	-3.390365000
		H	-3.400726000	-2.909167000	-3.071727000
		Cl	-1.320856000	-0.927887000	2.952889000
		O	-1.552665000	-0.936517000	4.415562000
		O	-0.604153000	0.343186000	2.551455000
		O	-2.635364000	-0.959677000	2.213529000
		O	-0.497068000	-2.102801000	2.536027000
g.1b	**1b**	N	-2.977219000	-1.277181000	0.544133000
		C	-4.195416000	-2.213480000	-1.226896000
		C	-2.929541000	-4.525161000	-1.005617000
		H	-3.467926000	-5.021860000	-1.805604000
		C	-1.934068000	-5.206940000	-0.295706000
		H	-1.704083000	-6.235390000	-0.549652000
		C	-1.229360000	-4.573872000	0.729846000
		H	-0.450639000	-5.108754000	1.260667000
		C	-1.497908000	-3.249376000	1.086414000
		H	-0.909275000	-2.756156000	1.850248000
		C	-2.497195000	-2.603566000	0.371682000
		C	-3.204407000	-3.210108000	-0.664853000
		C	-2.565186000	-0.464310000	1.688274000
		H	-1.516198000	-0.178098000	1.614329000
		H	-2.698933000	-1.061976000	2.592636000
		H	-3.191216000	0.420658000	1.740916000
		C	-3.901643000	-1.880066000	-2.707356000
		H	-4.601017000	-1.126070000	-3.076125000
		H	-4.008808000	-2.780643000	-3.317367000
		H	-2.889371000	-1.490700000	-2.823695000
		C	-5.650713000	-2.706542000	-1.058164000
		H	-6.364778000	-1.969728000	-1.433425000
		H	-5.881729000	-2.918018000	-0.011918000
		H	-5.791043000	-3.627111000	-1.629579000
		C	-3.912738000	-0.983601000	-0.353241000
		O	-1.686898000	0.546112000	-1.019222000
		O	-2.157041000	5.849169000	0.371676000
		C	-4.644647000	0.219621000	-0.497340000
		H	-5.663795000	0.043051000	-0.831742000
		C	-4.327894000	1.555012000	-0.345829000
		H	-5.207482000	2.196891000	-0.373931000
		C	-3.225391000	3.672615000	0.028517000
		H	-4.214339000	4.063197000	0.236923000
		C	-2.123330000	4.510230000	0.074986000
		C	-0.857686000	3.981123000	-0.185873000
		H	-0.007571000	4.651819000	-0.111036000
		C	-0.653539000	2.639301000	-0.515136000
		C	-1.805890000	1.722206000	-0.621321000
		C	-3.111990000	2.292510000	-0.268350000
		C	-3.408886000	6.435346000	0.691022000

		H	-4.110155000	6.370492000	-0.149306000
		H	-3.202635000	7.482922000	0.904579000
		H	-3.856510000	5.967945000	1.575699000
		C	0.697827000	2.213187000	-0.689933000
		H	1.422634000	3.014924000	-0.608598000
		C	1.158350000	0.933432000	-0.880067000
		H	0.415987000	0.151732000	-0.920120000
		N	2.899048000	-0.708620000	-1.049005000
		C	2.518552000	0.573676000	-0.952516000
		C	3.765301000	1.472120000	-0.955649000
		C	6.248449000	0.580455000	-1.084493000
		H	6.709630000	1.561512000	-1.056802000
		C	7.044816000	-0.568156000	-1.146151000
		H	8.123979000	-0.473363000	-1.170429000
		C	6.461747000	-1.835695000	-1.161890000
		H	7.092210000	-2.716484000	-1.193790000
		C	5.074791000	-1.991596000	-1.125577000
		H	4.633005000	-2.979086000	-1.116064000
		C	4.305652000	-0.835457000	-1.077328000
		C	4.871076000	0.437377000	-1.048178000
		C	2.006738000	-1.866778000	-0.993305000
		H	2.512053000	-2.716721000	-1.447189000
		H	1.100527000	-1.663599000	-1.560609000
		H	1.754836000	-2.090677000	0.047109000
		C	3.908699000	2.276918000	0.361188000
		H	3.167727000	3.074185000	0.428670000
		H	4.899424000	2.737184000	0.388769000
		H	3.790882000	1.624524000	1.226441000
		C	3.784811000	2.399901000	-2.193926000
		H	2.970017000	3.124640000	-2.163822000
		H	3.699015000	1.826919000	-3.120057000
		H	4.728677000	2.949595000	-2.220687000
		Cl	1.615654000	-0.746791000	2.783961000
		O	1.928417000	-0.834134000	4.228719000
		O	1.166690000	-2.093438000	2.266199000
		O	2.831416000	-0.332139000	2.005452000
		O	0.515131000	0.245223000	2.543171000
g.1c	**1c**	N	-3.889041000	-1.639336000	-0.621250000
		C	-5.282074000	0.152521000	0.014936000
		C	-7.347373000	-1.463540000	0.329232000
		H	-8.037823000	-0.681814000	0.627210000
		C	-7.782326000	-2.792335000	0.255846000
		H	-8.809885000	-3.037457000	0.496624000
		C	-6.899087000	-3.802270000	-0.124709000
		H	-7.246452000	-4.827568000	-0.177287000
		C	-5.568029000	-3.518633000	-0.440220000
		H	-4.894117000	-4.312370000	-0.734607000
		C	-5.157171000	-2.191841000	-0.360473000
		C	-6.030597000	-1.169772000	0.017274000
		C	-2.725377000	-2.424417000	-1.033489000
		H	-2.518134000	-2.262771000	-2.095117000
		H	-2.936969000	-3.477852000	-0.868565000
		H	-1.844169000	-2.155848000	-0.447080000
		C	-5.940161000	1.149799000	-0.964581000
		H	-5.396751000	2.094878000	-1.002517000
		H	-6.964137000	1.358665000	-0.644614000
		H	-5.977550000	0.738728000	-1.975521000
		C	-5.225717000	0.727127000	1.452234000
		H	-4.679174000	1.670144000	1.488797000
		H	-4.738471000	0.027658000	2.134006000
		H	-6.241471000	0.906128000	1.813723000

		C	-3.889113000	-0.290489000	-0.462281000
		O	-0.134695000	0.976766000	-1.766891000
		O	-0.171144000	5.938519000	0.477867000
		C	-2.751872000	0.467011000	-0.722503000
		H	-1.877465000	-0.048285000	-1.091909000
		C	-2.609631000	1.830436000	-0.479188000
		H	-3.462761000	2.378977000	-0.092199000
		C	-1.428522000	3.922577000	-0.111778000
		H	-2.380876000	4.362504000	0.160602000
		C	-0.254326000	4.638824000	0.048945000
		C	0.975737000	3.995813000	-0.154299000
		H	1.875804000	4.541702000	0.111833000
		C	1.070914000	2.692333000	-0.636804000
		C	-0.161943000	1.990496000	-1.061555000
		C	-1.425623000	2.584023000	-0.576930000
		C	-1.375900000	6.621386000	0.786867000
		H	-2.036988000	6.682292000	-0.085466000
		H	-1.082086000	7.626292000	1.085824000
		H	-1.908664000	6.139909000	1.615034000
		C	2.337364000	2.041140000	-0.608452000
		H	3.137043000	2.637517000	-0.182015000
		C	2.595158000	0.739884000	-0.975960000
		H	1.778212000	0.194286000	-1.423352000
		N	3.918266000	-1.247802000	-1.077669000
		C	3.782216000	0.036456000	-0.710702000
		C	5.040380000	0.484568000	0.042223000
		C	7.131034000	-1.059489000	0.511561000
		H	7.703503000	-0.297339000	1.028744000
		C	7.657356000	-2.346107000	0.352758000
		H	8.640276000	-2.577743000	0.745635000
		C	6.921744000	-3.336441000	-0.298886000
		H	7.337330000	-4.331580000	-0.405450000
		C	5.650585000	-3.071198000	-0.812090000
		H	5.084629000	-3.851764000	-1.302876000
		C	5.151640000	-1.784277000	-0.648830000
		C	5.870362000	-0.785334000	0.007407000
		C	2.881209000	-2.031013000	-1.751607000
		H	3.296594000	-2.995537000	-2.030677000
		H	2.559971000	-1.512201000	-2.655865000
		H	2.028635000	-2.174686000	-1.082675000
		C	4.695451000	0.853508000	1.507721000
		H	4.125170000	1.782125000	1.557755000
		H	5.620875000	0.988263000	2.073147000
		H	4.099689000	0.067308000	1.973629000
		C	5.776130000	1.636073000	-0.681240000
		H	5.183072000	2.551325000	-0.692060000
		H	6.011409000	1.368354000	-1.713759000
		H	6.714557000	1.849365000	-0.163792000
		Cl	0.730655000	-1.498255000	1.563984000
		O	0.217285000	-2.290696000	2.710039000
		O	0.214218000	-2.088811000	0.267384000
		O	2.233236000	-1.548228000	1.523801000
		O	0.280705000	-0.077827000	1.662424000
g.1d	**1d**	N	-5.822446000	0.286770000	0.131835000
		C	-4.262889000	-1.311285000	-0.642506000
		C	-6.030367000	-3.256049000	-0.395171000
		H	-5.358893000	-4.033270000	-0.742860000
		C	-7.339459000	-3.576793000	-0.016421000
		H	-7.680774000	-4.603485000	-0.074058000
		C	-8.204287000	-2.583474000	0.440408000
		H	-9.214323000	-2.843264000	0.735430000

		C	-7.790158000	-1.251437000	0.529771000
		H	-8.472341000	-0.493022000	0.892683000
		C	-6.486775000	-0.956828000	0.144506000
		C	-5.607537000	-1.939764000	-0.312032000
		C	-6.425333000	1.538474000	0.556630000
		H	-5.953670000	1.907997000	1.472067000
		H	-7.483838000	1.382638000	0.748547000
		H	-6.324404000	2.294128000	-0.226282000
		C	-3.152404000	-1.916505000	0.252531000
		H	-2.164761000	-1.509739000	0.035965000
		H	-3.105436000	-2.995453000	0.087515000
		H	-3.364083000	-1.748084000	1.310350000
		C	-3.939242000	-1.507906000	-2.143826000
		H	-2.983362000	-1.059710000	-2.414856000
		H	-4.718359000	-1.074775000	-2.775652000
		H	-3.880512000	-2.576949000	-2.361389000
		C	-4.532869000	0.165380000	-0.301199000
		O	0.105320000	0.797702000	-2.020704000
		O	-0.477446000	5.537798000	0.553737000
		C	-3.671749000	1.249143000	-0.359430000
		H	-4.049260000	2.202149000	-0.006975000
		C	-2.343421000	1.176935000	-0.794748000
		H	-1.979130000	0.237371000	-1.187861000
		C	-1.522384000	3.456362000	-0.187031000
		H	-2.515277000	3.789661000	0.086054000
		C	-0.430430000	4.267871000	0.043816000
		C	0.873731000	3.768238000	-0.165524000
		H	1.700789000	4.386685000	0.170001000
		C	1.118434000	2.520422000	-0.717009000
		C	-0.029030000	1.740397000	-1.238942000
		C	-1.358612000	2.161532000	-0.744857000
		C	-1.745582000	6.078616000	0.889242000
		H	-2.400491000	6.135214000	0.011955000
		H	-1.553875000	7.083797000	1.261037000
		H	-2.235403000	5.489873000	1.673405000
		C	2.435391000	1.975014000	-0.653093000
		H	3.166694000	2.613641000	-0.169346000
		C	2.789099000	0.702120000	-1.027648000
		H	2.025950000	0.115299000	-1.517088000
		N	4.189507000	-1.230600000	-1.020614000
		C	3.998877000	0.059100000	-0.708754000
		C	5.228868000	0.592156000	0.032635000
		C	7.397192000	-0.827929000	0.540035000
		H	7.932493000	-0.021335000	1.028789000
		C	7.987497000	-2.090511000	0.418754000
		H	8.983001000	-2.259040000	0.812082000
		C	7.301071000	-3.137246000	-0.197705000
		H	7.767535000	-4.112100000	-0.277474000
		C	6.015689000	-2.953731000	-0.710977000
		H	5.490590000	-3.775927000	-1.178606000
		C	5.451916000	-1.689820000	-0.583673000
		C	6.122290000	-0.634244000	0.034111000
		C	3.179590000	-2.088948000	-1.646271000
		H	3.587965000	-3.089766000	-1.752434000
		H	2.925202000	-1.702486000	-2.634794000
		H	2.287098000	-2.128643000	-1.017099000
		C	4.864205000	0.982038000	1.489106000
		H	4.265611000	1.893503000	1.516896000
		H	5.782941000	1.159177000	2.053588000
		H	4.290171000	0.188900000	1.969985000
		C	5.899847000	1.762453000	-0.721707000
		H	5.249837000	2.637430000	-0.764831000

		H	6.159406000	1.478322000	-1.743978000
		H	6.818839000	2.049627000	-0.205142000
		Cl	0.946441000	-1.346484000	1.573311000
		O	0.443839000	-2.030744000	2.791755000
		O	0.435934000	-2.046829000	0.339373000
		O	2.453403000	-1.382268000	1.541402000
		O	0.488717000	0.078838000	1.549616000
g.1a′	**1a′**	N	2.145169000	-2.370102000	-1.189351000
		C	2.156803000	-2.475874000	1.185359000
		C	-0.003330000	-3.996712000	1.196704000
		H	-0.059153000	-4.074721000	2.277519000
		C	-0.922274000	-4.692715000	0.395386000
		H	-1.684227000	-5.308983000	0.857928000
		C	-0.839539000	-4.611060000	-0.992843000
		H	-1.542821000	-5.163019000	-1.606522000
		C	0.145825000	-3.834887000	-1.617454000
		H	0.202141000	-3.785998000	-2.698014000
		C	1.053882000	-3.157590000	-0.806814000
		C	0.978453000	-3.231707000	0.591764000
		C	2.306385000	-1.892734000	-2.552691000
		H	1.498127000	-1.214716000	-2.856102000
		H	2.329181000	-2.740855000	-3.239494000
		H	3.256614000	-1.366278000	-2.640530000
		C	1.828711000	-1.632878000	2.422884000
		H	2.695390000	-1.042255000	2.732636000
		H	1.570071000	-2.290754000	3.256085000
		H	0.992635000	-0.956029000	2.250645000
		C	3.259615000	-3.500400000	1.546329000
		H	4.143724000	-3.005641000	1.956244000
		H	3.557016000	-4.098784000	0.682624000
		H	2.875549000	-4.183489000	2.306326000
		C	2.600852000	-1.602291000	-0.062311000
		O	1.767382000	-0.342052000	-0.027214000
		O	3.699946000	4.839762000	-0.020011000
		C	4.058566000	-1.270835000	-0.132082000
		H	4.725437000	-2.119350000	-0.208204000
		C	4.537664000	-0.024011000	-0.115004000
		H	5.607925000	0.146741000	-0.164260000
		C	4.164180000	2.438479000	-0.052441000
		H	5.238200000	2.573104000	-0.068308000
		C	3.302873000	3.541102000	-0.031512000
		C	1.934201000	3.314083000	-0.026314000
		H	1.275621000	4.174510000	-0.015194000
		C	1.381761000	2.012393000	-0.034010000
		C	2.276856000	0.903987000	-0.038855000
		C	3.661459000	1.133394000	-0.057538000
		C	5.096202000	5.134511000	-0.025487000
		H	5.591292000	4.726947000	0.861712000
		H	5.166982000	6.219796000	-0.010406000
		H	5.578826000	4.752909000	-0.930939000
		C	-0.053485000	1.935540000	-0.033276000
		H	-0.520513000	2.912193000	-0.024584000
		C	-0.876723000	0.840121000	-0.047162000
		H	-0.424488000	-0.139267000	-0.053427000
		N	-3.060363000	-0.176919000	-0.091535000
		C	-2.294399000	0.917667000	-0.039999000
		C	-3.197186000	2.160494000	0.043569000
		C	-5.838315000	2.089958000	0.138085000
		H	-5.972232000	3.164105000	0.195972000
		C	-6.951488000	1.243658000	0.142730000
		H	-7.946168000	1.668127000	0.204045000

		C	-6.797534000	-0.142467000	0.073167000
		H	-7.672656000	-0.780609000	0.083164000
		C	-5.530628000	-0.722563000	-0.007318000
		H	-5.419595000	-1.797986000	-0.053381000
		C	-4.442524000	0.141592000	-0.014886000
		C	-4.574703000	1.524604000	0.061037000
		C	-2.598948000	-1.564026000	-0.184382000
		H	-3.328825000	-2.134851000	-0.754134000
		H	-2.497675000	-1.999524000	0.811004000
		H	-1.644610000	-1.619570000	-0.699442000
		C	-3.045443000	3.061833000	-1.208249000
		H	-2.063822000	3.533236000	-1.259443000
		H	-3.796710000	3.853031000	-1.171175000
		H	-3.201457000	2.491960000	-2.126369000
		C	-2.962858000	2.955155000	1.352175000
		H	-1.977907000	3.421455000	1.379189000
		H	-3.061990000	2.311224000	2.228271000
		H	-3.711618000	3.745866000	1.429194000
g.1b′	**1b′**	N	-3.142942000	-1.131551000	0.897773000
		C	-3.654234000	-2.300621000	-1.066724000
		C	-2.601069000	-4.537075000	-0.121580000
		H	-2.817762000	-5.137927000	-0.997704000
		C	-1.960690000	-5.110697000	0.982699000
		H	-1.681768000	-6.157292000	0.956441000
		C	-1.682458000	-4.351712000	2.120707000
		H	-1.189875000	-4.814661000	2.967445000
		C	-2.035014000	-3.001307000	2.189192000
		H	-1.815378000	-2.416501000	3.073365000
		C	-2.668173000	-2.457697000	1.079685000
		C	-2.951581000	-3.196917000	-0.067237000
		C	-3.126384000	-0.146336000	1.970916000
		H	-2.147654000	0.329828000	2.040231000
		H	-3.360174000	-0.649691000	2.909184000
		H	-3.880714000	0.610246000	1.769548000
		C	-2.871190000	-2.166523000	-2.392183000
		H	-3.387922000	-1.487994000	-3.074258000
		H	-2.793857000	-3.143993000	-2.873805000
		H	-1.869871000	-1.773371000	-2.214315000
		C	-5.099515000	-2.787866000	-1.336630000
		H	-5.619245000	-2.115469000	-2.022412000
		H	-5.677098000	-2.864757000	-0.413190000
		H	-5.066893000	-3.775904000	-1.800373000
		C	-3.657802000	-0.965746000	-0.318355000
		O	-1.261869000	0.332499000	-0.468612000
		O	-1.719938000	5.749300000	0.405525000
		C	-4.234288000	0.216611000	-0.845936000
		H	-5.094288000	0.021361000	-1.481200000
		C	-3.893795000	1.544822000	-0.724132000
		H	-4.662275000	2.219256000	-1.097681000
		C	-2.792961000	3.617279000	-0.134899000
		H	-3.772024000	4.073540000	-0.219500000
		C	-1.686282000	4.407276000	0.168510000
		C	-0.431876000	3.809291000	0.226273000
		H	0.419209000	4.446305000	0.444680000
		C	-0.233462000	2.437738000	-0.004262000
		C	-1.390591000	1.559659000	-0.271070000
		C	-2.698957000	2.223440000	-0.324835000
		C	-2.967191000	6.431535000	0.317451000
		H	-3.392736000	6.356112000	-0.688891000
		H	-2.749198000	7.474433000	0.537539000
		H	-3.683605000	6.049558000	1.052644000

		C	1.105411000	1.964271000	0.027214000
		H	1.838442000	2.736521000	0.233130000
		C	1.559114000	0.675320000	-0.186972000
		H	0.806557000	-0.071177000	-0.394038000
		N	3.258352000	-0.997222000	-0.409413000
		C	2.906398000	0.280764000	-0.165482000
		C	4.173903000	1.103931000	0.110057000
		C	6.628196000	0.126668000	0.119894000
		H	7.110282000	1.067896000	0.358942000
		C	7.396457000	-1.028784000	-0.056328000
		H	8.473473000	-0.978542000	0.047340000
		C	6.788409000	-2.246116000	-0.364753000
		H	7.397473000	-3.131970000	-0.498121000
		C	5.402588000	-2.344668000	-0.505791000
		H	4.946025000	-3.296398000	-0.744646000
		C	4.661206000	-1.183001000	-0.326364000
		C	5.251667000	0.041174000	-0.017217000
		C	2.313789000	-2.066414000	-0.724123000
		H	2.864033000	-2.980962000	-0.924671000
		H	1.729668000	-1.804568000	-1.607988000
		H	1.636320000	-2.235705000	0.115085000
		C	4.170954000	1.699184000	1.538877000
		H	3.393405000	2.453653000	1.662942000
		H	5.135099000	2.172692000	1.735549000
		H	4.017794000	0.921323000	2.289638000
		C	4.380797000	2.204430000	-0.959943000
		H	3.610882000	2.974634000	-0.905379000
		H	4.372423000	1.781855000	-1.966587000
		H	5.349571000	2.683188000	-0.802722000
g.1c′	**1c′**	N	-4.300783000	-1.894888000	0.000013000
		C	-5.475166000	0.142439000	-0.000009000
		C	-7.803952000	-1.104427000	-0.000020000
		H	-8.401513000	-0.199683000	-0.000032000
		C	-8.428619000	-2.356076000	-0.000015000
		H	-9.510070000	-2.416966000	-0.000024000
		C	-7.670493000	-3.527184000	0.000000000
		H	-8.168513000	-4.489246000	0.000003000
		C	-6.274603000	-3.483007000	0.000010000
		H	-5.701108000	-4.400843000	0.000021000
		C	-5.677112000	-2.228128000	0.000005000
		C	-6.419275000	-1.047921000	-0.000009000
		C	-3.223664000	-2.880272000	0.000028000
		H	-2.601512000	-2.761354000	-0.889271000
		H	-3.652235000	-3.878211000	0.000039000
		H	-2.601518000	-2.761333000	0.889328000
		C	-5.682246000	0.989798000	-1.278793000
		H	-5.003191000	1.842405000	-1.315314000
		H	-6.705492000	1.370957000	-1.299400000
		H	-5.527115000	0.390085000	-2.177836000
		C	-5.682261000	0.989802000	1.278773000
		H	-5.003204000	1.842407000	1.315300000
		H	-5.527141000	0.390089000	2.177818000
		H	-6.705506000	1.370962000	1.299366000
		C	-4.107283000	-0.558049000	0.000004000
		O	0.035876000	-0.064819000	0.000007000
		O	0.092983000	5.437447000	0.000005000
		C	-2.815553000	-0.016873000	0.000005000
		H	-1.974832000	-0.694330000	0.000009000
		C	-2.516477000	1.337248000	0.000002000
		H	-3.343438000	2.039251000	-0.000001000
		C	-1.204942000	3.364721000	0.000003000

		H	-2.150990000	3.893020000	0.000001000
		C	-0.014475000	4.078733000	0.000004000
		C	1.192668000	3.378050000	0.000004000
		H	2.107537000	3.962211000	0.000004000
		C	1.263247000	1.979276000	0.000004000
		C	0.017842000	1.178997000	0.000005000
		C	-1.241154000	1.950683000	0.000003000
		C	-1.097573000	6.218519000	-0.000004000
		H	-1.698085000	6.028790000	-0.896186000
		H	-0.770460000	7.256109000	-0.000006000
		H	-1.698093000	6.028797000	0.896174000
		C	2.559349000	1.395578000	0.000003000
		H	3.366590000	2.119729000	0.000003000
		C	2.886190000	0.052991000	0.000003000
		H	2.060820000	-0.643489000	0.000004000
		N	4.417145000	-1.787305000	-0.000001000
		C	4.194347000	-0.458800000	0.000000000
		C	5.543815000	0.274624000	0.000000000
		C	7.901520000	-0.917001000	-0.000007000
		H	8.478296000	0.001044000	-0.000007000
		C	8.553954000	-2.154182000	-0.000010000
		H	9.636518000	-2.190350000	-0.000013000
		C	7.823354000	-3.342947000	-0.000010000
		H	8.343726000	-4.293042000	-0.000013000
		C	6.427027000	-3.331119000	-0.000007000
		H	5.874682000	-4.261797000	-0.000008000
		C	5.802097000	-2.089857000	-0.000004000
		C	6.515755000	-0.892553000	-0.000004000
		C	3.363176000	-2.799508000	0.000001000
		H	3.816484000	-3.786309000	0.000009000
		H	2.739197000	-2.695161000	-0.889475000
		H	2.739191000	-2.695151000	0.889472000
		C	5.729406000	1.127027000	1.279205000
		H	5.031617000	1.964266000	1.314354000
		H	6.743608000	1.531307000	1.299880000
		H	5.587640000	0.524418000	2.178530000
		C	5.729407000	1.127037000	-1.279197000
		H	5.031621000	1.964279000	-1.314339000
		H	5.587637000	0.524435000	-2.178528000
		H	6.743610000	1.531313000	-1.299871000
g.1d′	**1d′**	N	-5.960427000	0.359047000	0.000016000
		C	-4.587411000	-1.553907000	-0.000004000
		C	-6.684704000	-3.158660000	-0.000016000
		H	-6.106380000	-4.075800000	-0.000026000
		C	-8.082483000	-3.212127000	-0.000014000
		H	-8.583795000	-4.172309000	-0.000023000
		C	-8.836794000	-2.038688000	-0.000002000
		H	-9.918636000	-2.095354000	-0.000001000
		C	-8.220776000	-0.785213000	0.000009000
		H	-8.821192000	0.115314000	0.000018000
		C	-6.831207000	-0.758337000	0.000007000
		C	-6.061837000	-1.920607000	-0.000005000
		C	-6.418053000	1.743713000	0.000032000
		H	-6.061038000	2.264000000	0.891695000
		H	-7.503927000	1.762752000	0.000049000
		H	-6.061066000	2.264012000	-0.891637000
		C	-3.900440000	-2.094042000	1.278199000
		H	-2.840837000	-1.838614000	1.308427000
		H	-3.986764000	-3.182568000	1.300620000
		H	-4.377458000	-1.699736000	2.177843000
		C	-3.900441000	-2.094023000	-1.278216000

		H	-2.840838000	-1.838593000	-1.308441000
		H	-4.377461000	-1.699705000	-2.177853000
		H	-3.986764000	-3.182548000	-1.300653000
		C	-4.661053000	-0.018109000	0.000007000
		O	0.296029000	-0.401303000	0.000007000
		O	-0.192789000	5.067433000	-0.000017000
		C	-3.621035000	0.915565000	0.000008000
		H	-3.908078000	1.960358000	0.000012000
		C	-2.269001000	0.597722000	0.000004000
		H	-1.974564000	-0.443871000	0.000003000
		C	-1.286006000	2.881402000	-0.000005000
		H	-2.273993000	3.323036000	-0.000006000
		C	-0.170664000	3.704906000	-0.000010000
		C	1.108262000	3.132352000	-0.000008000
		H	1.954361000	3.812562000	-0.000011000
		C	1.328180000	1.753281000	-0.000003000
		C	0.167464000	0.832217000	0.000002000
		C	-1.166993000	1.474211000	0.000001000
		C	-1.451176000	5.731921000	-0.000011000
		H	-2.030764000	5.485427000	-0.896399000
		H	-1.224454000	6.795981000	-0.000015000
		H	-2.030754000	5.485430000	0.896384000
		C	2.677132000	1.299488000	-0.000001000
		H	3.413222000	2.096140000	-0.000005000
		C	3.117695000	-0.008402000	0.000003000
		H	2.352712000	-0.771283000	0.000004000
		N	4.791312000	-1.718238000	0.000000000
		C	4.464355000	-0.413051000	0.000004000
		C	5.749397000	0.426462000	0.000005000
		C	8.195207000	-0.572130000	0.000011000
		H	8.696941000	0.388944000	0.000017000
		C	8.943997000	-1.753426000	0.000007000
		H	10.026007000	-1.703176000	0.000009000
		C	8.310704000	-2.996912000	-0.000002000
		H	8.905370000	-3.902340000	-0.000005000
		C	6.918051000	-3.096786000	-0.000005000
		H	6.441626000	-4.068437000	-0.000011000
		C	6.196275000	-1.909201000	0.000001000
		C	6.811917000	-0.658490000	0.000008000
		C	3.820789000	-2.812544000	-0.000002000
		H	4.351819000	-3.759672000	0.000015000
		H	3.190420000	-2.758283000	-0.889164000
		H	3.190396000	-2.758266000	0.889141000
		C	5.863719000	1.291538000	1.279123000
		H	5.098404000	2.067596000	1.313487000
		H	6.840720000	1.778871000	1.299601000
		H	5.772399000	0.679578000	2.178649000
		C	5.863718000	1.291521000	-1.279128000
		H	5.098399000	2.067574000	-1.313504000
		H	5.772402000	0.679545000	-2.178643000
		H	6.840718000	1.778857000	-1.299611000

Compound 2

Key	Structure	Geometry			
g.2a	**2a**	N	5.259025000	0.388367000	1.133443000
		C	5.471378000	0.303013000	-1.233936000
		C	7.526472000	-1.348864000	-1.060860000
		H	7.661254000	-1.444784000	-2.133116000
		C	8.392194000	-2.019139000	-0.181345000
		H	9.192571000	-2.634695000	-0.575243000
		C	8.219321000	-1.896605000	1.196116000

		H	8.888075000	-2.420329000	1.870458000
		C	7.186670000	-1.115232000	1.732224000
		H	7.056641000	-1.038835000	2.804738000
		C	6.338832000	-0.456122000	0.845045000
		C	6.504579000	-0.572805000	-0.542620000
		C	4.661949000	0.422779000	2.460591000
		H	3.876284000	1.177730000	2.481248000
		H	5.417912000	0.704239000	3.195708000
		H	4.233231000	-0.545132000	2.748805000
		C	4.830482000	-0.323373000	-2.477806000
		H	4.427864000	-1.314698000	-2.273433000
		H	5.579108000	-0.412436000	-3.268953000
		H	4.024053000	0.310256000	-2.858068000
		C	6.137053000	1.644220000	-1.622871000
		H	6.564133000	2.152611000	-0.755569000
		H	5.422732000	2.315559000	-2.106229000
		H	6.945454000	1.446910000	-2.330036000
		O	3.530691000	-0.676748000	-0.074822000
		O	2.230224000	-2.940798000	0.038638000
		N	-5.137261000	-2.448343000	-0.025162000
		C	4.440644000	0.517293000	-0.049109000
		C	3.656573000	1.793779000	-0.084507000
		H	4.243113000	2.702642000	-0.061495000
		C	2.320778000	1.843029000	-0.119632000
		H	1.800835000	2.794662000	-0.139253000
		C	0.089799000	-1.785718000	-0.016093000
		H	-0.459295000	-2.715298000	0.017597000
		C	-0.612034000	-0.552928000	-0.067041000
		C	0.124029000	0.642553000	-0.109924000
		H	-0.396226000	1.591826000	-0.145138000
		C	1.516407000	0.631667000	-0.106333000
		C	2.198327000	-0.593569000	-0.062749000
		C	-4.669720000	-3.837218000	-0.013798000
		H	-4.164389000	-4.056885000	0.927573000
		H	-3.990116000	-4.007585000	-0.848206000
		H	-5.522735000	-4.499145000	-0.121142000
		C	1.565855000	-4.207076000	0.092942000
		H	2.357550000	-4.952141000	0.126361000
		H	0.950443000	-4.365936000	-0.796982000
		H	0.948068000	-4.288030000	0.991713000
		C	-4.343781000	-1.370889000	-0.044942000
		C	-5.205054000	-0.102516000	-0.064568000
		C	-7.845155000	-0.087792000	-0.025793000
		H	-7.940540000	0.991681000	-0.044932000
		C	-8.987624000	-0.894796000	0.008230000
		H	-9.968600000	-0.434935000	0.014983000
		C	-8.877094000	-2.286924000	0.035409000
		H	-9.771934000	-2.896964000	0.063937000
		C	-7.628032000	-2.911862000	0.027729000
		H	-7.556548000	-3.990957000	0.052839000
		C	-6.509430000	-2.087759000	-0.008749000
		C	-6.599935000	-0.697649000	-0.032974000
		C	1.471590000	-1.817500000	-0.009679000
		C	-4.962112000	0.774460000	1.188699000
		H	-5.069400000	0.188769000	2.103908000
		H	-5.700981000	1.578074000	1.208206000
		H	-3.973391000	1.231465000	1.173510000
		C	-4.993364000	0.704381000	-1.370429000
		H	-5.136208000	0.072464000	-2.249296000
		H	-3.999055000	1.147514000	-1.412238000
		H	-5.723508000	1.515122000	-1.409342000
		C	-2.045316000	-0.455246000	-0.073195000

		H	-2.416930000	0.561936000	-0.106487000
		C	-2.935794000	-1.497519000	-0.041780000
		H	-2.548338000	-2.507254000	-0.008467000
		Cl	-1.853590000	4.313736000	0.151656000
		O	-0.412673000	4.239809000	-0.254973000
		O	-2.535303000	3.028128000	-0.216494000
		O	-2.518568000	5.450976000	-0.557512000
		O	-1.947290000	4.521190000	1.631212000
g.2b	**2b**	N	4.735792000	-0.121612000	0.982586000
		C	6.107417000	0.808134000	-0.668847000
		C	8.170521000	-0.676964000	0.068742000
		H	8.859392000	-0.283516000	-0.669845000
		C	8.591944000	-1.658955000	0.972955000
		H	9.610518000	-2.025798000	0.927667000
		C	7.715900000	-2.174598000	1.931093000
		H	8.060653000	-2.936935000	2.619431000
		C	6.395485000	-1.724909000	2.015913000
		H	5.716811000	-2.130889000	2.754687000
		C	6.005153000	-0.751511000	1.106588000
		C	6.860750000	-0.226718000	0.140401000
		C	3.661857000	-0.352431000	1.943769000
		H	2.960972000	0.476361000	1.899323000
		H	4.096830000	-0.408498000	2.940867000
		H	3.143391000	-1.284332000	1.717545000
		C	6.041678000	0.449121000	-2.170387000
		H	5.589073000	-0.531834000	-2.317943000
		H	7.051346000	0.440851000	-2.586532000
		H	5.451162000	1.190110000	-2.713282000
		C	6.710595000	2.222335000	-0.475764000
		H	6.736640000	2.505257000	0.578349000
		H	6.137884000	2.969753000	-1.028304000
		H	7.732409000	2.229456000	-0.859946000
		O	3.272288000	-1.432511000	-1.019573000
		O	1.698434000	-3.556698000	-1.029757000
		N	-5.483654000	-2.163680000	-0.004616000
		C	4.717777000	0.725101000	-0.036102000
		C	3.625868000	1.546670000	-0.443148000
		H	3.936920000	2.542781000	-0.745585000
		C	2.283310000	1.299633000	-0.541196000
		H	1.685709000	2.189713000	-0.726262000
		C	-0.234790000	-2.170568000	-0.614935000
		H	-0.905207000	-3.018452000	-0.628650000
		C	-0.773657000	-0.852809000	-0.412184000
		C	0.116808000	0.233570000	-0.398279000
		H	-0.293825000	1.227949000	-0.262915000
		C	1.499418000	0.090115000	-0.534108000
		C	2.064061000	-1.234900000	-0.793885000
		C	-5.211653000	-3.589580000	-0.171142000
		H	-4.555106000	-3.945017000	0.624803000
		H	-4.743753000	-3.773920000	-1.139577000
		H	-6.145874000	-4.140238000	-0.125038000
		C	0.874682000	-4.722367000	-1.068378000
		H	1.547972000	-5.556443000	-1.255282000
		H	0.138326000	-4.657519000	-1.875249000
		H	0.360499000	-4.873283000	-0.114214000
		C	-4.540066000	-1.197567000	-0.021666000
		C	-5.215367000	0.168107000	0.177505000
		C	-7.809516000	0.523185000	0.516858000
		H	-7.748835000	1.601462000	0.611812000
		C	-9.049714000	-0.121106000	0.601595000
		H	-9.948481000	0.462441000	0.761781000

		C	-9.136964000	-1.509205000	0.481545000
		H	-10.103140000	-1.995212000	0.549096000
		C	-7.996200000	-2.289984000	0.275423000
		H	-8.079571000	-3.364985000	0.185505000
		C	-6.776480000	-1.627107000	0.194884000
		C	-6.671623000	-0.241266000	0.311662000
		C	1.101930000	-2.357165000	-0.808902000
		C	-4.731592000	0.867651000	1.470725000
		H	-4.840050000	0.210233000	2.335825000
		H	-5.336020000	1.761080000	1.641773000
		H	-3.690016000	1.179112000	1.394967000
		C	-5.026059000	1.081492000	-1.058527000
		H	-5.342813000	0.574267000	-1.972207000
		H	-3.988413000	1.394514000	-1.172128000
		H	-5.635353000	1.979687000	-0.937160000
		C	-2.150239000	-0.578330000	-0.232438000
		H	-2.381967000	0.472797000	-0.110388000
		C	-3.186017000	-1.500840000	-0.201176000
		H	-2.940222000	-2.547872000	-0.322561000
		Cl	-1.242736000	4.231290000	0.005042000
		O	0.024830000	4.004437000	-0.763057000
		O	-2.096023000	3.000195000	-0.078165000
		O	-1.983172000	5.392461000	-0.580240000
		O	-0.914809000	4.516446000	1.437863000
g.2c	**2c**	N	6.091932000	1.089921000	0.005883000
		C	4.992719000	-0.982078000	-0.102835000
		C	7.283898000	-2.294357000	-0.156948000
		H	6.834189000	-3.279432000	-0.206247000
		C	8.676643000	-2.156950000	-0.146357000
		H	9.303212000	-3.039937000	-0.187436000
		C	9.266488000	-0.892650000	-0.084432000
		H	10.346226000	-0.802663000	-0.078427000
		C	8.487219000	0.265679000	-0.030275000
		H	8.957709000	1.238817000	0.015272000
		C	7.106660000	0.102299000	-0.040501000
		C	6.500706000	-1.151473000	-0.104240000
		C	6.361860000	2.526498000	0.081254000
		H	5.869793000	2.953075000	0.955560000
		H	6.002467000	3.024781000	-0.820192000
		H	7.431786000	2.684300000	0.170151000
		C	4.373957000	-1.662003000	1.143632000
		H	4.777530000	-1.233792000	2.063549000
		H	4.616747000	-2.726561000	1.126236000
		H	3.288885000	-1.567744000	1.153845000
		C	4.386151000	-1.542445000	-1.412719000
		H	4.809777000	-1.041433000	-2.285640000
		H	3.302924000	-1.429505000	-1.432840000
		H	4.614148000	-2.607881000	-1.484925000
		O	2.258580000	3.838973000	0.052965000
		O	-0.028825000	5.154158000	0.086240000
		N	-6.110279000	1.071562000	0.000759000
		C	4.865081000	0.544680000	-0.032348000
		C	3.714113000	1.357202000	-0.010803000
		H	3.855643000	2.426543000	0.025012000
		C	2.413336000	0.899363000	-0.033047000
		H	2.232609000	-0.169548000	-0.066978000
		C	-1.262185000	3.081039000	0.026786000
		H	-2.212676000	3.595194000	0.041509000
		C	-1.244872000	1.641091000	-0.016035000
		C	-0.003623000	0.993676000	-0.037173000
		H	0.016035000	-0.089885000	-0.072416000

		C	1.219347000	1.681898000	-0.013835000
		C	1.223239000	3.151058000	0.030671000
		C	-6.372477000	2.507961000	0.072178000
		H	-6.004409000	3.005740000	-0.826600000
		H	-5.888246000	2.934696000	0.951469000
		H	-7.442247000	2.672807000	0.151245000
		C	-1.247261000	5.898711000	0.105216000
		H	-0.955070000	6.946337000	0.134889000
		H	-1.841595000	5.658425000	0.992051000
		H	-1.838770000	5.708367000	-0.795541000
		C	-4.881126000	0.517665000	-0.034462000
		C	-5.018980000	-1.009693000	-0.099875000
		C	-7.317444000	-2.307931000	-0.151728000
		H	-6.871933000	-3.295202000	-0.197053000
		C	-8.710016000	-2.164966000	-0.142885000
		H	-9.340532000	-3.045260000	-0.181410000
		C	-9.292938000	-0.897583000	-0.085886000
		H	-10.372265000	-0.801725000	-0.081052000
		C	-8.507702000	0.257306000	-0.035093000
		H	-8.974133000	1.232654000	0.006743000
		C	-7.127404000	0.088956000	-0.043470000
		C	-6.528697000	-1.169013000	-0.102314000
		C	-0.105519000	3.800072000	0.047896000
		C	-4.415549000	-1.579781000	-1.406495000
		H	-4.835991000	-1.079948000	-2.281682000
		H	-4.649586000	-2.644266000	-1.474743000
		H	-3.331546000	-1.473753000	-1.427513000
		C	-4.407063000	-1.689919000	1.149242000
		H	-4.811124000	-1.257427000	2.066990000
		H	-3.321485000	-1.601134000	1.162764000
		H	-4.654582000	-2.753531000	1.134320000
		C	-2.418705000	0.843361000	-0.035385000
		H	-2.235734000	-0.224286000	-0.068275000
		C	-3.723510000	1.307976000	-0.013919000
		H	-3.879936000	2.378063000	0.021591000
		Cl	-0.004536000	-3.209534000	0.224211000
		O	1.199271000	-2.423442000	-0.203066000
		O	-1.244022000	-2.469334000	-0.182042000
		O	0.011484000	-3.380572000	1.711137000
		O	0.014718000	-4.551919000	-0.435885000
g.2d	**2d**	N	-4.766408000	-1.322868000	-0.309323000
		C	-5.641382000	0.850710000	-0.135956000
		C	-8.122880000	-0.042746000	-0.319610000
		H	-8.591462000	0.931388000	-0.238983000
		C	-8.908718000	-1.191751000	-0.468379000
		H	-9.987951000	-1.101641000	-0.502208000
		C	-8.317348000	-2.452747000	-0.575792000
		H	-8.941499000	-3.330606000	-0.693157000
		C	-6.928943000	-2.603639000	-0.534897000
		H	-6.474831000	-3.581931000	-0.621699000
		C	-6.173704000	-1.446610000	-0.383373000
		C	-6.743924000	-0.181473000	-0.279304000
		C	-3.908226000	-2.503550000	-0.402189000
		H	-2.888253000	-2.268462000	-0.122385000
		H	-3.925689000	-2.888025000	-1.424333000
		H	-4.288791000	-3.267000000	0.276061000
		C	-5.776135000	1.587799000	1.219350000
		H	-5.726891000	0.885145000	2.053611000
		H	-6.743016000	2.093943000	1.255328000
		H	-4.996638000	2.337736000	1.353231000
		C	-5.687466000	1.838538000	-1.328014000

		H	-5.567909000	1.312493000	-2.277289000
		H	-4.912070000	2.600851000	-1.255837000
		H	-6.656385000	2.341854000	-1.336062000
		O	-2.127973000	4.383725000	0.260286000
		O	0.280470000	5.490034000	0.362547000
		N	5.944215000	0.903156000	-0.234097000
		C	-4.385871000	-0.041483000	-0.177847000
		C	-3.032687000	0.349367000	-0.102899000
		H	-2.287150000	-0.434114000	-0.154203000
		C	-2.618056000	1.655562000	0.024673000
		H	-3.360514000	2.439938000	0.080942000
		C	1.307267000	3.313675000	0.175912000
		H	2.303478000	3.730940000	0.211385000
		C	1.152032000	1.884269000	0.064483000
		C	-0.142698000	1.348231000	0.030744000
		H	-0.246670000	0.271327000	-0.047360000
		C	-1.284868000	2.155021000	0.086316000
		C	-1.152009000	3.617457000	0.202496000
		C	6.330995000	2.312979000	-0.211629000
		H	6.011243000	2.777490000	0.722440000
		H	5.882181000	2.839947000	-1.054914000
		H	7.410957000	2.389145000	-0.287590000
		C	1.564552000	6.113559000	0.417132000
		H	1.373046000	7.180626000	0.508470000
		H	2.134725000	5.919864000	-0.496470000
		H	2.133029000	5.766950000	1.285441000
		C	4.673480000	0.456680000	-0.171868000
		C	4.675074000	-1.077079000	-0.223090000
		C	6.844667000	-2.569888000	-0.407854000
		H	6.313919000	-3.515189000	-0.406326000
		C	8.241843000	-2.547761000	-0.492169000
		H	8.790805000	-3.479635000	-0.556902000
		C	8.933692000	-1.335025000	-0.492925000
		H	10.015282000	-1.332912000	-0.558396000
		C	8.255524000	-0.116055000	-0.409845000
		H	8.805764000	0.815420000	-0.410514000
		C	6.868340000	-0.164223000	-0.327413000
		C	6.161757000	-1.366403000	-0.325858000
		C	0.227988000	4.140365000	0.247226000
		C	4.099371000	-1.686276000	1.078112000
		H	4.615258000	-1.289283000	1.955100000
		H	4.241257000	-2.768857000	1.060026000
		H	3.032454000	-1.491113000	1.184217000
		C	3.936810000	-1.609686000	-1.475149000
		H	4.338858000	-1.161998000	-2.386346000
		H	2.867266000	-1.404625000	-1.432019000
		H	4.069610000	-2.691585000	-1.537830000
		C	2.253039000	0.993733000	-0.026535000
		H	1.983289000	-0.054166000	-0.072625000
		C	3.592381000	1.343467000	-0.071309000
		H	3.843644000	2.395186000	-0.037130000
		Cl	0.005476000	-3.169874000	0.810102000
		O	-0.458819000	-2.068288000	-0.102336000
		O	0.675377000	-2.567713000	2.004168000
		O	0.973082000	-4.045142000	0.078607000
		O	-1.176071000	-3.979288000	1.244388000
g.2a′	**2a′**	N	-4.954225000	-0.702754000	1.248483000
		C	-5.218070000	-0.903595000	-1.106800000
		C	-7.148848000	0.900244000	-1.116036000
		H	-7.301904000	0.869640000	-2.189685000
		C	-7.945212000	1.735951000	-0.316447000

		H	-8.710296000	2.352473000	-0.773806000
		C	-7.749038000	1.775987000	1.062795000
		H	-8.364303000	2.426702000	1.674523000
		C	-6.760182000	0.997053000	1.678922000
		H	-6.610606000	1.047037000	2.750442000
		C	-5.980918000	0.173052000	0.870451000
		C	-6.170985000	0.124810000	-0.517898000
		C	-4.329428000	-0.609544000	2.560064000
		H	-3.600231000	-1.412043000	2.669004000
		H	-5.086258000	-0.735949000	3.336015000
		H	-3.825783000	0.353073000	2.713033000
		C	-4.566144000	-0.488532000	-2.430817000
		H	-4.092474000	0.489996000	-2.363003000
		H	-5.326335000	-0.449649000	-3.214903000
		H	-3.813934000	-1.220746000	-2.738103000
		C	-5.985249000	-2.231618000	-1.309670000
		H	-6.423571000	-2.594469000	-0.377327000
		H	-5.332870000	-3.008403000	-1.716649000
		H	-6.796456000	-2.066559000	-2.021744000
		O	-3.185282000	0.071438000	-0.117383000
		O	-1.737226000	2.239269000	-0.261153000
		N	5.581339000	1.270362000	-0.073578000
		C	-4.176860000	-1.039155000	0.080090000
		C	-3.483444000	-2.362032000	0.196784000
		H	-4.130066000	-3.220316000	0.321181000
		C	-2.154248000	-2.506102000	0.179838000
		H	-1.710165000	-3.490876000	0.275677000
		C	0.319787000	0.949560000	-0.126345000
		H	0.930231000	1.837492000	-0.200322000
		C	0.938214000	-0.322454000	-0.010197000
		C	0.123471000	-1.463023000	0.083066000
		H	0.579021000	-2.442628000	0.177504000
		C	-1.265346000	-1.361829000	0.059973000
		C	-1.863120000	-0.097597000	-0.063530000
		C	5.207063000	2.684975000	-0.162447000
		H	4.648046000	2.979752000	0.726122000
		H	4.604423000	2.856170000	-1.054312000
		H	6.107288000	3.286792000	-0.228549000
		C	-0.990013000	3.456128000	-0.362206000
		H	-1.730688000	4.248728000	-0.439782000
		H	-0.358700000	3.455319000	-1.255063000
		H	-0.375625000	3.614189000	0.528435000
		C	4.716904000	0.251874000	-0.016448000
		C	5.488956000	-1.069709000	0.077126000
		C	8.122487000	-1.262679000	0.111235000
		H	8.144770000	-2.344195000	0.178198000
		C	9.317089000	-0.535233000	0.077690000
		H	10.264595000	-1.058946000	0.119073000
		C	9.301674000	0.858864000	-0.007763000
		H	10.236135000	1.406419000	-0.031608000
		C	8.098158000	1.565030000	-0.063385000
		H	8.100327000	2.644704000	-0.128396000
		C	6.926038000	0.819113000	-0.030242000
		C	6.921730000	-0.571481000	0.056955000
		C	-1.056281000	1.072862000	-0.151516000
		C	5.197035000	-1.805934000	1.408618000
		H	5.371324000	-1.151506000	2.264806000
		H	5.863701000	-2.665989000	1.493978000
		H	4.170448000	-2.169279000	1.454228000
		C	5.216398000	-1.977248000	-1.147835000
		H	5.411145000	-1.444854000	-2.080757000
		H	4.187726000	-2.337540000	-1.163724000

		H	5.877853000	-2.844589000	-1.103861000
		C	2.362450000	-0.504389000	0.017687000
		H	2.675696000	-1.537516000	0.097952000
		C	3.320112000	0.473845000	-0.044405000
		H	3.002736000	1.505502000	-0.118476000
g.2b′	**2b′**	N	-4.530777000	-0.488369000	0.990294000
		C	-5.940086000	-1.313507000	-0.683841000
		C	-7.926678000	0.263457000	0.071820000
		H	-8.630773000	-0.079360000	-0.677484000
		C	-8.301191000	1.248557000	0.992942000
		H	-9.298935000	1.668960000	0.950036000
		C	-7.405072000	1.699198000	1.965301000
		H	-7.713707000	2.464980000	2.666778000
		C	-6.110573000	1.179526000	2.047827000
		H	-5.416318000	1.534654000	2.798143000
		C	-5.766623000	0.205016000	1.121238000
		C	-6.642635000	-0.255910000	0.141111000
		C	-3.446778000	-0.323971000	1.954327000
		H	-2.785011000	-1.183383000	1.895898000
		H	-3.878200000	-0.263706000	2.952643000
		H	-2.886739000	0.586978000	1.741972000
		C	-5.847921000	-0.932632000	-2.178618000
		H	-5.345980000	0.026690000	-2.306713000
		H	-6.853657000	-0.867677000	-2.599025000
		H	-5.292036000	-1.692978000	-2.731185000
		C	-6.616852000	-2.697841000	-0.518148000
		H	-6.657898000	-3.000241000	0.530099000
		H	-6.084612000	-3.462927000	-1.086750000
		H	-7.637522000	-2.642584000	-0.901407000
		O	-3.013398000	0.763407000	-1.009518000
		O	-1.344970000	2.814082000	-1.037343000
		N	5.765337000	1.128148000	-0.010965000
		C	-4.552171000	-1.314694000	-0.043219000
		C	-3.502414000	-2.188455000	-0.460387000
		H	-3.864236000	-3.164506000	-0.771200000
		C	-2.151539000	-2.005639000	-0.561424000
		H	-1.604483000	-2.921935000	-0.772240000
		C	0.523581000	1.344790000	-0.616335000
		H	1.230794000	2.162175000	-0.630373000
		C	1.004667000	0.005701000	-0.408940000
		C	0.066838000	-1.040519000	-0.398660000
		H	0.428534000	-2.054612000	-0.259436000
		C	-1.307029000	-0.837028000	-0.540290000
		C	-1.813678000	0.512941000	-0.793172000
		C	5.551558000	2.562976000	-0.189280000
		H	4.906604000	2.949671000	0.601432000
		H	5.095227000	2.758240000	-1.161048000
		H	6.506859000	3.076024000	-0.142980000
		C	-0.470628000	3.942508000	-1.080981000
		H	-1.106772000	4.804154000	-1.272439000
		H	0.262312000	3.841077000	-1.887051000
		H	0.048763000	4.075056000	-0.127034000
		C	4.783527000	0.202273000	-0.017645000
		C	5.401954000	-1.188089000	0.195364000
		C	7.980993000	-1.648051000	0.525693000
		H	7.876758000	-2.722077000	0.630235000
		C	9.246831000	-1.054447000	0.599171000
		H	10.121656000	-1.672948000	0.760462000
		C	9.390604000	0.327802000	0.466520000
		H	10.376260000	0.774034000	0.525614000
		C	8.282242000	1.153176000	0.258252000

		H	8.409466000	2.222925000	0.158372000
		C	7.036072000	0.540335000	0.188712000
		C	6.874811000	-0.838838000	0.318646000
		C	-0.803095000	1.590815000	-0.812379000
		C	4.897077000	-1.847887000	1.501299000
		H	5.049421000	-1.188190000	2.357859000
		H	5.454840000	-2.770255000	1.676249000
		H	3.837980000	-2.100400000	1.444597000
		C	5.170516000	-2.108722000	-1.027514000
		H	5.520102000	-1.634113000	-1.946521000
		H	4.117046000	-2.361649000	-1.149686000
		H	5.727056000	-3.037936000	-0.888837000
		C	2.369502000	-0.318996000	-0.223929000
		H	2.564471000	-1.375708000	-0.089567000
		C	3.442150000	0.559348000	-0.199695000
		H	3.239996000	1.614053000	-0.332420000
g.2c′	**2c′**	N	-6.073329000	0.489815000	0.000004000
		C	-4.999234000	-1.599132000	0.000001000
		C	-7.308283000	-2.883268000	-0.000002000
		H	-6.872441000	-3.876027000	-0.000003000
		C	-8.698360000	-2.728453000	-0.000002000
		H	-9.336187000	-3.603932000	-0.000004000
		C	-9.272053000	-1.456405000	-0.000001000
		H	-10.350422000	-1.353718000	-0.000002000
		C	-8.478766000	-0.307408000	0.000001000
		H	-8.938453000	0.672224000	0.000002000
		C	-7.100763000	-0.487089000	0.000002000
		C	-6.510404000	-1.750030000	0.000000000
		C	-6.320373000	1.932567000	0.000007000
		H	-5.883939000	2.390804000	-0.888929000
		H	-5.883914000	2.390804000	0.888931000
		H	-7.391503000	2.110201000	0.000022000
		C	-4.394738000	-2.227985000	-1.278886000
		H	-4.815738000	-1.774359000	-2.178262000
		H	-4.623245000	-3.295678000	-1.300067000
		H	-3.310712000	-2.112659000	-1.312793000
		C	-4.394738000	-2.227988000	1.278886000
		H	-4.815738000	-1.774364000	2.178262000
		H	-3.310712000	-2.112661000	1.312793000
		H	-4.623244000	-3.295681000	1.300064000
		O	-2.271626000	3.189587000	0.000004000
		O	-0.021411000	4.544788000	-0.000008000
		N	6.137412000	0.486603000	0.000003000
		C	-4.850795000	-0.071601000	0.000002000
		C	-3.694585000	0.727460000	0.000002000
		H	-3.819516000	1.800393000	0.000003000
		C	-2.393736000	0.265344000	0.000001000
		H	-2.221043000	-0.806097000	0.000000000
		C	1.255722000	2.502373000	-0.000006000
		H	2.200086000	3.028330000	-0.000011000
		C	1.259605000	1.058067000	-0.000004000
		C	0.025115000	0.388278000	-0.000002000
		H	0.029716000	-0.698355000	-0.000001000
		C	-1.206356000	1.048993000	-0.000001000
		C	-1.235763000	2.530401000	0.000000000
		C	6.412909000	1.918678000	0.000009000
		H	5.991805000	2.388712000	0.891680000
		H	5.991806000	2.388720000	-0.891658000
		H	7.487257000	2.077394000	0.000010000
		C	1.164173000	5.331728000	-0.000002000
		H	0.831680000	6.367412000	0.000003000

		H	1.764223000	5.140008000	-0.896181000
		H	1.764221000	5.139997000	0.896174000
		C	4.896323000	-0.054450000	0.000000000
		C	5.022099000	-1.587012000	-0.000002000
		C	7.308138000	-2.909291000	-0.000001000
		H	6.852956000	-3.893408000	-0.000003000
		C	8.701300000	-2.782453000	0.000001000
		H	9.322017000	-3.670079000	0.000000000
		C	9.297870000	-1.521607000	0.000003000
		H	10.377980000	-1.438400000	0.000005000
		C	8.525718000	-0.357704000	0.000004000
		H	9.005364000	0.612503000	0.000007000
		C	7.144220000	-0.509425000	0.000003000
		C	6.531660000	-1.761509000	0.000000000
		C	0.091193000	3.206169000	-0.000005000
		C	4.412041000	-2.209840000	1.278751000
		H	4.841848000	-1.763172000	2.177472000
		H	4.626752000	-3.280475000	1.298376000
		H	3.329565000	-2.081823000	1.317729000
		C	4.412045000	-2.209835000	-1.278761000
		H	4.841856000	-1.763164000	-2.177478000
		H	3.329570000	-2.081816000	-1.317742000
		H	4.626756000	-3.280470000	-1.298389000
		C	2.434909000	0.278914000	-0.000002000
		H	2.269090000	-0.791485000	-0.000002000
		C	3.748018000	0.740027000	0.000000000
		H	3.903317000	1.811292000	0.000002000
g.2d′	**2d′**	N	-4.659442000	-1.892166000	0.074607000
		C	-5.645206000	0.237770000	-0.044689000
		C	-8.075757000	-0.793874000	-0.093848000
		H	-8.588419000	0.159704000	-0.146417000
		C	-8.808376000	-1.986191000	-0.078832000
		H	-9.890476000	-1.951404000	-0.120012000
		C	-8.158095000	-3.220244000	-0.012455000
		H	-8.739447000	-4.134480000	-0.003151000
		C	-6.764458000	-3.300031000	0.042160000
		H	-6.273754000	-4.262896000	0.091587000
		C	-6.059825000	-2.101865000	0.027629000
		C	-6.691965000	-0.861354000	-0.041069000
		C	-3.680524000	-2.977665000	0.151993000
		H	-3.039546000	-2.840863000	1.023047000
		H	-3.071921000	-3.002012000	-0.753098000
		H	-4.204131000	-3.923019000	0.250294000
		C	-5.820194000	1.149899000	1.194566000
		H	-5.742126000	0.574402000	2.119064000
		H	-6.808971000	1.611909000	1.161614000
		H	-5.076094000	1.946195000	1.219261000
		C	-5.724093000	1.049778000	-1.361033000
		H	-5.588899000	0.402282000	-2.229752000
		H	-4.969255000	1.835553000	-1.395351000
		H	-6.706734000	1.519908000	-1.434049000
		O	-2.118630000	3.918814000	0.008829000
		O	0.296852000	5.014982000	0.011106000
		N	5.922950000	0.266839000	-0.009572000
		C	-4.351894000	-0.585646000	0.031790000
		C	-3.015350000	-0.144786000	0.048462000
		H	-2.256569000	-0.916133000	0.080932000
		C	-2.619711000	1.174401000	0.023871000
		H	-3.372015000	1.952162000	0.000173000
		C	1.312201000	2.826015000	0.024265000
		H	2.311362000	3.237606000	0.023778000

		C	1.147340000	1.393210000	0.031686000
		C	-0.149416000	0.868386000	0.036139000
		H	-0.260059000	-0.210176000	0.041297000
		C	-1.289640000	1.679957000	0.028162000
		C	-1.147868000	3.146103000	0.017188000
		C	6.361541000	1.662071000	-0.012376000
		H	5.992028000	2.173913000	0.877263000
		H	5.996382000	2.169911000	-0.906286000
		H	7.446191000	1.695712000	-0.009284000
		C	1.584577000	5.634584000	0.011171000
		H	1.398292000	6.706355000	0.005923000
		H	2.154023000	5.356134000	-0.880616000
		H	2.149975000	5.364229000	0.908008000
		C	4.636680000	-0.130390000	0.004360000
		C	4.581727000	-1.664910000	0.003380000
		C	6.700331000	-3.240257000	-0.024252000
		H	6.135265000	-4.165342000	-0.017572000
		C	8.099669000	-3.270387000	-0.042246000
		H	8.616061000	-4.222828000	-0.049846000
		C	8.835664000	-2.083844000	-0.050728000
		H	9.918390000	-2.122788000	-0.065011000
		C	8.200429000	-0.839346000	-0.041050000
		H	8.783951000	0.071608000	-0.047891000
		C	6.810286000	-0.835847000	-0.022969000
		C	6.059868000	-2.010985000	-0.015169000
		C	0.237291000	3.662006000	0.017875000
		C	3.919543000	-2.213921000	1.290606000
		H	4.406215000	-1.813822000	2.182276000
		H	4.015414000	-3.301481000	1.307121000
		H	2.858519000	-1.967630000	1.337358000
		C	3.887682000	-2.211185000	-1.268247000
		H	4.350947000	-1.807866000	-2.170864000
		H	2.825439000	-1.966320000	-1.287435000
		H	3.984308000	-3.298548000	-1.290618000
		C	2.237170000	0.483425000	0.028769000
		H	1.948902000	-0.560259000	0.036247000
		C	3.583708000	0.797647000	0.014771000
		H	3.866417000	1.842061000	0.008015000

Table S3 The overview of the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method: total electronic energy (Hartree), total electronic energy with zero point vibrational energy (Hartree), enthalpy (Hartree) under standard conditions (T = 298.15 K, P = 1.0 atm.), dipole moment (Debye), the number of negative eigenvalues of the Hessian.

Compound 1								
Key	**Struc-ture**	**Charge**	**E_{tot}**	**E_0**	**$H_{298K,1atm}$**	**μ**	**λ**	**Point group**
o.1a	**1a**	0	-2299,750449	-2299,132143	-2299,090906	11,28	0	C_1
o.1b	**1b**	0	-2299,748640	-2299,131270	-2299,089334	10,62	0	C_1
o.1c	**1c**	0	-2299,751982	-2299,135150	-2299,092770	6,28	0	C_1
o.1d	**1d**	0	-2299,745330	-2299,128926	-2299,086264	7,08	0	C_1
o.1a′	**1a′**	1	-1538,764027	-1538,162486	-1538,126534	3,42	0	C_1
o.1b′	**1b′**	1	-1538,721027	-1538,119086	-1538,082649	2,51	0	C_S
o.1c′	**1c′**	1	-1538,777018	-1538,175269	-1538,139065	3,54	0	C_1
o.1d′	**1d′**	1	-1538,720004	-1538,118258	-1538,081747	0,55	0	C_S
Compound 2								
Key	**Struc-ture**	**Charge**	**E_{tot}**	**E_0**	**$H_{298K,1atm}$**	**μ**	**λ**	**Point Group**
o.2a	**2a**	0	-2299,746083	-2299,127954	-2299,086434	17,07	0	C_1
o.2b	**2b**	0	-2299,743633	-2299,126421	-2299,084207	11,95	0	C_1
o.2c	**2c**	0	-2299,760025	-2299,142191	-2299,099608	9,04	0	C_S
o.2d	**2d**	0	-2299,762607	-2299,144975	-2299,102435	5,60	0	C_1
o.2a′	**2a′**	1	-1538,708403	-1538,105669	-1538,070318	12,61	0	C_1
o.2b′	**2b′**	1	-1538,710367	-1538,108208	-1538,072181	3,22	0	C_1
o.2c′	**2c′**	1	-1538,719340	-1538,117277	-1538,080822	3,39	0	C_S
o.2d′	**2d′**	1	-1538,714791	-1538,112908	-1538,076362	7,12	0	C_S

Table S4 The summary of NBO deletion analysis for the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method.

Compound 1			
Structure	**E(L) (a.u.)**	**E(full) (a.u.)**	**E(NL) (a.u.)**
1a	-2295,754432665	-2299,750449259	-3,996016594
1b	-2295,519255276	-2299,748640110	-4,229384834
1c	-2295,731881732	-2299,751981685	-4,020099953
1d	-2295,762728332	-2299,745329545	-3,982601213
1a′	-1535,586914465	-1538,710456271	-3,123541806
1b′	-1535,521788048	-1538,708640872	-3,186852824
1c′	-1535,515982702	-1538,721009424	-3,205026722
1d′	-1535,524406342	-1538,720006085	-3,195599743
Compound 2			
Structure	**E(L) (a.u.)**	**E(full) (a.u.)**	**E(NL) (a.u.)**
2a	-2295,738053764	-2299,740615589	-4,002561825
2b	-2295,714392261	-2299,737429971	-4,023037710
2c	-2295,706498603	-2299,756171304	-4,049672701
2d	-2295,723843818	-2299,756626312	-4,032782494
2a′	-1535,581986540	-1538,707459583	-3,125473043
2b′	-1535,552170867	-1538,709458458	-3,157287591
2c′	-1535,519386810	-1538,719344032	-3,199957222
2d′	-1535,546695887	-1538,713546025	-3,166850138

Table S5 ESP, Mulliken and APT charges with hydrogens summed into heavy atoms for structures of compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method.

Compound 1					
Atom	**Charge**	**Structure**			
		1a	**1b**	**1c**	**1d**
N(1)	ESP	-0,308451	-0,015195	0,059724	0,105443
	Mulliken	0,277259	0,493398	0,272572	0,182441
	APT	-0,815375	-0,201451	-1,056345	-1,494976
C(3)	ESP	0,048817	0,320556	0,443390	0,193124
	Mulliken	0,582104	0,113939	0,534843	0,405261
	APT	0,101889	0,000377	0,129980	0,148610
C(4)	ESP	-0,021150	-0,047391	-0,016943	-0,055788
	Mulliken	-0,019424	-0,249454	-0,175501	-0,037336
	APT	0,088520	0,030063	0,148236	0,131257
C(5)	ESP	-0,100550	-0,033704	-0,020412	0,002843
	Mulliken	-0,281870	-0,262320	-0,323232	-0,379519
	APT	-0,147142	-0,025667	-0,174936	-0,176700
C(6)	ESP	0,026005	0,024493	0,021877	0,005814
	Mulliken	-0,115859	-0,176362	-0,128654	-0,054164
	APT	0,067242	-0,002508	0,011065	0,029713
C(7)	ESP	-0,084527	0,019446	-0,078257	-0,084204
	Mulliken	-0,113665	0,118326	-0,229960	-0,122591
	APT	-0,085417	0,055561	-0,074766	-0,062250
C(8)	ESP	0,209775	0,095442	0,159084	0,070914
	Mulliken	0,012997	0,372110	0,689590	0,469797
	APT	0,404152	0,283514	0,678039	0,531151
C(9)	ESP	0,010613	0,010692	-0,098247	0,081274
	Mulliken	-0,200226	0,445803	0,537473	0,470489
	APT	-0,138142	-0,097110	-0,209113	-0,136154
C(CH_3-N(1))	ESP	0,101182	0,164976	0,143868	0,067248
	Mulliken	0,243571	0,093482	0,156359	0,209362
	APT	0,297381	0,241525	0,260041	0,355023
C(CH_3-C(3))	ESP	-0,076111	-0,062586	-0,133897	0,049749
	Mulliken	0,010037	-0,077570	-0,200221	-0,261549
	APT	-0,003397	0,019539	0,013243	0,040264
C(C′H_3-C(3))	ESP	-0,071324	-0,116303	-0,052750	-0,061891
	Mulliken	0,031856	-0,062589	-0,174009	-0,192414
	APT	0,001777	0,038377	-0,008172	0,028631
C(2,2′)	ESP	0,844533	0,374939	0,026945	0,051596
	Mulliken	-0,366158	0,067563	-0,125198	-0,072280
	APT	0,879896	0,413905	1,400898	1,520259
O(1′)	ESP	-0,414951	-0,540961	-0,603858	-0,534701
	Mulliken	0,228190	-0,185819	-0,222464	-0,218505
	APT	-0,858227	-0,359678	-0,291538	-0,373233
O(2′)	ESP	-0,360899	-0,381275	-0,376802	-0,368613
	Mulliken	-0,142140	-0,144766	-0,154556	-0,146179
	APT	-1,022292	-1,060889	-1,018051	-0,935509
C(3′)	ESP	-0,312901	-0,316073	-0,039653	-0,113498
	Mulliken	-0,061791	-0,286066	0,292208	-0,179681
	APT	-0,128214	-0,671237	-1,187345	-1,333912
C(4′)	ESP	0,105836	0,152356	0,099331	0,134760
	Mulliken	0,287574	0,254312	-0,329271	0,301738
	APT	0,163441	0,918778	1,198701	1,482055
C(5′)	ESP	-0,132706	-0,179354	-0,225925	-0,122728
	Mulliken	0,330940	0,455914	0,610834	0,415783
	APT	0,047149	0,398065	0,449069	0,228118

C(6′)	ESP	0,466637	0,511589	0,528598	0,446120
	Mulliken	-0,731025	-0,670537	-0,277975	-0,720263
	APT	0,399975	-0,153391	-0,466474	-0,478449
C(7′)	ESP	-0,237275	-0,250584	-0,252061	-0,192125
	Mulliken	-0,629793	-0,367328	-0,185901	-0,271359
	APT	0,082045	0,385375	0,610992	0,772329
C(8′)	ESP	0,037905	-0,003953	0,019921	0,064482
	Mulliken	0,600350	0,230835	0,370853	0,584697
	APT	-0,462303	-0,639690	-0,719465	-0,735820
C(9′)	ESP	0,257496	0,470781	0,517457	0,417345
	Mulliken	-0,208219	-0,824677	-1,517281	-1,271516
	APT	0,396277	0,189094	0,192753	0,320255
C(10′)	ESP	-0,057973	-0,126279	-0,034621	-0,081670
	Mulliken	0,325992	0,638724	0,420336	0,553016
	APT	-0,044266	-0,577611	-0,844337	-0,807289
C(11′)	ESP	0,200775	0,198402	0,195341	0,200158
	Mulliken	0,131374	0,119260	0,132415	0,124099
	APT	0,514325	0,518544	0,491260	0,456723
C(12′)	ESP	0,169914	0,193879	0,143330	0,101714
	Mulliken	-0,093320	-0,228094	-0,304634	-0,208005
	APT	0,805458	1,005734	1,160705	1,188471
C(13′)	ESP	0,015797	-0,269428	-0,152979	-0,110215
	Mulliken	-0,157176	-0,092867	0,168563	0,218655
	APT	-0,728853	-0,982227	-1,125261	-1,149575
N(1″)	ESP	0,016668	-0,350690	-0,199527	-0,143403
	Mulliken	0,563344	0,294482	0,303843	0,313963
	APT	-0,623258	-0,803157	-0,885070	-0,881504
C(2″)	ESP	0,203444	0,654659	0,359722	0,344362
	Mulliken	-0,019772	0,556587	0,376387	0,340053
	APT	0,999659	1,250247	1,382090	1,408503
C(3″)	ESP	0,058747	-0,213572	0,235850	0,175447
	Mulliken	0,257135	0,278151	0,236225	0,205189
	APT	0,053045	0,081843	0,088096	0,088306
C(4″)	ESP	-0,061545	-0,047066	-0,008726	-0,001475
	Mulliken	-0,023753	-0,011652	-0,132656	-0,002037
	APT	0,074469	0,106519	0,118245	0,113403
C(5″)	ESP	-0,015127	-0,027576	-0,034764	-0,037971
	Mulliken	-0,268116	-0,378479	-0,362360	-0,365297
	APT	-0,071879	-0,111234	-0,131519	-0,129534
C(6″)	ESP	0,032566	0,025092	0,052551	0,047080
	Mulliken	-0,196302	-0,154232	-0,102528	-0,121799
	APT	-0,014053	-0,018155	-0,021692	-0,024092
C(7″)	ESP	-0,077347	-0,105049	-0,128393	-0,123081
	Mulliken	-0,191276	-0,091082	-0,222634	-0,066785
	APT	0,049690	0,010806	-0,004160	0,005674
C(8″)	ESP	0,188326	0,299775	0,294822	0,290811
	Mulliken	0,925252	0,590063	0,720884	0,592492
	APT	0,297373	0,439587	0,504871	0,482260
C(9″)	ESP	0,112668	0,171501	-0,045907	-0,027268
	Mulliken	0,163693	0,256551	0,385628	0,321906
	APT	-0,127759	-0,160631	-0,181414	-0,180912
C(CH_3-N(1″))	ESP	0,101120	0,241353	0,198176	0,182036
	Mulliken	0,211238	0,200593	0,270937	0,265102
	APT	0,322934	0,275712	0,278950	0,294401
C(CH_3-C(3″))	ESP	0,062096	0,082816	0,018893	0,036684
	Mulliken	-0,249039	-0,264327	-0,223670	-0,208208
	APT	0,072333	0,050159	0,025940	0,027738
C(C′H_3-C(3″))	ESP	-0,084464	-0,057905	-0,123283	-0,125687
	Mulliken	-0,218112	-0,150628	-0,177952	-0,205524
	APT	0,038666	0,024109	0,026866	0,032493

Cl(1′)	ESP	0,943293	0,968117	0,892105	0,850768
	Mulliken	-0,513375	-0,538990	-0,495370	-0,449391
	APT	2,161910	2,120521	1,863594	1,886086
O(3′)	ESP	-0,435283	-0,433049	-0,433555	-0,423495
	Mulliken	-0,082605	-0,075627	-0,098660	-0,121845
	APT	-0,776507	-0,764907	-0,674672	-0,680992
O(4′)	ESP	-0,482013	-0,491426	-0,520284	-0,484930
	Mulliken	-0,100962	-0,124002	-0,140318	-0,072402
	APT	-0,811459	-0,775720	-0,698205	-0,685090
O(5′)	ESP	-0,451668	-0,439461	-0,420435	-0,420136
	Mulliken	-0,108549	-0,115866	-0,133650	-0,166889
	APT	-0,777649	-0,747563	-0,661860	-0,682109
O(6′)	ESP	-0,427950	-0,471985	-0,409706	-0,406893
	Mulliken	-0,090377	-0,046755	-0,041294	-0,058505
	APT	-0,683413	-0,705128	-0,599241	-0,623623

Compound 2

Atom	Charge	Structure			
		2a	2b	2c	2d
N(1)	ESP	-0,311033	-0,230419	-0,095171	-0,081437
	Mulliken	0,355040	0,469282	0,169956	0,254664
	APT	-1,056806	-0,398645	-1,363398	-1,093143
C(3)	ESP	0,196725	0,307916	0,146242	0,158389
	Mulliken	0,509463	0,212669	0,477286	0,428044
	APT	0,115243	0,007422	0,114892	0,112981
C(4)	ESP	0,010103	-0,018670	-0,034653	-0,066142
	Mulliken	-0,019977	-0,302538	-0,065104	-0,028612
	APT	0,120634	0,083561	0,119057	0,135675
C(5)	ESP	-0,080740	-0,004147	-0,008453	0,005320
	Mulliken	-0,412832	-0,308125	-0,409580	-0,336834
	APT	-0,161328	-0,053090	-0,155067	-0,154724
C(6)	ESP	0,008877	0,002020	0,021912	0,016773
	Mulliken	-0,016470	-0,083355	-0,045268	-0,208589
	APT	0,047950	-0,032499	0,000381	-0,014838
C(7)	ESP	-0,120434	-0,065174	-0,123139	-0,105546
	Mulliken	-0,238046	-0,307876	-0,183907	-0,127395
	APT	-0,120038	-0,004558	0,001977	-0,016647
C(8)	ESP	0,308311	0,275649	0,237926	0,239545
	Mulliken	0,187167	0,571981	0,522156	0,617260
	APT	0,563410	0,417133	0,463691	0,586033
C(9)	ESP	-0,090369	-0,057816	0,047423	0,040067
	Mulliken	0,142239	0,472786	0,670478	0,539617
	APT	-0,141699	-0,138309	-0,151795	-0,200169
$C(CH_3$-N(1))	ESP	0,096323	0,283607	0,131982	0,156815
	Mulliken	0,153167	0,243382	0,219053	0,192408
	APT	0,251970	0,242864	0,361605	0,290434
$C(CH_3$-C(3))	ESP	-0,069758	-0,026257	-0,003055	-0,031563
	Mulliken	0,061383	-0,079317	-0,155835	-0,206318
	APT	-0,011666	0,055910	0,048071	0,020950
$C(C'H_3$-C(3))	ESP	-0,069149	-0,101950	-0,005648	-0,042644
	Mulliken	-0,048531	-0,056575	-0,171617	-0,139925
	APT	-0,028542	0,022359	0,050262	0,021749
O(1′)	ESP	-0,486469	-0,598199	-0,616023	-0,585519
	Mulliken	0,281896	-0,169568	-0,250910	-0,259564
	APT	-1,607431	-1,020623	-0,854617	-0,880971
O(2′)	ESP	-0,222876	-0,295780	-0,285915	-0,286002
	Mulliken	-0,143271	-0,121096	-0,154242	-0,136621
	APT	-0,829760	-0,867590	-0,962221	-0,984877

N(1″)	ESP	0,252006	0,001968	-0,033732	-0,002486
	Mulliken	0,209092	0,194454	0,191134	0,196338
	APT	-1,095152	-1,443530	-1,536973	-1,538274
C(2,2′)	ESP	0,614387	0,391796	0,258506	0,271873
	Mulliken	-0,791082	-0,037364	-0,181216	-0,106737
	APT	1,173336	0,811269	1,689884	1,573972
C(3′)	ESP	-0,215458	-0,199890	-0,157729	-0,147816
	Mulliken	0,120122	-0,328697	-0,032518	0,009773
	APT	-0,182275	-1,001546	-1,500185	-1,289662
C(4′)	ESP	0,121048	0,176490	0,254429	0,273948
	Mulliken	0,091058	0,435406	-0,269702	-0,213996
	APT	0,222988	1,073827	1,634091	1,462256
C(7′)	ESP	-0,206246	-0,163970	-0,041197	-0,070927
	Mulliken	0,128855	0,197439	0,076804	0,271434
	APT	0,170049	0,004145	-0,036479	-0,009925
C(6′)	ESP	0,069324	0,124970	-0,202753	-0,188516
	Mulliken	0,742377	0,235278	0,360159	0,505011
	APT	-1,001154	-1,188661	-1,407088	-1,363982
C(5′)	ESP	-0,049200	-0,058102	0,145901	0,162459
	Mulliken	-0,142749	-0,055788	0,035887	-0,340901
	APT	0,679131	1,268504	1,476818	1,337997
C(10′)	ESP	0,025312	-0,165249	-0,274362	-0,257606
	Mulliken	0,290915	0,847354	1,027747	1,117724
	APT	-0,424067	-1,143937	-1,583493	-1,659770
C(9′)	ESP	0,314716	0,577643	0,610089	0,538509
	Mulliken	-0,500560	-0,871857	-0,762833	-0,818717
	APT	1,254587	0,892538	0,843179	0,879325
C(CH_3-N(1″))	ESP	0,066808	0,089998	0,094084	0,085971
	Mulliken	0,229336	0,211991	0,182958	0,191891
	APT	0,312288	0,311317	0,345683	0,352769
C(11′)	ESP	0,159012	0,190950	0,193625	0,186148
	Mulliken	0,205765	0,196644	0,182537	0,156996
	APT	0,410986	0,397322	0,423380	0,425322
C(2″)	ESP	-0,028059	0,091416	0,274432	0,157244
	Mulliken	-0,156407	-0,169678	-0,245712	-0,108002
	APT	1,521166	1,633013	1,733449	1,702069
C(3″)	ESP	0,355004	0,271026	-0,030831	0,082595
	Mulliken	0,504698	0,514569	0,512737	0,395141
	APT	0,085801	0,147285	0,151899	0,150996
C(4″)	ESP	-0,032936	-0,036116	-0,097758	-0,073267
	Mulliken	-0,053928	-0,030345	-0,064838	-0,037970
	APT	0,116212	0,147758	0,139144	0,136841
C(5″)	ESP	0,014042	-0,008093	0,008353	-0,009539
	Mulliken	-0,370256	-0,429170	-0,410196	-0,404939
	APT	-0,114563	-0,177787	-0,179397	-0,179919
C(6″)	ESP	0,020344	0,013070	0,010996	0,030331
	Mulliken	-0,028673	-0,050679	-0,054392	-0,038917
	APT	-0,024005	0,010537	0,011000	0,013734
C(7″)	ESP	-0,049466	-0,112056	-0,109938	-0,146175
	Mulliken	-0,207984	-0,132835	-0,221213	-0,163266
	APT	0,020669	-0,068436	-0,041546	-0,035289
C(8″)	ESP	-0,027655	0,168059	0,142374	0,188789
	Mulliken	0,588216	0,483283	0,535291	0,496064
	APT	0,412129	0,610070	0,556531	0,534297
C(9″)	ESP	0,006683	0,008722	0,212379	0,160911
	Mulliken	0,594078	0,602258	0,685688	0,570904
	APT	-0,151662	-0,164185	-0,157784	-0,153685
C(8′)	ESP	0,292766	0,179249	0,149752	0,196728
	Mulliken	-0,751314	-0,689803	-0,539659	-0,775382
	APT	0,134317	0,371111	0,550752	0,605939

C(CH_3-C(3″))	ESP	0,006527	-0,002147	0,011248	0,003587
	Mulliken	-0,135532	-0,207805	-0,184676	-0,182965
	APT	0,067731	0,041007	0,039907	0,042839
C(C′H_3-C(3″))	ESP	-0,022126	-0,054049	0,014057	-0,014423
	Mulliken	-0,154572	-0,163825	-0,168128	-0,160421
	APT	0,067270	0,027132	0,038017	0,031042
C(12′)	ESP	0,222183	0,072698	0,257756	0,241743
	Mulliken	-0,127270	-0,304772	-0,292770	-0,130255
	APT	1,536736	1,476979	1,601092	1,524621
C(13′)	ESP	-0,158179	-0,116098	-0,222256	-0,154293
	Mulliken	-0,227282	-0,126683	-0,119757	-0,156768
	APT	-1,365000	-1,440696	-1,572387	-1,541618
Cl(1′)	ESP	1,126420	1,083411	1,102387	1,105823
	Mulliken	-0,282760	-0,335137	-0,397445	-0,411263
	APT	2,349539	2,199803	2,232116	2,035824
O(3′)	ESP	-0,515176	-0,499500	-0,524729	-0,555551
	Mulliken	-0,121196	-0,152906	-0,118421	-0,126827
	APT	-0,810654	-0,759256	-0,821719	-0,740774
O(4′)	ESP	-0,578820	-0,527330	-0,522138	-0,550034
	Mulliken	-0,231504	-0,108427	-0,126393	-0,123940
	APT	-0,931600	-0,802529	-0,823038	-0,734068
O(5′)	ESP	-0,454049	-0,450703	-0,477436	-0,456211
	Mulliken	-0,128271	-0,146362	-0,088676	-0,077209
	APT	-0,809700	-0,779618	-0,721807	-0,687675
O(6′)	ESP	-0,498721	-0,518943	-0,458937	-0,477872
	Mulliken	-0,104401	-0,118191	-0,134866	-0,120938
	APT	-0,767042	-0,767371	-0,757885	-0,697654

Table S6 The lengths of some bonds, distances (Å) and angles (°) for the structures **1a** and **2d** calculated by B3LYP/6-311++G(d,p) method and obtained from XRD data[14].

Structure 1a			**Structure 2d**		
Bond	**Calculations**	**XRD**	**Bond**	**Calculations**	**XRD**
C(2,2′)–N(1)	1,439	1,448(4)	C(2,2′)–N(1)	1.348	1,341(2)
C(2,2′)–O(1′)	1,500	1,478(4)	O(1′)–C(9′)	1.224	1,245(2)
O(1′)–C(9′)	1,348	1,367(4)	C(2,2′)–C(3)	1.537	1,529(2)
C(2,2′)–C(3)	1,589	1,574(5)	C(2,2′)–C(3′)	1.404	1,402(2)
C(2,2′)–C(3′)	1,498	1,497(5)	C(3′)–C(4′)	1.381	1,374(2)
C(3′)–C(4′)	1,336	1,317(5)	C(4′)–C(10′)	1.416	1,419(2)
C(4′)–C(10′)	1,451	1,451(5)	C(10′)–C(9′)	1.488	1,454(2)
C(9′)–C(10′)	1,403	1,398(5)	C(10′)–C(5′)	1.394	1,399(2)
C(9′)–C(8′)	1,422	1,411(5)	C(5′)–C(6′)	1.405	1,391(2)
C(8′)–C(12′)	1,444	1,459(4)	C(6′)–C(12′)	1.411	1,426(2)
C(12′)–C(13′)	1,362	1,357(4)	C(12′)–C(13′)	1.391	1,368(2)
C(2″)–C(13′)	1,423	1,431(4)	C(13′)–C(2″)	1.397	1,404(2)
C(2″)–C(3″)	1,535	1,519(4)	C(2″)–C(3″)	1.537	1,526(2)
C(2″)–N(1″)	1,331	1,325(4)	C(2″)–N(1″)	1.362	1,334(2)
C(6′)–O(2′)	1,367	1,368(4)	C(8′)–O(2′)	1,352	1,359(2)
Distance	**Calculations**	**XRD**	**Distance**	**Calculations**	**XRD**
Cl(1)–N(1″)	3,992	3,921(3)	Cl(1)–N(1)	4,956	5,0458(15)
Cl(1)–C(2″)	3,812	4,151(3)	Cl(1)–C(5′)	4,138	4,5176(17)
Cl(1)–C(13′)	3,673	4,289(4)	Cl(1)–C(12′)	4,373	4,6535(17)
Cl(1)–O(1′)	4,995	5,537(3)	Cl(1)–C(3″)	4,919	5,0332(17)
C(2,2′)–C(2″)	5,501	5,449(5)	C(2,2′)–C(2″)	9,027	9,010(3)
C(2,2′)–C(6′)	5,177	5,126(6)	C(2,2′)–C(8′)	6,243	6,204(3)
C(2″)–C(6′)	6,172	6,164(5)	C(2″)–C(8′)	5,790	5,763(3)
Angle	**Calculations**	**XRD**	**Angle**	**Calculations**	**XRD**
D(C(2,2′),C(6′), C(8′),C(2″))	-171,30	-168.6(5)	D(C(2,2′),C(8′), C(7′),C(2″))	6,86	54,8(13)

Table S7 The lengths of some bonds, distances (Å) and angles (°) for the structures of compounds **1** and **2** with and without perchlorate anion calculated by B3LYP/6-311++G(d,p) method.

Compound 1								
Structure / Bond	**1a**	**1a′**	**1b**	**1b′**	**1c**	**1c′**	**1d**	**1d′**
C(2,2′)–N(1)	1,439	1,438	1,329	1,331	1,358	1,351	1,366	1,353
C(2,2′)–O(1′)	1,500	1,511	-	-	-	-	-	-
O(1′)–C(9′)	1,348	1,346	1,247	1,249	1,235	1,244	1,232	1,240
C(2,2′)–C(3)	1,589	1,587	1,535	1,530	1,538	1,537	1,539	1,538
C(2,2′)–C(3′)	1,498	1,497	1,416	1,417	1,391	1,401	1,385	1,398
C(3′)–C(4′)	1,336	1,336	1,381	1,377	1,392	1,387	1,400	1,389
C(4′)–C(10′)	1,451	1,453	1,424	1,431	1,407	1,415	1,393	1,408
C(9′)–C(10′)	1,403	1,399	1,468	1,468	1,478	1,477	1,480	1,481
C(9′)–C(8′)	1,422	1,425	1,477	1,477	1,481	1,480	1,482	1,482
C(8′)–C(12′)	1,444	1,437	1,428	1,420	1,424	1,421	1,427	1,423
C(12′)–C(13′)	1,362	1,370	1,373	1,383	1,377	1,382	1,373	1,380
C(2″)–C(13′)	1,423	1,420	1,409	1,404	1,405	1,405	1,407	1,406
C(2″)–C(3″)	1,535	1,538	1,537	1,536	1,533	1,536	1,532	1,535
C(2″)–N(1″)	1,331	1,337	1,341	1,348	1,343	1,347	1,340	1,346
C(6′)–O(2′)	1,367	1,358	1,363	1,372	1,363	1,371	1,369	1,363
Structure / Distance	**1a**	**1a′**	**1b**	**1b′**	**1c**	**1c′**	**1d**	**1d′**
Cl(1)–N(1″)	3,992	-	4,042	-	4,148	-	4,154	-
Cl(1)–C(2″)	3,812	-	4,064	-	4,104	-	4,062	-
Cl(1)–C(13′)	3,673	-	4,057	-	3,865	-	3,789	-
Cl(1)–O(1′)	4,995	-	5,200	-	4,239	-	4,267	-
C(2,2′)–C(2″)	5,501	5,506	6,644	6,683	9,134	8,302	8,542	9,134
C(2,2′)–C(6′)	5,178	5,191	5,794	5,744	5,833	6,185	5,812	5,833
C(2″)–C(6′)	6,172	6,181	6,172	6,183	6,200	6,189	6,156	6,200
Structure / Angle	**1a**	**1a′**	**1b**	**1b′**	**1c**	**1c′**	**1d**	**1d′**
D(C(2,2′), C(6′), C(8′),C(2″))	-171,30	-179,47	-155,95	-178,91	-126,84	180,00	-116,25	180,00
Compound 2								
Structure / Bond	**2a**	**2a′**	**2b**	**2b′**	**2c**	**2c′**	**2d**	**2d′**
C(2,2′)–N(1)	1,440	1,424	1,328	1,322	1,352	1,345	1,348	1,348
C(2,2′)–O(1′)	1,509	1,538	-	-	-	-	-	-
O(1′)–C(9′)	1,327	1,314	1,237	1,235	1,231	1,227	1,223	1,224
C(2,2′)–C(3)	1,584	1,582	1,528	1,528	1,535	1,535	1,537	1,537
C(2,2′)–C(3′)	1,499	1,497	1,422	1,434	1,400	1,405	1,404	1,404
C(3′)–C(4′)	1,337	1,337	1,366	1,365	1,383	1,380	1,381	1,381
C(4′)–C(10′)	1,454	1,454	1,441	1,442	1,421	1,423	1,416	1,416
C(10′)–C(9′)	1,404	1,411	1,468	1,469	1,477	1,482	1,488	1,488
C(10′)–C(5′)	1,389	1,388	1,386	1,391	1,398	1,398	1,394	1,394
C(5′)–C(6′)	1,408	1,410	1,412	1,410	1,404	1,404	1,405	1,405
C(6′)–C(12′)	1,426	1,423	1,402	1,408	1,407	1,410	1,411	1,411
C(12′)–C(13′)	1,382	1,381	1,399	1,393	1,396	1,392	1,391	1,391
C(13′)–C(2″)	1,404	1,406	1,387	1,395	1,391	1,396	1,397	1,397
C(2″)–C(3″)	1,535	1,536	1,539	1,538	1,538	1,538	1,537	1,537
C(2″)–N(1″)	1,351	1,345	1,365	1,355	1,362	1,354	1,362	1,354
C(8′)–O(2′)	1,357	1,348	1,355	1,347	1,352	1,343	1,352	1,341

Structure / Distance	2a	2a′	2b	2b′	2c	2c′	2d	2d′
Cl(1)–N(1)	8,076	-	5,604	-	7,256	-	4,956	-
Cl(1)–C(5′)	3,886	-	3,643	-	3,996	-	4,138	-
Cl(1)–C(12′)	4,271	-	4,440	-	4,536	-	4,373	-
Cl(1)–C(3″)	4,955	-	5,563	-	5,284	-	4,919	-
C(2,2′)–C(2″)	8,968	9,005	9,207	9,490	9,662	9,747	9,027	9,082
C(2,2′)–C(8′)	3,783	3,806	4,733	4,777	5,941	5,930	6,243	6,251
C(2″)–C(8′)	5,836	5,837	5,814	5,811	5,820	5,807	5,790	5,801
Structure / Angle	**2a**	**2a′**	**2b**	**2b′**	**2c**	**2c′**	**2d**	**2d′**
D(C(2,2′), C(8′), C(7′),C(2″))	-18,09	3,833	-23,54	27,73	8,59	0,00	6,86	0,00

Table S8 The summary NBO results for 3-center 4-electron hyperbonds search in structures of compounds **1** and **2** with and without perchlorate anion calculated by B3LYP/6-311++G(d,p) method.

Compound 1								
Structure	**3c-4e hyperbond A–B :C ↔ A: B–C**	**%A–B / %B–C**	**Occupancy**	**Low occupancy n_C**	**High occupancy σ_{AB}***	***E(2)*, kcal/mol**	***E(NL)-E(L)*, kcal/mol**	***F(L,NL)*, kcal/mol**
1a	-	-	-	-	-	-	-	-
1a′	-	-	-	-	-	-	-	-
1b	C(3′)–C(4′) :C(10′) ↔ C(3′): C(4′)–C(10′) C(6′)–C(5′) :C(10′) ↔ C(6′): C(5′)–C(10′)	61,8 / 38,2 56,1 / 43,9	3,1465 3,1431	1,09383 1,09383	0,28753 0,37256	102,27 96,14	87,85 87,85	66,52 64,01
1b′	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	57,6 / 42,4	3,4519	1,52519	0,35268	57,47	181,98	72,16
1c	C(3′)–C(2,2′) :N(1) ↔ C(3′): C(2,2′)–N(1)	62,9 / 37,1	3,4874	1,54201	0,32175	57,77	181,98	69,03
1c′	C(3′)–C(2,2′) :N(1) ↔ C(3′): C(2,2′)–N(1)	59,2 / 40,8	3,4704	1,53345	0,34398	55,92	181,98	71,54
1d	C(3′)–C(2,2′) :N(1) ↔ C(3′): C(2,2′)–N(1)	65,3 / 34,7	3,5963	1,58542	0,31136	51,23	188,25	69,03
1d′	C(3′)–C(2,2′) :N(1) ↔ C(3′): C(2,2′)–N(1)	59,8 / 40,2	3,5270	1,54640	0,34693	57,23	181,98	87,85
Compound 2								
Structure	**3c-4e hyperbond A–B :C ↔ A: B–C**	**%A–B / %B–C**	**Occupancy**	**Low occupancy n_C**	**High occupancy σ_{AB}***	***E(2)*, kcal/mol**	***E(NL)-E(L)*, kcal/mol**	***F(L,NL)*, kcal/mol**
2a	-	-	-	-	-	-	-	-
2a′	-	-	-	-	-	-	-	-
2b	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	61,5 / 38,5	3,5650	1,56688	0,33745	56,56	181,98	72,16
2b′	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	59,6 / 40,4	3,5414	1,54603	0,35275	58,20	181,98	72,16
2c	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	60,8 / 39,2	3,5558	1,56320	0,34136	57,19	181,98	72,16
2c′	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	60,1 / 39,9	3,5383	1,54685	0,34822	57,01	181,98	71,54
2d	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	60,7 / 39,3	3,5539	1,56176	0,34326	57,27	181,98	72,16
2d′	C(13′)–C(2″) :N(1″) ↔ C(13′): C(2″)–N(1″)	58,7 / 41,3	3,5220	1,53843	0,35877	59,11	181,98	72,79