Application of the additivity of group energies to understand conformational preference: the Anomeric Effect

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Tables S1 – S18: Optimized Geometries at B3LYP/6-311++G(2d,2p) level and energies at QCISD/6-311++G(2d,2p) level in atomic units. The molecules are labeled according to Chart 1 of the manuscript.

Tables S19 – S32: Atomic charges and atomic energies at at QCISD/6-311++G(2d,2p) level

Table S33. Group charges and group energies.

Table S34. QTAIM and NBO group charges

Table S35. Deletion NBO energies

Table S1. Optimized Geometries of 1 with a QCISD energy of -2.3529971780E+02 a.u.

C1	6.0	-1.2987800000E-03	8.3740000000E-05	2.6690000000E-05
C2	6.0	2.8710000000E-04	-8.6385000000E-04	2.8976681100E+00
C3	6.0	2.6959239300E+00	1.7750400000E-03	3.9617617000E+00
C4	6.0	4.2662711100E+00	-2.1879019700E+00	2.8953283900E+00
C5	6.0	4.2646851000E+00	-2.1869545500E+00	-2.3132200000E-03
C6	6.0	1.5690481100E+00	-2.1895932100E+00	-1.0664066100E+00
H7	1.0	7.8472656000E-01	1.7907318600E+00	-6.7668539000E-01
H8	1.0	-1.9358883400E+00	-9.5821520000E-02	-7.1256622000E-01
H9	1.0	-9.9364561000E-01	-1.6846795100E+00	3.5755129100E+00
H10	1.0	-1.0503582000E+00	1.6252316100E+00	3.6129120000E+00
H11	1.0	3.6138962500E+00	1.7922160900E+00	3.4777920400E+00
H12	1.0	2.6492125900E+00	-9.1988310000E-02	6.0230437500E+00
H13	1.0	3.4802458600E+00	-3.9785502100E+00	3.5720410000E+00
H14	1.0	6.2008605400E+00	-2.0919963700E+00	3.6079215400E+00
H15	1.0	5.2586180200E+00	-5.0313887000E-01	-6.8015757000E-01
H16	1.0	5.3153305200E+00	-3.8130502600E+00	-7.1755673000E-01
H17	1.0	6.5107597000E-01	-3.9800339900E+00	-5.8243649000E-01
H18	1.0	1.6157595500E+00	-2.0958300000E+00	-3.1276888100E+00

Table S2. Optimized Geometries of 2 with a QCISD energy of -3.0703036111E+02 a.u.

C1	6.0	-1.3628515900E+00	-2.0222847500E+00	1.0673777900E+00
O2	8.0	1.3366996700E+00	-2.0137280700E+00	1.0763653300E+00
C3	6.0	2.2879556800E+00	4.6752958400E-01	1.0823066300E+00
O4	8.0	1.5528522100E+00	1.8639861700E+00	-1.0558221200E+00
C5	6.0	-1.1335012000E+00	2.0914959700E+00	-1.1945828200E+00
C6	6.0	-2.3656196500E+00	-5.1648105000E-01	-1.1791210800E+00
H7	1.0	-4.4190848800E+00	-3.3975008200E-01	-1.0659359300E+00
H8	1.0	-1.9018770700E+00	-1.5040027900E+00	-2.9280191500E+00
H9	1.0	-1.5377230700E+00	3.1264120500E+00	-2.9239978100E+00
H10	1.0	-1.8091217600E+00	3.2202974200E+00	4.1098141900E-01
H11	1.0	4.3346878200E+00	3.3129544700E-01	1.0419628600E+00
H12	1.0	1.6517340200E+00	1.4500303300E+00	2.8045255500E+00
H13	1.0	-2.0562355700E+00	-1.2126731600E+00	2.8484446700E+00
H14	1.0	-1.9347016200E+00	-3.9952514300E+00	9.9182465100E-01

Table S3. Optimized Geometries of 3 with a QCISD energy of -9.5224442370E+02

C1	6.0	-6.1842988500E-01	-1.1472716300E+00	3.0047212400E+00
H2	1.0	-6.1197269100E-01	-1.1384976300E+00	5.0742226900E+00
C3	6.0	2.1252691600E+00	-1.1608871100E+00	2.1092083800E+00
S4	16.0	2.5119808200E+00	-1.4727523900E+00	-1.3221091000E+00
C5	6.0	6.9497135200E-01	1.2876820600E+00	-2.3071175000E+00
H6	1.0	6.9525859100E-01	1.2920662300E+00	-4.3606696700E+00

H7	1.0	1.6226738200E+00	3.0005808500E+00	-1.6437934000E+00
S8	16.0	-2.6084834700E+00	1.2985933400E+00	-1.3176644600E+00
C9	6.0	-2.1312218000E+00	1.1431558100E+00	2.1127686200E+00
H10	1.0	-1.2388250800E+00	2.8975435400E+00	2.7303405700E+00
H11	1.0	-4.0322484900E+00	1.1067105500E+00	2.8981274600E+00
H12	1.0	3.1352824200E+00	-2.7730105900E+00	2.8921162400E+00
H13	1.0	3.1071330600E+00	5.4511040100E-01	2.7266026900E+00
H14	1.0	-1.5567790700E+00	-2.8800484500E+00	2.4019628600E+00

Table S4. Optimized Geometries of 4 with a QCISD energy of -6.2963420852E+02 a.u.

C1	6.0	2.6815119400E+00	-8.4868356600E-01	-1.1266131500E+00
H2	1.0	4.7492030300E+00	-8.4404428800E-01	-1.1131923100E+00
C3	6.0	1.7157522800E+00	1.8707967500E+00	-1.1257514300E+00
S4	16.0	-1.7537490000E+00	1.9779423300E+00	-1.0465416700E+00
C5	6.0	-2.0994706200E+00	-1.8102631500E-01	1.6555720600E+00
H6	1.0	-4.1112258200E+00	-5.1901328300E-01	1.8822295900E+00
H7	1.0	-1.3567421100E+00	7.5814300700E-01	3.3430011200E+00
O8	8.0	-9.1852595400E-01	-2.5278979900E+00	1.3030058500E+00
C9	6.0	1.7682318600E+00	-2.3466505700E+00	1.1640542900E+00
H10	1.0	2.4832494300E+00	-1.4855628500E+00	2.9121945800E+00
H11	1.0	2.4474958100E+00	-4.2858157200E+00	1.0854227900E+00
H12	1.0	2.2760598600E+00	2.8686042700E+00	-2.8339240200E+00
H13	1.0	2.4533426200E+00	2.9193755400E+00	4.9005134000E-01
H14	1.0	2.0706560700E+00	-1.8021921300E+00	-2.8487394700E+00

Table S5. Optimized Geometries of 5ax with a QCISD energy of -6.9438916634E+02 a.u.

C1	6.0	-1.3004504400E+00	3.5317000000E-04	1.5640943700E+00
C2	6.0	2.9357564000E-01	-2.3977549900E+00	1.4418076600E+00
C3	6.0	2.1730703600E+00	-2.3949881900E+00	-7.6089671000E-01
C4	6.0	3.8039693100E+00	-6.3795000000E-04	-7.6254958000E-01
C5	6.0	2.1742839800E+00	2.3945774500E+00	-7.6095895000E-01
C6	6.0	2.9371247000E-01	2.3983537300E+00	1.4409070300E+00
Cl7	17.0	-3.6491010100E+00	-2.2390000000E-05	-1.0324060000E+00
H8	1.0	-2.4838205100E+00	7.1028000000E-04	3.2410872000E+00
H9	1.0	1.3353237400E+00	-2.5013699500E+00	3.2290990700E+00
H10	1.0	-9.3148721000E-01	-4.0513172900E+00	1.3709845900E+00
H11	1.0	1.1341247100E+00	-2.5242415200E+00	-2.5393317400E+00
H12	1.0	3.3640557300E+00	-4.0750724100E+00	-6.4847595000E-01
H13	1.0	5.0210429700E+00	-9.2291000000E-04	9.1169033000E-01
H14	1.0	5.0608469200E+00	-9.3435000000E-04	-2.3981277600E+00
H15	1.0	1.1363475300E+00	2.5250590800E+00	-2.5398928900E+00
H16	1.0	3.3663031400E+00	4.0738647000E+00	-6.4745347000E-01
H17	1.0	1.3344796600E+00	2.5034329600E+00	3.2286738400E+00

H18	1.0	-9.3146739000E-01	4.0517526400E+00	1.3682259500E+00

Table S6. Optimized Geometries of 5eq with a QCISD energy of -6.9438978244E+02 a.u.

C1	6.0	1.1430817800E+00	-1.8500000000E-06	7.0584435000E-01
C2	6.0	-1.1260571000E-01	-2.3912247800E+00	-2.8335631000E-01
C3	6.0	-2.9426976700E+00	-2.3900096600E+00	3.7228298000E-01
C4	6.0	-4.2623899600E+00	1.3000000000E-07	-5.9197886000E-01
C5	6.0	-2.9426971800E+00	2.3900106600E+00	3.7227961000E-01
C6	6.0	-1.1260377000E-01	2.3912236200E+00	-2.8335254000E-01
H7	1.0	1.1546866900E+00	-3.8700000000E-06	2.7633121300E+00
Cl8	17.0	4.5188966700E+00	1.5000000000E-07	-1.2852872000E-01
H9	1.0	1.3046240000E-01	-2.4728879400E+00	-2.3321440400E+00
H10	1.0	8.1705679000E-01	-4.0524544500E+00	5.0274900000E-01
H11	1.0	-3.1714520600E+00	-2.5184148800E+00	2.4237556100E+00
H12	1.0	-3.8284156900E+00	-4.0757842000E+00	-4.1945570000E-01
H13	1.0	-4.2479145000E+00	-1.8000000000E-06	-2.6600205600E+00
H14	1.0	-6.2438517300E+00	2.4700000000E-06	-1.8428340000E-02
H15	1.0	-3.1714585500E+00	2.5184245400E+00	2.4237506500E+00
H16	1.0	-3.8284093800E+00	4.0757833400E+00	-4.1947016000E-01
H17	1.0	1.3047247000E-01	2.4728947400E+00	-2.3321388000E+00
H18	1.0	8.1705524000E-01	4.0524506500E+00	5.0276311000E-01

Table S7. Optimized Geometries of 6ax with a QCISD energy of -7.6612176155E+02 a.u.

C1	6.0	2.0324154500E+00	-2.3401466500E+00	-6.7682210000E-01
O2	8.0	3.2659153000E-01	-2.1883654200E+00	1.4404058200E+00
C3	6.0	-1.0216939000E+00	-6.0100000000E-06	1.6020288300E+00
O4	8.0	3.2657332000E-01	2.1883642300E+00	1.4404035800E+00
C5	6.0	2.0323962000E+00	2.3401571400E+00	-6.7682445000E-01
C6	6.0	3.7005511300E+00	1.2110000000E-05	-7.7826399000E-01
H7	1.0	4.8191042800E+00	1.5880000000E-05	-2.5106794100E+00
H8	1.0	5.0007642600E+00	1.8130000000E-05	8.2111813000E-01
H9	1.0	3.1122395900E+00	4.0584129500E+00	-3.6837822000E-01
H10	1.0	9.1731860000E-01	2.5508441700E+00	-2.3997224700E+00
H11	1.0	-2.0986414600E+00	-9.5700000000E-06	3.3376717800E+00
Cl12	17.0	-3.6170279800E+00	-1.7910000000E-05	-9.4013433000E-01
H13	1.0	9.1733948000E-01	-2.5508443300E+00	-2.3997198500E+00
H14	1.0	3.1122732500E+00	-4.0583931300E+00	-3.6837443000E-01

Table S8. Optimized Geometries of 6eq with a QCISD energy of -7.6611412824E+02 a.u.

C1	6.0	2.6930228600E+00	2.3411347500E+00	3.1981132000E-01
O2	8.0	5.0630770000E-02	2.1927218600E+00	-2.9609020000E-01
C3	6.0	-1.0236493100E+00	-3.1100000000E-06	6.7222065000E-01
O4	8.0	5.0636380000E-02	-2.1927300400E+00	-2.9607265000E-01

C5	6.0	2.6930302900E+00	-2.3411317500E+00	3.1982838000E-01
C6	6.0	4.0709677200E+00	-2.0000000000E-08	-6.3367066000E-01
H7	1.0	6.0244990600E+00	5.2100000000E-06	3.0203060000E-02
H8	1.0	4.0895016500E+00	-7.4800000000E-06	-2.6938134000E+00
H9	1.0	3.3682642900E+00	-4.0662249200E+00	-5.6589747000E-01
H10	1.0	2.9034102100E+00	-2.5353857300E+00	2.3727642500E+00
Cl11	17.0	-4.3010326700E+00	-1.0230000000E-05	-1.7897171000E-01
H12	1.0	-9.4584032000E-01	6.7700000000E-06	2.7424781100E+00
H13	1.0	2.9034022000E+00	2.5354029600E+00	2.3727462800E+00
H14	1.0	3.3682538600E+00	4.0662236200E+00	-5.6592516000E-01

Table S9. Optimized Geometries of 7ax with a QCISD energy of -1.4113232017E+03 a.u.

C1	6.0	3.9658169400E+00	4.2750000000E-05	9.9816546000E-01
H2	1.0	5.3312315800E+00	5.3710000000E-05	2.5518464100E+00
C3	6.0	2.3986548200E+00	2.4114887500E+00	1.1971831000E+00
S4	16.0	1.7034354000E-01	2.8985660000E+00	-1.4106318200E+00
C5	6.0	-1.6354512200E+00	-2.4410000000E-05	-1.2437174500E+00
H6	1.0	-2.8530245900E+00	-3.2300000000E-05	-2.8913533700E+00
S7	16.0	1.7042586000E-01	-2.8985621800E+00	-1.4106633200E+00
C8	6.0	2.3987234500E+00	-2.4114498800E+00	1.1971567400E+00
H9	1.0	1.3408877900E+00	-2.4745726500E+00	2.9631045800E+00
H10	1.0	3.6040460200E+00	-4.0775520200E+00	1.1280390300E+00
H11	1.0	3.6039299700E+00	4.0776260000E+00	1.1280834800E+00
H12	1.0	1.3408175900E+00	2.4745615300E+00	2.9631317100E+00
H13	1.0	5.0373025000E+00	6.7310000000E-05	-7.6184348000E-01
Cl14	17.0	-3.8543541500E+00	-7.0870000000E-05	1.4798451000E+00

Table S10. Optimized Geometries of 7eq with a QCISD energy of -1.4113194741E+03 a.u.

C1	6.0	4.4497266000E+00	-1.0000000000E-06	-4.6076886000E-01
H2	1.0	6.4386254900E+00	-1.6000000000E-06	1.0995375000E-01
C3	6.0	3.2375206500E+00	2.4119821500E+00	5.5073876000E-01
S4	16.0	-4.5740650000E-02	2.9153196200E+00	-4.7059761000E-01
C5	6.0	-1.4029312900E+00	-3.3000000000E-07	7.8888073000E-01
H6	1.0	-1.2583253000E+00	-9.3000000000E-07	2.8357409000E+00
S7	16.0	-4.5742030000E-02	-2.9153193700E+00	-4.7060011000E-01
C8	6.0	3.2375196000E+00	-2.4119843900E+00	5.5073661000E-01
H9	1.0	3.3060147300E+00	-2.4663040100E+00	2.6113754600E+00
H10	1.0	4.2277702000E+00	-4.0777233200E+00	-1.4137038000E-01
H11	1.0	4.2277721700E+00	4.0777212200E+00	-1.4136659000E-01
H12	1.0	3.3060157600E+00	2.4662998300E+00	2.6113776800E+00
H13	1.0	4.3994412900E+00	0.0000000000E+00	-2.5202832100E+00
Cl14	17.0	-4.7252107100E+00	7.9000000000E-07	6.5188720000E-02

Table S11. Optimized Geometries of 8ax with a QCISD energy of -3.6263792345E+02 a.u.

C1	6.0	1.8345645200E+00	2.3252743700E+00	5.9214798000E-01
O2	8.0	-4.1682751000E-01	2.2023954900E+00	-1.0050980700E+00
C3	6.0	-1.6317544000E+00	1.4121300000E-03	-1.2063759800E+00
O4	8.0	-4.1777749000E-01	-2.2004506000E+00	-1.0087176400E+00
C5	6.0	1.8300653100E+00	-2.3263116100E+00	5.9310321000E-01
C6	6.0	3.4514453100E+00	-2.2365100000E-03	1.9510736000E-01
H7	1.0	5.0203472100E+00	-3.0992300000E-03	1.5296541300E+00
H8	1.0	4.2400818800E+00	-3.7930500000E-03	-1.7072897200E+00
H9	1.0	2.7539285800E+00	-4.0633966200E+00	1.9540930000E-02
H10	1.0	1.2217530300E+00	-2.5238692900E+00	2.5561709300E+00
H11	1.0	-2.8678161200E+00	3.0156800000E-03	-2.8436534400E+00
N12	7.0	-3.9169470900E+00	1.1133000000E-04	1.1547489300E+00
H13	1.0	1.2299181500E+00	2.5264165500E+00	2.5559658600E+00
H14	1.0	2.7606491000E+00	4.0599283400E+00	1.4835880000E-02
H15	1.0	-5.0141070500E+00	1.5718318100E+00	9.7309429000E-01
H16	1.0	-5.0145552600E+00	-1.5710417600E+00	9.7085944000E-01
H17	1.0	-3.1406543800E+00	-1.1611700000E-03	2.9142094700E+00

Table S12. Optimized Geometries of 8eq with a QCISD energy of -3.6264645858E+02 a.u.

C1	6.0	2.1261228400E+00	2.3540730600E+00	3.2092516000E-01
O2	8.0	-5.8058601000E-01	2.1935212800E+00	-2.1270439000E-01
C3	6.0	-1.6081194100E+00	-1.2134000000E-04	7.0890693000E-01
O4	8.0	-5.8076214000E-01	-2.1936670400E+00	-2.1319665000E-01
C5	6.0	2.1258026800E+00	-2.3540115200E+00	3.2118978000E-01
C6	6.0	3.4460597800E+00	-7.2120000000E-05	-6.6746468000E-01
H7	1.0	5.4128569300E+00	-2.8866000000E-04	-5.1486940000E-02
H8	1.0	3.4316395600E+00	-1.1814000000E-04	-2.7267079200E+00
H9	1.0	2.7433321700E+00	-4.0688632600E+00	-6.1523400000E-01
H10	1.0	2.3654951400E+00	-2.5822578500E+00	2.3597616200E+00
N11	7.0	-4.2791847500E+00	2.1105000000E-04	-3.3801350000E-01
H12	1.0	-1.7486983100E+00	-5.4262000000E-04	2.7822852600E+00
H13	1.0	2.3662262600E+00	2.5827002300E+00	2.3594048500E+00
H14	1.0	2.7433607100E+00	4.0687980400E+00	-6.1593526000E-01
H15	1.0	-5.2317430200E+00	-1.5822397700E+00	2.2584161000E-01
H16	1.0	-5.2300317900E+00	1.5846659400E+00	2.2310127000E-01
H17	1.0	-4.1465546200E+00	-1.3736000000E-03	-2.2690709000E+00

Table S13. Optimized Geometries of 9ax with a QCISD energy of -9.5908815471E+02 a.u.

C1	6.0	2.8830600000E-03	-2.5941070800E+00	5.2879787000E-01
S2	16.0	-2.8698441000E+00	-1.1210320800E+00	-7.5905841000E-01
C3	6.0	-2.4346087000E+00	2.0392987400E+00	5.7140799000E-01
C4	6.0	-4.6147600000E-03	3.3577115500E+00	-2.8017311000E-01
C5	6.0	2.4289536600E+00	2.0451006600E+00	5.6991307000E-01

S6	16.0	2.8731855700E+00	-1.1153239400E+00	-7.5816748000E-01
Li7	3.0	3.3047700000E-03	-2.5719054400E+00	4.2613339800E+00
H8	1.0	5.3540600000E-03	-4.5013522800E+00	-2.5962375000E-01
H9	1.0	-2.4847755700E+00	1.9203379100E+00	2.6420706500E+00
H10	1.0	-4.0816764800E+00	3.1273466200E+00	-1.1718550000E-02
H11	1.0	-5.7329600000E-03	3.5179709700E+00	-2.3345458700E+00
H12	1.0	-6.1492100000E-03	5.2805024400E+00	4.9020238000E-01
H13	1.0	2.4809216800E+00	1.9279085300E+00	2.6406281900E+00
H14	1.0	4.0730010500E+00	3.1366753900E+00	-1.5075680000E-02

Table S14. Optimized Geometries of 1 with a QCISD energy of -9.5911221404E+02 a.u.

C1	6.0	1.2189600000E-03	-2.7016847500E+00	-9.9763801000E-01
S2	16.0	2.8306682400E+00	-1.1824589700E+00	7.6260050000E-02
C3	6.0	2.4180241800E+00	2.2567227000E+00	-4.2299255000E-01
C4	6.0	-2.1251700000E-03	3.3315451100E+00	7.2541453000E-01
C5	6.0	-2.4205673500E+00	2.2539532800E+00	-4.2401365000E-01
S6	16.0	-2.8293696700E+00	-1.1853656000E+00	7.7067770000E-02
Li7	3.0	3.3194100000E-03	-3.2301529100E+00	2.7079882400E+00
H8	1.0	1.2070300000E-03	-3.0851800600E+00	-3.0082306700E+00
H9	1.0	2.4809166000E+00	2.5906039700E+00	-2.4564150700E+00
H10	1.0	4.0811495900E+00	3.1301778300E+00	4.2219817000E-01
H11	1.0	-2.5280300000E-03	3.0018400000E+00	2.7648590100E+00
H12	1.0	-3.1338500000E-03	5.3822471700E+00	4.5361395000E-01
H13	1.0	-2.4825744300E+00	2.5865719700E+00	-2.4576421600E+00
H14	1.0	-4.0850758300E+00	3.1261729600E+00	4.1978514000E-01

Table S15. Optimized Geometries of Methylcyclohexane axial **with a QCISD energy of** -2.7451726306E+02 a.u.

C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
C2	6.0	0.0000000000E+00	0.0000000000E+00	2.9136685700E+00
C3	6.0	2.6670026200E+00	0.0000000000E+00	4.0503615200E+00
C4	6.0	4.2561583600E+00	2.1961924700E+00	3.0266779700E+00
C5	6.0	4.3210931300E+00	2.1973149700E+00	1.2972969900E-01
C6	6.0	1.6474878100E+00	2.1892307200E+00	-9.9117458500E-01
C7	6.0	7.7701759200E-01	-2.5639010500E+00	-1.1094827800E+00
H8	1.0	-1.9399229300E+00	3.5660266000E-01	-6.1872657200E-01
H9	1.0	-9.9678707200E-01	1.6885666800E+00	3.5722645800E+00
H10	1.0	-1.0723288700E+00	-1.6197447400E+00	3.6144810700E+00
H11	1.0	3.6142202800E+00	-1.7867133800E+00	3.6242396100E+00
H12	1.0	2.5457086600E+00	1.0796761300E-01	6.1077819500E+00
H13	1.0	3.4434740800E+00	3.9823408200E+00	3.6848128900E+00
H14	1.0	6.1729038000E+00	2.1098603300E+00	3.7869525900E+00
H15	1.0	5.3671340300E+00	5.4220589200E-01	-5.3177649300E-01
H16	1.0	5.3583732500E+00	3.8435839000E+00	-5.5816462900E-01
H17	1.0	7.2595341200E-01	3.9773840700E+00	-5.0959299800E-01

H18	1.0	1.7402601400E+00	2.1186078700E+00	-3.0529583900E+00
H19	1.0	2.6979431000E+00	-3.0982419000E+00	-5.9170726800E-01
H20	1.0	-4.7950666800E-01	-4.0595474800E+00	-4.4730384500E-01
H21	1.0	6.7954929700E-01	-2.5305284900E+00	-3.1695091400E+00

Table S16. Optimized Geometries of Methylcyclohexane equatorial **with a QCISD energy of** -2.7452023935E+02 a.u.

C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
C2	6.0	0.0000000000E+00	0.0000000000E+00	2.9027554000E+00
C3	6.0	2.6786584500E+00	0.0000000000E+00	4.0064348300E+00
C4	6.0	4.2549678300E+00	2.2012531600E+00	2.9796332400E+00
C5	6.0	4.2790051500E+00	2.2195230300E+00	8.4085254100E-02
C6	6.0	1.5951915300E+00	2.2059566800E+00	-1.0073978800E+00
H7	1.0	9.0381632600E-01	-1.7585734700E+00	-6.2297467600E-01
C8	6.0	-2.6848359600E+00	4.6440019700E-02	-1.0694961700E+00
H9	1.0	-1.0116667800E+00	1.6806222700E+00	3.5677575900E+00
H10	1.0	-1.0575738900E+00	-1.6302799600E+00	3.6023358000E+00
H11	1.0	3.6107790900E+00	-1.7839732800E+00	3.5269584000E+00
H12	1.0	2.5965177200E+00	7.9171966100E-02	6.0672000800E+00
H13	1.0	3.4596728100E+00	3.9846009400E+00	3.6644510900E+00
H14	1.0	6.1828702200E+00	2.1021351300E+00	3.7096627900E+00
H15	1.0	5.2969118000E+00	5.5128602600E-01	-5.9584198800E-01
H16	1.0	5.3190461600E+00	3.8605479800E+00	-6.1232418000E-01
H17	1.0	6.5212370200E-01	3.9845423600E+00	-5.1991090300E-01
H18	1.0	1.6671825400E+00	2.1325313800E+00	-3.0701851400E+00
H19	1.0	-3.6733649300E+00	1.7684869700E+00	-5.0347406500E-01
H20	1.0	-3.7900366200E+00	-1.5590297300E+00	-3.9456536800E-01
H21	1.0	-2.6733747700E+00	-1.8498529100E-02	-3.1310985700E+00

Table S17. Optimized Geometries of Tert-butylcyclohexane axial **with a QCISD energy of** -3.9216416548E+02 a.u.

C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
C2	6.0	0.0000000000E+00	0.0000000000E+00	2.9291907800E+00
C3	6.0	2.6175484900E+00	0.0000000000E+00	4.1896645700E+00
C4	6.0	4.3153067900E+00	2.1065967700E+00	3.1671621000E+00
C5	6.0	4.5106458900E+00	1.9772355700E+00	2.8471936700E-01
C6	6.0	1.8877475900E+00	2.0269126900E+00	-9.4962139700E-01
C7	6.0	1.0439603100E-01	-2.6685597500E+00	-1.3048785700E+00
H8	1.0	-1.8636195700E+00	7.0431415800E-01	-5.5754857800E-01
H9	1.0	-9.8143871600E-01	1.7168010700E+00	3.5367169500E+00
H10	1.0	-1.1228412500E+00	-1.5651014200E+00	3.6600026800E+00
H11	1.0	3.5554139000E+00	-1.8143411800E+00	3.9061376200E+00
H12	1.0	2.3786379700E+00	2.1085942100E-01	6.2295785800E+00
H13	1.0	3.5326767100E+00	3.9436789200E+00	3.7112029200E+00
H14	1.0	6.1908921000E+00	1.9865084600E+00	4.0197989800E+00
H15	1.0	5.5362890800E+00	2.7013068200E-01	-2.5669850800E-01

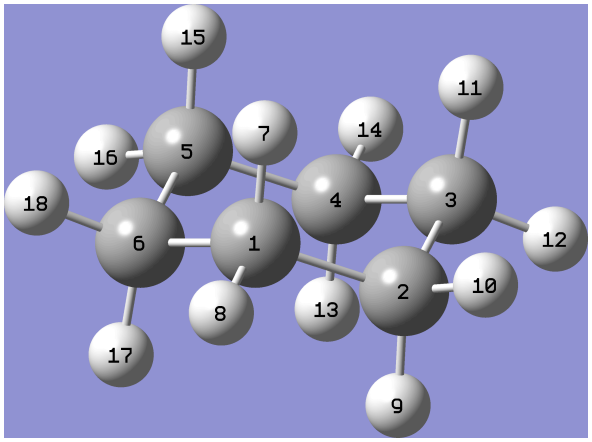
H16	1.0	5.6242142600E+00	3.5651422100E+00	-4.2325708000E-01
H17	1.0	1.0451319400E+00	3.8695109500E+00	-5.2746602800E-01
H18	1.0	2.0650568100E+00	1.9603263000E+00	-2.9988782100E+00
C19	6.0	2.3690003700E+00	-4.3322047200E+00	-5.4807916000E-01
H20	1.0	2.2912211300E+00	-6.1175499400E+00	-1.5803004900E+00
H21	1.0	2.3549786000E+00	-4.7877458800E+00	1.4592446300E+00
H22	1.0	4.1721770400E+00	-3.4458872600E+00	-9.9257298300E-01
C23	6.0	-2.3347509700E+00	-4.1214454500E+00	-6.3608559600E-01
H24	1.0	-2.3729045400E+00	-5.9407528300E+00	-1.6065053200E+00
H25	1.0	-2.4900770100E+00	-4.5015827600E+00	1.3815806700E+00
H26	1.0	-4.0122306200E+00	-3.0677341600E+00	-1.2126334800E+00
C27	6.0	1.4375335700E-01	-2.3469472600E+00	-4.1998634200E+00
H28	1.0	-1.3527793500E-01	-4.1713039900E+00	-5.1204472900E+00
H29	1.0	-1.3604724300E+00	-1.0872671600E+00	-4.8394998100E+00
H30	1.0	1.9361415900E+00	-1.5909434200E+00	-4.8745334400E+00

Table S18. Optimized Geometries of Tert-butylcyclohexane equatorial **with a QCISD energy of** -3.9217232896E+02 a.u,

C1	6.0	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00
C2	6.0	0.0000000000E+00	0.0000000000E+00	2.9123911200E+00
C3	6.0	2.6855918500E+00	0.0000000000E+00	4.0068297900E+00
C4	6.0	4.2593784600E+00	2.2163823000E+00	3.0196444100E+00
C5	6.0	4.2489301600E+00	2.2820313900E+00	1.2796280500E-01
C6	6.0	1.5551917000E+00	2.2741096600E+00	-9.4492353800E-01
H7	1.0	1.0155955200E+00	-1.7089152500E+00	-5.9437745100E-01
C8	6.0	-2.6874910300E+00	-2.2599234800E-01	-1.2223655700E+00
H9	1.0	-1.0024751500E+00	1.6717632300E+00	3.6037153000E+00
H10	1.0	-1.0173284000E+00	-1.6364801600E+00	3.6381876800E+00
H11	1.0	3.6215788800E+00	-1.7745907900E+00	3.5004285300E+00
H12	1.0	2.5994505800E+00	4.4491712100E-02	6.0687496500E+00
H13	1.0	3.4795810800E+00	3.9890247900E+00	3.7478447100E+00
H14	1.0	6.1953405200E+00	2.0878544700E+00	3.7236184200E+00
H15	1.0	5.2699000600E+00	6.3242519700E-01	-5.9180553300E-01
H16	1.0	5.2688550400E+00	3.9415907700E+00	-5.5497666100E-01
H17	1.0	6.1406650700E-01	4.0293250900E+00	-3.8882627000E-01
H18	1.0	1.6501957900E+00	2.2862927200E+00	-3.0022362500E+00
C19	6.0	-4.3564593600E+00	2.0910991300E+00	-6.6649884900E-01
H20	1.0	-6.2227245400E+00	1.8381101500E+00	-1.5081469600E+00
H21	1.0	-4.6281660700E+00	2.3754254300E+00	1.3560901500E+00
H22	1.0	-3.5588513100E+00	3.8208769500E+00	-1.4509298400E+00
C23	6.0	-4.0389135600E+00	-2.6041635600E+00	-2.2151558700E-01
H24	1.0	-2.8716864100E+00	-4.2881608700E+00	-4.6943253800E-01
H25	1.0	-4.5142344800E+00	-2.4499543400E+00	1.7752767600E+00
H26	1.0	-5.8004520100E+00	-2.9085511900E+00	-1.2497949500E+00
C27	6.0	-2.4326671300E+00	-5.2214644900E-01	-4.1088050800E+00
H28	1.0	-1.2221331300E+00	-2.1232906100E+00	-4.5883155200E+00

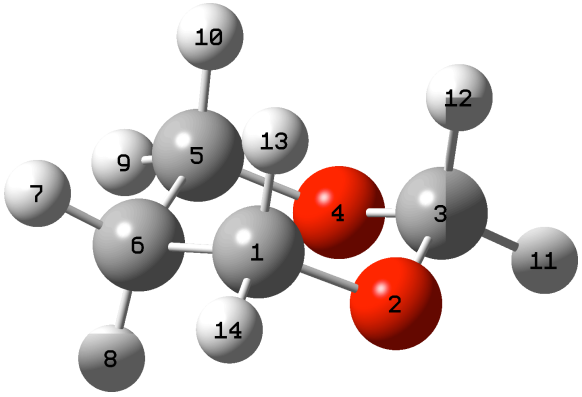
H29	1.0	-4.2812766000E+00	-8.5926603200E-01	-4.9588983800E+00
H30	1.0	-1.6457379200E+00	1.1569659300E+00	-5.0021258600E+00

Table S19. Atomic charges and atomic energies of 1



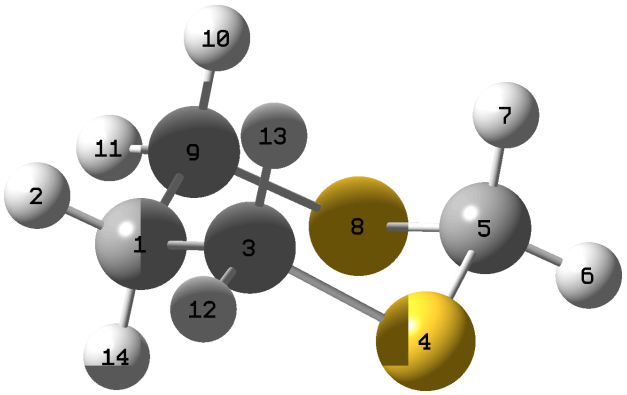
Atom	q(A)	E(A)
C1	0.07456	-37.90962
C2	0.07445	-37.90957
C3	0.07455	-37.90954
C4	0.07456	-37.90962
C5	0.07445	-37.90957
C6	0.07455	-37.90954
H7	-0.04095	-0.65447
H8	-0.03354	-0.65258
H9	-0.04096	-0.65445
H10	-0.03356	-0.65259
H11	-0.04096	-0.65444
H12	-0.03360	-0.65260
H13	-0.04095	-0.65447
H14	-0.03354	-0.65258
H15	-0.04096	-0.65445
H16	-0.03357	-0.65259
H17	-0.04096	-0.65444
H18	-0.03360	-0.65260
Total	0.003	-235.29972

Table S20. Atomic charges and atomic energies of 2



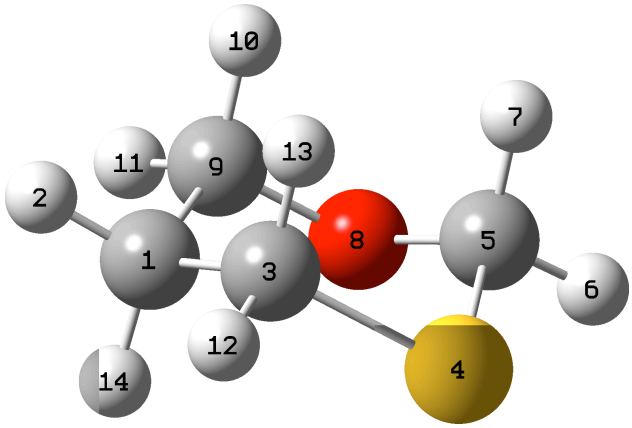
Atom	q(A)	E(A)
C1	0.533	-37.64530
O2	-1.077	-75.65091
C3	1.060	-37.31018
O4	-1.077	-75.65087
C5	0.533	-37.64524
C6	0.060	-37.96566
H7	-0.018	-0.64162
H8	-0.005	-0.64068
H9	0.010	-0.64348
H10	-0.024	-0.65103
H11	0.036	-0.63884
H12	-0.017	-0.65205
H13	-0.024	-0.65103
H14	0.010	-0.64348
Total	0.000	-307.030

Table S21. Atomic charges and atomic energies of 3



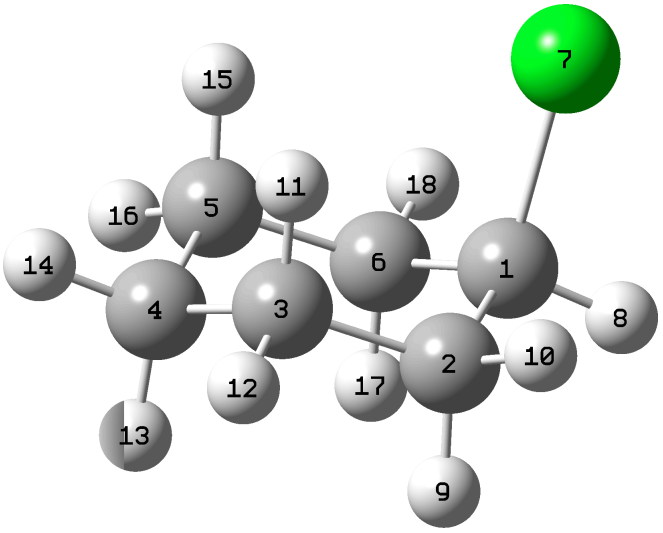
Atom	q(A)	E(A)
C1	0.088	-37.89852
H2	-0.02	-0.64595
C3	-0.043	-37.91603
S4	0.048	-397.74593
C5	-0.165	-37.93354
H6	0.044	-0.6217
H7	0.027	-0.62999
S8	0.048	-397.74595
C9	-0.043	-37.91607
H10	-0.003	-0.64044
H11	0.013	-0.63529
H12	0.013	-0.63529
H13	-0.003	-0.64045
H14	-0.002	-0.63922
Total	0.002	-952.244

Table S22. Atomic charges and atomic energies of 4



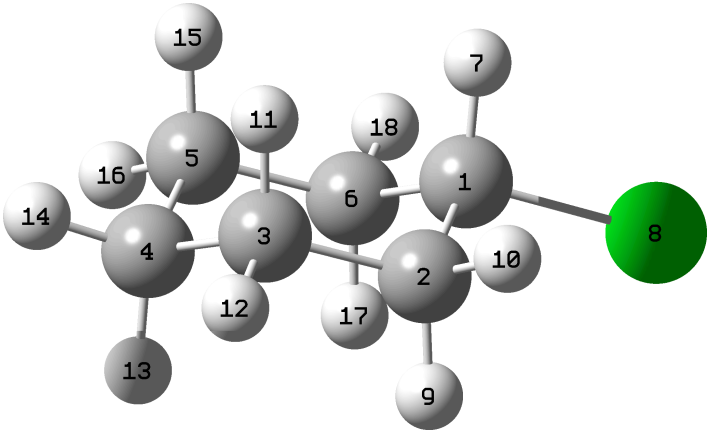
Atom	q(A)	E(A)
C1	0.075	-37.92512
H2	-0.019	-0.64349
C3	-0.045	-37.92081
S4	0.012	-397.83035
C5	0.473	-37.60271
H6	0.038	-0.63129
H7	0.005	-0.64106
O8	-1.070	-75.60580
C9	0.540	-37.62323
H10	-0.024	-0.65108
H11	0.010	-0.64365
H12	0.012	-0.63546
H13	-0.004	-0.64073
H14	-0.003	-0.63954
Total	0.001	-629.634

Table S23. Atomic charges and atomic energies of 5ax



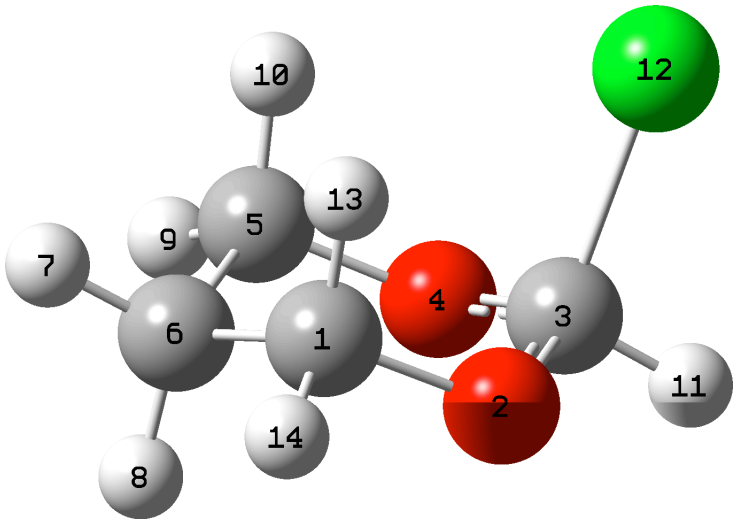
Atom	q(A)	E(A)
C1	0.132	-37.83770
C2	0.077	-37.91537
C3	0.072	-37.90175
C4	0.075	-37.89902
C5	0.072	-37.90173
C6	0.077	-37.91535
Cl7	-0.299	-459.89467
H8	0.019	-0.64328
H9	-0.027	-0.64767
H10	-0.007	-0.64284
H11	-0.018	-0.64743
H12	-0.027	-0.65000
H13	-0.042	-0.65456
H14	-0.027	-0.64986
H15	-0.018	-0.64743
H16	-0.027	-0.65001
H17	-0.027	-0.64767
H18	-0.007	-0.64284
Total	0.000	-694.38919

Table S24. Atomic charges and atomic energies of 5eq



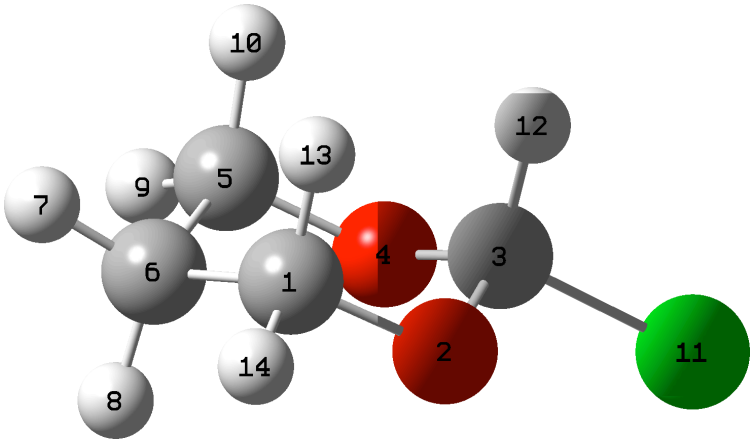
Atom	q(A)	E(A)
C1	0.131	-37.84453
C2	0.079	-37.91782
C3	0.071	-37.89914
C4	0.074	-37.90063
C5	0.071	-37.89914
C6	0.079	-37.91782
H7	0.012	-0.64382
Cl8	-0.29	-459.88764
H9	-0.017	-0.64507
H10	-0.01	-0.64385
H11	-0.035	-0.6523
H12	-0.022	-0.6477
H13	-0.034	-0.65201
H14	-0.026	-0.64944
H15	-0.035	-0.6523
H16	-0.022	-0.6477
H17	-0.017	-0.64507
H18	-0.01	-0.64385
Total	-0.001	-694.38983

Table S25. Atomic charges and atomic energies of 6ax



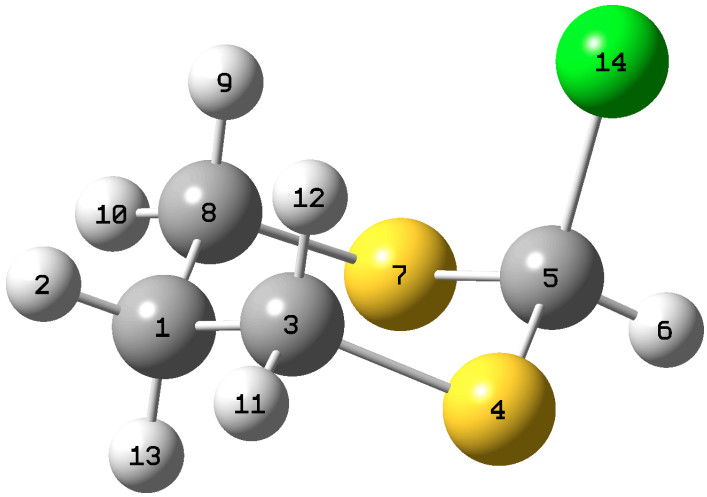
Atom	q(A)	E(A)
C1	0.503	-37.64797
O2	-1.092	-75.68394
C3	1.29	-37.0781
O4	-1.092	-75.68394
C5	0.503	-37.64797
C6	0.064	-37.9489
H7	-0.004	-0.63642
H8	-0.003	-0.63996
H9	0.022	-0.63897
H10	0.016	-0.63872
H11	0.09	-0.62213
Cl12	-0.335	-459.97713
H13	0.016	-0.63872
H14	0.022	-0.63897
Total	0.00000	-766.12184

Table S26. Atomic charges and atomic energies of 6eq



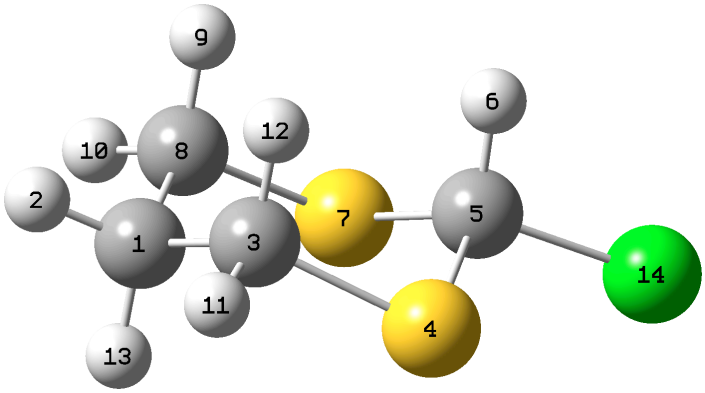
Atom	q(A)	E(A)
C1	0.512	-37.64043
O2	-1.059	-75.63733
C3	1.171	-37.17158
O4	-1.059	-75.63733
C5	0.512	-37.64043
C6	0.061	-37.95014
H7	-0.01	-0.63798
H8	0.003	-0.63751
H9	0.023	-0.63792
H10	-0.015	-0.64786
Cl11	-0.182	-459.95163
H12	0.033	-0.63828
H13	-0.015	-0.64786
H14	0.023	-0.63792
Total	-0.002	-766.114

Table S27. Atomic charges and atomic energies of 7ax



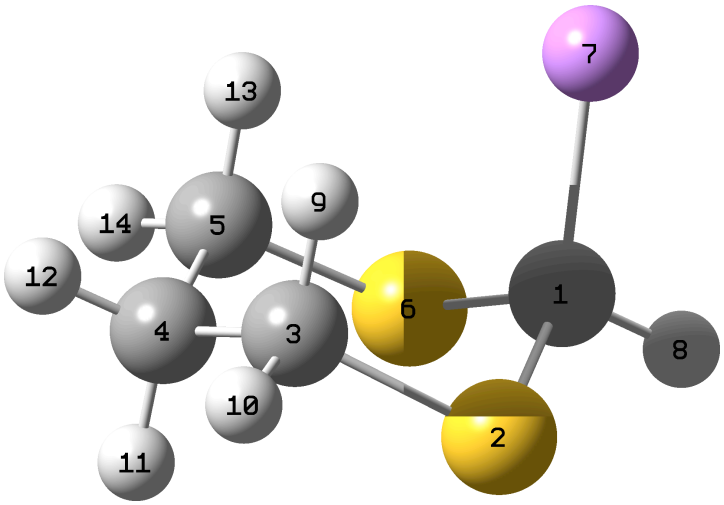
Atom	q(A)	E(A)
C1	0.09089	-37.89749
H2	-0.01349	-0.64347
C3	-0.04660	-37.92084
S4	0.11237	-397.72912
C5	-0.11856	-37.85353
H6	0.08361	-0.61493
S7	0.11237	-397.72913
C8	-0.04660	-37.92084
H9	0.01767	-0.63318
H10	0.01815	-0.63274
H11	0.01815	-0.63274
H12	0.01767	-0.63318
H13	-0.00175	-0.63947
Cl14	-0.24340	-459.84264
Total	0.001	-1411.323

Table S28. Atomic charges and atomic energies of 7eq



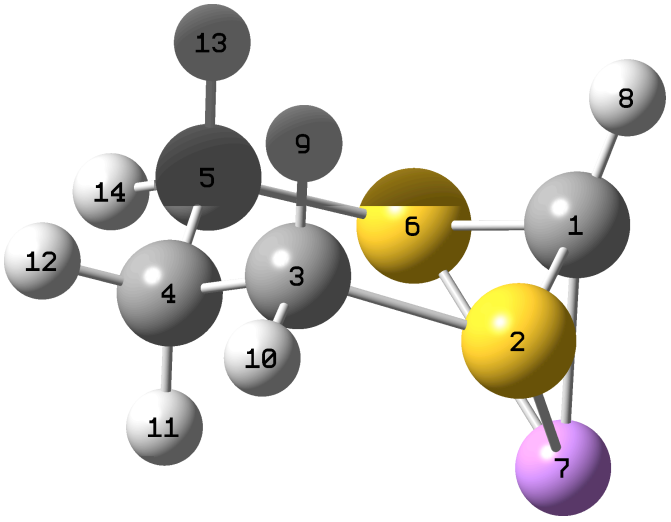
Atom	q(A)	E(A)
C1	0.08830	-37.89951
H2	-0.01455	-0.64333
C3	-0.04760	-37.91657
S4	0.09504	-397.72783
C5	-0.09374	-37.85239
H6	0.06436	-0.62355
S7	0.09504	-397.72783
C8	-0.04759	-37.91657
H9	0.00069	-0.63895
H10	0.01956	-0.63201
H11	0.01956	-0.63201
H12	0.00069	-0.63895
H13	0.00203	-0.63764
Cl14	-0.18262	-459.83205
Total	-0.001	-1411.319

Table S31. Atomic charges and atomic energies of 8ax



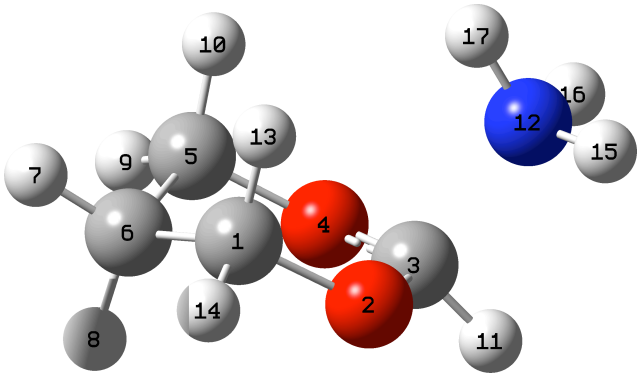
Atom	q(A)	E(A)
C1	-0.677	-38.00269
S2	-0.033	-397.74121
C3	-0.043	-37.91128
C4	0.087	-37.89844
C5	-0.043	-37.91116
S6	-0.033	-397.74117
Li7	0.918	-7.36369
H8	-0.015	-0.63801
H9	-0.063	-0.65652
H10	0.002	-0.63881
H11	-0.003	-0.63878
H12	-0.035	-0.65116
H13	-0.063	-0.65652
H14	0.002	-0.63885
Total	0.002	-959.088

Table S32. Atomic charges and atomic energies of 8eq



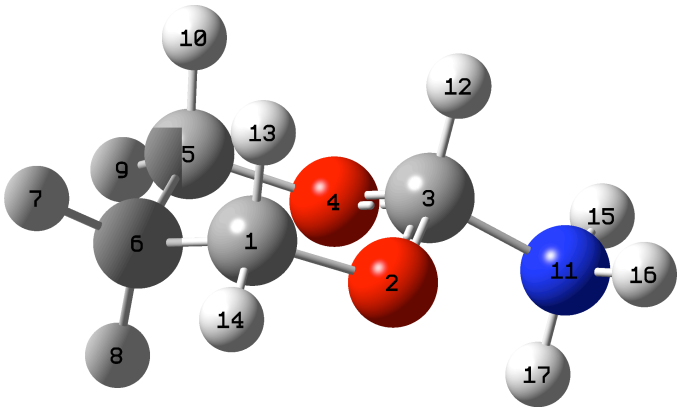
Atom	q(A)	E(A)
C1	-0.61491	-38.01286
S2	-0.10788	-397.76444
C3	-0.05320	-37.92338
C4	0.08969	-37.89336
C5	-0.05323	-37.92341
S6	-0.10765	-397.76428
Li7	0.89521	-7.35216
H8	0.00740	-0.62974
H9	-0.00150	-0.63831
H10	0.00009	-0.63835
H11	-0.02908	-0.64753
H12	-0.02297	-0.64784
H13	-0.00149	-0.63831
H14	0.00010	-0.63833
Total	0.001	-959.11229

Table S29. Atomic charges and atomic energies of 9ax



Atom	q(A)	E(A)
C1	0.46198	-37.68956
O2	-1.10755	-75.75193
C3	1.49598	-36.98120
O4	-1.10743	-75.75193
C5	0.46205	-37.68960
C6	0.06389	-37.97467
H7	0.04309	-0.61723
H8	0.03577	-0.62435
H9	0.07462	-0.61711
H10	0.00769	-0.64222
H11	0.11187	-0.61157
N12	-0.90523	-55.06054
H13	0.00787	-0.64215
H14	0.07460	-0.61713
H15	0.43186	-0.45314
H16	0.43185	-0.45314
H17	0.41761	-0.46059
Total	1.001	-362.63805

Table S30. Atomic charges and atomic energies of 9eq



Atom	q(A)	E(A)
C1	0.46173	-37.68445
O2	-1.08093	-75.69087
C3	1.40463	-37.09623
O4	-1.08087	-75.69082
C5	0.46172	-37.68446
C6	0.06213	-37.96867
H7	0.03664	-0.61966
H8	0.02332	-0.62978
H9	0.06557	-0.62046
H10	0.02121	-0.63518
N11	-0.92075	-55.14542
H12	0.06238	-0.62252
H13	0.02122	-0.63518
H14	0.06557	-0.62046
H15	0.46293	-0.43601
H16	0.46296	-0.43600
H17	0.47046	-0.43026
Total	1.000	-362.646

Table S33. Group charges and group energies.

	E(ring)	E(subst)	q(ring)	q(subst)
5ax	-234.49453	-459.89467	0.29894	-0.29897
5eq	-234.50219	-459.88764	0.28900	-0.29000
6ax	-306.14471	-459.97713	0.33500	-0.33500
6eq	-306.16257	-459.95163	0.18000	-0.18200
7ax	-951.48067	-459.84264	0.24390	-0.24340
7eq	-951.48715	-459.83205	0.18178	-0.18262
8ax	-951.72461	-7.36369	-0.91617	0.91772
8eq	-951.76012	-7.35216	-0.89465	0.89521
9ax	-306.21064	-56.42741	0.62444	0.37609
9eq	-306.19875	-56.44769	0.52432	0.47560

Table S34. QTAIM and NBO group charges

	q(ring)		q(Substituent)	
	AIM	NBO	AIM	NBO
5ax	0.29894	0.1137	-0.29897	-0.1137
5eq	0.28900	0.0938	-0.29000	-0.0938
6ax	0.33500	0.2061	-0.33500	-0.2062
6eq	0.18000	0.0220	-0.18200	-0.0221
7ax	0.24390	0.0775	-0.24340	-0.0775
7eq	0.18178	-0.0071	-0.18262	0.0071
8ax	-0.91617	-0.8373	0.91772	0.8373
8eq	-0.89465	-0.6459	0.89521	0.6459
9ax	0.62444	0.5225	0.37609	0.4775
9eq	0.52432	0.3463	0.47560	0.6537

Table S35. Deletion NBO energies

	E_{total}	E_{Lewis}	$E_{no\text{-}Lewis}$
5ax	-695.58350	-695.17049	-0.41301
5eq	-695.58470	-695.17218	-0.41251
6ax	-767.40535	-766.88587	-0.51948
6eq	-767.39535	-766.90487	-0.49048
7ax	-1413.35206	-1412.94180	-0.41026
7eq	-1413.34755	-1412.95028	-0.39727
8ax	-960.63280	-960.23956	-0.39325
8eq	-960.65965	-960.17536	-0.48429
9ax	-363.50828	-362.95788	-0.55040
9eq	-363.51213	-363.03088	-0.48125