

Supporting Information

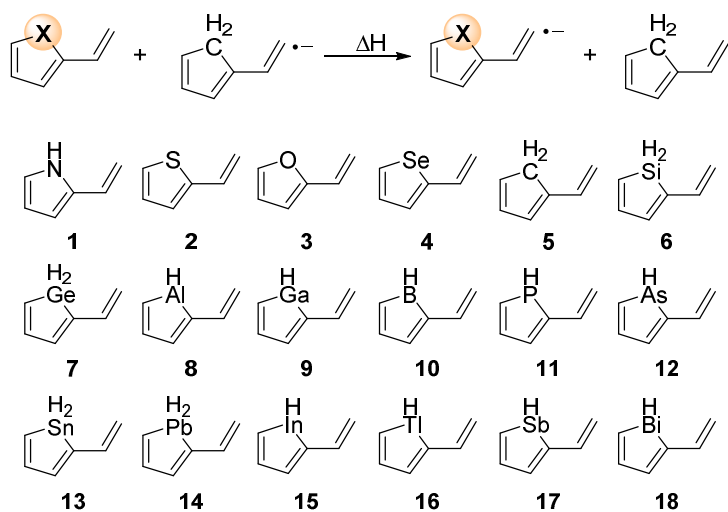
Antiaromaticity-Promoted Radical Anion Stability in α -Vinyl Heterocyclics

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Table S1. NICS(1)_{zz} (ppm) and RSE values (kcal/mol) of compounds **1-18** and their corresponding radical anions.



	1	2	3	4	5	6	7	8	9
NICS(1)_{zz,original}	-26.2	-22.3	-23.4	-17.5	-8.6	2.2	1.7	11.6	12.0
NICS(1)_{zz,rad.anion}	-19.3	-8.9	-15.9	-7.5	-4.3	-0.2	-0.6	-2.3	-2.2
RSE	11.5	1.6	6.7	-1.8	0.0	-15.8	-13.4	-24.2	-23.9
	10	11	12	13	14	15	16	17	18
NICS(1)_{zz,original}	35.3	-9.8	-5.1	2.7	1.1	9.5	7.5	-1.5	0.3
NICS(1)_{zz,rad.anion}	5.6	-6.6	-4.7	-0.1	-0.6	-1.6	-1.2	-3.2	-2.7
RSE	-35.7	-9.9	-10.7	-14.5	-12.9	-22.5	-20.7	-13.3	-12.9

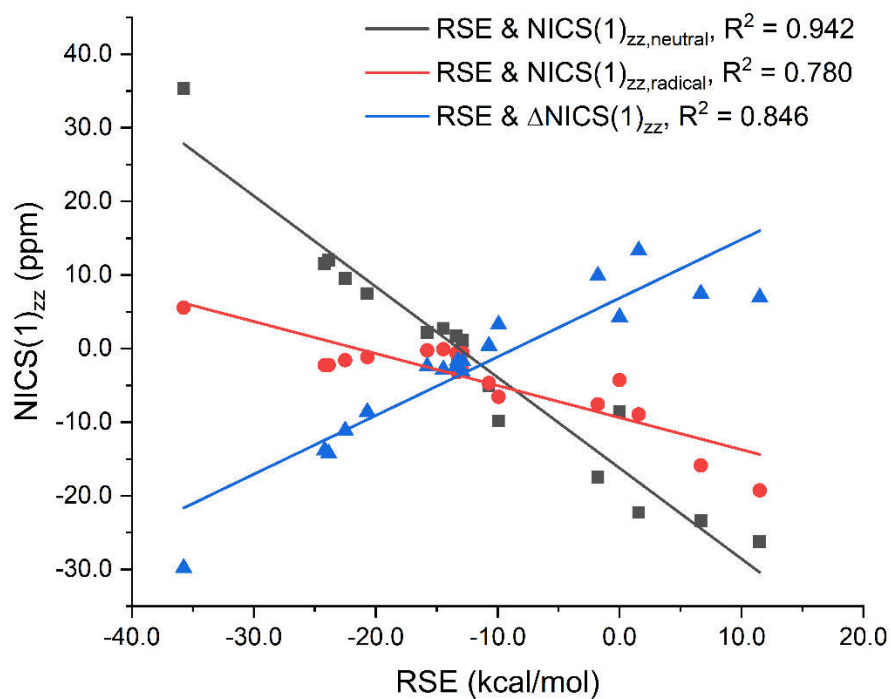
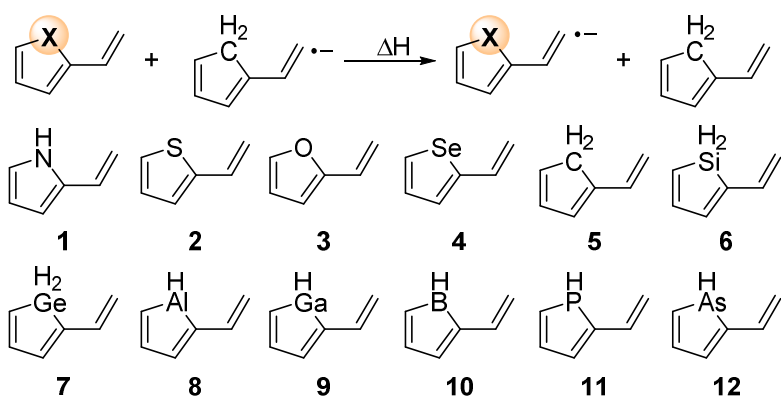


Figure S1. Linear correlation between $\text{NICS}(1)_{zz}$ values and RSE values, $\Delta\text{NICS}(1)_{zz} = \text{NICS}(1)_{zz,\text{radical}} - \text{NICS}(1)_{zz,\text{neutral}}$.

Table S2. RSE values (kcal/mol) of radical anions **1-12** at different computational levels.



	1	2	3	4	5	6
RSE_a	11.5	1.6	6.7	-1.8	0.0	-15.8
RSE_b	10.7	1.8	9.2	-1.1	0.0	-14.3
RSE_c	16.4	1.7	9.9	-1.4	0.0	-17.2
	7	8	9	10	11	12
RSE_a	-13.4	-24.2	-23.9	-35.7	-9.9	-10.7
RSE_b	-11.6	-24.2	-21.8	-36.4	-9.3	-9.3
RSE_c	-15.3	-26.0	-25.4	-37.8	-10.3	-12.1

a. (U)OPBE/6-311++G(d,p)~SDD//B3LYP/6-311G(d,p)~SDD level; b. (U)CCSD(T)/6-311++G(d,p)~SDD//B3LYP/6-311G(d,p)~SDD level; c. (U)OPBE/cc-pvtz//B3LYP/6-311G(d,p)~SDD level.

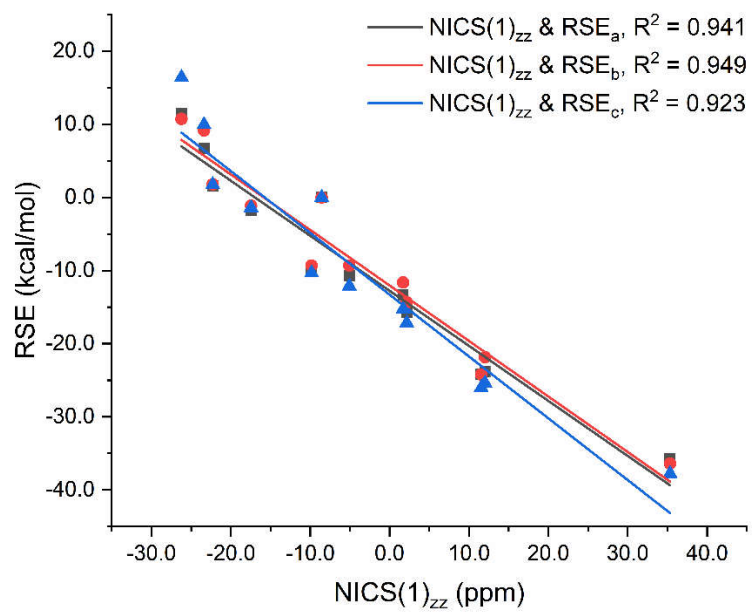


Figure S2. Linear correlation between NICS(1)_{zz} values and RSE values at different computational levels.

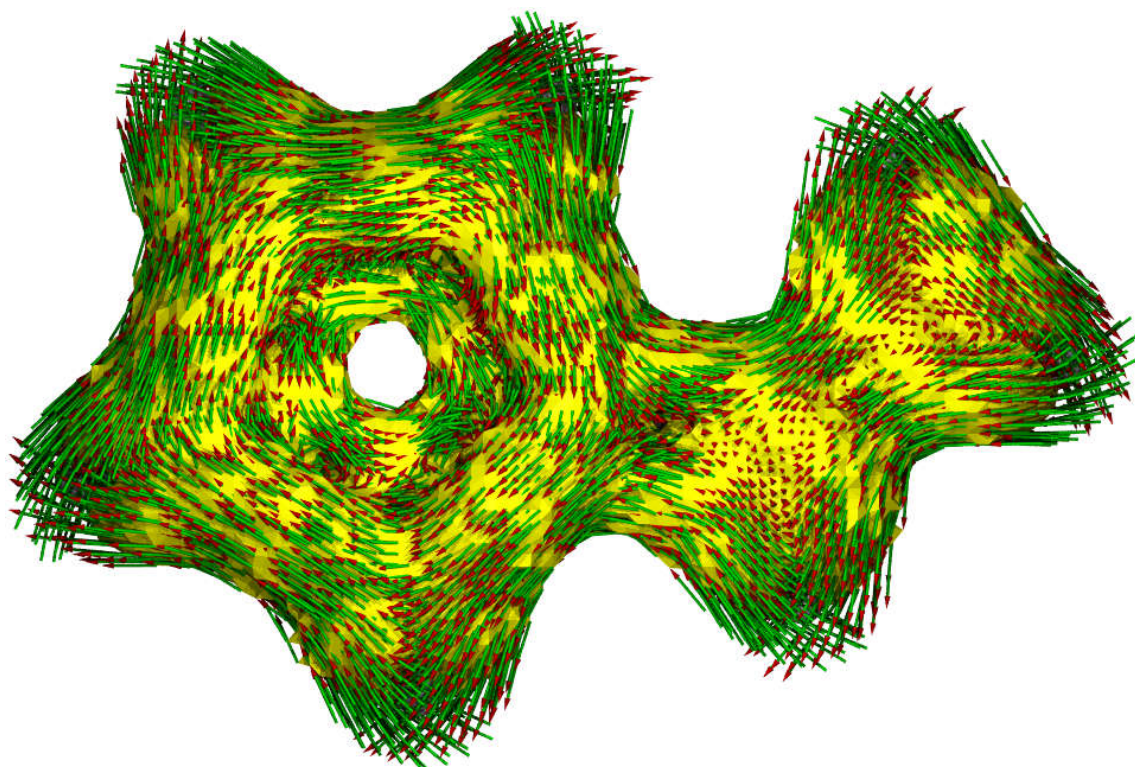


Figure S3. Computed ACID plots of **1** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

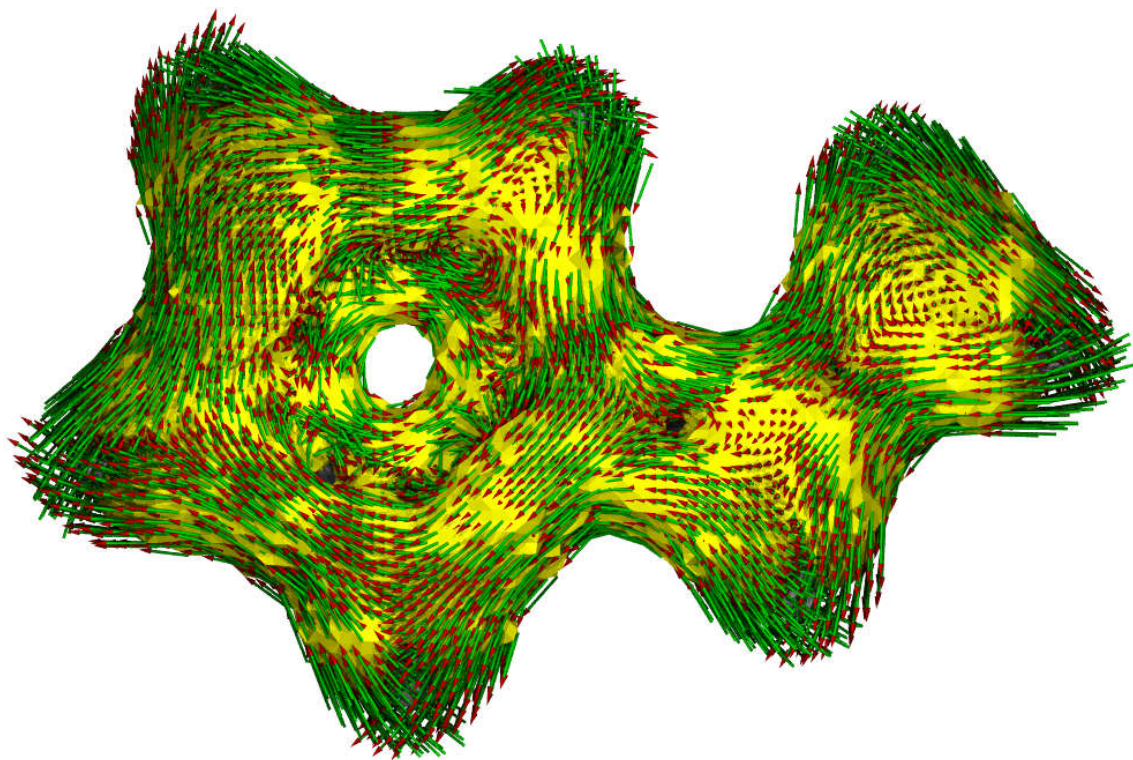


Figure S4. Computed ACID plots of **1rad.anion** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

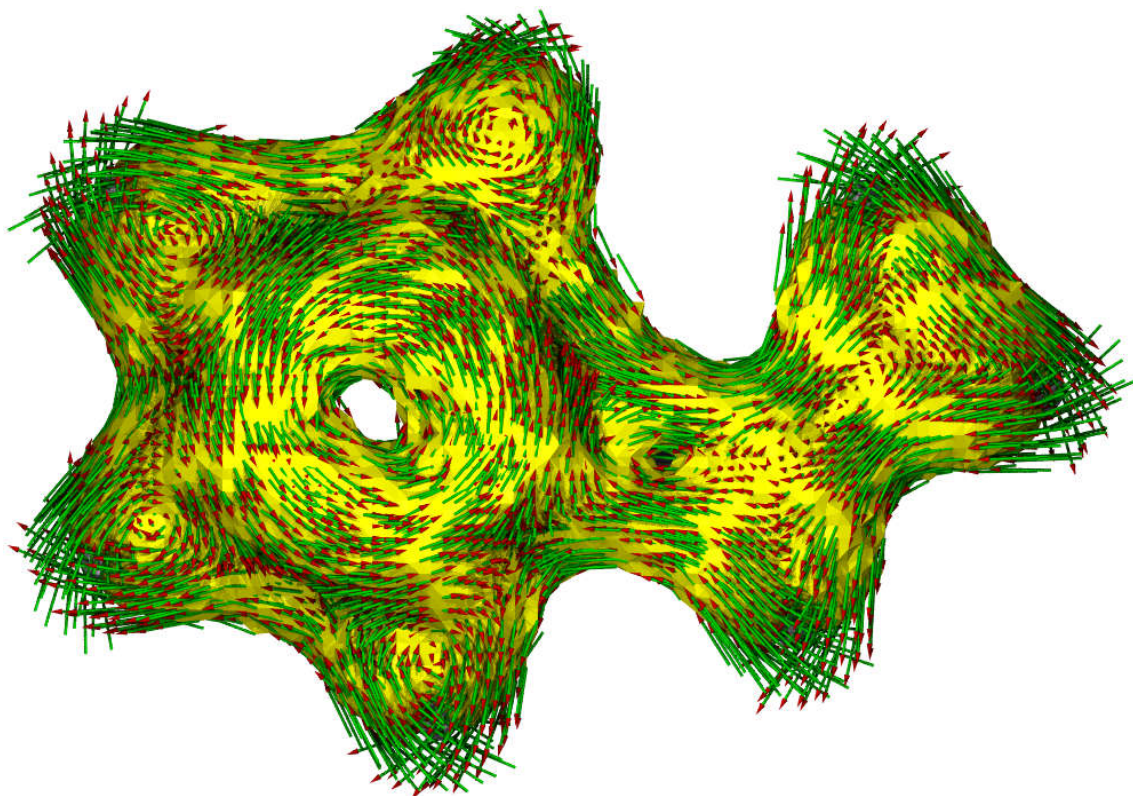


Figure S5. Computed ACID plots of **10** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

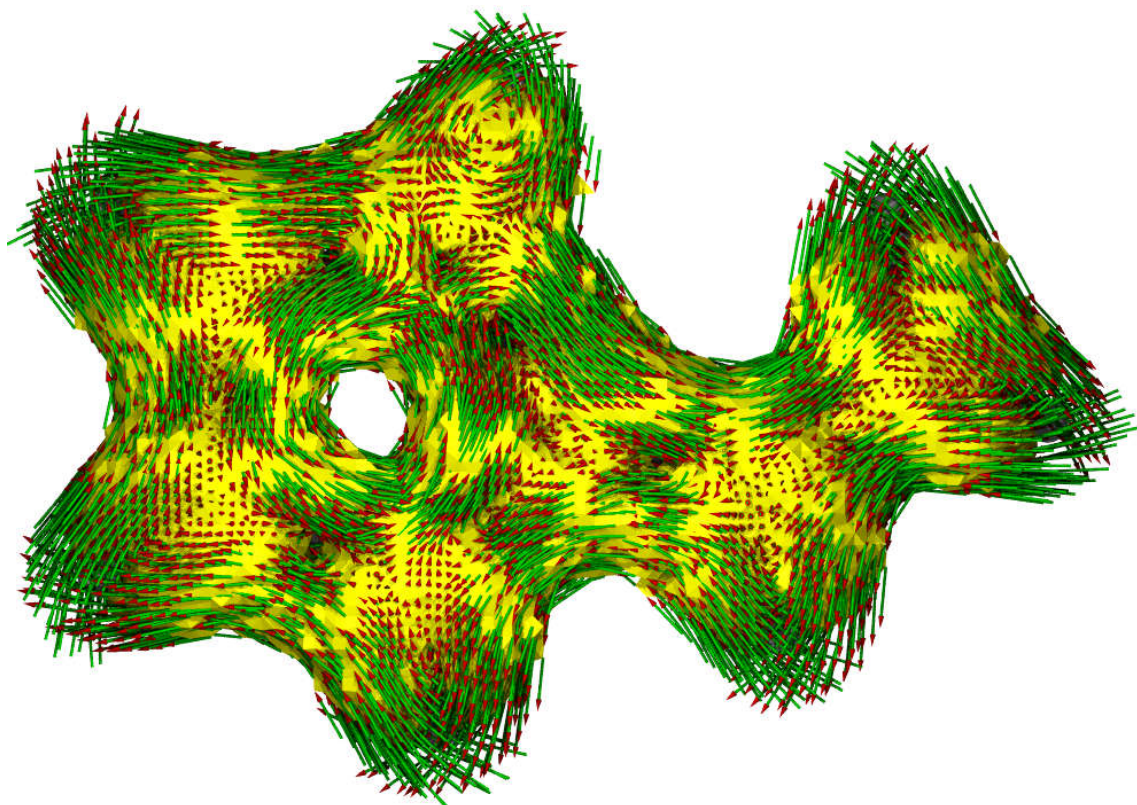


Figure S6. Computed ACID plots of **10rad.anion** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

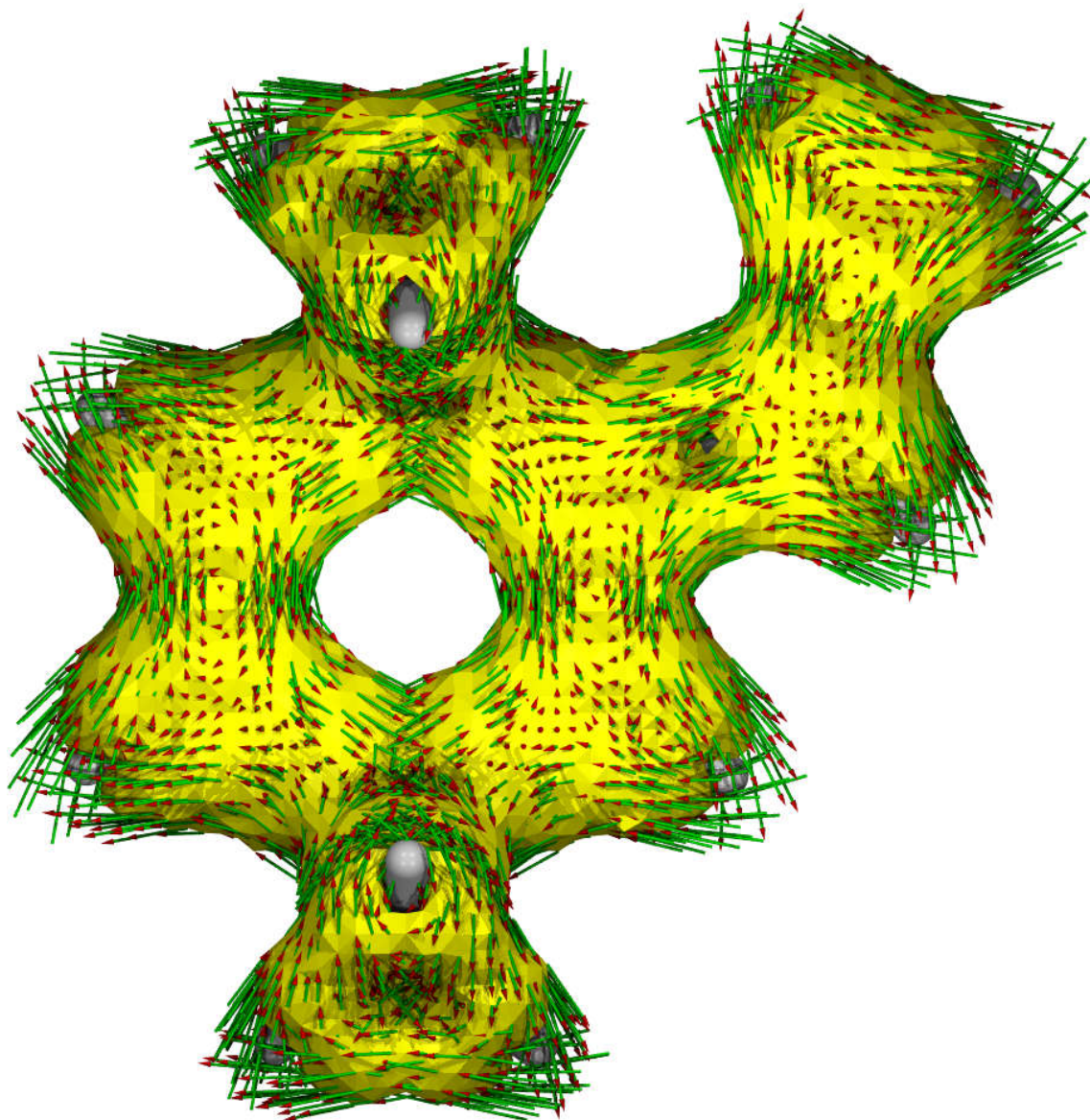


Figure S7. Computed ACID plots of **19** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

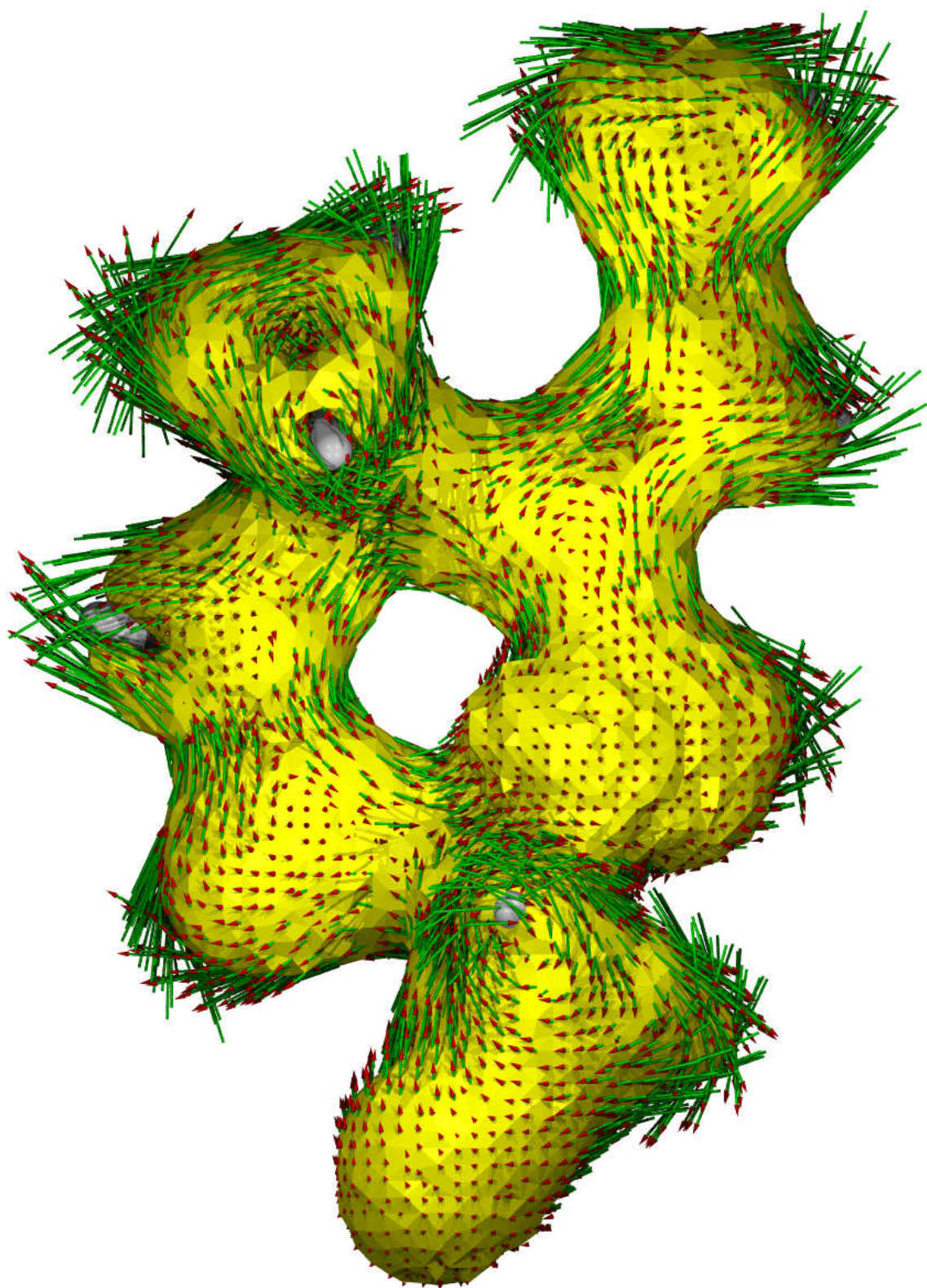


Figure S8. Computed ACID plots of **19rad.anion** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

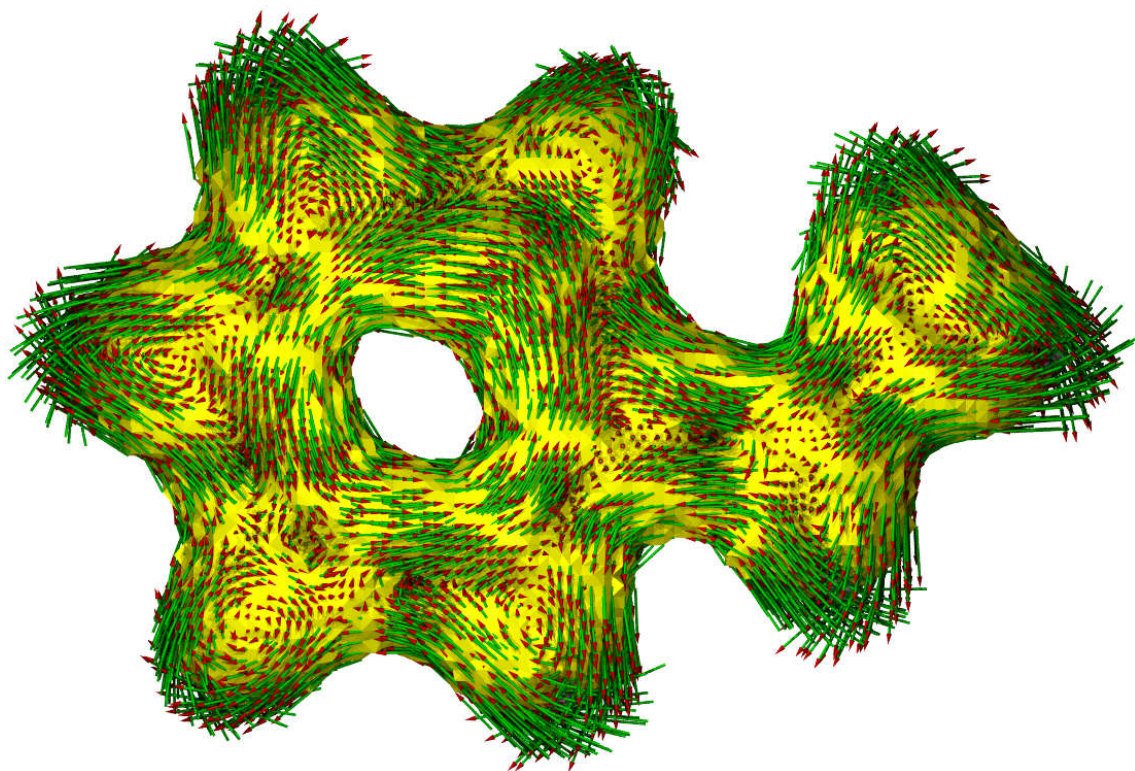


Figure S9. Computed ACID plots of **20** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

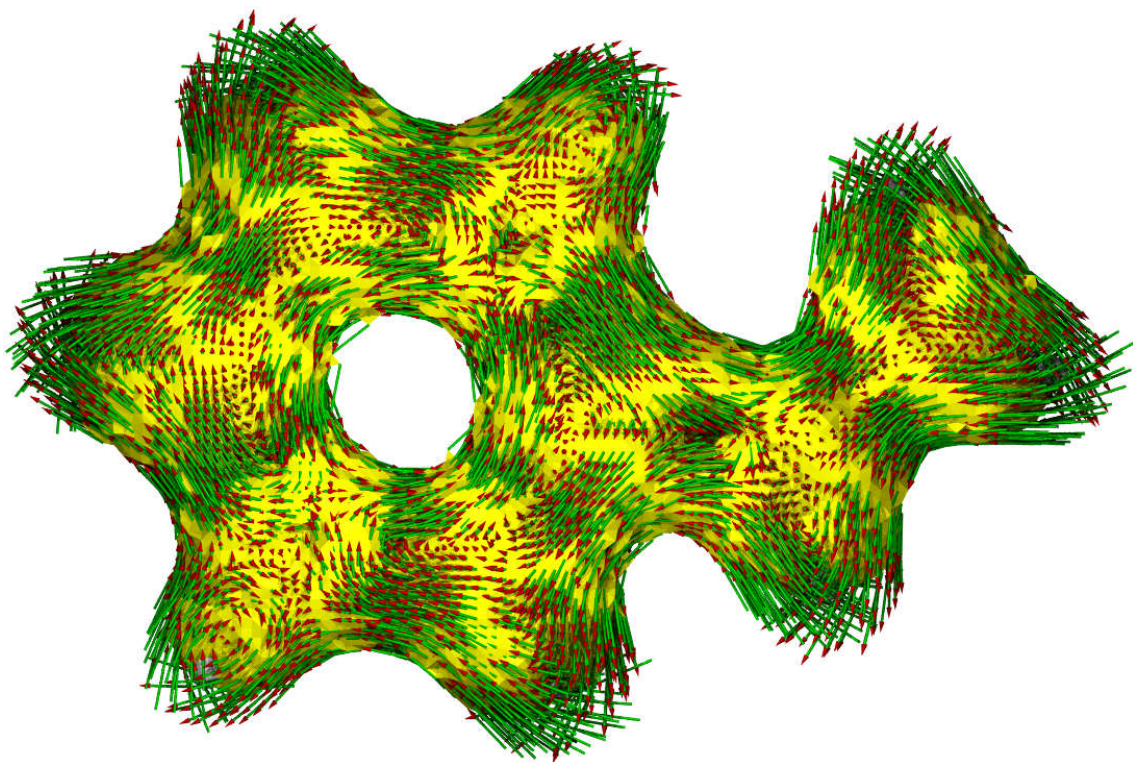


Figure S10. Computed ACID plots of **20rad.anion** with isosurface values of 0.03 a.u. Aromatic species exhibit clockwise ring currents. Antiaromatic species exhibit anticlockwise ring currents.

Cartesian Coordinates of Models Described in the Text.

1

The number of imaginary frequencies is 0

E (OPBE) = -287.5310483 a.u.

C -0.23338700 0.28243100 0.00000400
C 0.82943500 1.17588800 0.00000000
H 0.73354900 2.25099100 0.00000200
C 1.68503200 -0.90476600 -0.00000900
H 2.29522300 -1.79352500 -0.00001400
C 2.03352700 0.42908700 -0.00000100
H 3.03945900 0.81823200 0.00000000
N 0.31706300 -0.98343500 -0.00000500
H -0.21073500 -1.83964100 -0.00000600
C -1.65415700 0.55495700 0.00001000
H -1.89635500 1.61418600 0.00002200
C -2.65892400 -0.33056500 0.00000100
H -3.69087600 -0.00406700 0.00000600
H -2.49886400 -1.40431700 -0.00001100

1.rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -287.5069998 a.u.

C -0.24717100 0.34094600 0.02690000
C 0.89271000 1.18857300 0.03567000
H 0.86202000 2.27018400 0.05114200
C 1.66254400 -0.95054000 -0.05397300
H 2.24775600 -1.85458800 0.04483400
C 2.04923800 0.37547800 -0.00882100
H 3.07587300 0.72367800 0.01979300
N 0.25368400 -0.98359200 0.06124800
H -0.29212200 -1.68029900 -0.43377200
C -1.62974500 0.59995900 -0.03602300
H -1.89864400 1.64477500 -0.19347000
C -2.65926600 -0.35608300 -0.00192000
H -3.69899300 -0.04816700 -0.06394200
H -2.48153600 -1.36043800 0.37568400

2

The number of imaginary frequencies is 0

E (OPBE) = -630.3565388 a.u.

C -0.37627000 0.43025700 0.00000300
C 0.61074900 1.38803700 0.00000600
H 0.38853000 2.44772800 0.00001300
C 1.94281400 -0.50912300 -0.00000700

H 2.79333900 -1.17313000 -0.00001300
C 1.92882700 0.85538400 0.00000000
H 2.82595100 1.46005300 0.00000000
C -1.80933700 0.66727400 0.00000800
H -2.07795500 1.72126000 0.00001400
C -2.78646900 -0.24513600 0.00000500
H -3.82703700 0.05367800 0.00000900
H -2.58522600 -1.31109400 -0.00000100
S 0.33878200 -1.16991600 -0.00000700

2.rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -630.3493881 a.u.

C -0.39986900 0.46569800 0.00000300
C 0.66073000 1.40819600 0.00000600
H 0.46720800 2.47595500 0.00001200
C 1.97136700 -0.53772500 -0.00000800
H 2.81756600 -1.20676800 -0.00001300
C 1.94405000 0.84628900 0.00000000
H 2.85260900 1.44321000 0.00000100
C -1.78922900 0.68152900 0.00000800
H -2.06311600 1.73953600 0.00001400
C -2.82596100 -0.23497300 0.00000500
H -3.85941800 0.09400000 0.00000900
H -2.64625900 -1.30499400 0.00000000
S 0.31655500 -1.18843900 -0.00000700

3

The number of imaginary frequencies is 0

E (OPBE) = -307.3753266 a.u.

C -0.21766400 0.32156700 0.00000200
C 0.85703400 1.17071000 0.00000200
H 0.81042800 2.24828200 0.00000700
C 1.58946100 -0.93243700 -0.00001000
H 2.08663700 -1.88766800 -0.00001700
C 2.02902000 0.35356400 0.00000100
H 3.05707600 0.67865000 0.00000400
C -1.64121500 0.56575700 0.00000700
H -1.91308500 1.61725300 0.00001300
C -2.59624700 -0.37022800 0.00000400
H -3.64401800 -0.09793600 0.00000700
H -2.35371200 -1.42603100 -0.00000200
O 0.22929300 -0.97326800 -0.00000700

3.rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -307.3591149 a.u.

C -0.23911000 0.33110800 0.00032600
C 0.89365400 1.18022600 0.00051200
H 0.86506900 2.26043800 -0.00108100
C 1.61822500 -0.94991600 -0.00090900
H 2.12159100 -1.90246000 0.00249500
C 2.04064700 0.35491700 -0.00023100
H 3.07398300 0.68004400 -0.00041400
C -1.61976600 0.56888000 -0.00008100
H -1.87807400 1.62843800 -0.00000300
C -2.66418700 -0.36000300 0.00070200
H -3.69874200 -0.03288200 -0.00338300
H -2.47312800 -1.42668400 -0.00151700
O 0.22656500 -0.99477000 0.00024800

4

The number of imaginary frequencies is 0

E (OPBE) = -241.5662565 a.u.

C -0.56929600 0.71556300 -0.00013000
C 0.32125100 1.75370400 0.00012000
H -0.01763800 2.78352100 0.00023800
C 1.96058100 0.06841000 -0.00006400
H 2.91866200 -0.42768800 -0.00008800
C 1.70588700 1.40165200 -0.00027600
H 2.49701100 2.14167000 -0.00039000
C -2.01403000 0.81909300 -0.00014900
H -2.38000700 1.84434100 -0.00013000
C -2.90490700 -0.17835500 -0.00014800
H -3.96855800 0.02297700 -0.00013700
H -2.60711500 -1.22159700 -0.00013700
Se 0.36943300 -0.95951800 0.00013300

4.rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -241.5646113 a.u.

C -0.58878600 0.76152700 0.00025300
C 0.38758100 1.78134400 0.00012900
H 0.08471600 2.82485600 0.00001400
C 2.00358500 0.03316700 0.00039600
H 2.95463300 -0.47521400 0.00050100
C 1.73541200 1.38709000 0.00010200

H 2.54287000 2.11695600 -0.00002900
C -1.98766800 0.84823000 0.00029400
H -2.35396000 1.87919900 0.00043500
C -2.94192800 -0.15159800 0.00017900
H -3.99962000 0.08713800 0.00022900
H -2.67144600 -1.20239500 0.00002100
Se 0.34687200 -0.97615000 -0.00027300

5

The number of imaginary frequencies is 0

E (OPBE) = -271.4624510 a.u.

C 0.26957400 0.27147400 -0.00000200
C -0.73542800 1.18636700 -0.00000300
H -0.60291100 2.26148600 -0.00000900
C -1.83322500 -0.82356700 0.00000900
H -2.59454400 -1.59155200 0.00001500
C -2.02873600 0.50941200 0.00000000
H -2.98585300 1.01499200 -0.00000200
C 1.68927800 0.55856700 -0.00000700
H 1.94697900 1.61586200 -0.00001300
C 2.68152700 -0.34178400 -0.00000500
H 3.71986600 -0.03374700 -0.00000800
H 2.49083400 -1.40965900 0.00000200
H -0.05219600 -1.69078100 -0.87813500
H -0.05219200 -1.69077000 0.87815500
C -0.35465300 -1.10644100 0.00000700

5.rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -271.4572554 a.u.

C 0.27545700 0.29488000 -0.00000200
C -0.80833100 1.20347600 -0.00000400
H -0.71093400 2.28481500 -0.00001000
C -1.81400800 -0.87293600 0.00000900
H -2.56400100 -1.65516300 0.00001500
C -2.03551900 0.49115300 0.00000000
H -3.01652600 0.96151900 -0.00000100
C 1.65539100 0.57005900 -0.00000700
H 1.91355300 1.63358900 -0.00001300
C 2.71350400 -0.32009200 -0.00000400
H 3.74122500 0.02944600 -0.00000800
H 2.55956200 -1.39475000 0.00000200
H 0.03098200 -1.69478000 -0.87625300
H 0.03098500 -1.69476900 0.87627400

C -0.31730200 -1.11152400 0.00000700

6

The number of imaginary frequencies is 0

E (OPBE) = -522.8065937 a.u.

C 0.47768900 0.41498200 -0.00000300
C -0.45794200 1.39891700 -0.00000600
H -0.19536000 2.45488100 -0.00001300
C -2.14252800 -0.32755700 0.00000700
H -3.15167500 -0.71891400 0.00001200
C -1.87604200 0.99474500 0.00000000
H -2.64901600 1.75933000 -0.00000200
C 1.90638400 0.66416300 -0.00000900
H 2.20750200 1.71176500 -0.00001500
C 2.86335000 -0.27340100 -0.00000600
H 3.91386700 -0.00905100 -0.00001100
H 2.62836900 -1.33314000 0.00000000
H -0.25024300 -2.05189000 -1.20398100
H -0.25023600 -2.05187700 1.20400400
Si -0.49133400 -1.21372900 0.00000800

6rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -522.8275171 a.u.

C 0.47259100 0.40232700 -0.00002300
C -0.51204600 1.41860000 0.00006200
H -0.24134900 2.47513000 0.00006600
C -2.13351100 -0.36734600 0.00008800
H -3.14379300 -0.76110700 0.00010200
C -1.86956300 1.00594000 -0.00013500
H -2.66782600 1.74986400 -0.00023700
C 1.87329400 0.64812800 -0.00003400
H 2.15318800 1.70897100 0.00028000
Si -0.48795700 -1.20759000 0.00009800
H -0.20225300 -2.12955000 1.16792100
H -0.20222300 -2.12966700 -1.16762600
C 2.91071200 -0.23976300 -0.00019000
H 3.94187100 0.09868000 -0.00007400
H 2.74492400 -1.31336900 -0.00040400

7

The number of imaginary frequencies is 0

E (OPBE) = -237.1705130 a.u.

C 0.68780900 0.67759700 -0.00000700

C -0.14020500 1.74882300 -0.00001200

H 0.24069100 2.76810400 -0.00001900

C -2.05334200 0.26002900 -0.00000300

H -3.10549800 0.00803600 -0.00000300

C -1.59734000 1.52509300 0.00000500

H -2.25963800 2.38738400 0.00000700

C 2.13247400 0.76291100 -0.00001200

H 2.54749700 1.77126700 -0.00002100

C 2.98098800 -0.27384500 -0.00000900

H 4.05408200 -0.12655400 -0.00001500

H 2.62937500 -1.30071100 -0.00000100

H -0.34861200 -1.82834500 -1.25718000

H -0.34860400 -1.82833000 1.25720600

Ge -0.48348700 -0.93920300 0.00000800

7rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -237.1873968 a.u.

C 0.68161700 0.67326000 -0.00000600

C -0.20761300 1.76783400 -0.00000100

H 0.16778600 2.79163000 -0.00000400

C -2.06264700 0.19965300 0.00001300

H -3.11220900 -0.06722600 0.00002100

C -1.60565600 1.51364000 -0.00001400

H -2.30022900 2.35547100 -0.00002200

C 2.09467700 0.75861500 -0.00001100

H 2.48701800 1.78350800 -0.00001300

C 3.03265900 -0.23768300 -0.00001100

H 4.09382300 -0.01142600 -0.00001200

H 2.75101300 -1.28674200 -0.00000800

H -0.29699100 -1.91879600 -1.22084500

H -0.29698400 -1.91878400 1.22086600

Ge -0.47160800 -0.93061100 0.00000600

8

The number of imaginary frequencies is 0

E (OPBE) = -475.1164665 a.u.

C -0.52189700 0.33812700 0.00000300

C 0.41214100 1.32183200 0.00000600

H 0.14085900 2.37870800 0.00001200

C 2.26750800 -0.30741400 -0.00000800

H 3.32596800 -0.54032600 -0.00001100

C 1.86328400 0.98243000 0.00000000

H 2.56308200 1.81841000 0.00000200

C -1.94503800 0.61533700 0.00000900
H -2.23897900 1.66681100 0.00001500
C -2.91354200 -0.31246400 0.00000700
H -3.96211400 -0.03914500 0.00001100
H -2.68444000 -1.37370400 0.00000000
H 0.23200500 -2.83944400 -0.00001700
Al 0.58837600 -1.29987700 -0.00000900

8rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -475.1521162 a.u.

C -0.51705900 0.27648100 -0.00009200
C 0.41188300 1.31905600 0.00018600
H 0.08242700 2.36374400 0.00036900
C 2.26604700 -0.28017900 -0.00039300
H 3.33763500 -0.46804100 -0.00063300
C 1.82272200 1.03648000 0.00010900
H 2.51422300 1.88444800 0.00021400
C -1.92677000 0.57040700 -0.00012500
H -2.18146100 1.63947700 -0.00013100
C -2.97442100 -0.28578100 -0.00011800
H -3.99937000 0.07287900 -0.00013100
H -2.82671500 -1.36207100 -0.00009300
H 0.33550900 -2.89059600 0.00052600
Al 0.63410300 -1.31220200 0.00019100

9

The number of imaginary frequencies is 0

E (OPBE) = -234.8093332 a.u.

C -0.72496200 0.62218200 0.00021400
C 0.09755600 1.69547000 -0.00002900
H -0.28524900 2.71638700 -0.00040900
C 2.10573800 0.27012000 0.00058000
H 3.17878100 0.12142400 0.00085400
C 1.57508600 1.50809700 -0.00002300
H 2.18949900 2.40783800 -0.00036200
C -2.16866600 0.72026100 0.00024800
H -2.58780500 1.72848500 0.00029600
C -3.01846800 -0.31733300 0.00021100
H -4.09216500 -0.17181900 0.00024000
H -2.66212400 -1.34271400 0.00015000
H 0.34798900 -2.52380700 -0.00066300
Ga 0.53914100 -0.96543800 -0.00023600

9rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -234.8444494 a.u.

C -0.72962600 0.55504200 0.00004100
C 0.07368500 1.69112900 -0.00003400
H -0.37017300 2.69182900 -0.00009400
C 2.08657300 0.30729200 0.00007800
H 3.17034300 0.21460600 0.00011900
C 1.50780800 1.56380800 0.00002100
H 2.10624400 2.47919300 0.00000300
C -2.16237000 0.66186500 0.00005300
H -2.55164500 1.68986600 0.00005500
C -3.09276000 -0.32122700 0.00005300
H -4.15492200 -0.09580800 0.00005800
H -2.80734500 -1.36931000 0.00004600
H 0.45765500 -2.55564000 -0.00012800
Ga 0.58225800 -0.96136100 -0.00004300

10

The number of imaginary frequencies is 0

E (OPBE) = -257.5634036 a.u.

C -0.30634900 -0.21599900 -0.00000200
C 0.68473700 -1.13591400 -0.00000500
H 0.55551700 -2.21441600 -0.00001100
C 1.96573900 0.85783700 0.00000900
H 2.83404500 1.50365700 0.00001400
C 2.03811800 -0.48935400 0.00000300
H 2.95070200 -1.07966200 0.00000200
C -1.72271900 -0.51252400 -0.00000600
H -1.99943300 -1.56655500 -0.00001300
C -2.70155600 0.40549200 -0.00000400
H -3.74578500 0.11638700 -0.00000800
H -2.48449600 1.46763400 0.00000200
H -0.06288500 2.28363300 0.00001300
B 0.44090200 1.20641900 0.00000800

10rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -257.6173990 a.u.

C -0.29047300 -0.14166800 -0.00000100
C 0.70484700 -1.12112100 -0.00000700
H 0.51961900 -2.19649000 -0.00001500
C 1.96186200 0.84946400 0.00000800
H 2.85871100 1.46689700 0.00001300

C 2.02401200 -0.53813000 0.00000400
H 2.93490600 -1.13806400 0.00000500
C -1.69048300 -0.47790300 -0.00000500
H -1.91079000 -1.55281900 -0.00001200
C -2.76284200 0.34757500 -0.00000300
H -3.77687300 -0.04224100 -0.00000800
H -2.64468700 1.42656300 0.00000200
H -0.01099300 2.34290200 0.00001200
B 0.46971500 1.23679000 0.00000700

11

The number of imaginary frequencies is 0

E (OPBE) = -574.0834263 a.u.

C -0.41737500 0.42596100 0.02999000
C 0.53634100 1.39852400 -0.01537200
H 0.29469700 2.45639700 -0.05082400
C 2.02984800 -0.42420500 0.04285000
H 2.96650800 -0.96493900 0.03677000
C 1.90567600 0.92175200 -0.01749000
H 2.74928100 1.60229500 -0.06277300
H 0.22336100 -1.67001400 1.23803700
C -1.84867300 0.66602700 0.05465700
H -2.13635000 1.71009800 0.16824900
C -2.81425200 -0.25618500 -0.04151800
H -3.86046600 0.02087700 -0.00277100
H -2.59289300 -1.31034700 -0.17286400
P 0.40043200 -1.21570700 -0.09816900

11rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -574.0946659 a.u.

C -0.41976800 0.43013300 -0.01285700
C 0.59011100 1.41782700 0.03169900
H 0.35617400 2.48071500 0.03594900
C 2.02799900 -0.46190200 -0.01769000
H 2.95998500 -1.00529400 -0.11060200
C 1.90876800 0.92552800 0.01696100
H 2.77170300 1.59010200 -0.00571700
H 0.16627800 -1.63828000 1.31076100
C -1.81738400 0.66401400 -0.00615000
H -2.09239900 1.72353100 0.03287300
C -2.85454200 -0.23001500 -0.01447700
H -3.88545700 0.10861200 -0.01025900
H -2.68588700 -1.30146600 -0.05900800

P 0.38656600 -1.22876200 -0.07859400

12

The number of imaginary frequencies is 0

E (OPBE) = -238.9945894 a.u.

C -0.62198900 0.70851700 0.02710900
C 0.22524000 1.76662500 -0.01815700
H -0.13588200 2.79128700 -0.05455500
C 2.00003200 0.17847800 0.05292700
H 3.01599100 -0.19298300 0.05109300
C 1.65199300 1.47734600 -0.01225000
H 2.38080900 2.28171600 -0.05249200
H 0.33322600 -1.28124000 1.43776400
C -2.06717400 0.79883300 0.03679300
H -2.46620800 1.81113800 0.09731500
C -2.92950500 -0.22424800 -0.01803500
H -3.99974500 -0.05968200 0.00034200
H -2.59519700 -1.25401200 -0.09080600
As 0.42167900 -0.97968300 -0.05451500

12rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -239.0070049 a.u.

C -0.61937900 0.71496200 -0.00485000
C 0.29196900 1.78802800 0.02274100
H -0.05502800 2.82070200 0.02015900
C 2.01075400 0.12368500 0.00357100
H 3.01999400 -0.26427900 -0.05059000
C 1.66668500 1.46660100 0.01710900
H 2.42210500 2.25308900 -0.00206000
H 0.26492000 -1.33504000 1.47829300
C -2.02946200 0.80308300 -0.00934000
H -2.41132400 1.83078000 -0.00438600
C -2.97454700 -0.18998900 0.00144000
H -4.03382000 0.04427600 -0.00846800
H -2.70021900 -1.24041500 -0.00639900
As 0.40658300 -0.98022200 -0.04880500

13

The number of imaginary frequencies is 0

E (OPBE) = -236.7225007 a.u.

C 1.00214100 0.75409900 -0.00001400
C 0.38068000 1.95703700 -0.00001700
H 0.95774800 2.88134500 -0.00002200

C -1.87224900 0.97121000 -0.00003000
H -2.95263500 1.04034600 -0.00004000
C -1.09089200 2.06667200 0.00001600
H -1.51589900 3.06895700 0.00002300
C 2.44123500 0.59921400 -0.00002200
H 3.01944400 1.52461200 -0.00003200
C 3.10773100 -0.56302200 -0.00001900
H 4.19037200 -0.59655600 -0.00002900
H 2.59101400 -1.51810900 -0.00001100
H -0.65435400 -1.74260500 -1.39202700
H -0.65434700 -1.74258100 1.39206800
Sn -0.57586400 -0.75253300 0.00001200

13rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -236.7412165 a.u.

C 0.98666900 0.75483100 -0.00000900
C 0.29588600 1.98373900 -0.00002300
H 0.86116600 2.91793900 -0.00003400
C -1.91193900 0.88945300 -0.00002000
H -2.99443000 0.93236600 -0.00002700
C -1.12506900 2.03825100 0.00002000
H -1.59561900 3.02430000 0.00003000
C 2.39691400 0.61972800 -0.00001600
H 2.94276900 1.57262300 -0.00003100
C 3.17214600 -0.50634000 -0.00001200
H 4.25526400 -0.44547300 -0.00002400
H 2.73365900 -1.50080100 0.00001000
H -0.61954200 -1.87136500 -1.34389400
H -0.61953500 -1.87134900 1.34392500
Sn -0.55702700 -0.74872400 0.00000800

14

The number of imaginary frequencies is 0

E (OPBE) = -236.7411239 a.u.

C 1.35356400 0.71962500 -0.00003700
C 0.99839700 2.02354700 -0.00003400
H 1.76165200 2.80140800 -0.00003800
C -1.42115300 1.57059800 -0.00008400
H -2.45963700 1.87624100 -0.00011000
C -0.41137200 2.45530200 0.00004400
H -0.60035700 3.52763100 0.00006700
C 2.72539500 0.26106700 -0.00003200
H 3.48365100 1.04626300 -0.00004500

C 3.13701900 -1.01376600 -0.00003500
H 4.18972100 -1.26885300 -0.00004700
H 2.43400100 -1.84103100 -0.00002900
H -0.85737100 -1.43088300 -1.42916600
H -0.85734700 -1.43084500 1.42922700
Pb -0.55348100 -0.48022200 0.00001500

14rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -236.7568897 a.u.

C 1.32363000 0.76081800 -0.00000300
C 0.86447300 2.09029800 0.00002300
H 1.59680400 2.90006600 0.00002900
C -1.52703700 1.46983200 0.00008600
H -2.57983600 1.72259700 0.00012300
C -0.51880900 2.42209400 -0.00007700
H -0.77983800 3.48334700 -0.00011500
C 2.67345800 0.34780000 0.00000300
H 3.39200600 1.17871300 0.00001500
C 3.22013300 -0.90840900 -0.00000100
H 4.29503800 -1.05355700 0.00000700
H 2.59957200 -1.80027700 -0.00001000
H -0.82988300 -1.58379900 -1.38647300
H -0.82986600 -1.58381100 1.38646200
Pb -0.52535500 -0.49216900 -0.00000300

15

The number of imaginary frequencies is 0

E (OPBE) = -234.6094881 a.u.

C 1.00955100 0.70429000 -0.00006100
C 0.36504600 1.89390800 -0.00013500
H 0.92100800 2.83327200 -0.00003200
C -1.92466400 0.91872800 0.00015900
H -3.00086500 1.04829400 0.00012100
C -1.11923700 1.99943200 -0.00004400
H -1.52407900 3.01203200 -0.00017600
C 2.45365800 0.59819000 0.00015100
H 3.01010400 1.53837700 0.00045500
C 3.15178000 -0.54675400 -0.00004900
H 4.23531800 -0.55283700 0.00007100
H 2.65591200 -1.51299900 -0.00029900
H -0.72350600 -2.48368900 0.00004900
In -0.59572900 -0.76100500 -0.00000600

15rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -234.6428332 a.u.

C 1.04901900 0.62455400 0.04102200
C 0.50067400 1.87779600 0.00384700
H 1.14723700 2.76415600 -0.04783300
C -1.83170600 1.07953300 0.06997300
H -2.89326700 1.32796000 0.03821700
C -0.94223500 2.10895700 0.00584800
H -1.26563900 3.15434400 -0.05708800
C 2.48832700 0.48414200 0.03592400
H 3.05998200 1.42210800 0.08419500
C 3.20503500 -0.65503200 -0.01406500
H 4.29102200 -0.64492400 -0.00779200
H 2.71603000 -1.62330400 -0.06526500
H -0.89044100 -2.17194600 1.03753500
In -0.67305300 -0.76220600 -0.03749500

16

The number of imaginary frequencies is 0

E (OPBE) = -234.6667293 a.u.

C -1.33914400 0.71044700 0.00002400
C -0.94761800 2.00226000 0.00002600
H -1.68252100 2.80894800 0.00003500
C 1.48406400 1.50453700 0.00002400
H 2.51743400 1.83097200 0.00002200
C 0.48310700 2.40179400 0.00001400
H 0.68238700 3.47366800 0.00001500
C -2.72804400 0.30670500 0.00003000
H -3.46436000 1.11433900 0.00003800
C -3.18111700 -0.95543100 0.00002700
H -4.24136100 -1.17879100 0.00003200
H -2.50072000 -1.80164100 0.00002000
H 1.01787000 -2.13468500 -0.00005800
Tl 0.55609600 -0.49302100 -0.00001200

16rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -234.6968727 a.u.

C 1.42896200 0.58108700 0.04515900
C 1.18332600 1.91824200 0.00965000
H 2.01768900 2.63252500 -0.03652800
C -1.27725700 1.71353500 0.06325700
H -2.24809000 2.21026800 0.02085700

C -0.16833000 2.48804300 0.00624800
H -0.22691600 3.58158300 -0.05342400
C 2.79404700 0.10670600 0.03209500
H 3.57293500 0.88315000 0.06839900
C 3.21699500 -1.17024700 -0.01560600
H 4.27402600 -1.41993500 -0.01948100
H 2.50885800 -1.99219900 -0.05545300
H -1.12899000 -1.64665900 1.24165000
Tl -0.63995000 -0.47003600 -0.02482500

17

The number of imaginary frequencies is 0

E (OPBE) = -238.2088348 a.u.

C -0.94805900 0.79585300 0.02026200
C -0.32360100 1.99806700 -0.01258900
H -0.89622200 2.92404000 -0.03608600
C 1.84451300 0.92081300 0.04004100
H 2.92678200 0.89360500 0.03334700
C 1.13475800 2.06294500 -0.01018100
H 1.61806200 3.03718000 -0.04167000
H 0.52802800 -1.03143000 1.65793200
C -2.38673800 0.63226400 0.02606900
H -2.95974500 1.55944800 0.06793800
C -3.05849400 -0.52579300 -0.01294000
H -4.14114500 -0.55139500 -0.00139400
H -2.54979700 -1.48349700 -0.06315600
Sb 0.54705400 -0.79711500 -0.03766400

17rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -238.2255264 a.u.

C -0.93092700 0.80608300 0.00747600
C -0.23416300 2.02849100 0.02932300
H -0.78779900 2.96886900 0.02789100
C 1.88335300 0.83957700 -0.01034900
H 2.96355700 0.77896000 -0.06631400
C 1.17926900 2.03519300 0.01342400
H 1.70600800 2.99172700 -0.00474600
H 0.47837100 -1.15360500 1.70005500
C -2.33865300 0.66302700 -0.00639700
H -2.88268400 1.61608600 -0.00070300
C -3.11399600 -0.46482700 -0.01030400
H -4.19685500 -0.40223900 -0.02512600
H -2.67695600 -1.45933800 -0.01754000

Sb 0.52406000 -0.79972000 -0.03436400

18

The number of imaginary frequencies is 0

E (OPBE) = -238.1684833 a.u.

C -1.35086900 0.72808000 0.02168200

C -1.03727500 2.04381800 -0.01013500

H -1.82490900 2.79720600 -0.03661800

C 1.36033500 1.60530500 0.03936200

H 2.40462800 1.89373900 0.03790700

C 0.35360400 2.49386500 -0.00495000

H 0.54460900 3.56590800 -0.03150300

H 0.60864300 -0.69639600 1.78007100

C -2.70535100 0.21966500 0.01269300

H -3.48894600 0.97956500 0.01808800

C -3.07493300 -1.06790400 -0.00015900

H -4.11864200 -1.35709500 -0.00476000

H -2.34667900 -1.87323300 -0.00690300

Bi 0.56564100 -0.49935800 -0.02538800

18rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -238.1844724 a.u.

C -1.31531000 0.76687400 0.00418300

C -0.91624700 2.11202200 0.02596400

H -1.67779700 2.89516100 0.03267600

C 1.45152300 1.51334500 -0.00884600

H 2.50962300 1.74904600 0.01183700

C 0.45248300 2.47145700 0.02143400

H 0.70962300 3.53399800 0.02914700

H 0.61014700 -0.90420300 1.83333900

C -2.65197400 0.30304800 -0.01726000

H -3.39974800 1.10659700 -0.05276000

C -3.15068300 -0.97034100 0.00937000

H -4.21901300 -1.15612800 -0.01638300

H -2.49936200 -1.83877600 0.05332100

Bi 0.53913000 -0.51282100 -0.02530400

19

The number of imaginary frequencies is 0

E (OPBE) = -467.9754746 a.u.

C 0.48435900 1.83495300 0.00000000

C -0.75974300 0.98787900 0.00000000

C -0.83801600 -0.35673800 0.00000000

C 0.42400500 -1.22761600 0.00000000

C 1.67190000 -0.36777800 0.00000000

C 1.71015100 0.95964700 0.00000000

H -1.69142900 1.55197100 0.00000000

H 2.60576100 -0.92653300 0.00000000

H 2.66989300 1.47217000 0.00000000

C -2.19704300 -0.92649000 0.00000000

H -2.97053700 -0.16033600 0.00000000

C -2.62187400 -2.19518800 0.00000000

H -1.96561100 -3.05408700 0.00000000

H -3.68448000 -2.40917800 0.00000000

C 0.48923500 -2.11552600 1.27092200

H 0.46075000 -1.49630100 2.17036600

H -0.33469100 -2.82680700 1.32437600

H 1.42508500 -2.68272700 1.28041000

C 0.48923500 -2.11552600 -1.27092200

H -0.33469100 -2.82680700 -1.32437600

H 0.46075000 -1.49630100 -2.17036600

H 1.42508500 -2.68272700 -1.28041000

C 0.48923500 2.73884500 1.25885800

H 1.37983300 3.37497400 1.27127200

H -0.38975000 3.39083400 1.27236400

H 0.48493200 2.13711100 2.17018900

C 0.48923500 2.73884500 -1.25885800

H -0.38975000 3.39083400 -1.27236400

H 1.37983300 3.37497400 -1.27127200

H 0.48493200 2.13711100 -2.17018900

19rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -467.9606072 a.u.

C 1.89869500 -0.24233300 0.00023700

C 0.67479600 -1.11187600 0.00363600

C -0.67210200 -0.69034600 0.00075100

C -0.97888700 0.81430500 0.00007500

C 0.27276600 1.66364800 -0.00022900

C 1.52724900 1.21854600 -0.00032200

H 0.86990300 -2.18437800 0.00470300

H 0.09305900 2.74072900 -0.00070600

H 2.35370400 1.93125800 -0.00089900

C -1.72482100 -1.64175800 0.00011500

H -1.34988200 -2.66954200 0.00026700

C -3.11817800 -1.55256200 -0.00009300

H -3.67904500 -0.62655700 -0.00009500

H -3.70973100 -2.46300600 -0.00031100
C -1.77947200 1.20930600 -1.27032600
H -1.17345500 1.01705000 -2.15991700
H -2.69684900 0.62424800 -1.35641200
H -2.04086200 2.27693400 -1.25698400
C -1.77958700 1.20978100 1.27030300
H -2.69687800 0.62456700 1.35642700
H -1.17349600 1.01786200 2.15990400
H -2.04112000 2.27738300 1.25665900
C 2.77690200 -0.52071400 -1.25564300
H 3.69474600 0.08800800 -1.26847000
H 3.07359100 -1.57543700 -1.27816500
H 2.20655600 -0.31189300 -2.16356000
C 2.78194800 -0.51862100 1.25284600
H 3.07838300 -1.57339700 1.27618700
H 3.70001800 0.08981100 1.26049200
H 2.21551800 -0.30790700 2.16279000

C 2.41587500 -0.20587300 0.00005300
H -0.19697900 2.31500400 0.00004600
H 2.07980800 -2.30810200 -0.00002800
H 3.50203300 -0.35777900 0.00011400
C -2.00318500 0.46450500 -0.00010600
H -2.28622200 1.52242800 -0.00049800
C -3.00887300 -0.42823300 0.00016700
H -2.82124200 -1.49600100 0.00050800
H -4.04595400 -0.10461600 0.00004500
H -0.61293000 -2.18939500 -0.00022900
H 2.51703000 2.19306700 0.00014300
B 0.07595700 -1.19517600 -0.00011800
B 1.81146900 1.20720900 0.00007100

20

The number of imaginary frequencies is 0

E (OPBE) = -283.0063489 a.u.

C -0.25189500 -1.35878500 0.02163500
C 0.57859200 -0.27552900 0.01126200
C -1.62757200 1.32167300 -0.04013200
C -2.42519700 0.23036800 -0.03002700
H 0.20150200 -2.35196900 0.02094400
H -2.07579500 2.31464300 -0.07642200
H -3.50735700 0.36028400 -0.05882200
C 2.02865100 -0.46959500 -0.02033300
H 2.36140300 -1.50692600 -0.04905500
C 2.96058500 0.49417300 -0.02699500
H 2.70370600 1.54565300 0.00284600
H 4.01555100 0.24774500 -0.06027700
H 0.59200200 2.13050000 0.24626300
H -2.49740600 -2.17082800 0.03312400
B -0.08110400 1.16144500 0.07181800
B -1.79341300 -1.20603100 0.01797000

20rad.anion

The number of imaginary frequencies is 0

E (OPBE) = -283.0811366 a.u.

C 0.28685300 1.32894800 0.00001400
C -0.55662700 0.22190100 -0.00007700
C 1.60384600 -1.32037600 -0.00002800