SUPPORTING INFORMATION

The Nucleophilicity N Index in Organic Chemistry

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Table S1. Nucleophilicity (N), inverse of the electrophilicity (N') and Roy's nucleophilicity (N'') indices of substituted unsaturated bicyclic systems. A corresponds to an electron acceptor substituent group and D corresponds to an electron donor one.

А	D	N(eV)	А	D	N'(eV)	А	D	$N^{"}(eV)$
COMe	NH ₂	3.93	CN	NH ₂	0.77	COMe	NH ₂	2.89
CHO	NH ₂	3.81	COMe	NH ₂	0.74	CN	\mathbf{NH}_{2}	2.85
CN	NH_2	3.63	CN	OMe	0.69	CHO	\mathbf{NH}_{2}	2.71
NO ₂	NH_2	3.53	CN	Me	0.68	COMe	OMe	2.65
COMe	OMe	3.52	COMe	OMe	0.67	CN	OMe	2.62
COMe	OH	3.49	CN	OH	0.67	COMe	OH	2.61
СНО	OMe	3.39	COMe	Me	0.67	CN	OH	2.56
СНО	OH	3.32	CHO	NH2	0.66	COMe	Me	2.53
CN	OMe	3.26	COMe	OH	0.65	CHO	OMe	2.49
CN	ОН	3.17	CHO	Me	0.61	CN	Me	2.48
NO ₂	OMe	3.13	CHO	OH	0.61	CHO	OH	2.48
NO ₂	OH	3.06	CHO	OMe	0.60	CHO	Me	2.39
COMe	Me	3.04	NO ₂	NH_2	0.44	NO_2	\mathbf{NH}_{2}	2.15
СНО	Me	2.92	NO ₂	Me	0.43	NO_2	OMe	2.02
CN	Me	2.74	NO ₂	OMe	0.42	NO_2	ОН	1.98
NO ₂	Me	2.57	NO ₂	OH	0.40	NO ₂	Me	1.97

Table S2. Nucleophilicity (N), inverse of the electrophilicity (N') and Roy's nucleophilicity (N'') indices of some alkenes.

	N(eV)	<i>N</i> '(eV)	$N^{"}(eV)$
bicyclo[2.2.1]hepta-2,5-diene (11)	3.22	1.36	3.39
bicyclo[2.2.1]heptene (12)	2.84	1.79	3.54
cyclohexene (13)	2.77	1.98	3.61
but-2-ene (14)	2.76	1.82	3.52
Propene (15)	2.32	1.67	3.28
Ethene (16)	1.86	1.37	2.95

Table S3. Total energies (E, in au) of reagents and TSs associated with the nucleophilic attacks of twelve substituted methoxy bicyclo[2.2.1]hepta-2,5-dienes **10-IIIa-I** on dicyanoethylene.

	А	R	TS
10-IIIe	CHO-BF ₃	-823.903289	-1086.949073
10-IIIf	CHO-BH ₃	-525.974761	-789.021845
10-IIIa	NO_2	-590.500499	-853.549580
10-IIIg	COCF ₃	-836.359578	-1099.409540
10-IIId	CN	-478.246619	-741.296361
10-IIIh	CFO	-598.586018	-861.636241
10-IIIb	СНО	-499.326189	-762.377831
10-IIIi	CF ₃	-723.039378	-986.091326
10-IIIc	COMe	-538.649556	-801.702338
10-IIIj	COOMe	-613.880231	-876.933439
10-IIIk	CONH ₂	-554.703302	-817.757020
10-IIII	Н	-385.997423	-649.053317

The total energy of dicyanoethylene is -263.062684 au.



Figure S1. Transition structures involved in the nucleophilic attacks of twelve substituted methoxy bicyclo[2.2.1]hepta-2,5-dienes **10-IIIa-I** on dicyanoethylene. The distances are given in Å.

Complete citation for reference 29.

- Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.;
- Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.;
- Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.;
- Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.;
- Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H.
- P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin,
- A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.;
- Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M.
- C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.;
- Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.;
- Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.;
- Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.;
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B3LYP/6-31G* computed total energies, unique frequency imaginary, and cartesian coordinates of TSs associated with the nucleophilic attracts of twelve substituted methoxy bicyclo[2.2.1]hepta-2,5-dienes **10-IIIa-I** on dicyanoethylene.

TS-10-IIIa

E(RB+HF-LYP) = -853.549579967 A.U.1 imaginary frequency -270.2369 cm⁻¹

С	0.18724500	0.62809600	-0.36554000
С	-0.72394900	1.52985800	0.47521100
С	-1.29056800	-0.62348400	0.89694700
С	-0.08132500	-0.72253500	-0.07307600
С	-0.85427800	0.61703600	1.73148000
Η	-1.62924000	0.97235200	2.41545800
Η	0.08796300	0.49363300	2.27115800
С	-2.12338500	1.31364900	-0.13457400
С	-2.43824800	0.04032300	0.13299400
Η	-0.40903600	2.56235400	0.61718500
Η	-1.54892600	-1.53896700	1.42610700
С	2.71486800	-0.96091300	0.42270600
С	1.46212000	-1.50600300	0.81493100
Η	1.15118200	-1.29769000	1.83521700
Η	1.29058600	-2.54042400	0.52645700
Η	-0.10918900	-1.43497700	-0.89285700
0	1.08775400	0.97796000	-1.24466000
С	1.54957100	2.34645600	-1.32699800
Н	0.70600000	3.03069700	-1.44881500
Η	2.12911600	2.57096500	-0.42482900
Η	2.18852200	2.37619100	-2.20817600
Η	-2.69112000	2.02893400	-0.71531900
0	-3.68007600	-1.85821300	-0.10073800
С	3.06483300	0.30361500	0.94579000
Ν	3.21682600	1.37667900	1.39143100
С	3.48181600	-1.52788200	-0.62635200
Ν	4.10073900	-2.01293100	-1.48957500
Ν	-3.62699800	-0.64503400	-0.31815200
0	-4.49418300	0.01983200	-0.88568000

TS-10-IIIb

E(RB+HF-LYP) = -762.377830718 A.U.1 imaginary frequency -269.5495 cm⁻¹

С	-0.06639400	0.63625000	-0.41304200
С	-1.02244500	1.53873200	0.36857100
С	-1.62020100	-0.60948800	0.75925300
С	-0.35604200	-0.71065700	-0.13290400
С	-1.23570800	0.63075300	1.61623800
Н	-2.05248200	0.99169900	2.24676700
Н	-0.33155600	0.50836700	2.21852500

С	-2.38159400	1.30849000	-0.32370700
С	-2.73723900	0.03122900	-0.08551300
H	-0.71772800	2.57243700	0.52516900
H	-1.90348300	-1.52600400	1.27647900
С	2.42131300	-0.97440100	0.49222100
С	1.14560800	-1.48274100	0.85481700
Н	0.79804500	-1.23197600	1.85295900
Н	0.96052200	-2.52154900	0.59200600
H	-0.32239100	-1.42961900	-0.94655400
0	0.87769700	0.98263900	-1.24999300
С	1.35146900	2.34713500	-1.30402900
Н	0.51859100	3.03983900	-1.45029400
Н	1.90103400	2.56149100	-0.38081900
Н	2.02239000	2.38003000	-2.16124400
Н	-2.90160100	2.04460500	-0.92779000
С	-3.93640200	-0.65834600	-0.56816200
0	-4.17589500	-1.83036700	-0.33840500
Н	-4.63294700	-0.03489900	-1.16840900
С	2.79347700	0.28917000	1.00368500
Ν	2.97674100	1.36220900	1.43702700
С	3.20461400	-1.58107600	-0.52228100
N	3.83532300	-2.09976600	-1.35709800

TS-10-IIIc

E(RB+HF-LYP) = -801.702338198 A.U.1 imaginary frequency -265.1688 cm⁻¹

С	0.21778900	0.64552000	-0.32916400
С	-0.68943200	1.54003600	0.51592400
С	-1.25209100	-0.60877200	0.93612200
С	-0.04895300	-0.70204600	-0.03629200
С	-0.81713100	0.62873600	1.77115700
Н	-1.59260800	0.98475600	2.45446200
Н	0.12458200	0.50804300	2.31363200
С	-2.09197400	1.30613500	-0.08689000
С	-2.42845100	0.02759600	0.16719100
Н	-0.38061200	2.57523600	0.65508400
Н	-1.49792900	-1.52877800	1.46512400
С	2.77276500	-0.96944500	0.38473000
С	1.52797300	-1.46982500	0.84813200
Н	1.25591900	-1.20876800	1.86665600
Н	1.31679200	-2.50873700	0.60666600
Η	-0.06307800	-1.42120600	-0.85017900
0	1.10114000	0.99913400	-1.22822200
С	1.57011700	2.36371200	-1.30531100
Н	0.72964100	3.05912700	-1.37574600
Н	2.19353500	2.56784200	-0.42778300
Η	2.16953400	2.40645100	-2.21367400
Н	-2.64273400	2.04858000	-0.65345200
С	-3.64033400	-0.72747000	-0.22606500
0	-3.72807400	-1.91627000	0.04658200
С	3.19707800	0.29108000	0.86298300

N	3.43125300	1.36124700	1.27828900
С	3.46872500	-1.58313200	-0.68793600
Ν	4.02716700	-2.10709300	-1.56965300
С	-4.74485300	0.00757000	-0.96426000
Η	-5.10322500	0.86359500	-0.38048600
Η	-4.37897200	0.39475100	-1.92298700
Η	-5.57168600	-0.68105100	-1.14657200

TS-10-IIId

E(RB+HF-LYP) = -741.296360968 A.U. 1 imaginary frequency -265.2931 cm⁻¹

С	-0.13204200	0.56338400	-0.41118700
С	-1.10356700	1.45048600	0.36710900
С	-1.60068100	-0.70396400	0.83922800
С	-0.35762800	-0.78771300	-0.08213200
С	-1.24883500	0.57683700	1.64606000
Н	-2.06345900	0.92330100	2.28681100
Н	-0.32504100	0.50461300	2.22608000
С	-2.47002000	1.15577900	-0.28415800
С	-2.77164400	-0.12549000	-0.00090200
Η	-0.83706900	2.49933500	0.48630300
Н	-1.83262100	-1.61043700	1.39917900
С	2.42915000	-0.91459500	0.49016800
С	1.18198200	-1.47367700	0.88299500
Н	0.84504300	-1.22325600	1.88545400
Η	1.04625400	-2.52646900	0.64587200
Н	-0.32704300	-1.52371900	-0.88091200
0	0.77591700	0.91719300	-1.28071100
С	1.18928100	2.29863300	-1.39657800
Н	0.32405000	2.94753600	-1.55433900
Η	1.74318200	2.57083000	-0.49143600
Н	1.84365600	2.32563600	-2.26648500
Η	-3.03148200	1.84881500	-0.89893300
С	2.73893800	0.38004500	0.96232600
Ν	2.86085800	1.47399000	1.36440000
С	3.22846600	-1.50913200	-0.51849500
Ν	3.87336600	-2.01874100	-1.34804600
С	-3.90703400	-0.86583200	-0.41793700
N	-4.82722400	-1.50414800	-0.73791100

TS-10-IIIe

E(RB+HF-LYP) = -1086.94907283 A.U.1 imaginary frequency -278.2504 cm⁻¹

С	-1.43116700	-0.74410600	-0.44584700
С	-0.85805500	-1.96847400	0.27111200
С	0.28374800	-0.14304900	0.98444300
С	-0.80353400	0.42440900	0.03310800
С	-0.51883000	-1.30396300	1.63965100
Н	0.09451300	-1.95336500	2.26989300
Н	-1.40974400	-0.99072500	2.18926800

С	0.56430400	-2.07032400	-0.30066000
С	1.24935300	-0.98667200	0.13198500
H	-1.45590200	-2.87804500	0.26590500
H	0.75903000	0.58509100	1.64123400
С	-3.41665100	1.38389200	0.54058000
С	-2.07322500	1.49406400	1.00137500
H	-1.88025600	1.08732400	1.99075200
H	-1.61022800	2.46742500	0.85480700
H	-0.53468100	1.19063700	-0.68954300
0	-2.34072700	-0.70315500	-1.38286700
С	-3.17112800	-1.85534800	-1.65854800
Η	-2.55338900	-2.73021900	-1.87782900
H	-3.82548300	-2.02558000	-0.79656600
H	-3.75598400	-1.57877200	-2.53429300
H	0.91611100	-2.85457700	-0.96333100
С	2.61703000	-0.68509100	-0.19186600
0	3.17883600	0.33450400	0.24259000
H	3.18064600	-1.37224500	-0.83375500
С	-4.11788100	0.20845400	0.88514300
Ν	-4.56254000	-0.83545300	1.17894800
С	-3.95678100	2.27552600	-0.41922500
N	-4.38511600	3.02244200	-1.20800700
В	4.83500000	0.66553500	-0.16138300
F	5.15756200	-0.38606400	-0.97459800
F	5.41264500	0.65498100	1.06011800
F	4.72157000	1.86327700	-0.77568400

TS-10-IIIf

E(RB+HF-LYP) = -789.021844740 A.U.1 imaginary frequency -275.2749 cm⁻¹

С	-0.39526700	-0.70789500	-0.43784300
С	0.37174600	-1.79682800	0.31500400
С	1.27713700	0.20494900	0.87321900
С	0.08729300	0.56020100	-0.05725200
С	0.66741300	-1.01131100	1.62761500
Н	1.38779400	-1.53282800	2.26332900
Н	-0.23621700	-0.78771000	2.20032000
С	1.77250700	-1.74182300	-0.31486600
С	2.31820500	-0.55098400	0.02516200
H	-0.09483900	-2.77755800	0.38894000
H	1.67091800	1.03021900	1.46590600
С	-2.61567700	1.20034600	0.51843400
С	-1.28455300	1.51203200	0.91374400
H	-0.99964200	1.19071800	1.91215000
H	-0.95765000	2.52560200	0.69270400
H	0.21785700	1.31189900	-0.83130400
0	-1.34203900	-0.84768200	-1.32800900
С	-2.01855600	-2.11546200	-1.49335900
Н	-1.29816000	-2.91194200	-1.69763900
Н	-2.60348100	-2.31777800	-0.58948600
Н	-2.67601400	-1.97488500	-2.34985200

H	2.20129100	-2.51039400	-0.94947600
С	3.61485200	-0.07931300	-0.37239400
0	4.03430500	1.03838500	-0.01936500
H	4.25817900	-0.71258300	-0.99603800
С	-3.14659700	-0.03126100	0.95972600
Ν	-3.44706700	-1.10101000	1.33228700
С	-3.30052200	1.95305800	-0.46813000
Ν	-3.84954700	2.58815600	-1.27975100
В	5.47491400	1.60010500	-0.42969000
H	5.98324300	0.73022800	-1.10688200
H	6.00719400	1.80027700	0.63863400
Η	5.21523900	2.62630300	-1.01597900

TS- 9-IIIg E(RB+HF-LYP) = -1099.40953954 A.U.1 imaginary frequency -264.7031 cm⁻¹

С	-0.99279400	0.61087900	0.22838000
С	-0.14747500	1.46699400	-0.71574900
С	0.31959900	-0.70487100	-1.14431400
С	-0.79008000	-0.75088100	-0.06243700
С	-0.15927800	0.52968100	-1.95938200
Н	0.55718500	0.85218400	-2.71932100
Н	-1.15097100	0.42551100	-2.40711800
С	1.29445600	1.21042100	-0.23940400
С	1.57538400	-0.08257900	-0.50045600
Н	-0.44178400	2.50729500	-0.84541900
Н	0.49187800	-1.63901300	-1.67815400
С	-3.62789400	-0.94233100	-0.23787000
С	-2.43725500	-1.49966100	-0.77850300
Н	-2.24622300	-1.28723400	-1.82678500
Н	-2.24550300	-2.53819400	-0.51891200
Н	-0.70806900	-1.44908900	0.76600300
0	-1.78025800	1.00118600	1.19618200
С	-2.20099800	2.38079600	1.29767500
H	-1.33617200	3.04923800	1.30176000
Н	-2.88016100	2.59848000	0.46611100
H	-2.72996600	2.44563000	2.24734500
Н	1.91881600	1.94283800	0.25713100
С	2.79020400	-0.84669800	-0.20959200
0	2.90481500	-2.03432300	-0.44429100
С	-4.03323700	0.32291300	-0.71809100
Ν	-4.24147800	1.39355400	-1.14626000
С	-4.26423500	-1.50195300	0.89880700
Ν	-4.77465000	-1.98219600	1.83292800
С	3.98130800	-0.07589000	0.41861800
F	5.01552200	-0.88073800	0.64577200
F	3.61064600	0.49222900	1.58966800
F	4.37840700	0.91929100	-0.40550000

TS-10-IIIh

E(RB+HF-LYP) = -861.636240523 A.U.1 imaginary frequency -266.5353 cm⁻¹

С	0.20783300	0.62850200	-0.34324600
С	-0.70529100	1.51659400	0.50432700
С	-1.25944900	-0.63978800	0.91212300
С	-0.05233800	-0.72449300	-0.05849200
С	-0.83037800	0.59588100	1.75509000
Н	-1.60782200	0.94316500	2.44049600
Н	0.11215500	0.47657000	2.29564400
С	-2.10350300	1.28520100	-0.10166800
С	-2.43054000	0.00491900	0.14810700
Н	-0.39927100	2.55124500	0.65070800
Н	-1.50168200	-1.56209600	1.43998700
С	2.75243800	-0.96621300	0.40097900
С	1.50379800	-1.49932500	0.82109000
Н	1.21083100	-1.27667200	1.84340800
Н	1.32054700	-2.53580500	0.54758500
Н	-0.07109600	-1.43210600	-0.88275600
0	1.09731900	0.98938000	-1.23068500
С	1.55570500	2.35887100	-1.30384700
Н	0.70980700	3.04465300	-1.39829700
Н	2.15466800	2.57200800	-0.41157600
Н	2.17608300	2.40192700	-2.19778200
Н	-2.67158200	2.01687700	-0.66337000
С	-3.63689000	-0.71023000	-0.26161700
0	-3.89253800	-1.86331800	-0.07010100
С	3.12868600	0.29581700	0.91236000
Ν	3.30983300	1.36665800	1.35223800
С	3.49110500	-1.54466300	-0.66210800
Ν	4.08567000	-2.03980900	-1.53675700
F	-4.50738500	0.09970800	-0.92274700

TS-10-IIIi

E(RB+HF-LYP) = -986.091325798 A.U.1 imaginary frequency -262.9245 cm⁻¹

С	0.50987600	0.67374500	-0.37061600
С	-0.35909200	1.67531100	0.39139600
С	-1.02141400	-0.40298500	0.98125500
С	0.17883000	-0.63378900	0.02670500
С	-0.53078700	0.87679500	1.71563100
Н	-1.29027100	1.32196000	2.36317800
Н	0.40259400	0.75062500	2.27073200
С	-1.77104000	1.46409500	-0.20237200
С	-2.15545400	0.23525900	0.15561900
Н	-0.00180900	2.70219700	0.45217800
Н	-1.30597500	-1.26015500	1.59309300
С	2.98167800	-0.99415500	0.49427000
С	1.71314400	-1.40359900	0.98134600
Н	1.44723700	-1.05419700	1.97498400

Н	1.45913000	-2.44802000	0.81689900
Н	0.12415900	-1.41154800	-0.72951700
0	1.41683700	0.90999400	-1.28204900
С	1.94371300	2.24301500	-1.47135100
Н	1.13331600	2.96190100	-1.61604900
Н	2.56367200	2.49707800	-0.60466000
Н	2.55558500	2.18031600	-2.37003800
Н	-2.29338900	2.16905400	-0.83725700
С	-3.40192200	-0.48197800	-0.22021400
С	3.45454600	0.28102100	0.87931300
Ν	3.72679700	1.36984100	1.21515200
С	3.65866600	-1.71938600	-0.51927900
Ν	4.20020200	-2.33539500	-1.35047600
F	-4.22005600	0.27415800	-0.97716300
F	-4.09289400	-0.86857000	0.87683300
F	-3.11176200	-1.60673900	-0.91746000

TS-10-IIIj

E(RB+HF-LYP) = -876.933439177 A.U.1 imaginary frequency -264.2800 cm⁻¹

С	0.56164300	0.65111400	-0.32146500
С	-0.26850100	1.63004800	0.51006600
С	-0.88330300	-0.46635800	1.09252100
С	0.26418900	-0.66477900	0.06840900
С	-0.36046900	0.80170700	1.82528200
Н	-1.08579600	1.22810000	2.52312900
Н	0.60336600	0.67632600	2.32609800
С	-1.70839100	1.41698800	-0.00518000
С	-2.07045600	0.17209100	0.34643700
Н	0.08475900	2.65862800	0.56972900
Н	-1.13291600	-1.34192500	1.69122000
С	3.09737500	-1.01613700	0.35438700
С	1.86557600	-1.43468200	0.92012600
Н	1.66151500	-1.09400000	1.93084200
Н	1.60159600	-2.47748600	0.76199400
Н	0.18498000	-1.43235200	-0.69588000
0	1.40885100	0.91564700	-1.28335300
С	1.91426400	2.25598700	-1.47317400
Н	1.09271900	2.97371100	-1.54128000
Н	2.59279300	2.49223700	-0.64617500
Н	2.46191800	2.22180300	-2.41398700
Н	-2.27320800	2.13359300	-0.58875200
С	3.59756800	0.25366500	0.72311200
Ν	3.89924800	1.33644900	1.05309800
С	3.70413800	-1.72641300	-0.71298300
N	4.18795700	-2.32994200	-1.58787800
С	-3.32152300	-0.55281000	0.05812700
0	-3.51846800	-1.71002500	0.37627800
0	-4.22068200	0.21373600	-0.59740000
С	-5.46502700	-0.43519500	-0.91159700
Н	-5.96631700	-0.76508700	0.00208000

Н	-6.06246900	0.31612000	-1.42827600
Н	-5.29347900	-1.30145600	-1.55589200

TS-10-IIIk

E(RB+HF-LYP) = -817.757019619 A.U.1 imaginary frequency -261.8483 cm⁻¹

С	0.20246500	0.62367300	-0.37669000
С	-0.69640400	1.58238300	0.40727800
С	-1.27801500	-0.52615500	0.97088600
С	-0.07856800	-0.69743500	0.00398400
С	-0.82879700	0.75909800	1.71991400
H	-1.59713100	1.16892800	2.38099200
H	0.11359900	0.66183900	2.26566900
С	-2.10200100	1.32231800	-0.18024900
С	-2.44704100	0.06955700	0.16255700
H	-0.37586600	2.62109000	0.47722000
H	-1.52813000	-1.40844800	1.55931500
С	2.75122400	-0.93743300	0.46393500
С	1.50521700	-1.41657300	0.94273600
H	1.21927100	-1.09796600	1.94087000
H	1.29652800	-2.46673200	0.75448600
H	-0.10422000	-1.47406300	-0.75439800
0	1.09269300	0.90989200	-1.29278500
С	1.56319900	2.26502000	-1.46358100
Н	0.72372600	2.95156200	-1.60137000
H	2.17067900	2.53663200	-0.59341300
Н	2.17860400	2.24014900	-2.36186400
Н	-2.62304800	2.00810100	-0.83931100
С	3.16256300	0.35259800	0.87017500
Ν	3.38489700	1.44769400	1.22211400
С	3.46553200	-1.60958800	-0.56088300
Ν	4.04227300	-2.18059400	-1.40052600
С	-3.61219900	-0.75593100	-0.25039900
0	-3.53865000	-1.97906900	-0.26146500
Ν	-4.72997500	-0.07195200	-0.65582500
H	-4.87582100	0.88546200	-0.37054700
Н	-5.55396000	-0.62837900	-0.84195600

TS-10-IIII

E(RB+HF-LYP) = -649.053317342 A.U.1 imaginary frequency -263.6964 cm⁻¹

С	-0.70061700	0.38219100	-0.43497900
С	-1.93883900	0.80166100	0.35517500
С	-1.92624400	-1.45386800	0.24144800
С	-0.61345000	-1.01722600	-0.45931000
С	-1.98627400	-0.37912200	1.36509900
Н	-2.92416100	-0.39316200	1.92574700
Н	-1.13994000	-0.39702700	2.05814500
С	-3.11775900	0.37904200	-0.55854200
С	-3.10629600	-0.95695400	-0.61945700

H	-1.95900700	1.81655900	0.75022100
H	-1.96149700	-2.50118900	0.54710000
С	2.10798100	-0.67056700	0.44474400
С	0.99932400	-1.53809800	0.59570300
H	0.52436300	-1.55126600	1.57176400
Η	1.10276600	-2.52632600	0.15476900
Η	-0.28397500	-1.50899700	-1.36944900
0	0.16714700	1.14121500	-1.05620800
С	0.22872000	2.55959900	-0.78920300
Η	-0.75996200	3.01571400	-0.88458500
H	0.65053100	2.70886300	0.21065700
H	0.90180800	2.96158100	-1.54540800
H	-3.76202200	1.07558400	-1.08214200
С	2.12923300	0.52618400	1.19888300
Ν	2.03904900	1.50924900	1.82889400
С	3.06641900	-0.86784900	-0.58285700
N	3.84441500	-1.05525100	-1.43334100
Η	-3.76352700	-1.59800200	-1.19624800