Manipulation of N-Heterocyclic Carbene Reactivity with Practical Oriented Electric Fields

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Supplementary Information

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S1. General Remarks

Throughout this document, the following abbreviations are used:

ZPVE = Zero-Point Vibrational Energy
TC = Thermal Corrections
S = Entropy
TS = Temperature in Kelvin * Entropy
H = Enthalpy
G = Gibbs Free Energy
G_{soln} = Gibbs Free Energy in Solution
HOMO = Highest Occupied Molecular Orbital
LUMO = Lowest Unoccupied Molecular Orbital
GEI = Global Electrophilicity Index
N = Nucleophilicity Index
eV = Electron Volts

All raw log files used in this article can be found at: https://github.com/Ecaloota/CarbenesElectricFields

S2. Supplementary Figures Showing Electrostatic Switches on GEI and N

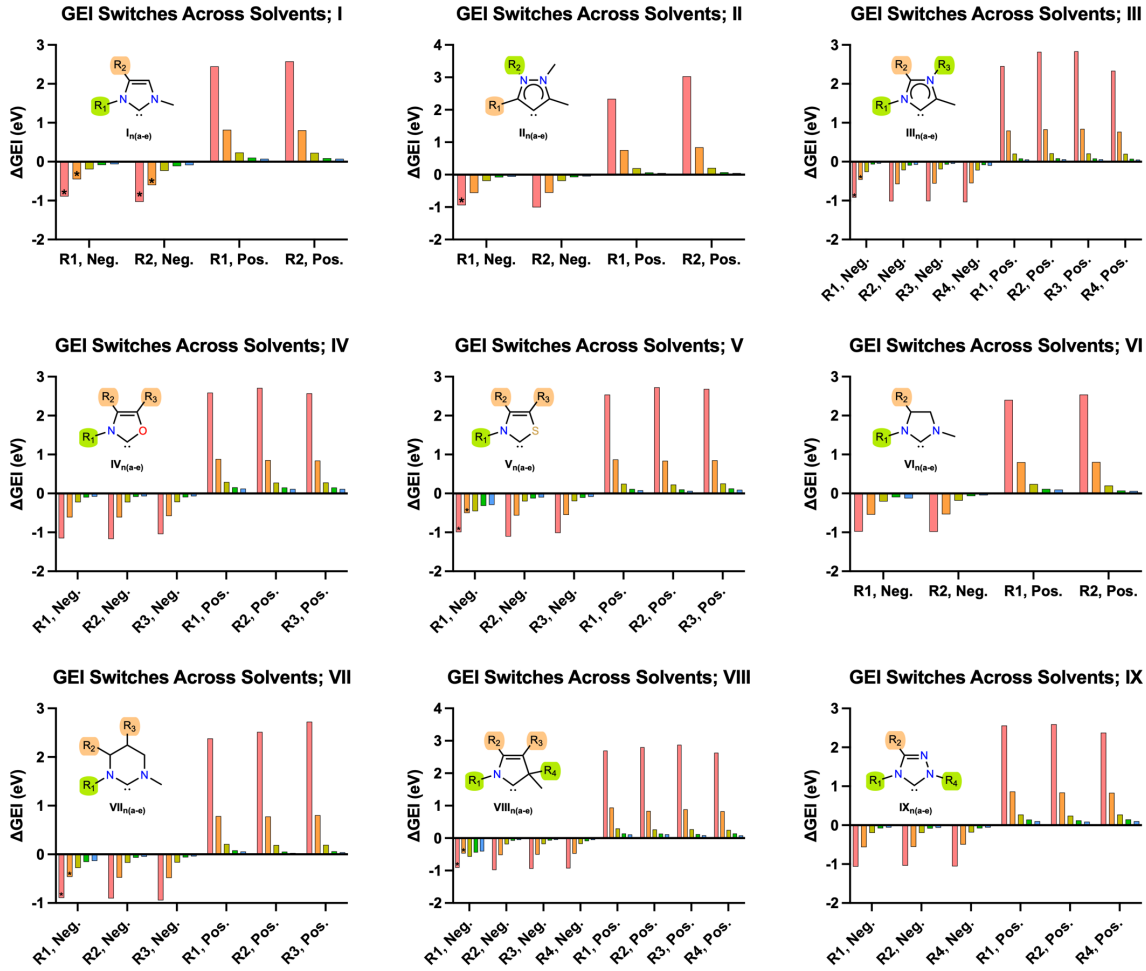


Figure S1. The DLEF-induced electrostatic GEI switches, in eV, for each of the carbenes in the test set (inlaid), with D-LEFs sampled at each position and across multiple solvents. Red = Gas, Orange = Toluene, Yellow = DCM, Green = MeCN, Blue = Water. A positive switch value indicates that the GEI increased after incorporation of the charged D-LEF.

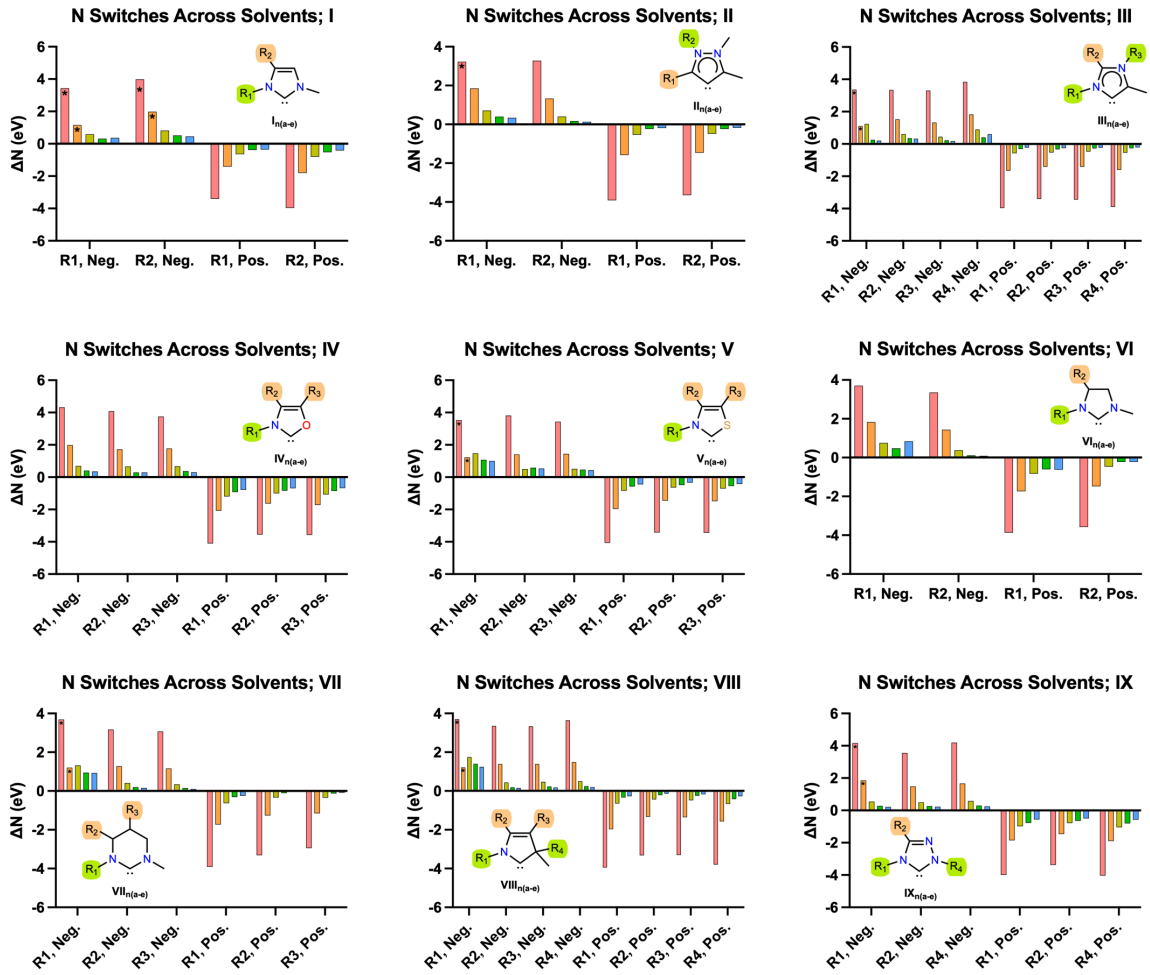


Figure S2. The DLEF-induced electrostatic N switches, in eV, for each of the carbenes in the test set (inlaid), with D-LEFs sampled at each position and across multiple solvents. Red = Gas, Orange = Toluene, Yellow = DCM, Green = MeCN, Blue = Water. A positive switch value indicates that the N increased after incorporation of the charged D-LEF.

S3. Electronic Energies of Singlet & Triplet NHCs in Test Set under EEFs Across Different Solvents

Table S1. I_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.774650	-304.777500	-304.777680
– 0.0025	-304.775040	-304.777420	-304.777550
– 0.0020	-304.775440	-304.777360	-304.777440
– 0.0015	-304.775860	-304.777310	-304.777360
– 0.0010	-304.776310	-304.777280	-304.777300
– 0.0005	-304.776770	-304.777250	-304.777260
+ 0.0000	-304.777250	-304.777250	-304.777250
+ 0.0005	-304.777750	-304.777250	-304.777260
+ 0.0010	-304.778270	-304.777280	-304.777300
+ 0.0015	-304.778810	-304.777310	-304.777360
+ 0.0020	-304.779370	-304.777360	-304.777440
+ 0.0025	-304.779950	-304.777420	-304.777550
+ 0.0030	-304.780540	-304.777500	-304.777680

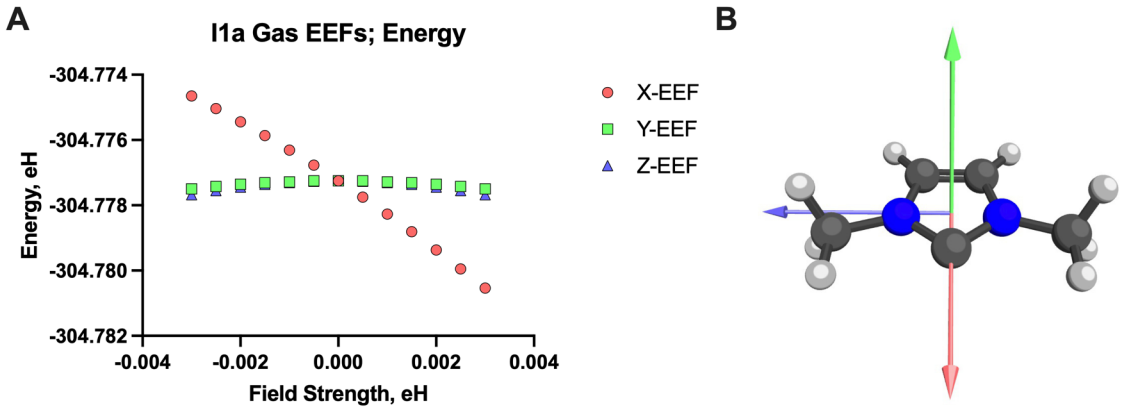


Figure S3. I_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S2. I_{1a} Under EEFs in SMD Toluene.
Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.790506	-304.794008	-304.794216
– 0.0025	-304.790984	-304.793920	-304.794065
– 0.0020	-304.791485	-304.793849	-304.793941
– 0.0015	-304.792009	-304.793793	-304.793845
– 0.0010	-304.792557	-304.793753	-304.793776
– 0.0005	-304.793127	-304.793729	-304.793735
+ 0.0000	-304.793721	-304.793721	-304.793721
+ 0.0005	-304.794338	-304.793729	-304.793735
+ 0.0010	-304.794978	-304.793753	-304.793776
+ 0.0015	-304.795642	-304.793793	-304.793845
+ 0.0020	-304.796329	-304.793849	-304.793941
+ 0.0025	-304.797039	-304.793920	-304.794065
+ 0.0030	-304.797772	-304.794008	-304.794216

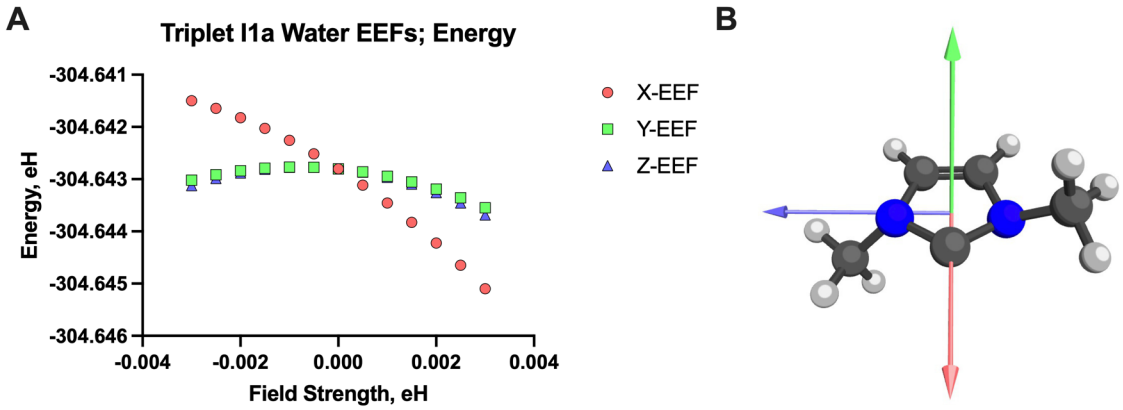


Figure S4. I_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S3. I_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.794609	-304.798860	-304.799073
– 0.0025	-304.795194	-304.798757	-304.798905
– 0.0020	-304.795805	-304.798673	-304.798768
– 0.0015	-304.796444	-304.798608	-304.798661
– 0.0010	-304.797110	-304.798561	-304.798585
– 0.0005	-304.797803	-304.798533	-304.798539
+ 0.0000	-304.798523	-304.798523	-304.798523
+ 0.0005	-304.799271	-304.798533	-304.798539
+ 0.0010	-304.800046	-304.798561	-304.798585
+ 0.0015	-304.800848	-304.798608	-304.798661
+ 0.0020	-304.801677	-304.798673	-304.798768
+ 0.0025	-304.802534	-304.798757	-304.798905
+ 0.0030	-304.803418	-304.798860	-304.799073

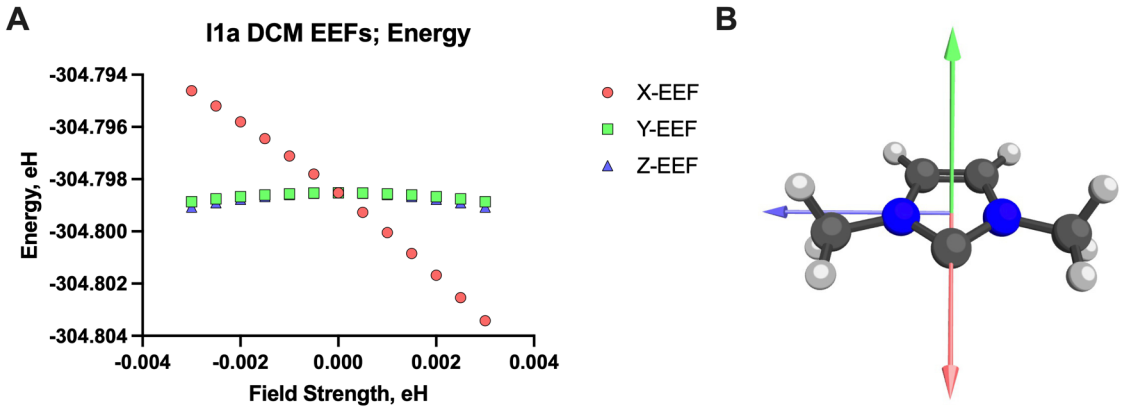


Figure S5. I_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S4. I_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.794685	-304.799256	-304.799465
– 0.0025	-304.795315	-304.799146	-304.799291
– 0.0020	-304.795974	-304.799056	-304.799149
– 0.0015	-304.796661	-304.798986	-304.799039
– 0.0010	-304.797377	-304.798936	-304.798960
– 0.0005	-304.798122	-304.798906	-304.798912
+ 0.0000	-304.798896	-304.798896	-304.798896
+ 0.0005	-304.799699	-304.798906	-304.798912
+ 0.0010	-304.800531	-304.798936	-304.798960
+ 0.0015	-304.801392	-304.798986	-304.799039
+ 0.0020	-304.802282	-304.799056	-304.799149
+ 0.0025	-304.803201	-304.799146	-304.799291
+ 0.0030	-304.804149	-304.799256	-304.799465

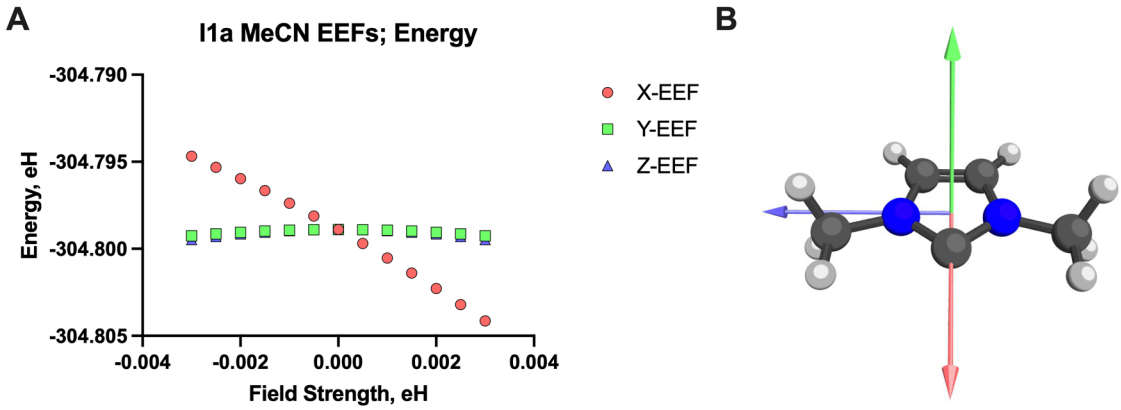


Figure S6. I_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S5. I_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.779810	-304.784448	-304.784656
– 0.0025	-304.780449	-304.784336	-304.784481
– 0.0020	-304.781118	-304.784245	-304.784337
– 0.0015	-304.781815	-304.784174	-304.784226
– 0.0010	-304.782542	-304.784123	-304.784147
– 0.0005	-304.783298	-304.784093	-304.784099
+ 0.0000	-304.784083	-304.784083	-304.784083
+ 0.0005	-304.784897	-304.784093	-304.784099
+ 0.0010	-304.785741	-304.784123	-304.784147
+ 0.0015	-304.786614	-304.784174	-304.784226
+ 0.0020	-304.787517	-304.784245	-304.784337
+ 0.0025	-304.788449	-304.784336	-304.784481
+ 0.0030	-304.789410	-304.784448	-304.784656

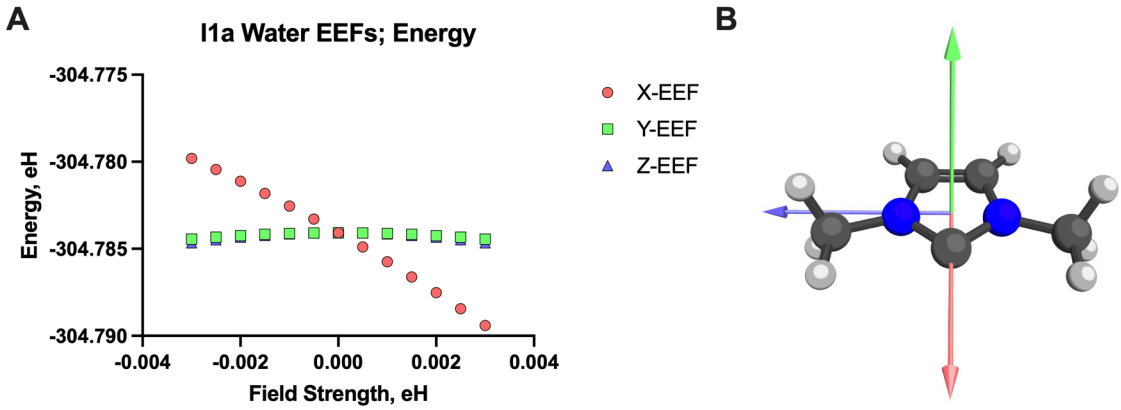


Figure S7. I_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S6. $^3I_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.639620	-304.640570	-304.640640
– 0.0025	-304.639700	-304.640500	-304.640540
– 0.0020	-304.639800	-304.640440	-304.640460
– 0.0015	-304.639930	-304.640410	-304.640410
– 0.0010	-304.640070	-304.640390	-304.640390
– 0.0005	-304.640230	-304.640390	-304.640380
+ 0.0000	-304.640410	-304.640410	-304.640410
+ 0.0005	-304.640600	-304.640440	-304.640450
+ 0.0010	-304.640820	-304.640490	-304.640520
+ 0.0015	-304.641060	-304.640570	-304.640620
+ 0.0020	-304.641310	-304.640650	-304.640740
+ 0.0025	-304.641580	-304.640760	-304.640890
+ 0.0030	-304.641880	-304.640890	-304.641060

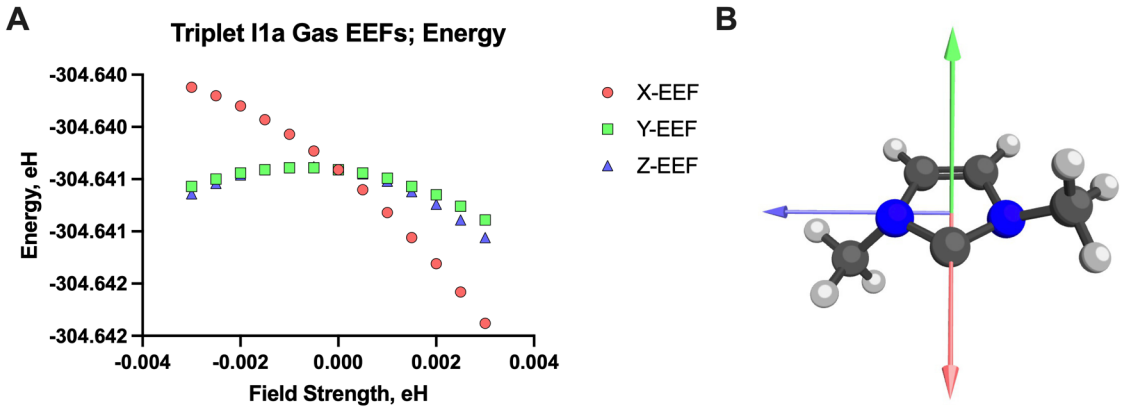


Figure S8. $^3I_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S7. $^3I_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.651446	-304.652611	-304.652702
– 0.0025	-304.651555	-304.652529	-304.652585
– 0.0020	-304.651686	-304.652467	-304.652497
– 0.0015	-304.651838	-304.652427	-304.652437
– 0.0010	-304.652013	-304.652407	-304.652406
– 0.0005	-304.652210	-304.652408	-304.652404
+ 0.0000	-304.652429	-304.652429	-304.652429
+ 0.0005	-304.652671	-304.652471	-304.652483
+ 0.0010	-304.652934	-304.652534	-304.652566
+ 0.0015	-304.653220	-304.652618	-304.652677
+ 0.0020	-304.653528	-304.652723	-304.652816
+ 0.0025	-304.653858	-304.652848	-304.652984
+ 0.0030	-304.654211	-304.652995	-304.653181

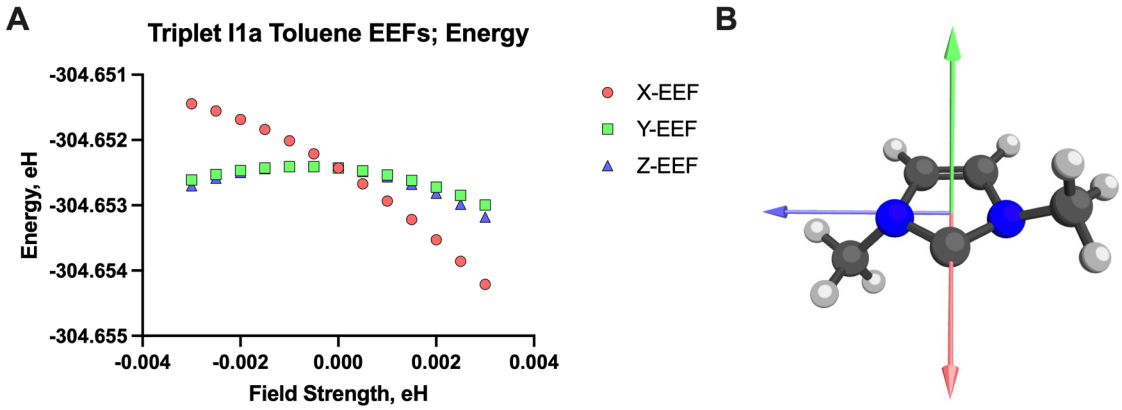


Figure S9. $^3I_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S8. $^3I_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.653509	-304.654909	-304.655011
– 0.0025	-304.653645	-304.654814	-304.654881
– 0.0020	-304.653806	-304.654744	-304.654782
– 0.0015	-304.653992	-304.654698	-304.654715
– 0.0010	-304.654205	-304.654677	-304.654681
– 0.0005	-304.654443	-304.654679	-304.654678
+ 0.0000	-304.654706	-304.654706	-304.654706
+ 0.0005	-304.654996	-304.654758	-304.654767
+ 0.0010	-304.655311	-304.654834	-304.654860
+ 0.0015	-304.655652	-304.654934	-304.654984
+ 0.0020	-304.656019	-304.655059	-304.655141
+ 0.0025	-304.656412	-304.655209	-304.655329
+ 0.0030	-304.656830	-304.655383	-304.655549

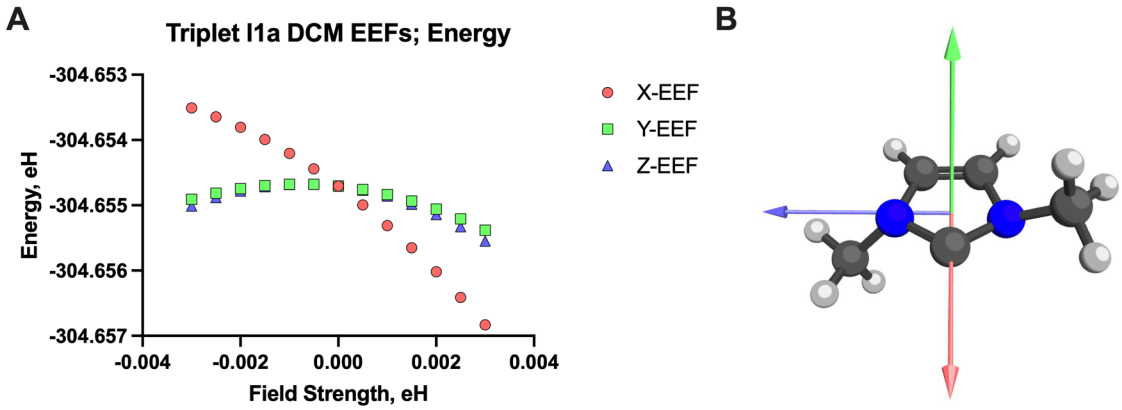


Figure S10. $^3I_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S9. $^3I_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.652722	-304.654222	-304.654326
– 0.0025	-304.652869	-304.654122	-304.654191
– 0.0020	-304.653043	-304.654047	-304.654088
– 0.0015	-304.653244	-304.653999	-304.654019
– 0.0010	-304.653472	-304.653976	-304.653983
– 0.0005	-304.653728	-304.653980	-304.653980
+ 0.0000	-304.654010	-304.654010	-304.654010
+ 0.0005	-304.654320	-304.654066	-304.654073
+ 0.0010	-304.654656	-304.654148	-304.654170
+ 0.0015	-304.655020	-304.654257	-304.654299
+ 0.0020	-304.655412	-304.654392	-304.654462
+ 0.0025	-304.655831	-304.654553	-304.654658
+ 0.0030	-304.656278	-304.654741	-304.654887

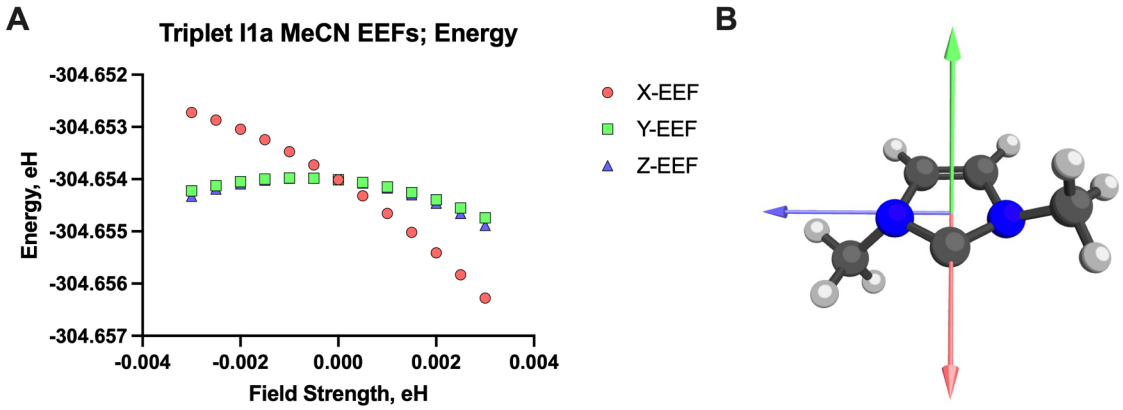


Figure S11. $^3I_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S10. $^3I_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.641496	-304.643017	-304.643121
– 0.0025	-304.641645	-304.642915	-304.642984
– 0.0020	-304.641822	-304.642840	-304.642881
– 0.0015	-304.642026	-304.642791	-304.642812
– 0.0010	-304.642258	-304.642768	-304.642775
– 0.0005	-304.642516	-304.642772	-304.642772
+ 0.0000	-304.642803	-304.642803	-304.642803
+ 0.0005	-304.643116	-304.642860	-304.642866
+ 0.0010	-304.643458	-304.642943	-304.642964
+ 0.0015	-304.643827	-304.643054	-304.643094
+ 0.0020	-304.644223	-304.643191	-304.643258
+ 0.0025	-304.644648	-304.643355	-304.643455
+ 0.0030	-304.645100	-304.643546	-304.643686

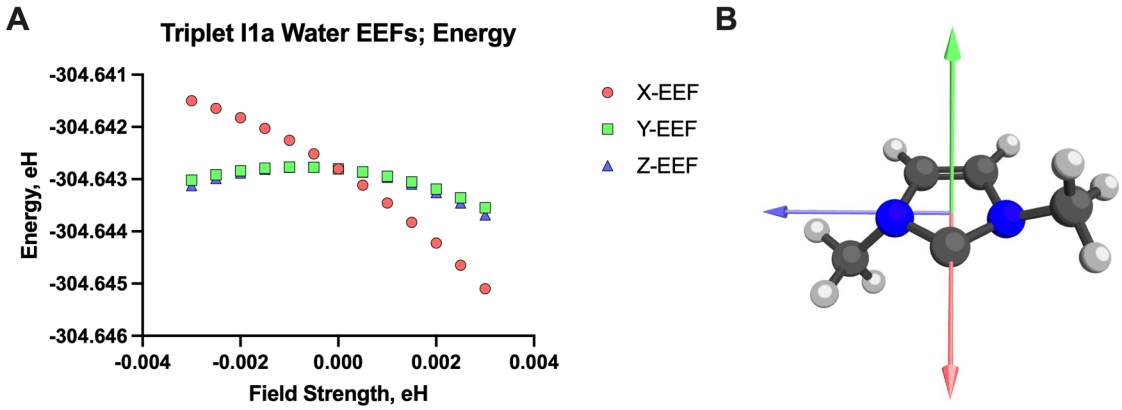


Figure S12. $^3I_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S11. II_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.318743	-383.326955	-383.327197
– 0.0025	-383.319982	-383.326854	-383.327022
– 0.0020	-383.321251	-383.326771	-383.326878
– 0.0015	-383.322549	-383.326707	-383.326767
– 0.0010	-383.323877	-383.326661	-383.326687
– 0.0005	-383.325236	-383.326633	-383.326640
+ 0.0000	-383.326624	-383.326624	-383.326624
+ 0.0005	-383.328041	-383.326633	-383.326639
+ 0.0010	-383.329489	-383.326660	-383.326687
+ 0.0015	-383.330966	-383.326706	-383.326767
+ 0.0020	-383.332473	-383.326771	-383.326878
+ 0.0025	-383.334010	-383.326853	-383.327022
+ 0.0030	-383.335577	-383.326954	-383.327197

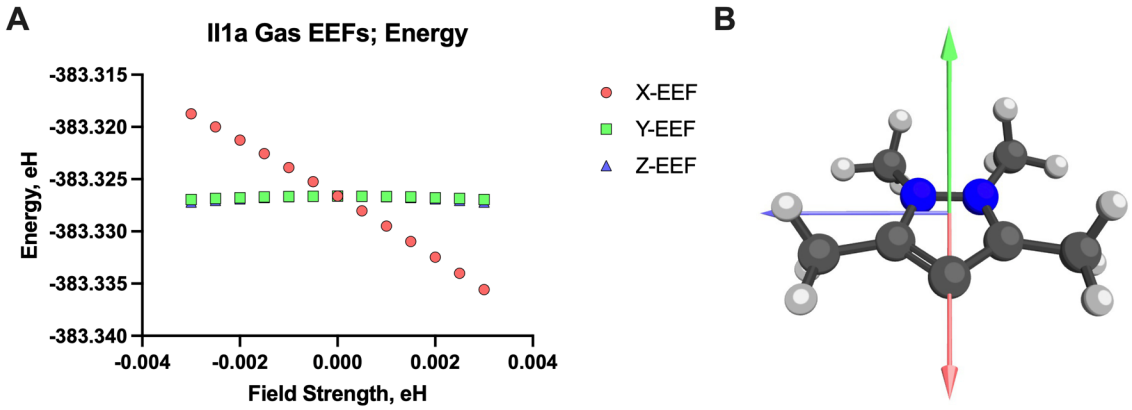


Figure S13. II_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S12. II_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.337191	-383.347277	-383.347555
– 0.0025	-383.338719	-383.347159	-383.347352
– 0.0020	-383.340283	-383.347062	-383.347186
– 0.0015	-383.341882	-383.346987	-383.347056
– 0.0010	-383.343516	-383.346933	-383.346964
– 0.0005	-383.345186	-383.346901	-383.346909
+ 0.0000	-383.346890	-383.346890	-383.346890
+ 0.0005	-383.348630	-383.346901	-383.346908
+ 0.0010	-383.350404	-383.346933	-383.346964
+ 0.0015	-383.352214	-383.346986	-383.347056
+ 0.0020	-383.354060	-383.347062	-383.347185
+ 0.0025	-383.355940	-383.347158	-383.347352
+ 0.0030	-383.357857	-383.347276	-383.347555

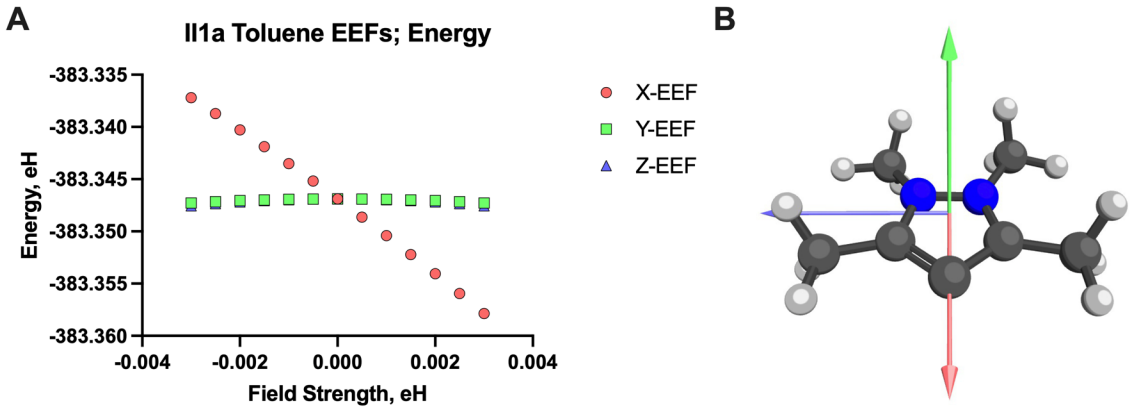


Figure S14. II_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S13. II_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.349230	-383.361245	-383.361527
– 0.0025	-383.351054	-383.361104	-383.361299
– 0.0020	-383.352918	-383.360988	-383.361113
– 0.0015	-383.354823	-383.360898	-383.360969
– 0.0010	-383.356769	-383.360834	-383.360865
– 0.0005	-383.358755	-383.360795	-383.360803
+ 0.0000	-383.360782	-383.360782	-383.360782
+ 0.0005	-383.362851	-383.360795	-383.360803
+ 0.0010	-383.364960	-383.360834	-383.360865
+ 0.0015	-383.367110	-383.360898	-383.360968
+ 0.0020	-383.369302	-383.360988	-383.361113
+ 0.0025	-383.371535	-383.361103	-383.361299
+ 0.0030	-383.373809	-383.361244	-383.361526

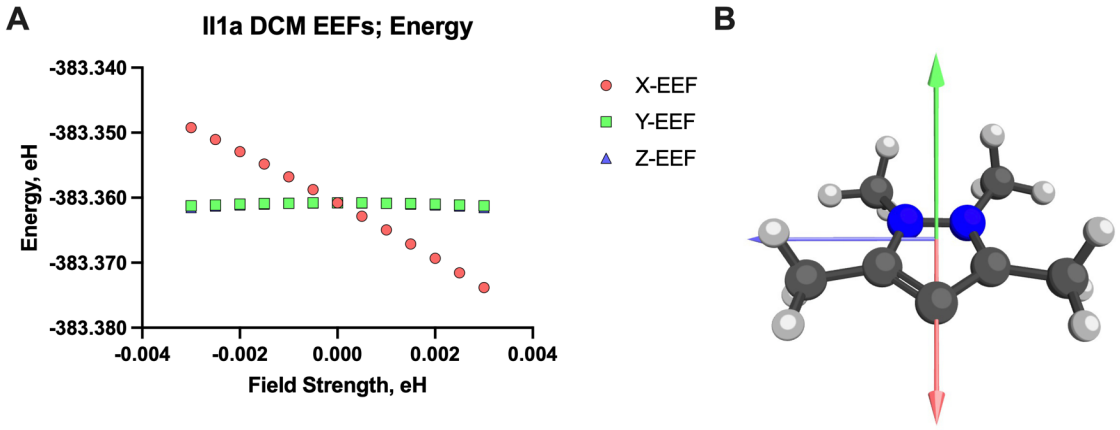


Figure S15. II_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S14. II_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.351554	-383.364356	-383.364628
– 0.0025	-383.353496	-383.364203	-383.364392
– 0.0020	-383.355482	-383.364078	-383.364198
– 0.0015	-383.357510	-383.363980	-383.364048
– 0.0010	-383.359582	-383.363911	-383.363941
– 0.0005	-383.361697	-383.363869	-383.363876
+ 0.0000	-383.363855	-383.363855	-383.363855
+ 0.0005	-383.366056	-383.363869	-383.363876
+ 0.0010	-383.368301	-383.363910	-383.363941
+ 0.0015	-383.370589	-383.363980	-383.364048
+ 0.0020	-383.372921	-383.364077	-383.364198
+ 0.0025	-383.375297	-383.364202	-383.364391
+ 0.0030	-383.377717	-383.364355	-383.364627

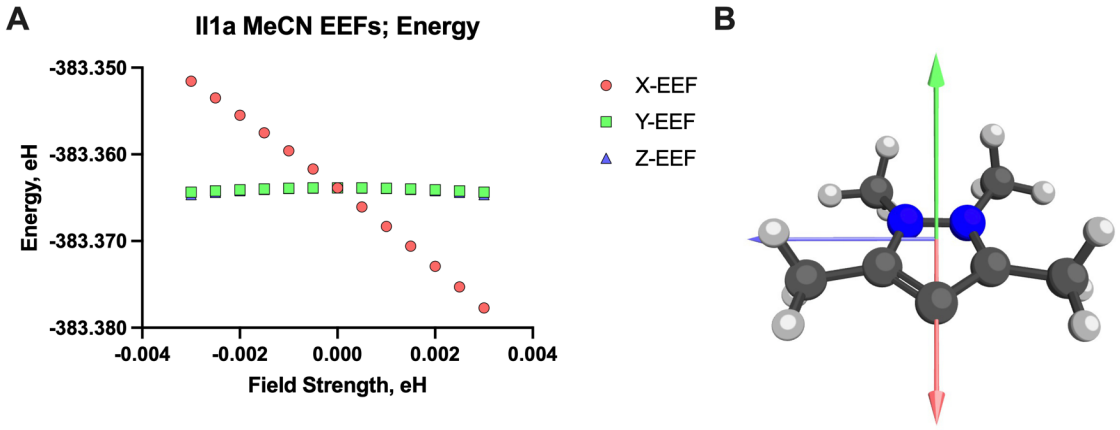


Figure S16. II_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S15. II_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.344099	-383.357064	-383.357333
– 0.0025	-383.346066	-383.356908	-383.357095
– 0.0020	-383.348076	-383.356781	-383.356900
– 0.0015	-383.350130	-383.356682	-383.356749
– 0.0010	-383.352228	-383.356611	-383.356641
– 0.0005	-383.354369	-383.356568	-383.356576
+ 0.0000	-383.356554	-383.356554	-383.356554
+ 0.0005	-383.358783	-383.356568	-383.356576
+ 0.0010	-383.361056	-383.356610	-383.356641
+ 0.0015	-383.363372	-383.356681	-383.356749
+ 0.0020	-383.365733	-383.356780	-383.356900
+ 0.0025	-383.368139	-383.356907	-383.357095
+ 0.0030	-383.370588	-383.357063	-383.357333

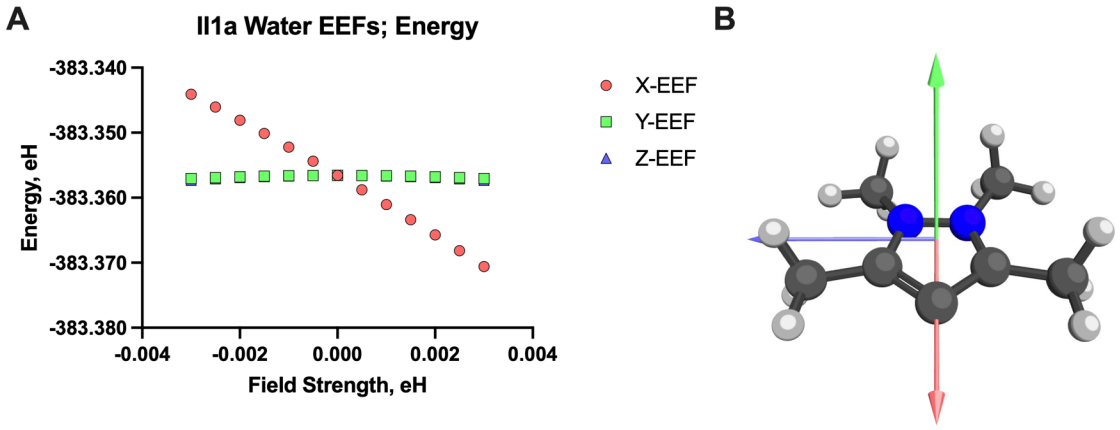


Figure S17. II_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S16. ^{3}II$_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.257891	-383.259314	-383.259560
– 0.0025	-383.257998	-383.259199	-383.259370
– 0.0020	-383.258132	-383.259105	-383.259214
– 0.0015	-383.258294	-383.259032	-383.259094
– 0.0010	-383.258482	-383.258980	-383.259007
– 0.0005	-383.258697	-383.258949	-383.258956
+ 0.0000	-383.258938	-383.258938	-383.258938
+ 0.0005	-383.259207	-383.258949	-383.258956
+ 0.0010	-383.259502	-383.258980	-383.259007
+ 0.0015	-383.259824	-383.259032	-383.259094
+ 0.0020	-383.260173	-383.259105	-383.259214
+ 0.0025	-383.260549	-383.259199	-383.259370
+ 0.0030	-383.260951	-383.259314	-383.259560

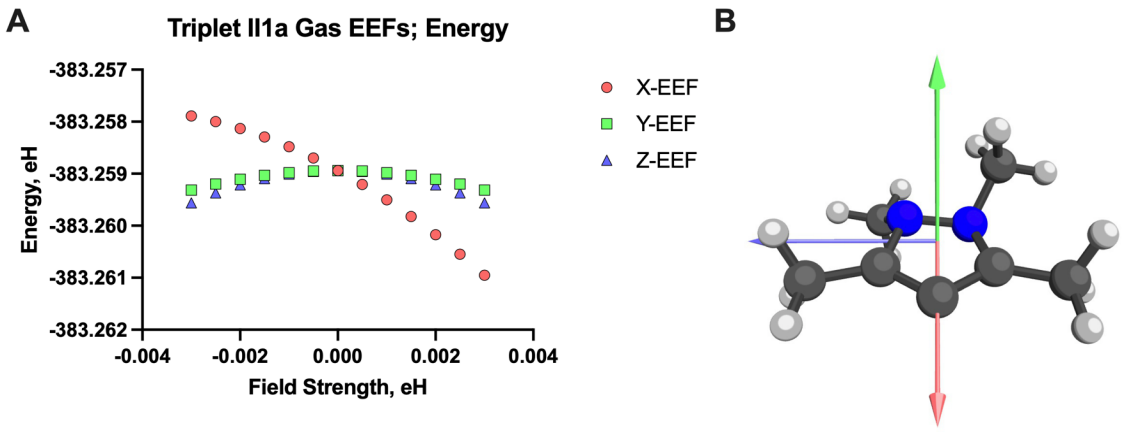


Figure S18. ^{3}II$_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S17. ^{3}II$_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.266340	-383.268094	-383.268388
– 0.0025	-383.266479	-383.267959	-383.268163
– 0.0020	-383.266650	-383.267849	-383.267980
– 0.0015	-383.266853	-383.267763	-383.267837
– 0.0010	-383.267088	-383.267702	-383.267734
– 0.0005	-383.267355	-383.267665	-383.267673
+ 0.0000	-383.267653	-383.267653	-383.267653
+ 0.0005	-383.267983	-383.267665	-383.267673
+ 0.0010	-383.268344	-383.267702	-383.267734
+ 0.0015	-383.268738	-383.267763	-383.267837
+ 0.0020	-383.269163	-383.267849	-383.267980
+ 0.0025	-383.269620	-383.267959	-383.268163
+ 0.0030	-383.270109	-383.268094	-383.268388

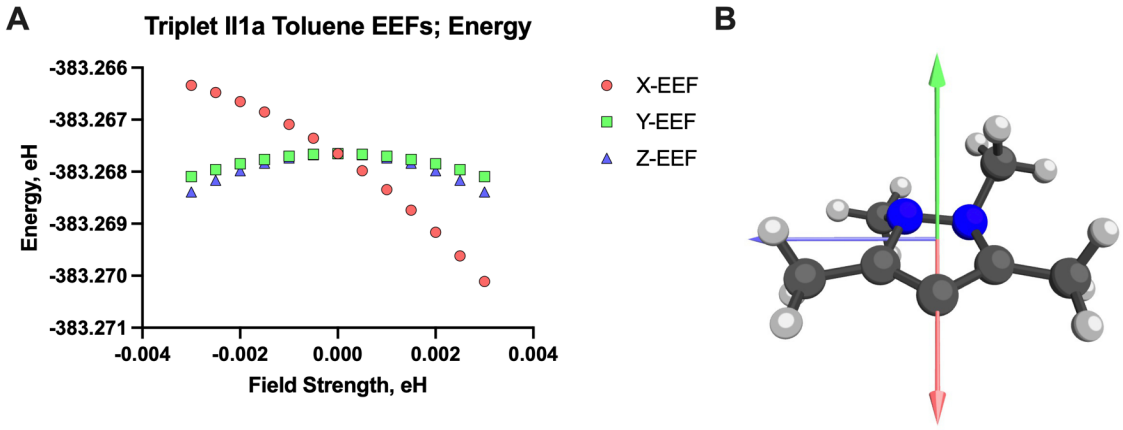


Figure S19. ^{3}II$_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S18. ^{3}II$_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.269263	-383.271360	-383.271674
– 0.0025	-383.269433	-383.271200	-383.271417
– 0.0020	-383.269640	-383.271068	-383.271207
– 0.0015	-383.269883	-383.270966	-383.271044
– 0.0010	-383.270163	-383.270893	-383.270927
– 0.0005	-383.270480	-383.270849	-383.270858
+ 0.0000	-383.270834	-383.270834	-383.270834
+ 0.0005	-383.271225	-383.270849	-383.270858
+ 0.0010	-383.271652	-383.270893	-383.270927
+ 0.0015	-383.272116	-383.270966	-383.271044
+ 0.0020	-383.272617	-383.271068	-383.271207
+ 0.0025	-383.273155	-383.271200	-383.271417
+ 0.0030	-383.273730	-383.271360	-383.271674

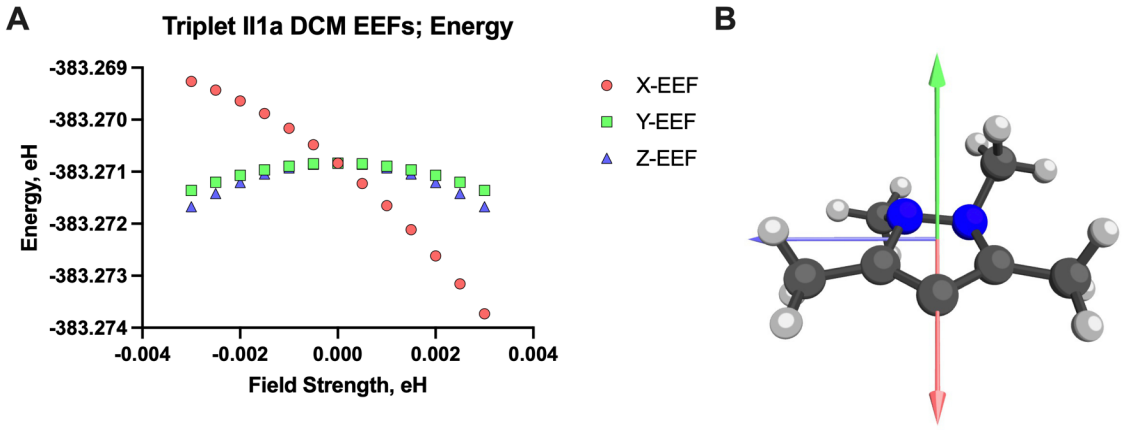


Figure S20. ^{3}II$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S19. ^{3}II$_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.268017	-383.270259	-383.270568
– 0.0025	-383.268199	-383.270085	-383.270300
– 0.0020	-383.268420	-383.269943	-383.270080
– 0.0015	-383.268679	-383.269832	-383.269909
– 0.0010	-383.268977	-383.269753	-383.269788
– 0.0005	-383.269314	-383.269706	-383.269714
+ 0.0000	-383.269690	-383.269690	-383.269690
+ 0.0005	-383.270105	-383.269706	-383.269714
+ 0.0010	-383.270558	-383.269753	-383.269788
+ 0.0015	-383.271050	-383.269832	-383.269909
+ 0.0020	-383.271582	-383.269943	-383.270080
+ 0.0025	-383.272152	-383.270085	-383.270300
+ 0.0030	-383.272761	-383.270259	-383.270568

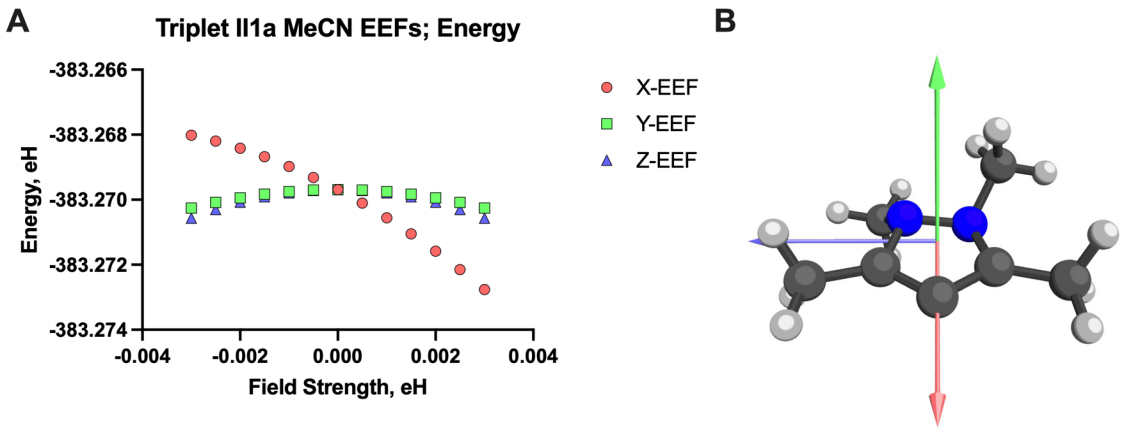


Figure S21. ^{3}II$_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S20. ^{3}II$_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-383.261106	-383.263379	-383.263686
– 0.0025	-383.261291	-383.263202	-383.263415
– 0.0020	-383.261514	-383.263057	-383.263194
– 0.0015	-383.261777	-383.262945	-383.263021
– 0.0010	-383.262079	-383.262864	-383.262898
– 0.0005	-383.262420	-383.262816	-383.262825
+ 0.0000	-383.262800	-383.262800	-383.262800
+ 0.0005	-383.263220	-383.262816	-383.262825
+ 0.0010	-383.263678	-383.262864	-383.262898
+ 0.0015	-383.264176	-383.262945	-383.263021
+ 0.0020	-383.264714	-383.263057	-383.263194
+ 0.0025	-383.265291	-383.263202	-383.263415
+ 0.0030	-383.265908	-383.263379	-383.263686

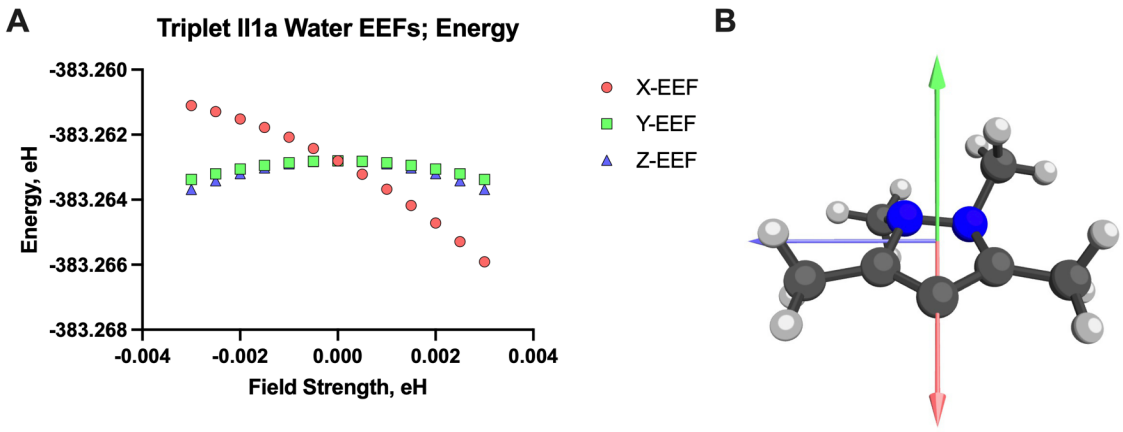


Figure S22. ^{3}II$_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S21. III_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-344.053960	-344.060360	-344.061350
– 0.0025	-344.054920	-344.060270	-344.061070
– 0.0020	-344.055900	-344.060200	-344.060810
– 0.0015	-344.056900	-344.060140	-344.060580
– 0.0010	-344.057930	-344.060100	-344.060390
– 0.0005	-344.058990	-344.060080	-344.060210
+ 0.0000	-344.060070	-344.060070	-344.060070
+ 0.0005	-344.061170	-344.060080	-344.059950
+ 0.0010	-344.062300	-344.060100	-344.059870
+ 0.0015	-344.063460	-344.060140	-344.059800
+ 0.0020	-344.064640	-344.060200	-344.059770
+ 0.0025	-344.065840	-344.060270	-344.059770
+ 0.0030	-344.067070	-344.060360	-344.059790

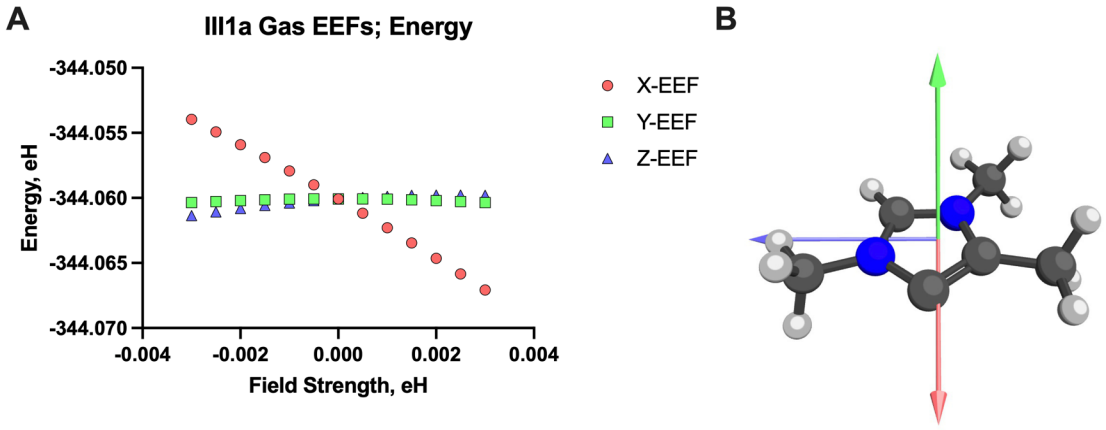


Figure S23. III_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S22. III_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-344.072781	-344.080615	-344.081793
– 0.0025	-344.073957	-344.080513	-344.081460
– 0.0020	-344.075163	-344.080429	-344.081160
– 0.0015	-344.076398	-344.080364	-344.080892
– 0.0010	-344.077662	-344.080317	-344.080656
– 0.0005	-344.078956	-344.080289	-344.080451
+ 0.0000	-344.080280	-344.080280	-344.080280
+ 0.0005	-344.081632	-344.080289	-344.080140
+ 0.0010	-344.083015	-344.080317	-344.080032
+ 0.0015	-344.084427	-344.080363	-344.079956
+ 0.0020	-344.085868	-344.080428	-344.079912
+ 0.0025	-344.087339	-344.080512	-344.079901
+ 0.0030	-344.088839	-344.080615	-344.079922

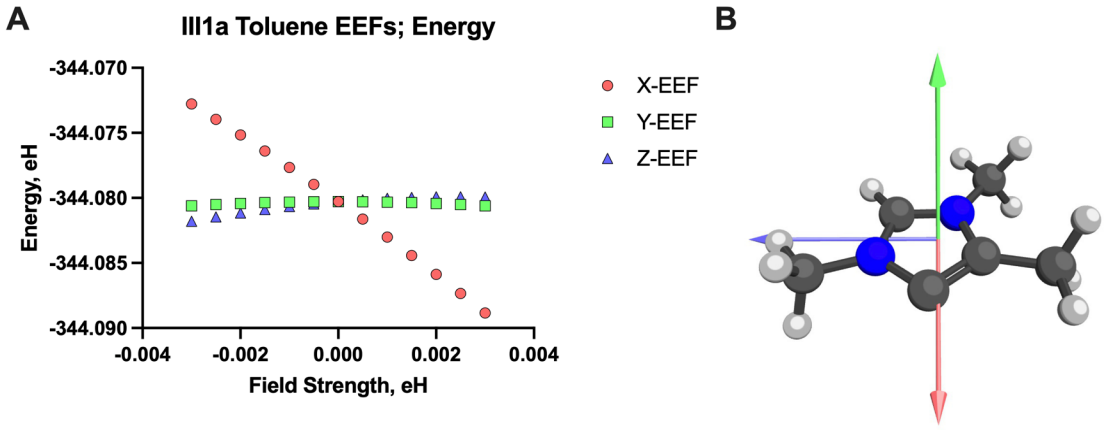


Figure S24. III_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S23. III_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-344.081754	-344.091123	-344.092466
– 0.0025	-344.083164	-344.091002	-344.092086
– 0.0020	-344.084608	-344.090902	-344.091743
– 0.0015	-344.086086	-344.090825	-344.091435
– 0.0010	-344.087598	-344.090769	-344.091162
– 0.0005	-344.089144	-344.090736	-344.090926
+ 0.0000	-344.090725	-344.090725	-344.090725
+ 0.0005	-344.092340	-344.090736	-344.090560
+ 0.0010	-344.093989	-344.090769	-344.090431
+ 0.0015	-344.095673	-344.090824	-344.090337
+ 0.0020	-344.097391	-344.090902	-344.090279
+ 0.0025	-344.099144	-344.091001	-344.090258
+ 0.0030	-344.100931	-344.091123	-344.090272

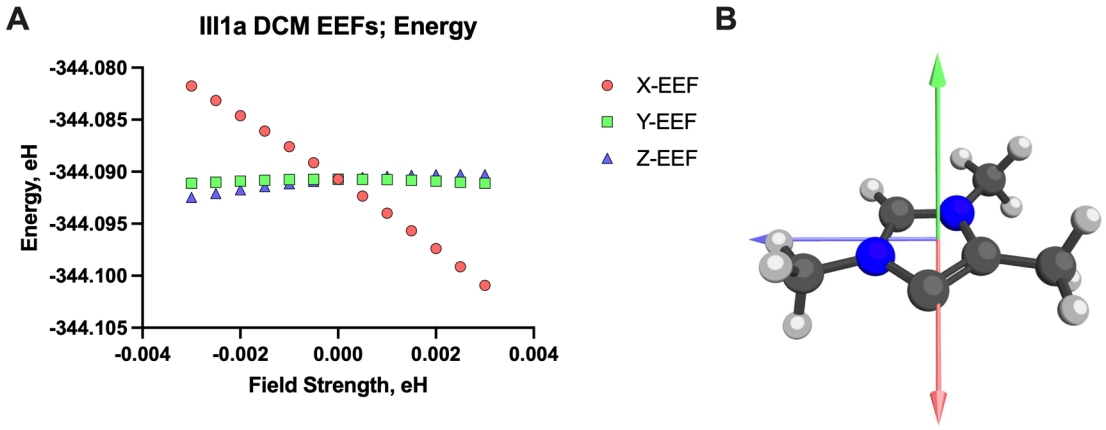


Figure S25. III_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S24. III_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-344.083408	-344.093415	-344.094815
– 0.0025	-344.084914	-344.093284	-344.094417
– 0.0020	-344.086456	-344.093176	-344.094057
– 0.0015	-344.088034	-344.093093	-344.093733
– 0.0010	-344.089648	-344.093033	-344.093447
– 0.0005	-344.091299	-344.092998	-344.093198
+ 0.0000	-344.092986	-344.092986	-344.092986
+ 0.0005	-344.094709	-344.092998	-344.092811
+ 0.0010	-344.096468	-344.093033	-344.092673
+ 0.0015	-344.098264	-344.093093	-344.092572
+ 0.0020	-344.100097	-344.093176	-344.092508
+ 0.0025	-344.101966	-344.093283	-344.092481
+ 0.0030	-344.103871	-344.093415	-344.092492

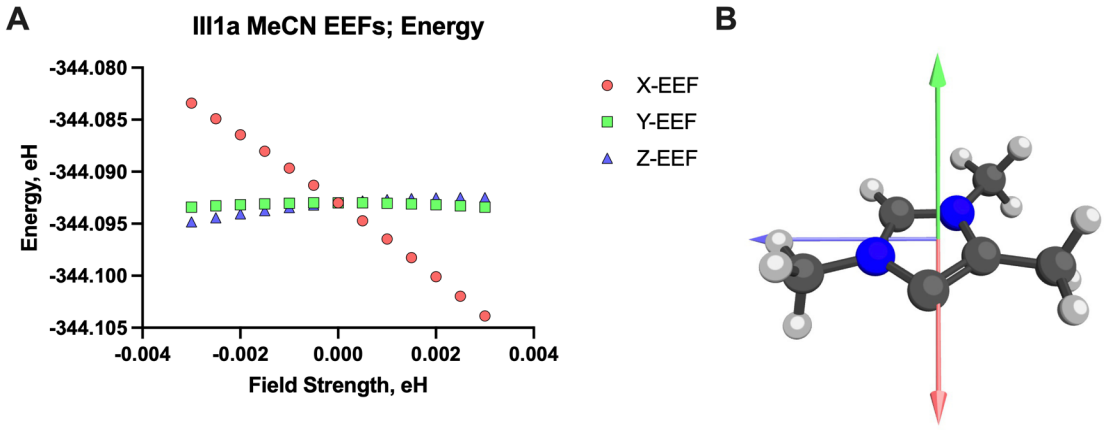


Figure S26. III_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S25. III_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-344.071019	-344.081158	-344.082569
– 0.0025	-344.072545	-344.081025	-344.082168
– 0.0020	-344.074107	-344.080916	-344.081804
– 0.0015	-344.075706	-344.080831	-344.081477
– 0.0010	-344.077341	-344.080770	-344.081188
– 0.0005	-344.079013	-344.080734	-344.080936
+ 0.0000	-344.080722	-344.080722	-344.080722
+ 0.0005	-344.082468	-344.080734	-344.080545
+ 0.0010	-344.084250	-344.080770	-344.080405
+ 0.0015	-344.086069	-344.080831	-344.080303
+ 0.0020	-344.087925	-344.080916	-344.080238
+ 0.0025	-344.089818	-344.081025	-344.080210
+ 0.0030	-344.091748	-344.081158	-344.080220

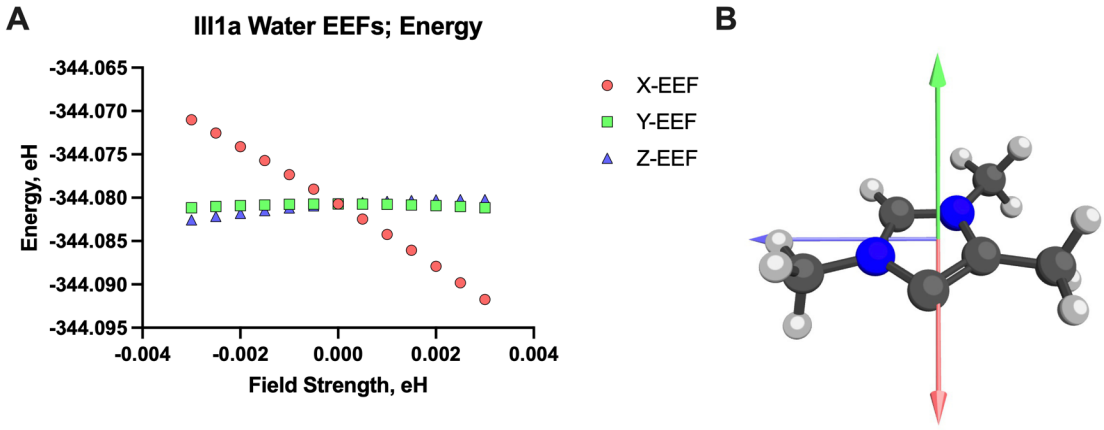


Figure S27. III_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S26. ^{3}III$_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-343.957880	-343.958870	-343.957190
– 0.0025	-343.957790	-343.958630	-343.957210
– 0.0020	-343.957730	-343.958410	-343.957250
– 0.0015	-343.957690	-343.958210	-343.957330
– 0.0010	-343.957680	-343.958030	-343.957430
– 0.0005	-343.957690	-343.957870	-343.957570
+ 0.0000	-343.957730	-343.957730	-343.957730
+ 0.0005	-343.957790	-343.957600	-343.957920
+ 0.0010	-343.957880	-343.957500	-343.958140
+ 0.0015	-343.958000	-343.957410	-343.958390
+ 0.0020	-343.958140	-343.957350	-343.958660
+ 0.0025	-343.958310	-343.957300	-343.958970
+ 0.0030	-343.958500	-343.957270	-343.959300

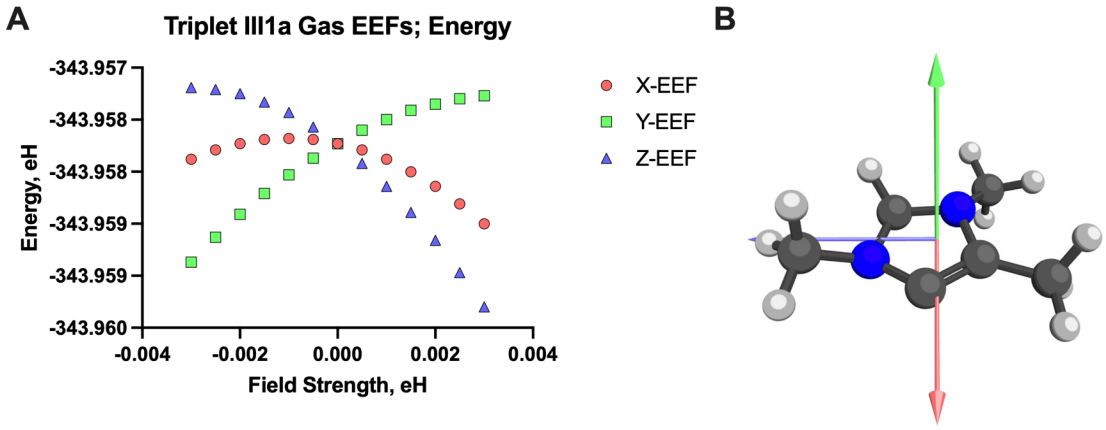


Figure S28. ^{3}III$_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S27. ^{3}III$_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-343.969539	-343.970753	-343.968655
– 0.0025	-343.969434	-343.970468	-343.968691
– 0.0020	-343.969361	-343.970205	-343.968761
– 0.0015	-343.969318	-343.969964	-343.968864
– 0.0010	-343.969306	-343.969746	-343.969001
– 0.0005	-343.969325	-343.969550	-343.969172
+ 0.0000	-343.969376	-343.969376	-343.969376
+ 0.0005	-343.969457	-343.969224	-343.969613
+ 0.0010	-343.969570	-343.969094	-343.969884
+ 0.0015	-343.969714	-343.968987	-343.970189
+ 0.0020	-343.969890	-343.968902	-343.970527
+ 0.0025	-343.970097	-343.968839	-343.970900
+ 0.0030	-343.970337	-343.968799	-343.971305

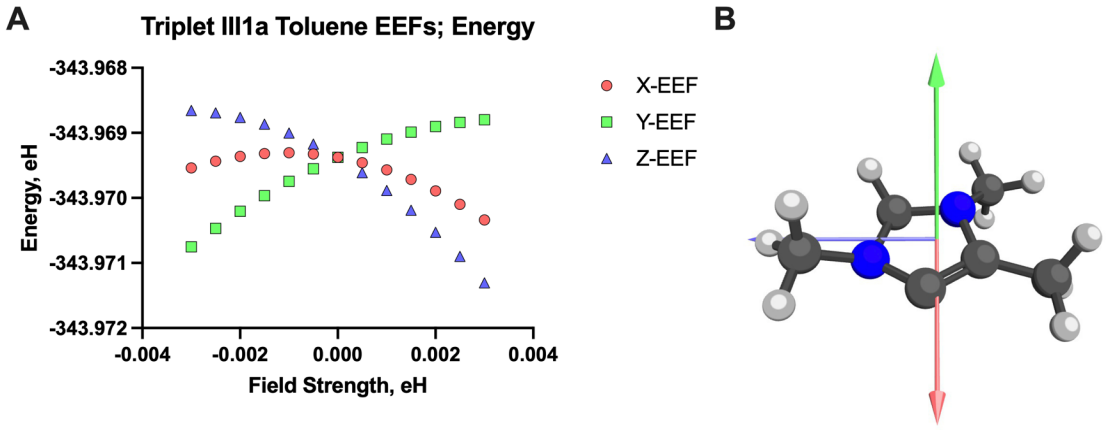


Figure S29. ^{3}III$_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S28. ^{3}III$_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-343.972307	-343.973797	-343.971192
– 0.0025	-343.972182	-343.973447	-343.971250
– 0.0020	-343.972093	-343.973125	-343.971345
– 0.0015	-343.972040	-343.972829	-343.971478
– 0.0010	-343.972025	-343.972561	-343.971649
– 0.0005	-343.972046	-343.972320	-343.971858
+ 0.0000	-343.972105	-343.972105	-343.972105
+ 0.0005	-343.972201	-343.971917	-343.972390
+ 0.0010	-343.972334	-343.971756	-343.972712
+ 0.0015	-343.972505	-343.971621	-343.973072
+ 0.0020	-343.972714	-343.971513	-343.973471
+ 0.0025	-343.972962	-343.971431	-343.973907
+ 0.0030	-343.973249	-343.971376	-343.974382

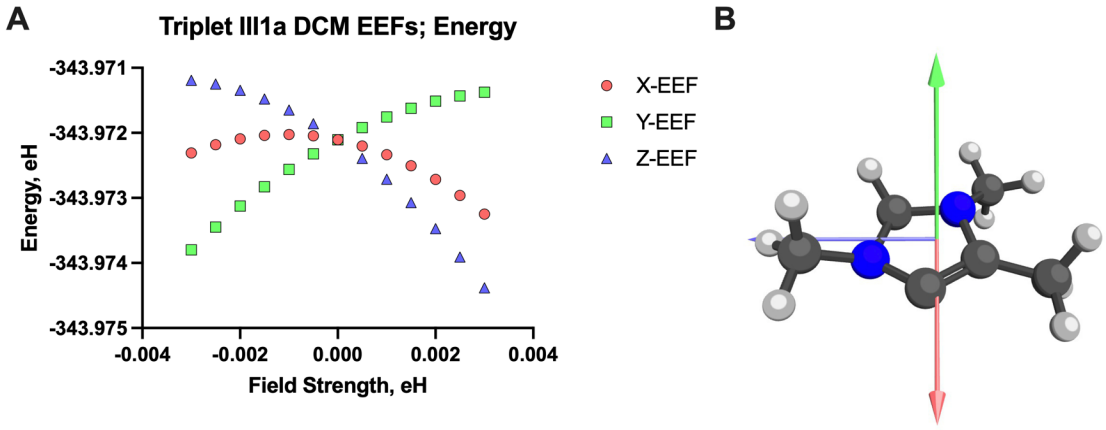


Figure S30. ^{3}III$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S29. ^{3}III$_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-343.971506	-343.973126	-343.970285
– 0.0025	-343.971370	-343.972744	-343.970351
– 0.0020	-343.971273	-343.972392	-343.970457
– 0.0015	-343.971215	-343.972069	-343.970603
– 0.0010	-343.971196	-343.971776	-343.970788
– 0.0005	-343.971216	-343.971512	-343.971013
+ 0.0000	-343.971277	-343.971277	-343.971277
+ 0.0005	-343.971377	-343.971071	-343.971580
+ 0.0010	-343.971517	-343.970894	-343.971923
+ 0.0015	-343.971698	-343.970745	-343.972306
+ 0.0020	-343.971920	-343.970626	-343.972728
+ 0.0025	-343.972183	-343.970535	-343.973190
+ 0.0030	-343.972490	-343.970474	-343.973691

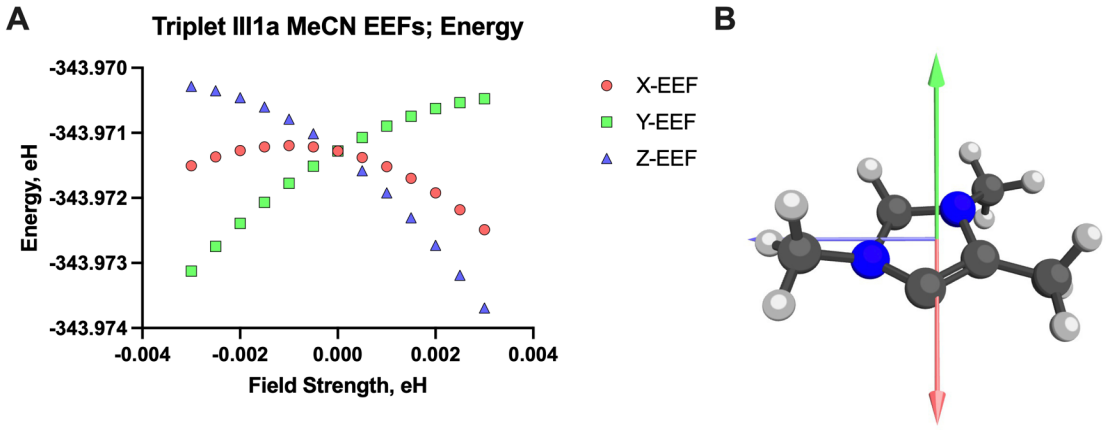


Figure S31. ^{3}III$_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S30. ^{3}III$_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-343.960505	-343.962154	-343.959261
– 0.0025	-343.960367	-343.961765	-343.959329
– 0.0020	-343.960268	-343.961406	-343.959438
– 0.0015	-343.960208	-343.961077	-343.959586
– 0.0010	-343.960189	-343.960778	-343.959774
– 0.0005	-343.960209	-343.960509	-343.960002
+ 0.0000	-343.960269	-343.960269	-343.960269
+ 0.0005	-343.960370	-343.960059	-343.960577
+ 0.0010	-343.960512	-343.959879	-343.960924
+ 0.0015	-343.960694	-343.959727	-343.961311
+ 0.0020	-343.960919	-343.959606	-343.961738
+ 0.0025	-343.961186	-343.959513	-343.962205
+ 0.0030	-343.961496	-343.959450	-343.962712

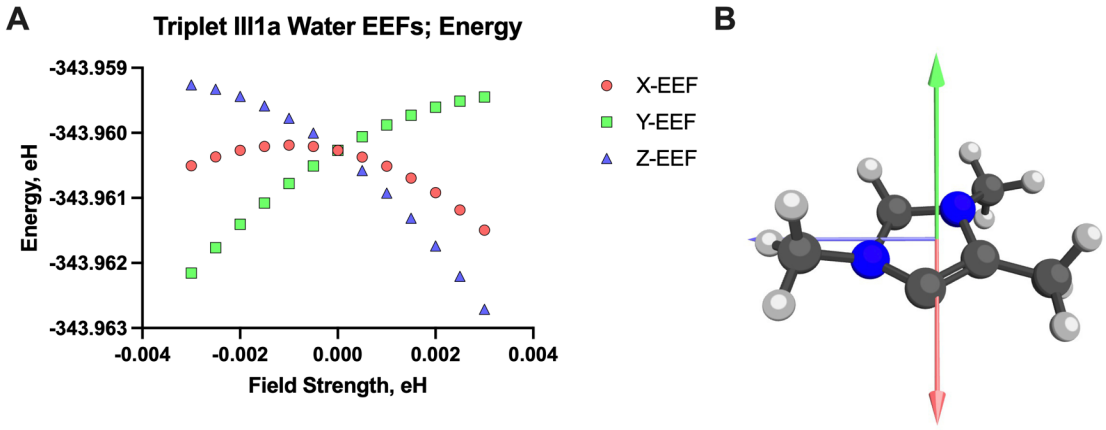


Figure S32. ^{3}III$_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S31. IV_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.324170	-285.327970	-285.324870
– 0.0025	-285.324730	-285.327920	-285.325310
– 0.0020	-285.325310	-285.327870	-285.325770
– 0.0015	-285.325900	-285.327830	-285.326250
– 0.0010	-285.326520	-285.327800	-285.326750
– 0.0005	-285.327140	-285.327790	-285.327260
+ 0.0000	-285.327780	-285.327780	-285.327780
+ 0.0005	-285.328440	-285.327790	-285.328330
+ 0.0010	-285.329110	-285.327800	-285.328890
+ 0.0015	-285.329800	-285.327830	-285.329470
+ 0.0020	-285.330510	-285.327870	-285.330060
+ 0.0025	-285.331230	-285.327920	-285.330670
+ 0.0030	-285.331970	-285.327970	-285.331300

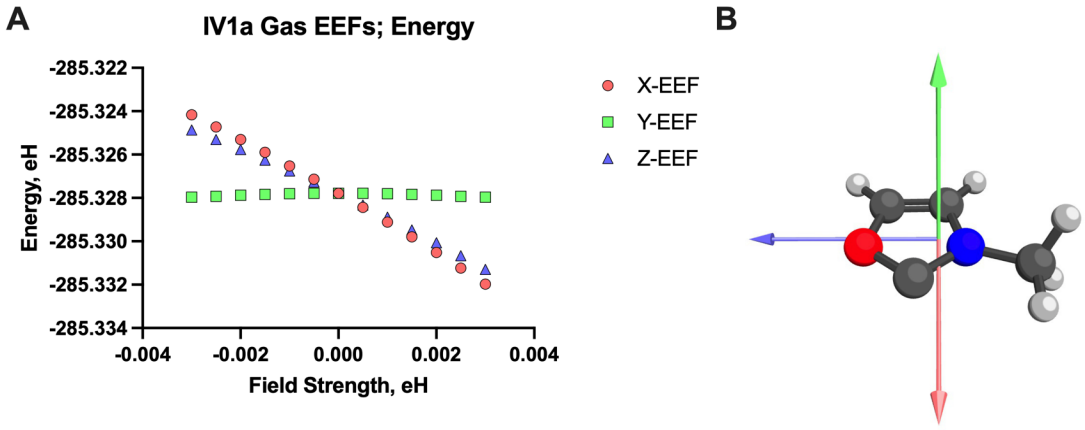


Figure S33. IV_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S32. IV_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.331779	-285.336274	-285.332671
– 0.0025	-285.332446	-285.336208	-285.333188
– 0.0020	-285.333132	-285.336154	-285.333723
– 0.0015	-285.333835	-285.336112	-285.334278
– 0.0010	-285.334558	-285.336081	-285.334852
– 0.0005	-285.335298	-285.336063	-285.335445
+ 0.0000	-285.336057	-285.336057	-285.336057
+ 0.0005	-285.336835	-285.336063	-285.336689
+ 0.0010	-285.337630	-285.336081	-285.337339
+ 0.0015	-285.338445	-285.336111	-285.338009
+ 0.0020	-285.339277	-285.336153	-285.338698
+ 0.0025	-285.340129	-285.336208	-285.339406
+ 0.0030	-285.340998	-285.336274	-285.340133

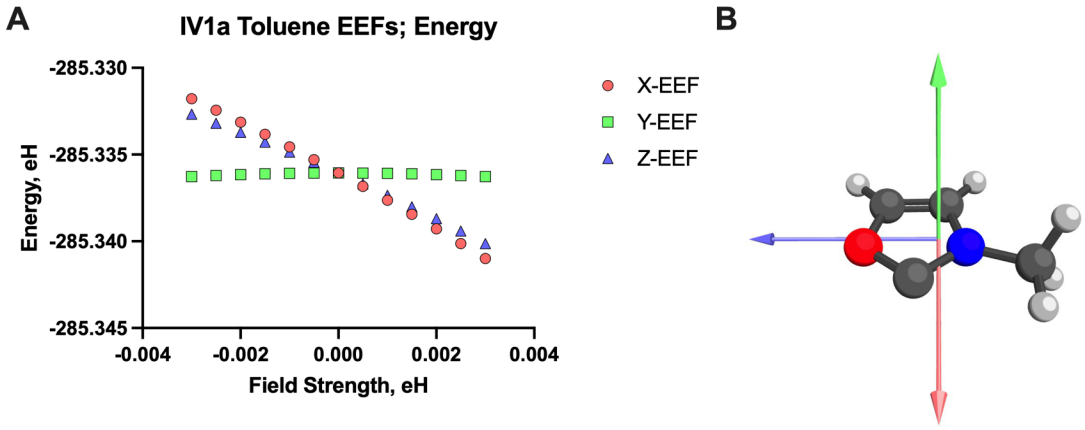


Figure S34. IV_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S33. IV_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.336482	-285.341712	-285.337658
– 0.0025	-285.337259	-285.341636	-285.338239
– 0.0020	-285.338057	-285.341573	-285.338841
– 0.0015	-285.338877	-285.341525	-285.339464
– 0.0010	-285.339717	-285.341490	-285.340108
– 0.0005	-285.340579	-285.341469	-285.340774
+ 0.0000	-285.341462	-285.341462	-285.341462
+ 0.0005	-285.342366	-285.341469	-285.342171
+ 0.0010	-285.343292	-285.341490	-285.342901
+ 0.0015	-285.344238	-285.341524	-285.343653
+ 0.0020	-285.345207	-285.341573	-285.344426
+ 0.0025	-285.346196	-285.341635	-285.345220
+ 0.0030	-285.347207	-285.341712	-285.346036

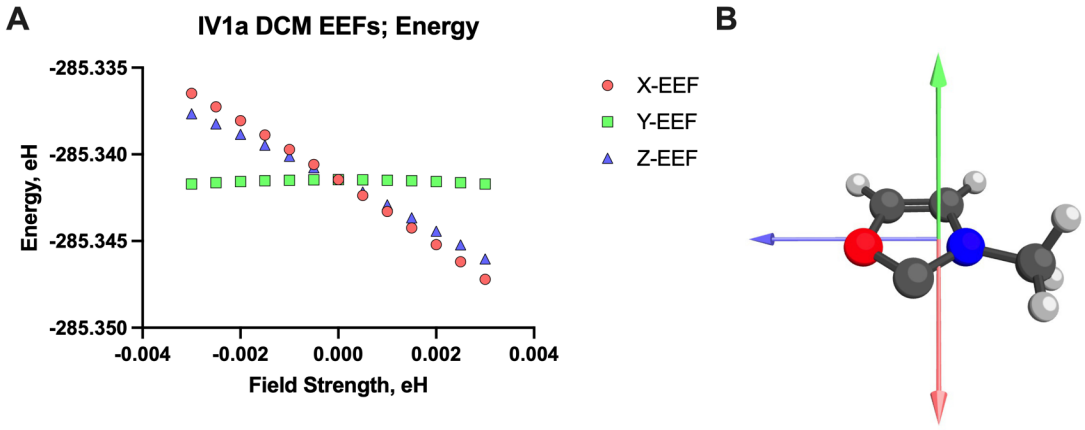


Figure S35. IV_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S34. IV_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.337325	-285.342832	-285.338627
– 0.0025	-285.338143	-285.342752	-285.339229
– 0.0020	-285.338983	-285.342685	-285.339852
– 0.0015	-285.339846	-285.342634	-285.340498
– 0.0010	-285.340731	-285.342597	-285.341166
– 0.0005	-285.341638	-285.342575	-285.341856
+ 0.0000	-285.342568	-285.342568	-285.342568
+ 0.0005	-285.343520	-285.342575	-285.343302
+ 0.0010	-285.344494	-285.342597	-285.344058
+ 0.0015	-285.345491	-285.342634	-285.344836
+ 0.0020	-285.346510	-285.342685	-285.345637
+ 0.0025	-285.347552	-285.342751	-285.346459
+ 0.0030	-285.348617	-285.342832	-285.347304

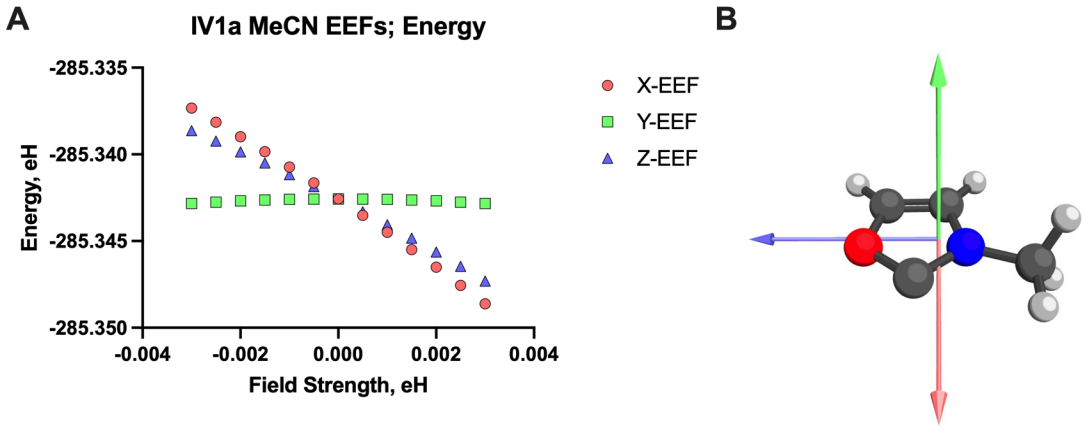


Figure S36. IV_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S35. IV_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.329471	-285.335099	-285.330738
– 0.0025	-285.330308	-285.335016	-285.331362
– 0.0020	-285.331167	-285.334949	-285.332009
– 0.0015	-285.332048	-285.334896	-285.332679
– 0.0010	-285.332952	-285.334858	-285.333372
– 0.0005	-285.333879	-285.334835	-285.334089
+ 0.0000	-285.334828	-285.334828	-285.334828
+ 0.0005	-285.335800	-285.334835	-285.335590
+ 0.0010	-285.336794	-285.334858	-285.336376
+ 0.0015	-285.337812	-285.334895	-285.337184
+ 0.0020	-285.338852	-285.334948	-285.338015
+ 0.0025	-285.339915	-285.335016	-285.338870
+ 0.0030	-285.341001	-285.335099	-285.339748

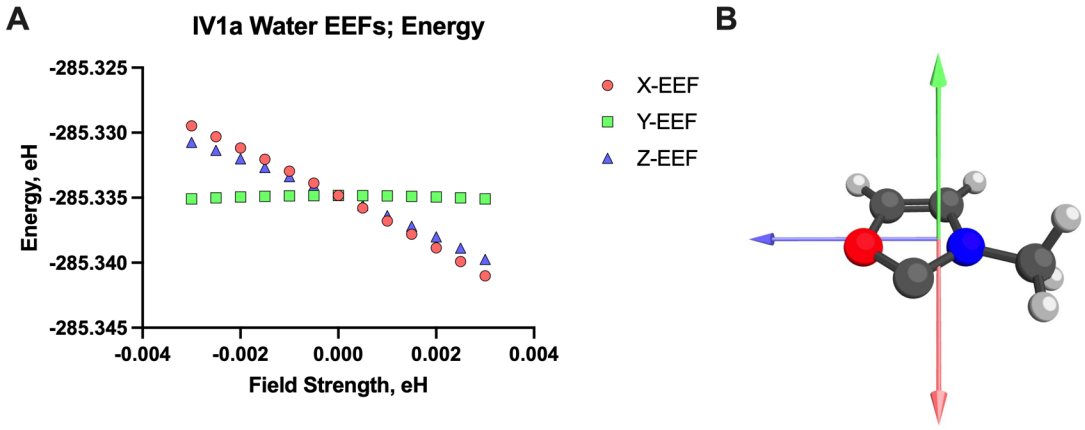


Figure S37. IV_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S36. $^3IV_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.199380	-285.202250	-285.199620
– 0.0025	-285.199620	-285.202010	-285.199810
– 0.0020	-285.199880	-285.201800	-285.200020
– 0.0015	-285.200150	-285.201590	-285.200250
– 0.0010	-285.200430	-285.201400	-285.200500
– 0.0005	-285.200730	-285.201210	-285.200770
+ 0.0000	-285.201050	-285.201050	-285.201050
+ 0.0005	-285.201370	-285.200890	-285.201340
+ 0.0010	-285.201720	-285.200750	-285.201660
+ 0.0015	-285.202080	-285.200610	-285.201990
+ 0.0020	-285.202450	-285.200500	-285.202330
+ 0.0025	-285.202840	-285.200390	-285.202700
+ 0.0030	-285.203240	-285.200300	-285.203080

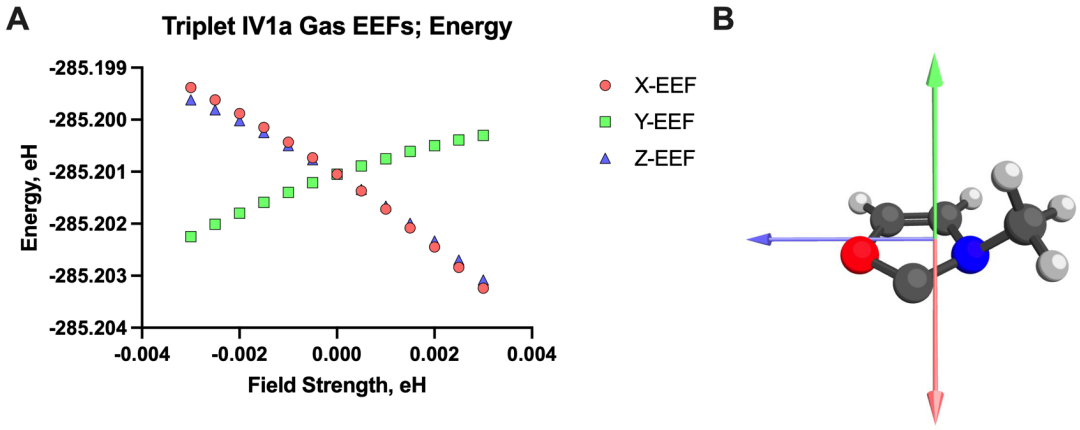


Figure S38. $^3IV_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S37. $^3IV_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.203386	-285.206747	-285.203683
– 0.0025	-285.203668	-285.206476	-285.203909
– 0.0020	-285.203967	-285.206219	-285.204155
– 0.0015	-285.204283	-285.205976	-285.204421
– 0.0010	-285.204616	-285.205747	-285.204706
– 0.0005	-285.204966	-285.205533	-285.205010
+ 0.0000	-285.205333	-285.205333	-285.205333
+ 0.0005	-285.205718	-285.205148	-285.205676
+ 0.0010	-285.206119	-285.204976	-285.206038
+ 0.0015	-285.206538	-285.204820	-285.206419
+ 0.0020	-285.206975	-285.204677	-285.206820
+ 0.0025	-285.207428	-285.204550	-285.207239
+ 0.0030	-285.207899	-285.204437	-285.207678

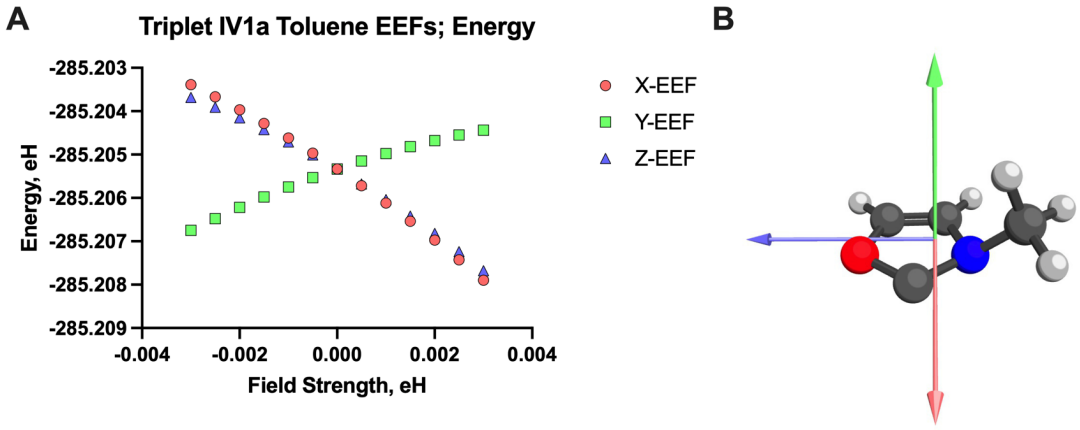


Figure S39. $^3IV_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S38. $^3IV_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.205387	-285.209258	-285.205786
– 0.0025	-285.205711	-285.208944	-285.206037
– 0.0020	-285.206053	-285.208646	-285.206311
– 0.0015	-285.206416	-285.208365	-285.206606
– 0.0010	-285.206798	-285.208101	-285.206922
– 0.0005	-285.207200	-285.207853	-285.207261
+ 0.0000	-285.207621	-285.207621	-285.207621
+ 0.0005	-285.208062	-285.207406	-285.208003
+ 0.0010	-285.208523	-285.207208	-285.208407
+ 0.0015	-285.209004	-285.207026	-285.208832
+ 0.0020	-285.209505	-285.206861	-285.209279
+ 0.0025	-285.210026	-285.206713	-285.209748
+ 0.0030	-285.210566	-285.206582	-285.210239

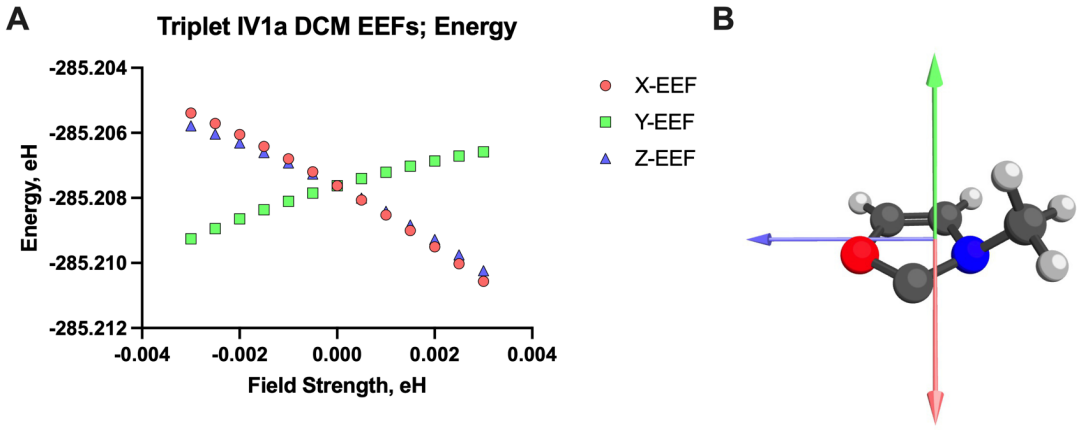


Figure S40. $^3IV_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S39. $^3IV_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.205254	-285.209321	-285.205705
– 0.0025	-285.205592	-285.208989	-285.205963
– 0.0020	-285.205951	-285.208674	-285.206243
– 0.0015	-285.206330	-285.208377	-285.206547
– 0.0010	-285.206730	-285.208098	-285.206872
– 0.0005	-285.207150	-285.207836	-285.207220
+ 0.0000	-285.207591	-285.207591	-285.207591
+ 0.0005	-285.208053	-285.207364	-285.207985
+ 0.0010	-285.208536	-285.207155	-285.208400
+ 0.0015	-285.209039	-285.206963	-285.208839
+ 0.0020	-285.209564	-285.206789	-285.209299
+ 0.0025	-285.210110	-285.206633	-285.209783
+ 0.0030	-285.210677	-285.206494	-285.210288

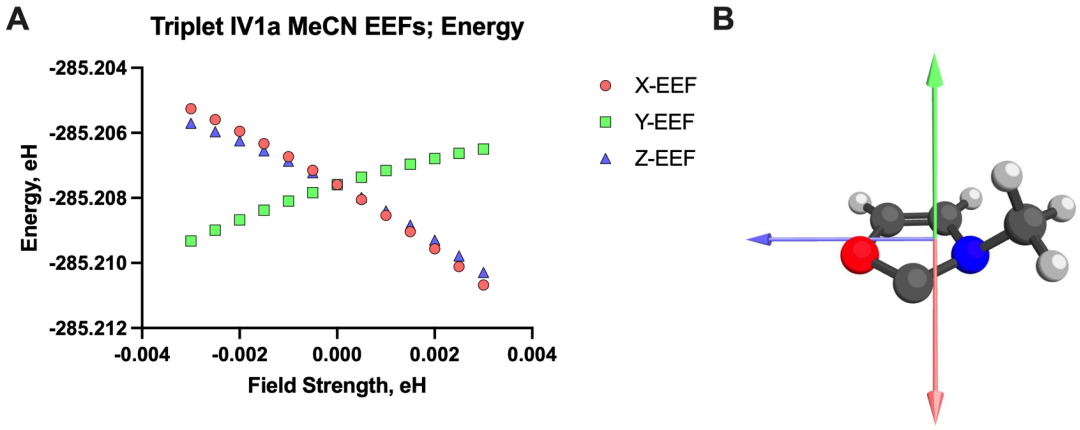


Figure S41. $^3IV_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S40. $^3IV_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-285.199594	-285.203752	-285.199959
– 0.0025	-285.199943	-285.203416	-285.200240
– 0.0020	-285.200313	-285.203097	-285.200545
– 0.0015	-285.200703	-285.202796	-285.200873
– 0.0010	-285.201115	-285.202513	-285.201225
– 0.0005	-285.201547	-285.202248	-285.201601
+ 0.0000	-285.202000	-285.202000	-285.202000
+ 0.0005	-285.202474	-285.201770	-285.202422
+ 0.0010	-285.202969	-285.201558	-285.202868
+ 0.0015	-285.203486	-285.201364	-285.203338
+ 0.0020	-285.204023	-285.201188	-285.203830
+ 0.0025	-285.204582	-285.201030	-285.204346
+ 0.0030	-285.205163	-285.200890	-285.204886

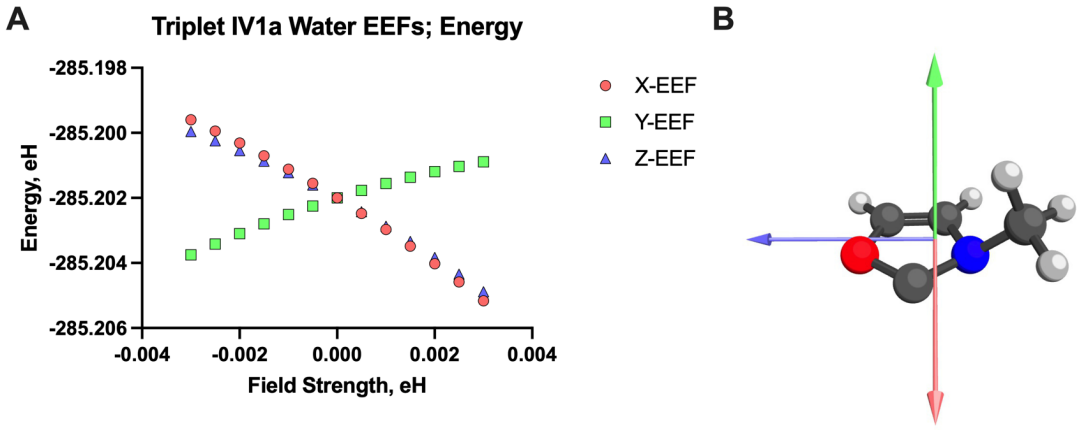


Figure S42. $^3IV_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S41. V_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.300800	-608.304300	-608.301800
– 0.0025	-608.301300	-608.304230	-608.302120
– 0.0020	-608.301820	-608.304170	-608.302470
– 0.0015	-608.302350	-608.304130	-608.302830
– 0.0010	-608.302900	-608.304100	-608.303220
– 0.0005	-608.303480	-608.304080	-608.303640
+ 0.0000	-608.304070	-608.304070	-608.304070
+ 0.0005	-608.304680	-608.304080	-608.304530
+ 0.0010	-608.305320	-608.304100	-608.305010
+ 0.0015	-608.305970	-608.304130	-608.305510
+ 0.0020	-608.306640	-608.304170	-608.306040
+ 0.0025	-608.307330	-608.304230	-608.306590
+ 0.0030	-608.308040	-608.304300	-608.307160

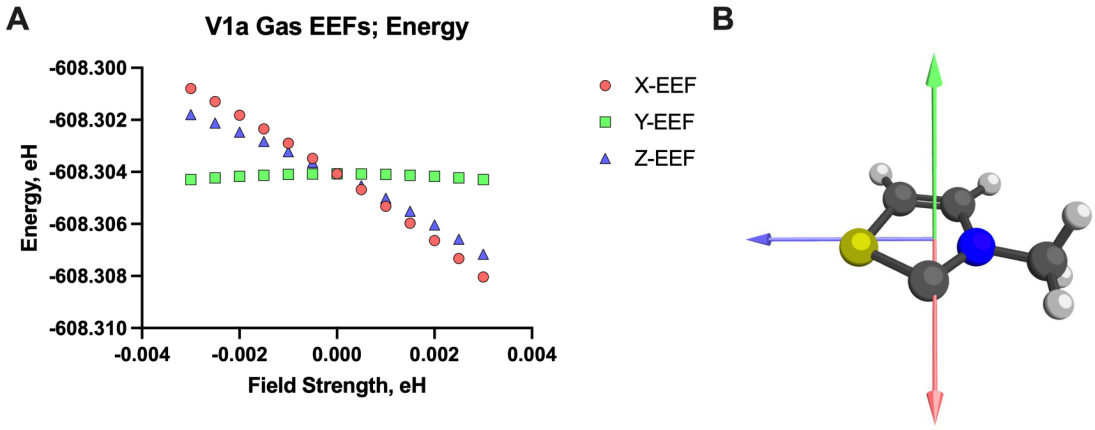


Figure S43. V_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S42. V_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.308696	-608.312966	-608.309960
– 0.0025	-608.309305	-608.312884	-608.310351
– 0.0020	-608.309938	-608.312818	-608.310769
– 0.0015	-608.310594	-608.312766	-608.311212
– 0.0010	-608.311273	-608.312729	-608.311682
– 0.0005	-608.311975	-608.312707	-608.312177
+ 0.0000	-608.312699	-608.312699	-608.312699
+ 0.0005	-608.313447	-608.312707	-608.313248
+ 0.0010	-608.314218	-608.312729	-608.313822
+ 0.0015	-608.315012	-608.312766	-608.314423
+ 0.0020	-608.315830	-608.312818	-608.315050
+ 0.0025	-608.316670	-608.312884	-608.315704
+ 0.0030	-608.317533	-608.312966	-608.316384

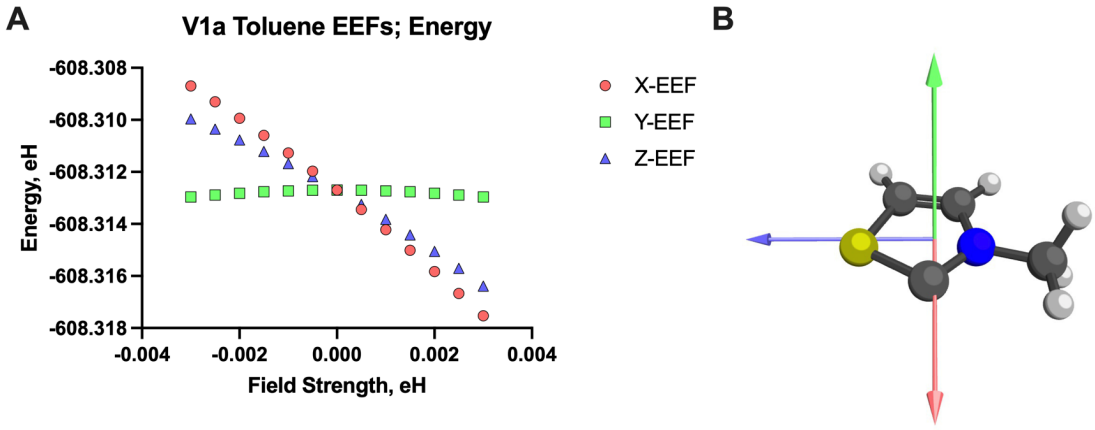


Figure S44. V_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S43. V_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.313102	-608.318196	-608.314766
– 0.0025	-608.313832	-608.318102	-608.315213
– 0.0020	-608.314589	-608.318024	-608.315689
– 0.0015	-608.315373	-608.317964	-608.316194
– 0.0010	-608.316184	-608.317921	-608.316729
– 0.0005	-608.317022	-608.317896	-608.317293
+ 0.0000	-608.317887	-608.317887	-608.317887
+ 0.0005	-608.318779	-608.317896	-608.318510
+ 0.0010	-608.319698	-608.317921	-608.319163
+ 0.0015	-608.320644	-608.317964	-608.319845
+ 0.0020	-608.321618	-608.318024	-608.320557
+ 0.0025	-608.322618	-608.318102	-608.321299
+ 0.0030	-608.323646	-608.318196	-608.322070

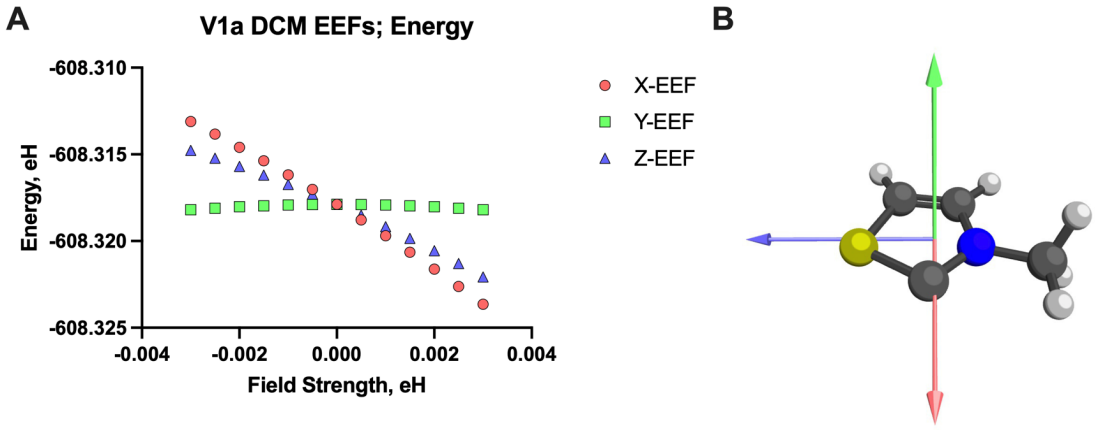


Figure S45. V_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S44. V_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.313265	-608.318699	-608.315117
– 0.0025	-608.314045	-608.318599	-608.315583
– 0.0020	-608.314853	-608.318517	-608.316079
– 0.0015	-608.315690	-608.318453	-608.316606
– 0.0010	-608.316555	-608.318407	-608.317164
– 0.0005	-608.317448	-608.318380	-608.317752
+ 0.0000	-608.318371	-608.318371	-608.318371
+ 0.0005	-608.319322	-608.318380	-608.319020
+ 0.0010	-608.320302	-608.318407	-608.319701
+ 0.0015	-608.321310	-608.318453	-608.320411
+ 0.0020	-608.322348	-608.318517	-608.321153
+ 0.0025	-608.323414	-608.318599	-608.321926
+ 0.0030	-608.324510	-608.318699	-608.322729

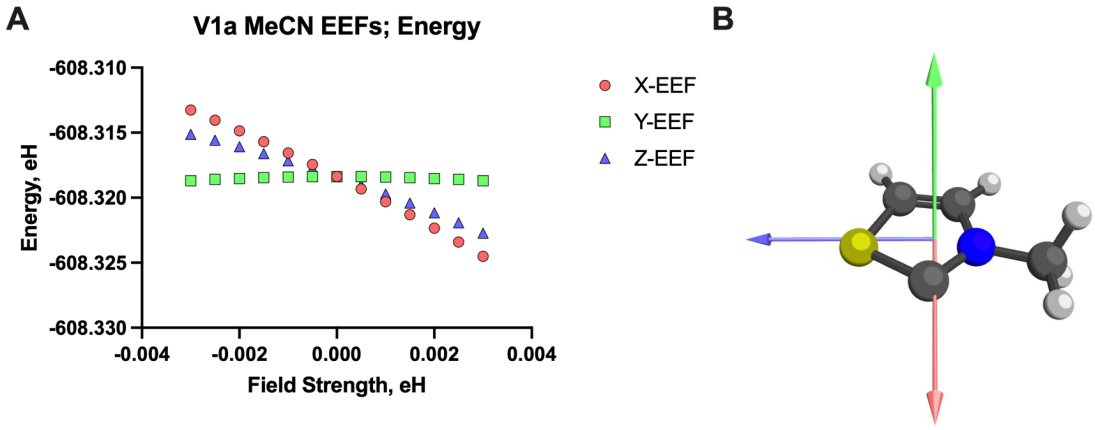


Figure S46. V_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S45. V_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.305354	-608.310858	-608.307246
– 0.0025	-608.306144	-608.310757	-608.307715
– 0.0020	-608.306963	-608.310674	-608.308216
– 0.0015	-608.307810	-608.310609	-608.308747
– 0.0010	-608.308686	-608.310563	-608.309309
– 0.0005	-608.309592	-608.310535	-608.309902
+ 0.0000	-608.310526	-608.310526	-608.310526
+ 0.0005	-608.311489	-608.310535	-608.311181
+ 0.0010	-608.312482	-608.310563	-608.311866
+ 0.0015	-608.313503	-608.310609	-608.312583
+ 0.0020	-608.314554	-608.310674	-608.313330
+ 0.0025	-608.315634	-608.310757	-608.314109
+ 0.0030	-608.316743	-608.310858	-608.314919

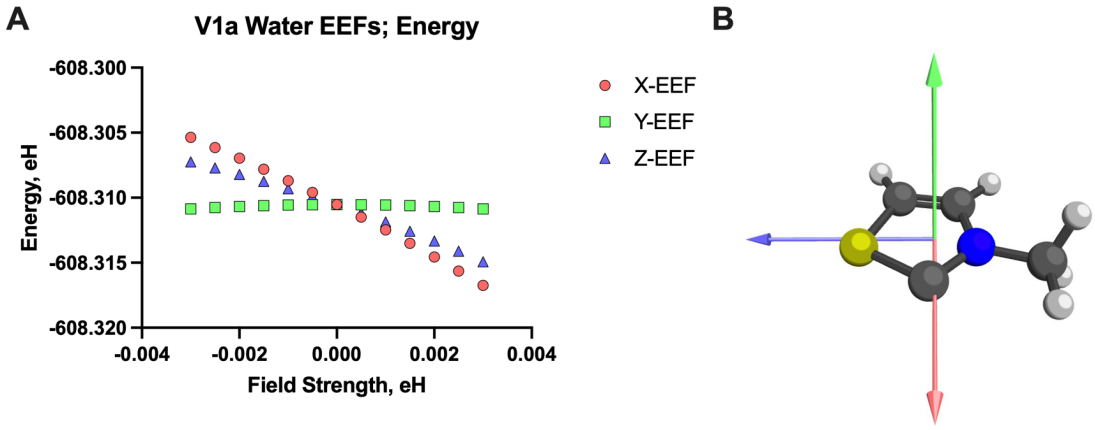


Figure S47. V_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S46. $^3V_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.195360	-608.197090	-608.193970
– 0.0025	-608.195470	-608.196930	-608.194300
– 0.0020	-608.195600	-608.196770	-608.194650
– 0.0015	-608.195750	-608.196640	-608.195030
– 0.0010	-608.195910	-608.196510	-608.195430
– 0.0005	-608.196100	-608.196400	-608.195860
+ 0.0000	-608.196300	-608.196300	-608.196300
+ 0.0005	-608.196530	-608.196220	-608.196780
+ 0.0010	-608.196770	-608.196160	-608.197270
+ 0.0015	-608.197030	-608.196100	-608.197800
+ 0.0020	-608.197310	-608.196060	-608.198340
+ 0.0025	-608.197610	-608.196040	-608.198910
+ 0.0030	-608.197930	-608.196030	-608.199500

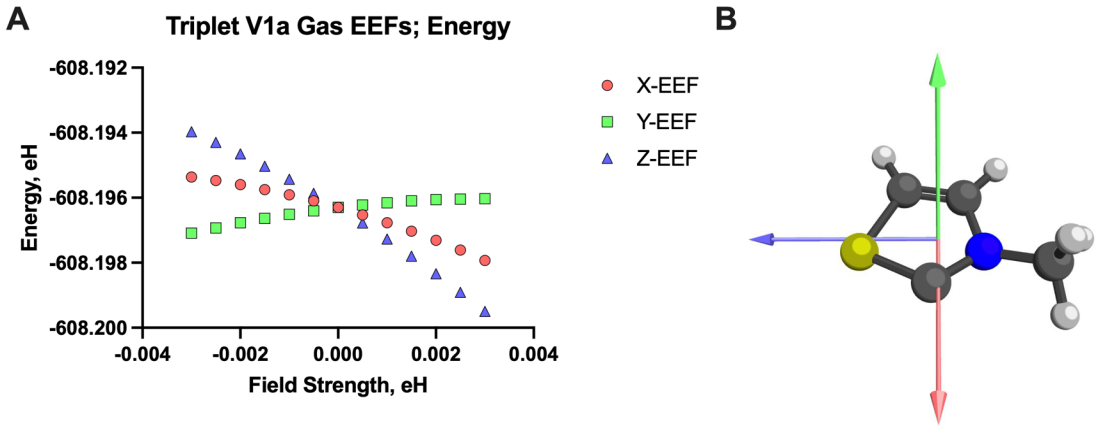


Figure S48. $^3V_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S47. $^3V_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.201184	-608.203300	-608.199525
– 0.0025	-608.201323	-608.203101	-608.199927
– 0.0020	-608.201484	-608.202918	-608.200357
– 0.0015	-608.201668	-608.202752	-608.200814
– 0.0010	-608.201874	-608.202602	-608.201299
– 0.0005	-608.202102	-608.202469	-608.201812
+ 0.0000	-608.202352	-608.202352	-608.202352
+ 0.0005	-608.202625	-608.202252	-608.202920
+ 0.0010	-608.202921	-608.202169	-608.203517
+ 0.0015	-608.203238	-608.202102	-608.204140
+ 0.0020	-608.203579	-608.202052	-608.204792
+ 0.0025	-608.203942	-608.202019	-608.205471
+ 0.0030	-608.204327	-608.202002	-608.206178

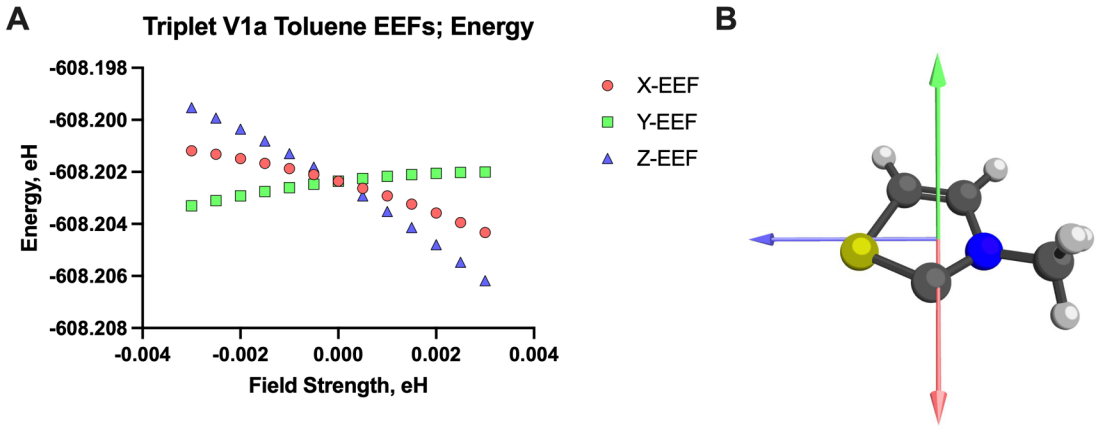


Figure S49. $^3V_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S48. $^3V_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.203769	-608.206264	-608.201954
– 0.0025	-608.203937	-608.206033	-608.202411
– 0.0020	-608.204131	-608.205821	-608.202900
– 0.0015	-608.204351	-608.205629	-608.203420
– 0.0010	-608.204598	-608.205456	-608.203972
– 0.0005	-608.204870	-608.205302	-608.204554
+ 0.0000	-608.205168	-608.205168	-608.205168
+ 0.0005	-608.205492	-608.205053	-608.205813
+ 0.0010	-608.205843	-608.204957	-608.206489
+ 0.0015	-608.206220	-608.204881	-608.207196
+ 0.0020	-608.206623	-608.204825	-608.207935
+ 0.0025	-608.207053	-608.204788	-608.208705
+ 0.0030	-608.207509	-608.204771	-608.209506

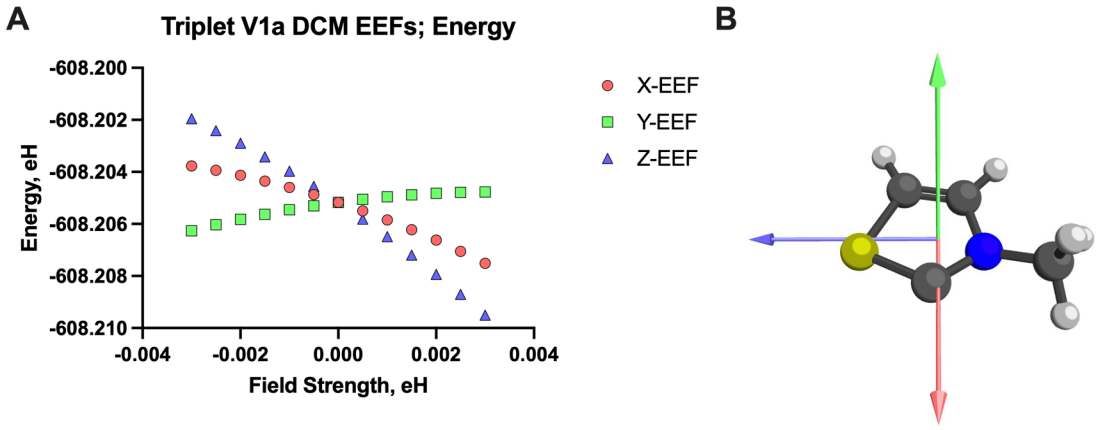


Figure S50. $^3V_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S49. $^3V_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.203204	-608.205849	-608.201352
– 0.0025	-608.203384	-608.205606	-608.201828
– 0.0020	-608.203592	-608.205383	-608.202337
– 0.0015	-608.203827	-608.205180	-608.202878
– 0.0010	-608.204089	-608.204998	-608.203452
– 0.0005	-608.204379	-608.204837	-608.204058
+ 0.0000	-608.204697	-608.204697	-608.204697
+ 0.0005	-608.205042	-608.204577	-608.205368
+ 0.0010	-608.205415	-608.204478	-608.206071
+ 0.0015	-608.205816	-608.204400	-608.206807
+ 0.0020	-608.206245	-608.204342	-608.207576
+ 0.0025	-608.206702	-608.204306	-608.208377
+ 0.0030	-608.207188	-608.204290	-608.209211

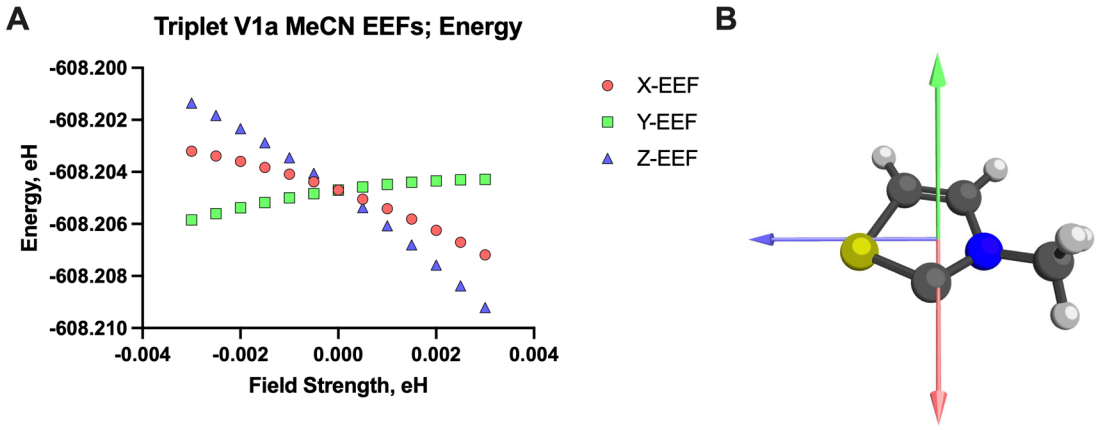


Figure S51. $^3V_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S50. $^3V_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-608.195915	-608.198590	-608.194056
– 0.0025	-608.196097	-608.198344	-608.194536
– 0.0020	-608.196308	-608.198119	-608.195049
– 0.0015	-608.196545	-608.197914	-608.195594
– 0.0010	-608.196811	-608.197731	-608.196172
– 0.0005	-608.197105	-608.197568	-608.196783
+ 0.0000	-608.197426	-608.197426	-608.197426
+ 0.0005	-608.197776	-608.197306	-608.198103
+ 0.0010	-608.198154	-608.197206	-608.198811
+ 0.0015	-608.198560	-608.197127	-608.199553
+ 0.0020	-608.198994	-608.197070	-608.200327
+ 0.0025	-608.199457	-608.197033	-608.201134
+ 0.0030	-608.199948	-608.197018	-608.201975

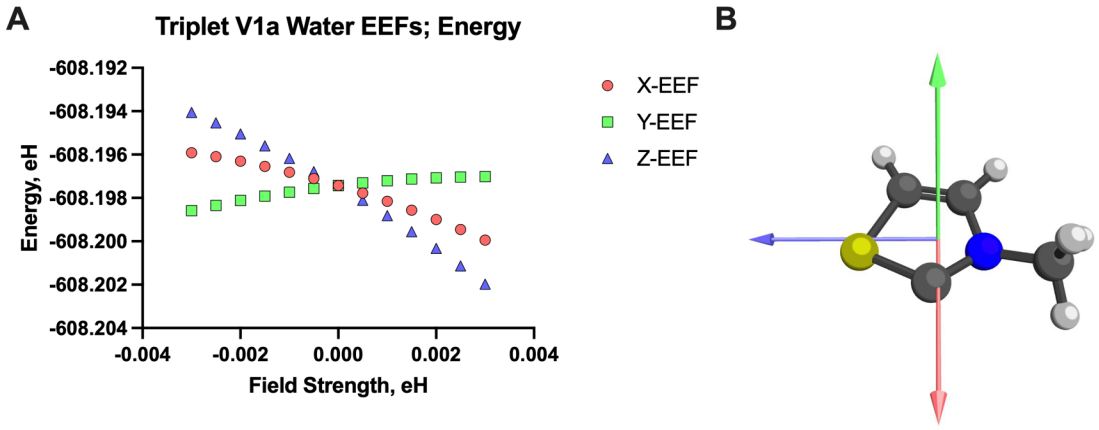


Figure S52. $^3V_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S51. VI_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.970126	-305.973592	-305.973754
– 0.0025	-305.970608	-305.973508	-305.973620
– 0.0020	-305.971110	-305.973440	-305.973511
– 0.0015	-305.971632	-305.973386	-305.973426
– 0.0010	-305.972174	-305.973348	-305.973366
– 0.0005	-305.972736	-305.973325	-305.973329
+ 0.0000	-305.973317	-305.973317	-305.973317
+ 0.0005	-305.973919	-305.973325	-305.973329
+ 0.0010	-305.974540	-305.973348	-305.973366
+ 0.0015	-305.975181	-305.973386	-305.973426
+ 0.0020	-305.975841	-305.973440	-305.973511
+ 0.0025	-305.976522	-305.973508	-305.973620
+ 0.0030	-305.977222	-305.973592	-305.973754

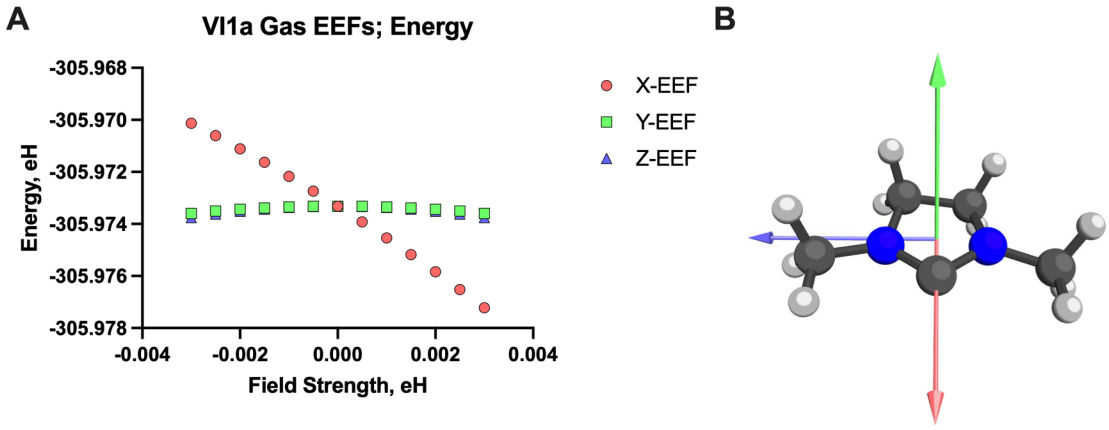


Figure S53. VI_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S52. VI_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.985037	-305.989279	-305.989463
– 0.0025	-305.985633	-305.989181	-305.989309
– 0.0020	-305.986252	-305.989101	-305.989183
– 0.0015	-305.986894	-305.989039	-305.989085
– 0.0010	-305.987559	-305.988995	-305.989015
– 0.0005	-305.988247	-305.988968	-305.988973
+ 0.0000	-305.988959	-305.988959	-305.988959
+ 0.0005	-305.989694	-305.988968	-305.988973
+ 0.0010	-305.990452	-305.988995	-305.989015
+ 0.0015	-305.991233	-305.989039	-305.989085
+ 0.0020	-305.992038	-305.989101	-305.989183
+ 0.0025	-305.992866	-305.989181	-305.989309
+ 0.0030	-305.993717	-305.989279	-305.989463

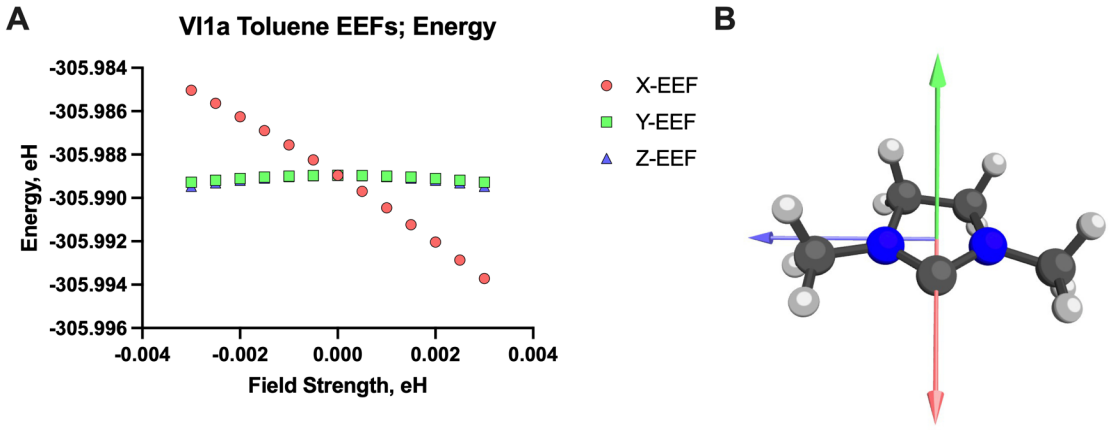


Figure S54. VI_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S53. VI_{1a} Under EEFs in SMD Dichloromethane.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.988595	-305.993675	-305.993861
– 0.0025	-305.989312	-305.993560	-305.993689
– 0.0020	-305.990056	-305.993466	-305.993549
– 0.0015	-305.990827	-305.993393	-305.993439
– 0.0010	-305.991624	-305.993341	-305.993361
– 0.0005	-305.992448	-305.993309	-305.993315
+ 0.0000	-305.993299	-305.993299	-305.993299
+ 0.0005	-305.994177	-305.993309	-305.993315
+ 0.0010	-305.995081	-305.993341	-305.993361
+ 0.0015	-305.996012	-305.993393	-305.993439
+ 0.0020	-305.996970	-305.993466	-305.993549
+ 0.0025	-305.997955	-305.993560	-305.993689
+ 0.0030	-305.998966	-305.993675	-305.993861

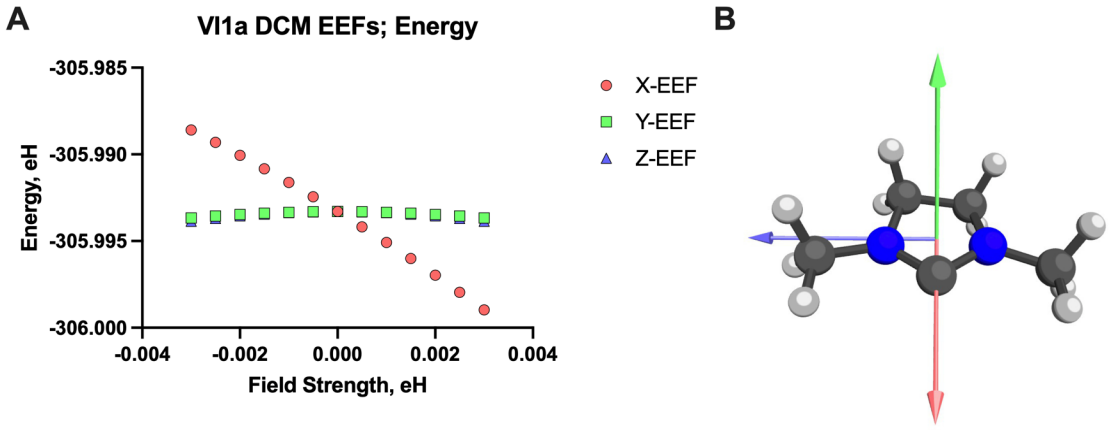


Figure S55. VI_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S54. VI_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.988428	-305.993855	-305.994037
– 0.0025	-305.989195	-305.993733	-305.993859
– 0.0020	-305.989990	-305.993632	-305.993713
– 0.0015	-305.990814	-305.993554	-305.993599
– 0.0010	-305.991666	-305.993498	-305.993518
– 0.0005	-305.992546	-305.993465	-305.993470
+ 0.0000	-305.993454	-305.993454	-305.993454
+ 0.0005	-305.994390	-305.993465	-305.993470
+ 0.0010	-305.995355	-305.993498	-305.993518
+ 0.0015	-305.996347	-305.993554	-305.993599
+ 0.0020	-305.997369	-305.993632	-305.993713
+ 0.0025	-305.998418	-305.993733	-305.993859
+ 0.0030	-305.999496	-305.993855	-305.994037

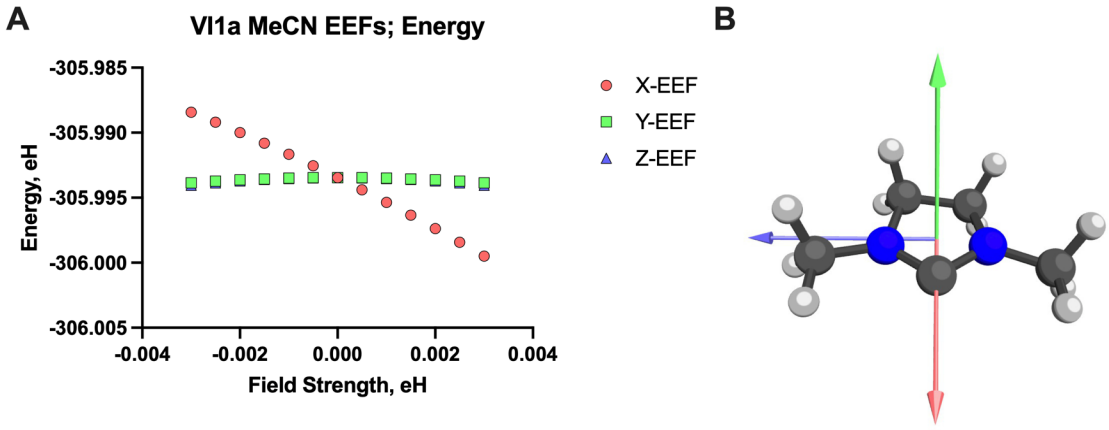


Figure S56. VI_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S55. VI_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.975625	-305.981125	-305.981305
– 0.0025	-305.976402	-305.981000	-305.981125
– 0.0020	-305.977208	-305.980898	-305.980978
– 0.0015	-305.978043	-305.980819	-305.980864
– 0.0010	-305.978906	-305.980763	-305.980783
– 0.0005	-305.979797	-305.980729	-305.980734
+ 0.0000	-305.980717	-305.980717	-305.980717
+ 0.0005	-305.981666	-305.980729	-305.980734
+ 0.0010	-305.982643	-305.980763	-305.980783
+ 0.0015	-305.983649	-305.980819	-305.980864
+ 0.0020	-305.984683	-305.980898	-305.980978
+ 0.0025	-305.985745	-305.981000	-305.981125
+ 0.0030	-305.986837	-305.981125	-305.981305

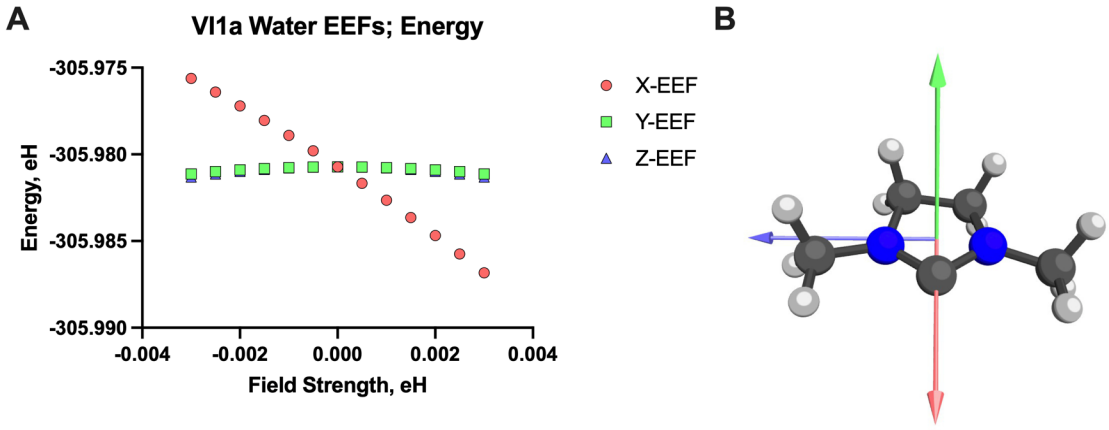


Figure S57. VI_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S56. ^{3}VI$_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.858380	-305.859994	-305.860271
– 0.0025	-305.858551	-305.859898	-305.860119
– 0.0020	-305.858742	-305.859820	-305.859990
– 0.0015	-305.858952	-305.859761	-305.859884
– 0.0010	-305.859182	-305.859721	-305.859799
– 0.0005	-305.859430	-305.859700	-305.859738
+ 0.0000	-305.859698	-305.859698	-305.859698
+ 0.0005	-305.859985	-305.859715	-305.859681
+ 0.0010	-305.860291	-305.859751	-305.859686
+ 0.0015	-305.860617	-305.859805	-305.859714
+ 0.0020	-305.860962	-305.859879	-305.859764
+ 0.0025	-305.861326	-305.859972	-305.859837
+ 0.0030	-305.861710	-305.860084	-305.859932

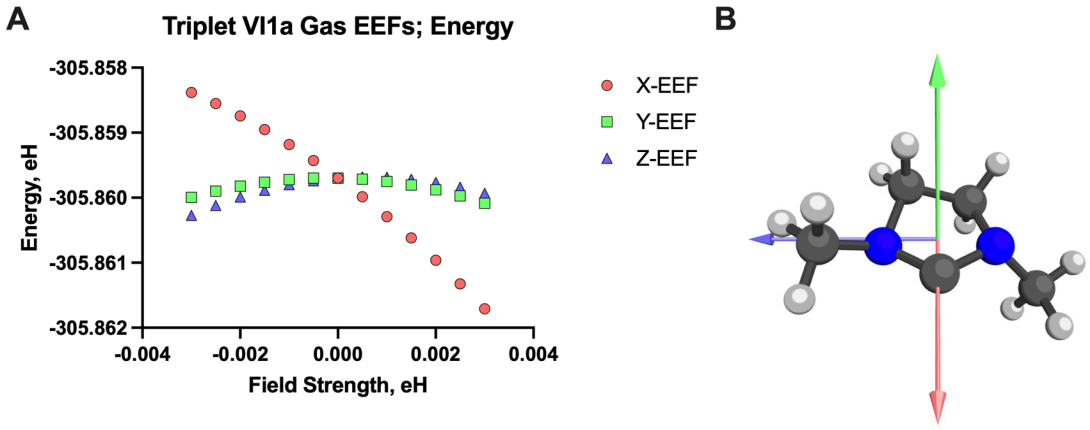


Figure S58. ^{3}VI$_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S57. $^3VI_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.869624	-305.871607	-305.871904
– 0.0025	-305.869838	-305.871492	-305.871730
– 0.0020	-305.870075	-305.871399	-305.871582
– 0.0015	-305.870334	-305.871327	-305.871460
– 0.0010	-305.870615	-305.871278	-305.871363
– 0.0005	-305.870920	-305.871251	-305.871292
+ 0.0000	-305.871246	-305.871246	-305.871246
+ 0.0005	-305.871595	-305.871263	-305.871226
+ 0.0010	-305.871967	-305.871303	-305.871232
+ 0.0015	-305.872362	-305.871364	-305.871264
+ 0.0020	-305.872779	-305.871448	-305.871321
+ 0.0025	-305.873219	-305.871555	-305.871404
+ 0.0030	-305.873681	-305.871683	-305.871513

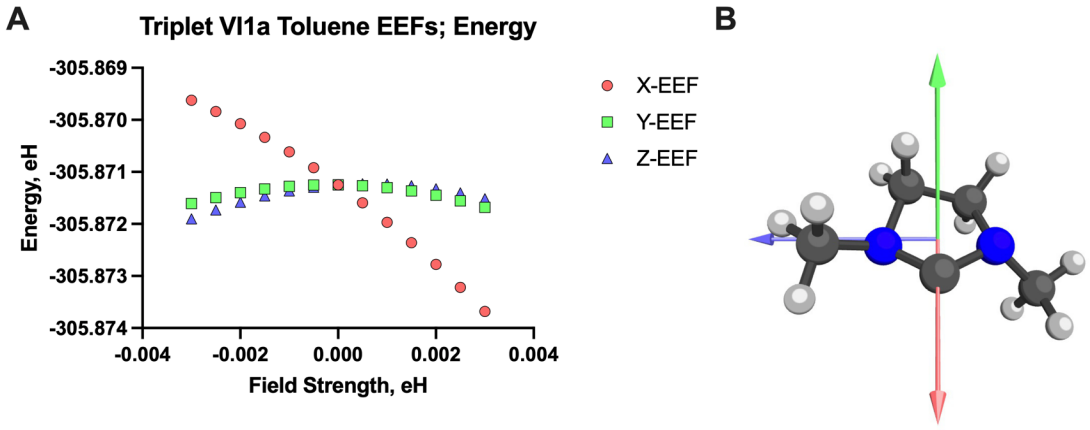


Figure S59. $^3VI_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S58. ^{3}VI$_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.871809	-305.874179	-305.874485
– 0.0025	-305.872068	-305.874042	-305.874291
– 0.0020	-305.872352	-305.873931	-305.874125
– 0.0015	-305.872662	-305.873846	-305.873988
– 0.0010	-305.872998	-305.873787	-305.873879
– 0.0005	-305.873359	-305.873754	-305.873799
+ 0.0000	-305.873748	-305.873748	-305.873748
+ 0.0005	-305.874162	-305.873767	-305.873725
+ 0.0010	-305.874602	-305.873812	-305.873730
+ 0.0015	-305.875068	-305.873883	-305.873764
+ 0.0020	-305.875561	-305.873981	-305.873827
+ 0.0025	-305.876080	-305.874105	-305.873919
+ 0.0030	-305.876625	-305.874256	-305.874039

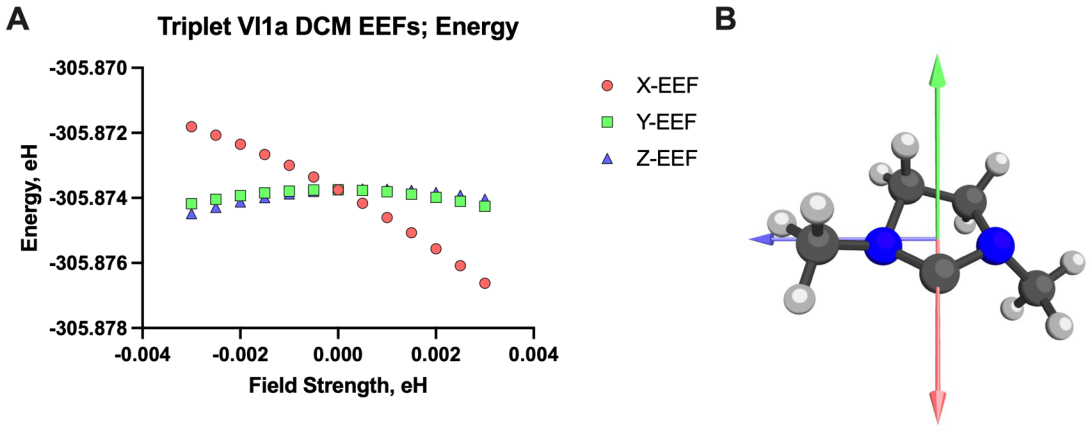


Figure S60. ^{3}VI$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S59. ^{3}VI$_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.870894	-305.873422	-305.873729
– 0.0025	-305.871170	-305.873276	-305.873527
– 0.0020	-305.871474	-305.873157	-305.873355
– 0.0015	-305.871805	-305.873067	-305.873212
– 0.0010	-305.872163	-305.873004	-305.873099
– 0.0005	-305.872548	-305.872969	-305.873015
+ 0.0000	-305.872961	-305.872961	-305.872961
+ 0.0005	-305.873402	-305.872982	-305.872937
+ 0.0010	-305.873870	-305.873031	-305.872942
+ 0.0015	-305.874366	-305.873107	-305.872977
+ 0.0020	-305.874890	-305.873212	-305.873042
+ 0.0025	-305.875441	-305.873345	-305.873136
+ 0.0030	-305.876020	-305.873507	-305.873260

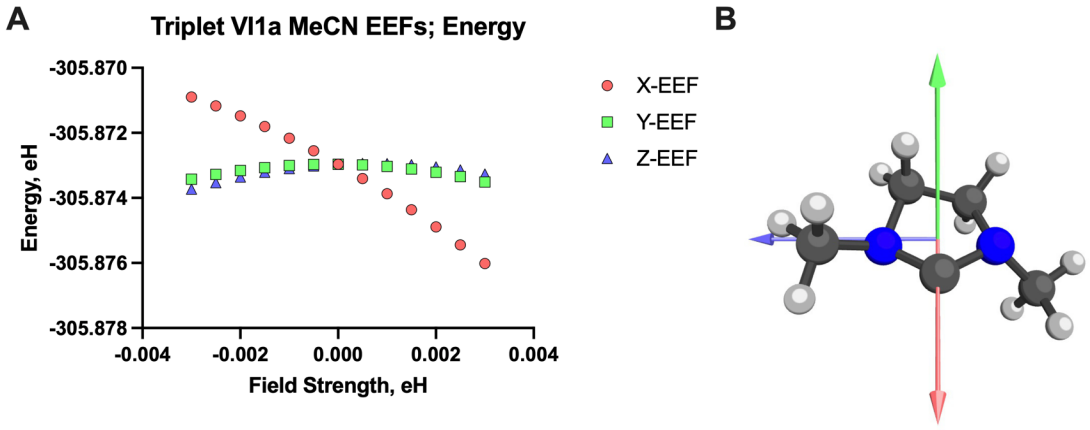


Figure S61. ^{3}VI$_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S60. ^{3}VI$_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-305.863685	-305.866245	-305.866552
– 0.0025	-305.863964	-305.866097	-305.866349
– 0.0020	-305.864272	-305.865977	-305.866175
– 0.0015	-305.864607	-305.865885	-305.866031
– 0.0010	-305.864969	-305.865821	-305.865917
– 0.0005	-305.865360	-305.865785	-305.865833
+ 0.0000	-305.865778	-305.865778	-305.865778
+ 0.0005	-305.866224	-305.865799	-305.865754
+ 0.0010	-305.866698	-305.865849	-305.865759
+ 0.0015	-305.867200	-305.865926	-305.865794
+ 0.0020	-305.867730	-305.866033	-305.865859
+ 0.0025	-305.868288	-305.866168	-305.865954
+ 0.0030	-305.868875	-305.866332	-305.866079

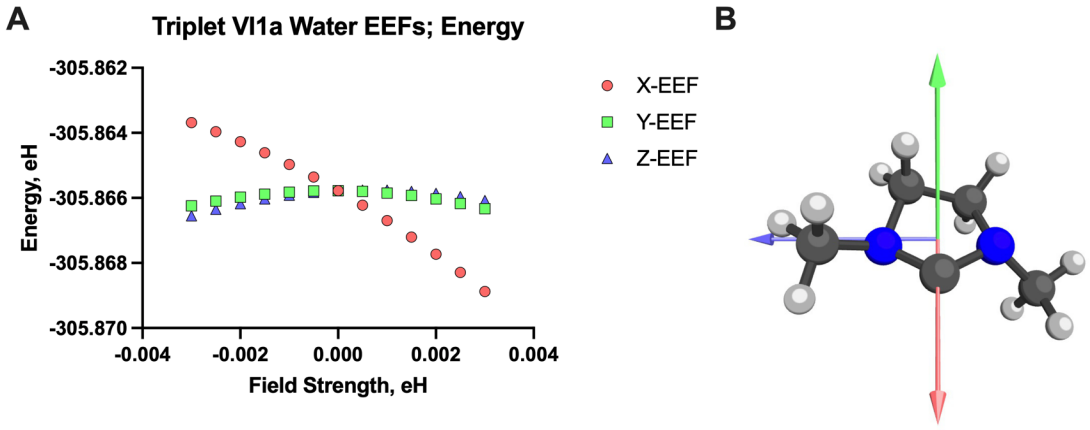


Figure S62. ^{3}VI$_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S61. VII_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.278395	-345.281889	-345.282081
– 0.0025	-345.278870	-345.281794	-345.281930
– 0.0020	-345.279367	-345.281717	-345.281806
– 0.0015	-345.279888	-345.281658	-345.281710
– 0.0010	-345.280431	-345.281617	-345.281641
– 0.0005	-345.280997	-345.281593	-345.281600
+ 0.0000	-345.281587	-345.281587	-345.281587
+ 0.0005	-345.282199	-345.281598	-345.281600
+ 0.0010	-345.282834	-345.281627	-345.281641
+ 0.0015	-345.283492	-345.281674	-345.281710
+ 0.0020	-345.284174	-345.281738	-345.281806
+ 0.0025	-345.284878	-345.281820	-345.281930
+ 0.0030	-345.285606	-345.281920	-345.282080

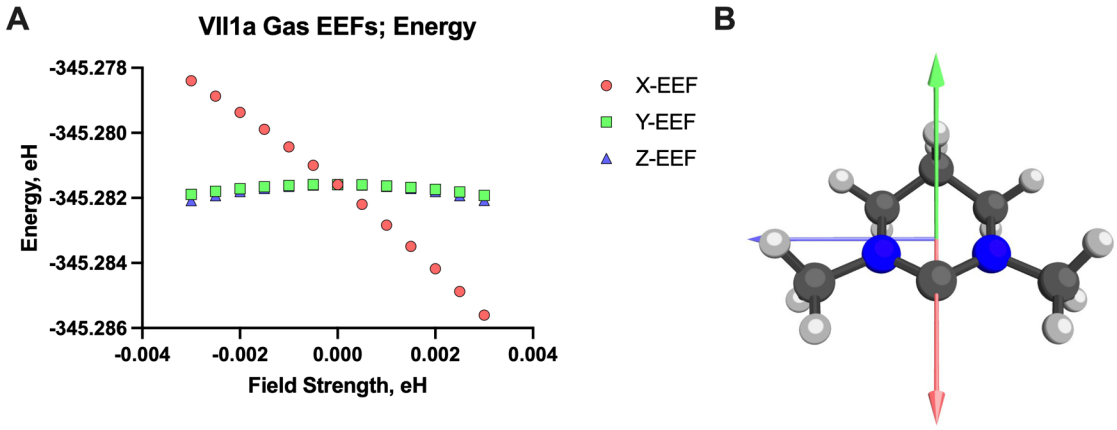


Figure S63. VII_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S62. VII_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.293356	-345.297623	-345.297860
– 0.0025	-345.293943	-345.297515	-345.297685
– 0.0020	-345.294558	-345.297427	-345.297541
– 0.0015	-345.295199	-345.297361	-345.297429
– 0.0010	-345.295868	-345.297315	-345.297349
– 0.0005	-345.296563	-345.297290	-345.297301
+ 0.0000	-345.297285	-345.297285	-345.297285
+ 0.0005	-345.298034	-345.297301	-345.297301
+ 0.0010	-345.298810	-345.297338	-345.297349
+ 0.0015	-345.299613	-345.297396	-345.297429
+ 0.0020	-345.300443	-345.297474	-345.297541
+ 0.0025	-345.301300	-345.297573	-345.297685
+ 0.0030	-345.302184	-345.297693	-345.297860

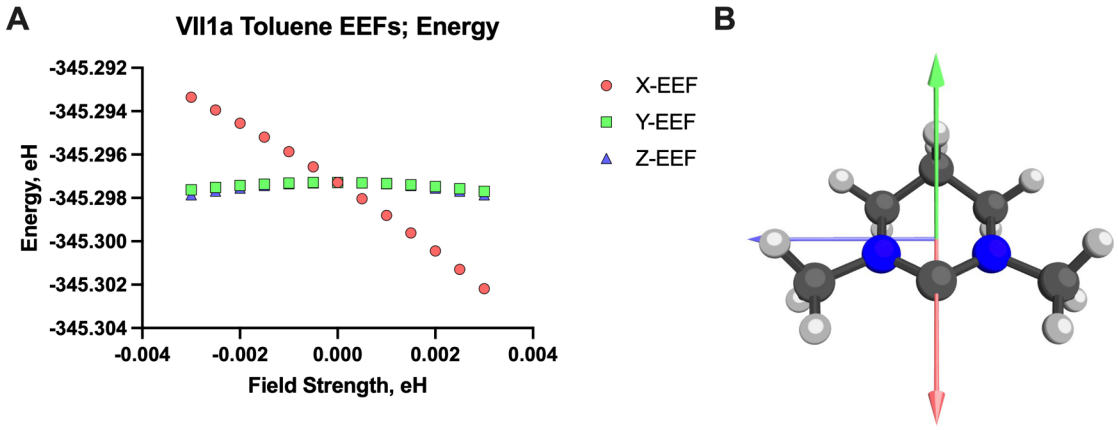


Figure S64. VII_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S63. VII_{1a} Under EEFs in SMD Dichloromethane.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.297096	-345.302196	-345.302478
– 0.0025	-345.297808	-345.302073	-345.302280
– 0.0020	-345.298550	-345.301975	-345.302118
– 0.0015	-345.299324	-345.301902	-345.301992
– 0.0010	-345.300128	-345.301853	-345.301901
– 0.0005	-345.300963	-345.301829	-345.301847
+ 0.0000	-345.301829	-345.301829	-345.301829
+ 0.0005	-345.302727	-345.301854	-345.301847
+ 0.0010	-345.303655	-345.301904	-345.301901
+ 0.0015	-345.304614	-345.301978	-345.301992
+ 0.0020	-345.305605	-345.302076	-345.302118
+ 0.0025	-345.306626	-345.302199	-345.302280
+ 0.0030	-345.307679	-345.302347	-345.302478

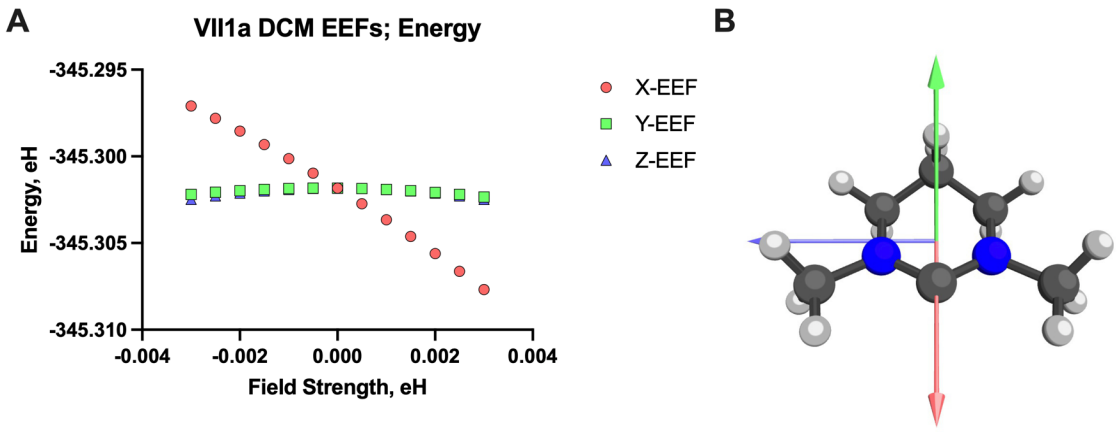


Figure S65. VII_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S64. VII_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.296859	-345.302306	-345.302606
– 0.0025	-345.297623	-345.302178	-345.302399
– 0.0020	-345.298419	-345.302075	-345.302231
– 0.0015	-345.299248	-345.302000	-345.302099
– 0.0010	-345.300110	-345.301950	-345.302006
– 0.0005	-345.301004	-345.301927	-345.301949
+ 0.0000	-345.301931	-345.301931	-345.301931
+ 0.0005	-345.302890	-345.301960	-345.301949
+ 0.0010	-345.303882	-345.302016	-345.302006
+ 0.0015	-345.304907	-345.302099	-345.302099
+ 0.0020	-345.305964	-345.302208	-345.302231
+ 0.0025	-345.307055	-345.302343	-345.302399
+ 0.0030	-345.308178	-345.302505	-345.302606

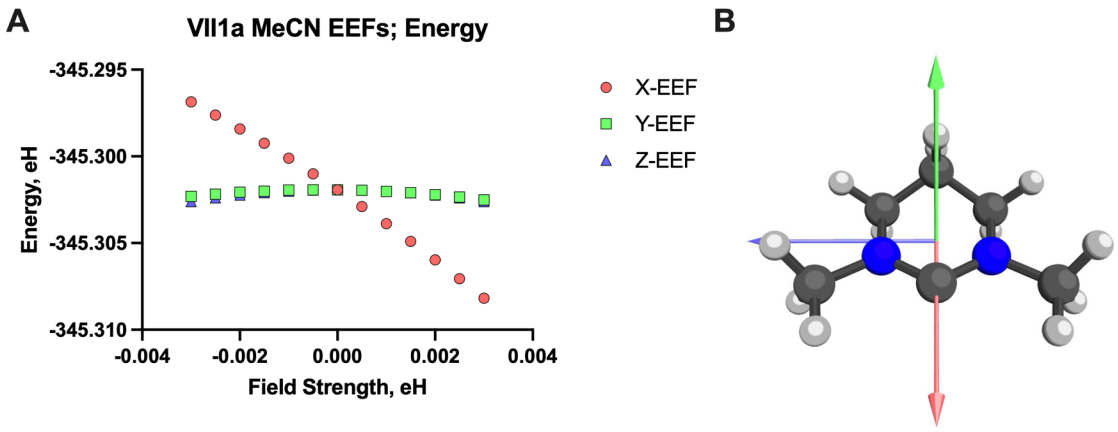


Figure S66. VII_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S65. VII_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.284153	-345.289672	-345.289976
– 0.0025	-345.284928	-345.289542	-345.289768
– 0.0020	-345.285736	-345.289439	-345.289597
– 0.0015	-345.286576	-345.289363	-345.289465
– 0.0010	-345.287449	-345.289314	-345.289371
– 0.0005	-345.288356	-345.289291	-345.289314
+ 0.0000	-345.289295	-345.289295	-345.289295
+ 0.0005	-345.290267	-345.289326	-345.289314
+ 0.0010	-345.291272	-345.289384	-345.289371
+ 0.0015	-345.292311	-345.289468	-345.289465
+ 0.0020	-345.293382	-345.289579	-345.289598
+ 0.0025	-345.294487	-345.289717	-345.289768
+ 0.0030	-345.295625	-345.289882	-345.289976

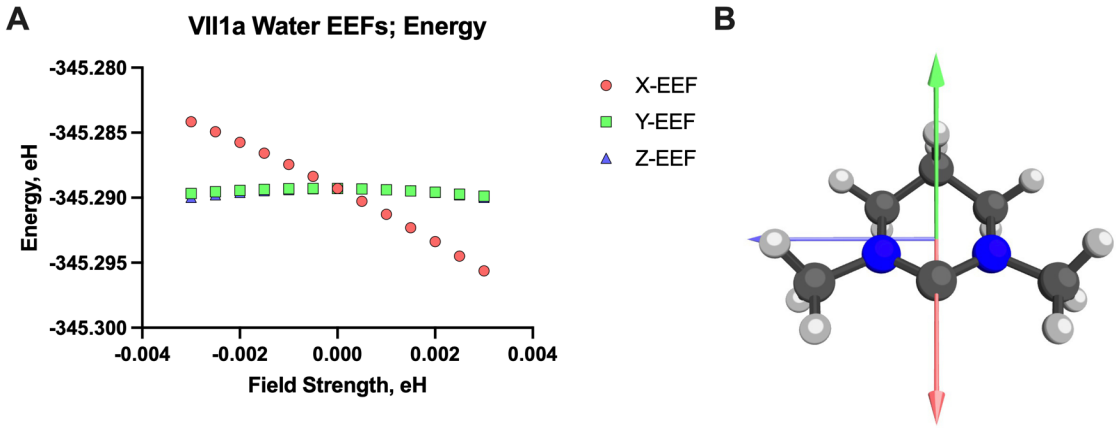


Figure S67. VII_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S66. ^{3}VII$_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.183650	-345.185481	-345.184515
– 0.0025	-345.183655	-345.185186	-345.184367
– 0.0020	-345.183683	-345.184912	-345.184245
– 0.0015	-345.183735	-345.184659	-345.184150
– 0.0010	-345.183809	-345.184427	-345.184082
– 0.0005	-345.183907	-345.184217	-345.184042
+ 0.0000	-345.184028	-345.184028	-345.184028
+ 0.0005	-345.184173	-345.183861	-345.184042
+ 0.0010	-345.184340	-345.183716	-345.184082
+ 0.0015	-345.184531	-345.183592	-345.184150
+ 0.0020	-345.184746	-345.183491	-345.184245
+ 0.0025	-345.184984	-345.183411	-345.184367
+ 0.0030	-345.185246	-345.183354	-345.184516

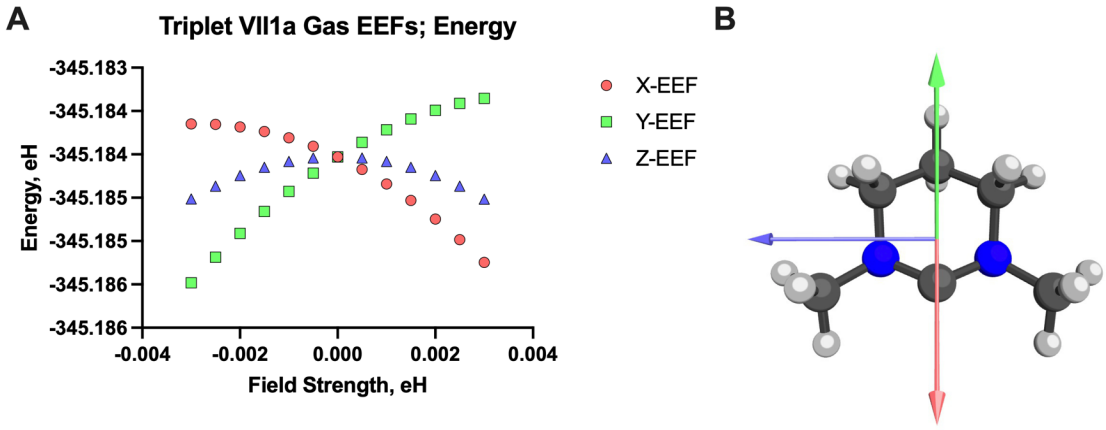


Figure S68. ^{3}VII$_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S67. ^{3}VII$_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.195257	-345.197561	-345.196293
– 0.0025	-345.195267	-345.197193	-345.196120
– 0.0020	-345.195305	-345.196850	-345.195979
– 0.0015	-345.195370	-345.196532	-345.195869
– 0.0010	-345.195462	-345.196239	-345.195791
– 0.0005	-345.195581	-345.195971	-345.195744
+ 0.0000	-345.195728	-345.195728	-345.195728
+ 0.0005	-345.195903	-345.195511	-345.195744
+ 0.0010	-345.196104	-345.195320	-345.195791
+ 0.0015	-345.196334	-345.195154	-345.195870
+ 0.0020	-345.196590	-345.195014	-345.195980
+ 0.0025	-345.196875	-345.194901	-345.196121
+ 0.0030	-345.197187	-345.194814	-345.196294

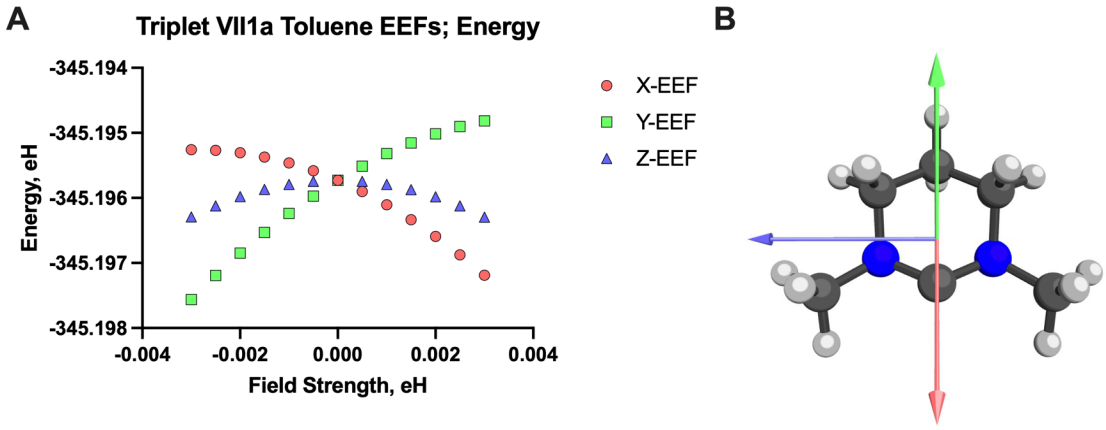


Figure S69. ^{3}VII$_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S68. ^{3}VII$_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.197734	-345.200567	-345.198919
– 0.0025	-345.197746	-345.200112	-345.198725
– 0.0020	-345.197791	-345.199687	-345.198567
– 0.0015	-345.197867	-345.199292	-345.198444
– 0.0010	-345.197975	-345.198927	-345.198356
– 0.0005	-345.198114	-345.198591	-345.198303
+ 0.0000	-345.198286	-345.198286	-345.198286
+ 0.0005	-345.198489	-345.198011	-345.198303
+ 0.0010	-345.198725	-345.197766	-345.198356
+ 0.0015	-345.198993	-345.197553	-345.198444
+ 0.0020	-345.199293	-345.197370	-345.198568
+ 0.0025	-345.199625	-345.197218	-345.198726
+ 0.0030	-345.199990	-345.197097	-345.198920

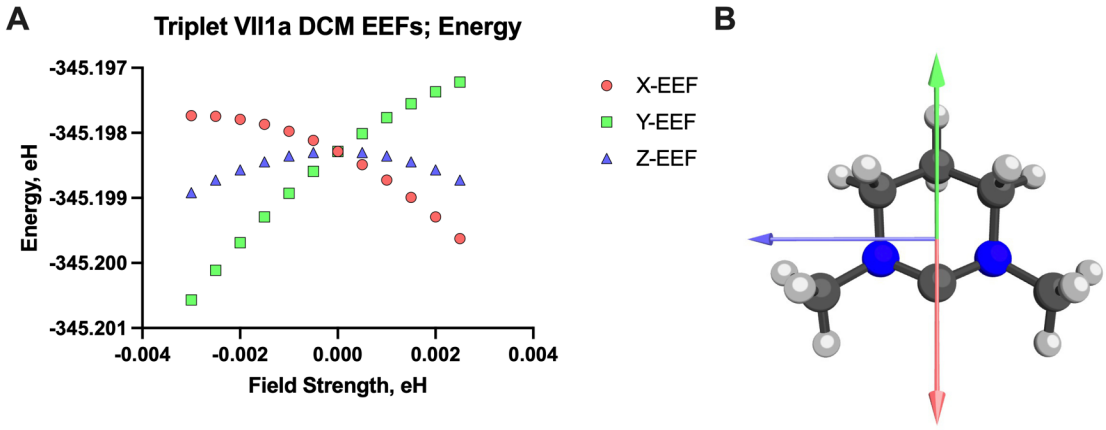


Figure S70. ^{3}VII$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S69. ^{3}VII$_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.196825	-345.199886	-345.198060
– 0.0025	-345.196837	-345.199391	-345.197859
– 0.0020	-345.196882	-345.198929	-345.197694
– 0.0015	-345.196961	-345.198499	-345.197566
– 0.0010	-345.197074	-345.198101	-345.197475
– 0.0005	-345.197221	-345.197735	-345.197420
+ 0.0000	-345.197402	-345.197402	-345.197402
+ 0.0005	-345.197616	-345.197101	-345.197420
+ 0.0010	-345.197865	-345.196833	-345.197475
+ 0.0015	-345.198148	-345.196598	-345.197566
+ 0.0020	-345.198465	-345.196397	-345.197695
+ 0.0025	-345.198817	-345.196229	-345.197859
+ 0.0030	-345.199203	-345.196095	-345.198061

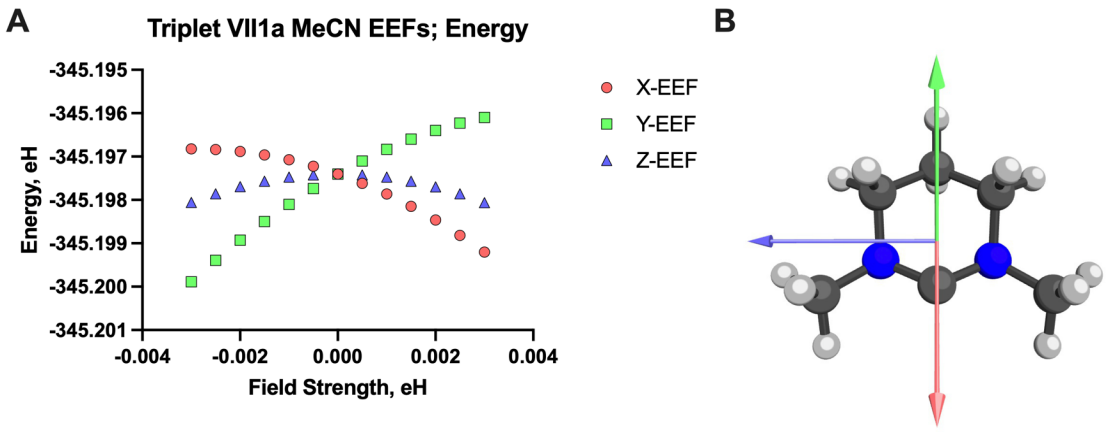


Figure S71. ^{3}VII$_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S70. ^{3}VII$_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-345.188908	-345.192017	-345.190152
– 0.0025	-345.188919	-345.191514	-345.189949
– 0.0020	-345.188965	-345.191043	-345.189783
– 0.0015	-345.189045	-345.190605	-345.189654
– 0.0010	-345.189158	-345.190200	-345.189562
– 0.0005	-345.189306	-345.189828	-345.189507
+ 0.0000	-345.189489	-345.189489	-345.189489
+ 0.0005	-345.189706	-345.189183	-345.189507
+ 0.0010	-345.189957	-345.188910	-345.189563
+ 0.0015	-345.190243	-345.188671	-345.189655
+ 0.0020	-345.190564	-345.188466	-345.189784
+ 0.0025	-345.190919	-345.188294	-345.189950
+ 0.0030	-345.191310	-345.188158	-345.190153

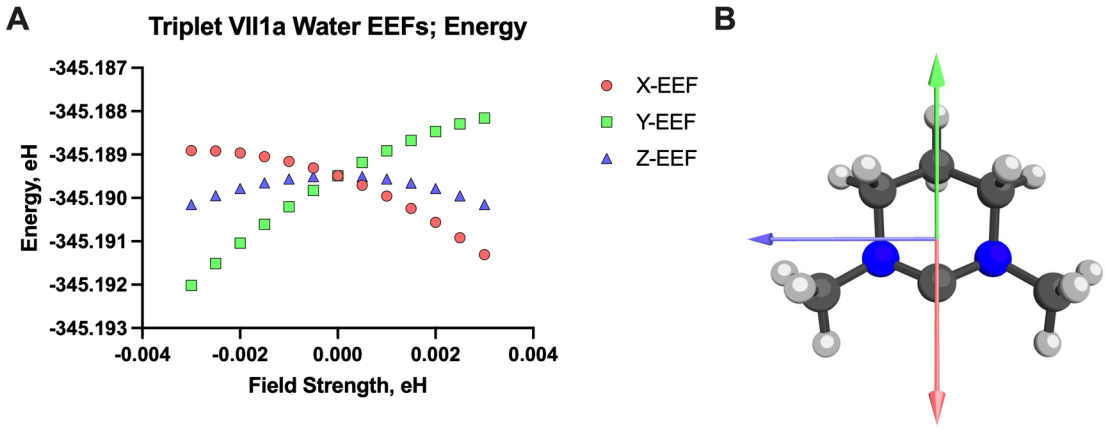


Figure S72. ^{3}VII$_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S71. $VIII_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.995390	-327.998327	-327.997199
– 0.0025	-327.995767	-327.998222	-327.997261
– 0.0020	-327.996166	-327.998136	-327.997350
– 0.0015	-327.996587	-327.998069	-327.997467
– 0.0010	-327.997030	-327.998021	-327.997611
– 0.0005	-327.997496	-327.997993	-327.997783
+ 0.0000	-327.997983	-327.997983	-327.997983
+ 0.0005	-327.998493	-327.997993	-327.998211
+ 0.0010	-327.999024	-327.998021	-327.998465
+ 0.0015	-327.999578	-327.998069	-327.998748
+ 0.0020	-328.000154	-327.998136	-327.999058
+ 0.0025	-328.000753	-327.998222	-327.999395
+ 0.0030	-328.001373	-327.998327	-327.999761

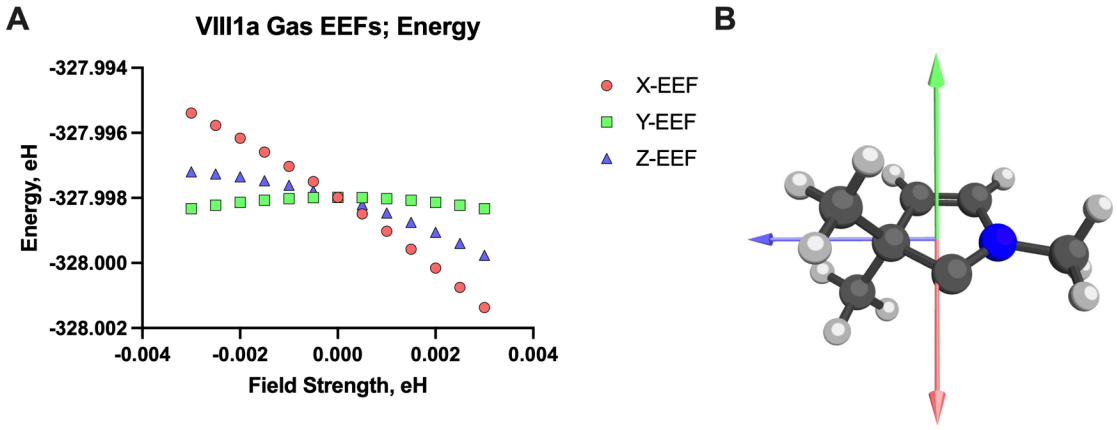


Figure S73. $VIII_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S72. $VIII_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-328.006387	-328.009991	-328.008681
– 0.0025	-328.006855	-328.009869	-328.008752
– 0.0020	-328.007349	-328.009768	-328.008855
– 0.0015	-328.007870	-328.009690	-328.008991
– 0.0010	-328.008417	-328.009635	-328.009159
– 0.0005	-328.008990	-328.009601	-328.009358
+ 0.0000	-328.009590	-328.009590	-328.009590
+ 0.0005	-328.010216	-328.009601	-328.009854
+ 0.0010	-328.010869	-328.009635	-328.010151
+ 0.0015	-328.011548	-328.009691	-328.010479
+ 0.0020	-328.012254	-328.009769	-328.010840
+ 0.0025	-328.012985	-328.009869	-328.011232
+ 0.0030	-328.013744	-328.009991	-328.011657

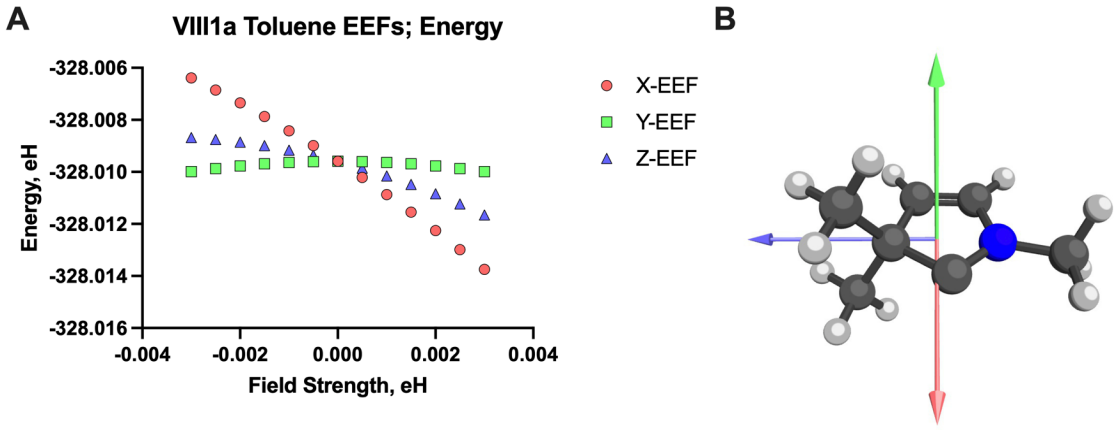


Figure S74. $VIII_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S73. VIII $_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-328.011023	-328.015402	-328.013943
– 0.0025	-328.011598	-328.015260	-328.014017
– 0.0020	-328.012203	-328.015143	-328.014128
– 0.0015	-328.012839	-328.015052	-328.014275
– 0.0010	-328.013507	-328.014987	-328.014459
– 0.0005	-328.014206	-328.014948	-328.014679
+ 0.0000	-328.014936	-328.014936	-328.014936
+ 0.0005	-328.015697	-328.014949	-328.015228
+ 0.0010	-328.016489	-328.014988	-328.015557
+ 0.0015	-328.017313	-328.015052	-328.015923
+ 0.0020	-328.018169	-328.015143	-328.016325
+ 0.0025	-328.019055	-328.015260	-328.016763
+ 0.0030	-328.019974	-328.015403	-328.017237

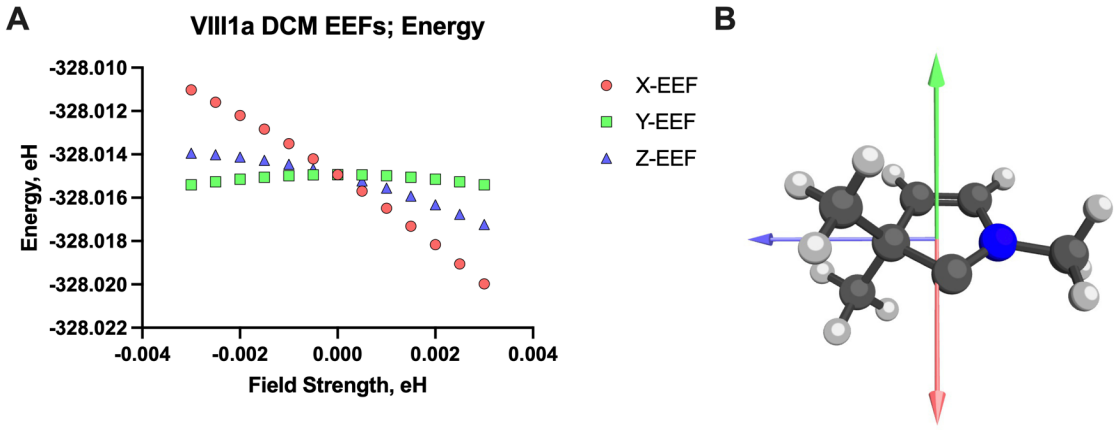


Figure S75. VIII$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S74. $VIII_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-328.010761	-328.015482	-328.013971
– 0.0025	-328.011382	-328.015330	-328.014045
– 0.0020	-328.012036	-328.015205	-328.014157
– 0.0015	-328.012723	-328.015109	-328.014307
– 0.0010	-328.013444	-328.015040	-328.014495
– 0.0005	-328.014197	-328.014998	-328.014721
+ 0.0000	-328.014985	-328.014985	-328.014985
+ 0.0005	-328.015805	-328.014999	-328.015287
+ 0.0010	-328.016659	-328.015040	-328.015626
+ 0.0015	-328.017547	-328.015109	-328.016004
+ 0.0020	-328.018468	-328.015206	-328.016420
+ 0.0025	-328.019423	-328.015330	-328.016873
+ 0.0030	-328.020412	-328.015482	-328.017365

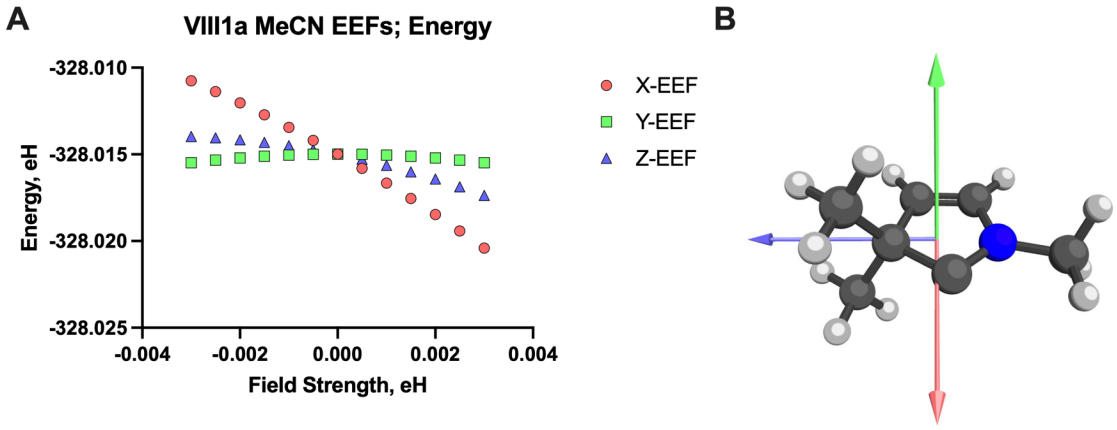


Figure S76. $VIII_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S75. $VIII_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-328.000709	-328.005502	-328.003981
– 0.0025	-328.001340	-328.005348	-328.004055
– 0.0020	-328.002004	-328.005222	-328.004167
– 0.0015	-328.002702	-328.005124	-328.004317
– 0.0010	-328.003434	-328.005054	-328.004506
– 0.0005	-328.004199	-328.005012	-328.004733
+ 0.0000	-328.004998	-328.004998	-328.004998
+ 0.0005	-328.005832	-328.005012	-328.005302
+ 0.0010	-328.006699	-328.005054	-328.005644
+ 0.0015	-328.007600	-328.005124	-328.006024
+ 0.0020	-328.008535	-328.005222	-328.006442
+ 0.0025	-328.009504	-328.005348	-328.006899
+ 0.0030	-328.010508	-328.005502	-328.007394

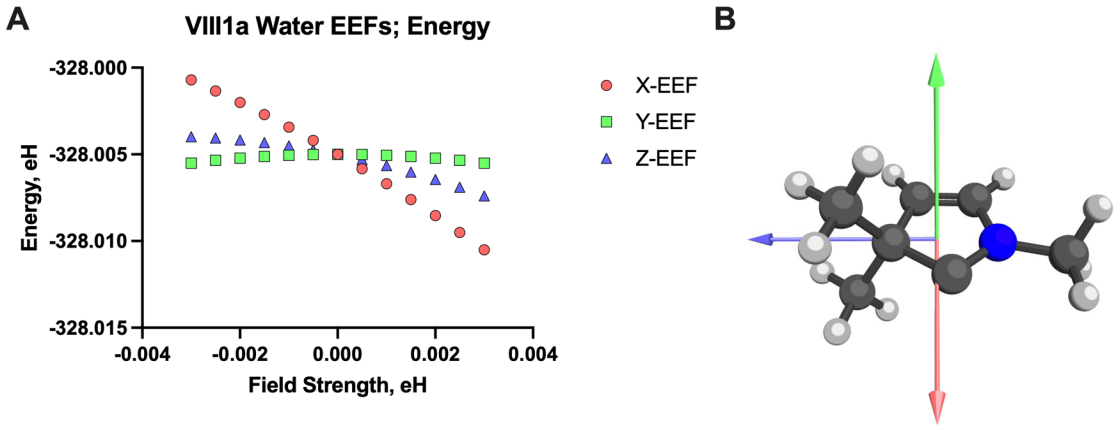


Figure S77. $VIII_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S76. ^{3}VIII$_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.923106	-327.924137	-327.922553
– 0.0025	-327.923080	-327.923944	-327.922603
– 0.0020	-327.923077	-327.923772	-327.922683
– 0.0015	-327.923095	-327.923619	-327.922790
– 0.0010	-327.923136	-327.923487	-327.922926
– 0.0005	-327.923198	-327.923375	-327.923090
+ 0.0000	-327.923283	-327.923283	-327.923283
+ 0.0005	-327.923389	-327.923211	-327.923504
+ 0.0010	-327.923518	-327.923160	-327.923753
+ 0.0015	-327.923668	-327.923128	-327.924031
+ 0.0020	-327.923841	-327.923117	-327.924337
+ 0.0025	-327.924035	-327.923127	-327.924671
+ 0.0030	-327.924252	-327.923157	-327.925035

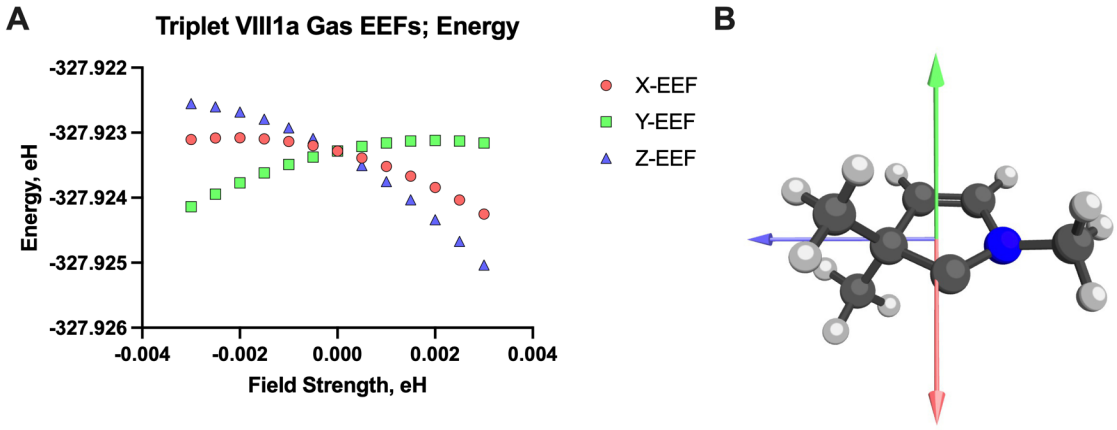


Figure S78. ^{3}VIII$_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S77. ^{3}VIII$_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.930927	-327.932164	-327.930346
– 0.0025	-327.930900	-327.931937	-327.930398
– 0.0020	-327.930898	-327.931734	-327.930484
– 0.0015	-327.930924	-327.931554	-327.930602
– 0.0010	-327.930975	-327.931398	-327.930754
– 0.0005	-327.931053	-327.931266	-327.930939
+ 0.0000	-327.931157	-327.931157	-327.931157
+ 0.0005	-327.931287	-327.931071	-327.931407
+ 0.0010	-327.931443	-327.931010	-327.931691
+ 0.0015	-327.931626	-327.930972	-327.932008
+ 0.0020	-327.931835	-327.930957	-327.932358
+ 0.0025	-327.932070	-327.930967	-327.932741
+ 0.0030	-327.932332	-327.931000	-327.933158

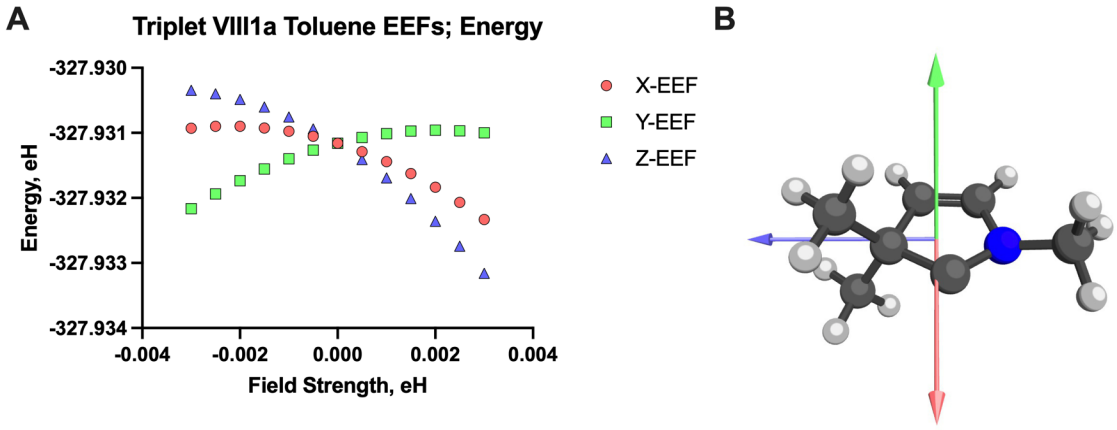


Figure S79. ^{3}VIII$_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S78. ^{3}VIII$_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.932928	-327.934402	-327.932392
– 0.0025	-327.932900	-327.934137	-327.932438
– 0.0020	-327.932904	-327.933901	-327.932522
– 0.0015	-327.932939	-327.933691	-327.932643
– 0.0010	-327.933004	-327.933510	-327.932801
– 0.0005	-327.933101	-327.933355	-327.932996
+ 0.0000	-327.933229	-327.933229	-327.933229
+ 0.0005	-327.933388	-327.933130	-327.933499
+ 0.0010	-327.933578	-327.933059	-327.933806
+ 0.0015	-327.933799	-327.933015	-327.934151
+ 0.0020	-327.934051	-327.932999	-327.934533
+ 0.0025	-327.934334	-327.933012	-327.934952
+ 0.0030	-327.934649	-327.933052	-327.935409

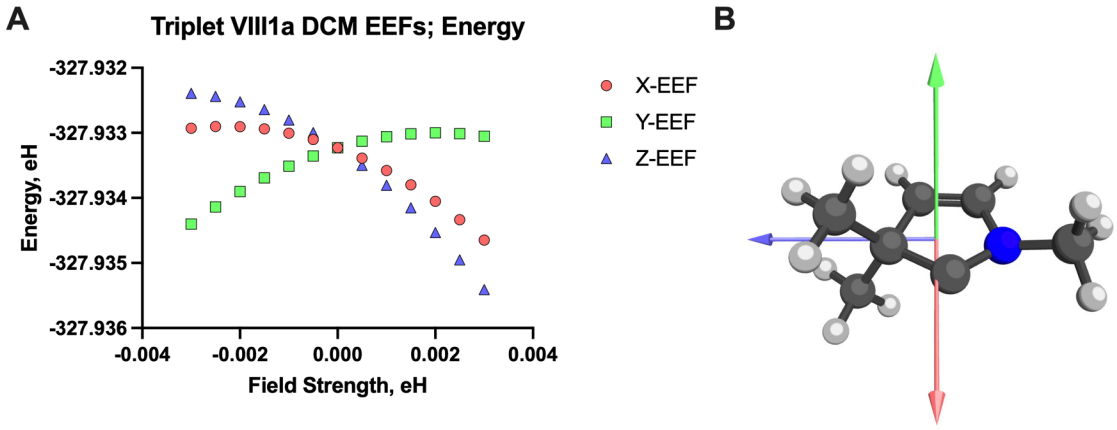


Figure S80. ^{3}VIII$_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S79. ^{3}VIII$_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.931658	-327.933237	-327.931161
– 0.0025	-327.931631	-327.932956	-327.931203
– 0.0020	-327.931637	-327.932705	-327.931283
– 0.0015	-327.931676	-327.932483	-327.931402
– 0.0010	-327.931749	-327.932290	-327.931560
– 0.0005	-327.931854	-327.932127	-327.931757
+ 0.0000	-327.931993	-327.931993	-327.931993
+ 0.0005	-327.932165	-327.931888	-327.932268
+ 0.0010	-327.932370	-327.931814	-327.932581
+ 0.0015	-327.932608	-327.931768	-327.932934
+ 0.0020	-327.932880	-327.931753	-327.933325
+ 0.0025	-327.933184	-327.931767	-327.933755
+ 0.0030	-327.933522	-327.931811	-327.934225

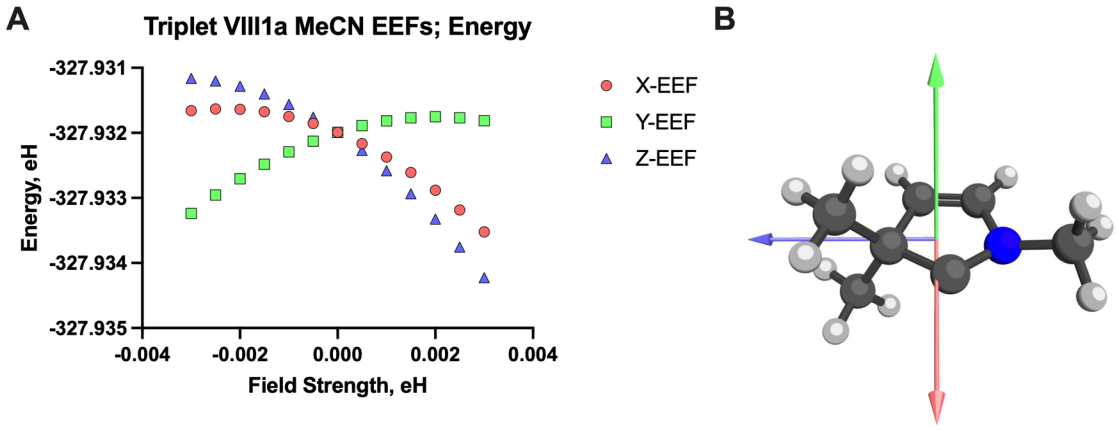


Figure S81. ^{3}VIII$_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table S80. ^{3}VIII$_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-327.922035	-327.923637	-327.921547
– 0.0025	-327.922008	-327.923352	-327.921588
– 0.0020	-327.922015	-327.923098	-327.921667
– 0.0015	-327.922055	-327.922873	-327.921786
– 0.0010	-327.922129	-327.922678	-327.921944
– 0.0005	-327.922236	-327.922512	-327.922141
+ 0.0000	-327.922377	-327.922377	-327.922377
+ 0.0005	-327.922552	-327.922271	-327.922652
+ 0.0010	-327.922760	-327.922196	-327.922967
+ 0.0015	-327.923002	-327.922150	-327.923321
+ 0.0020	-327.923277	-327.922135	-327.923714
+ 0.0025	-327.923587	-327.922149	-327.924147
+ 0.0030	-327.923930	-327.922194	-327.924618

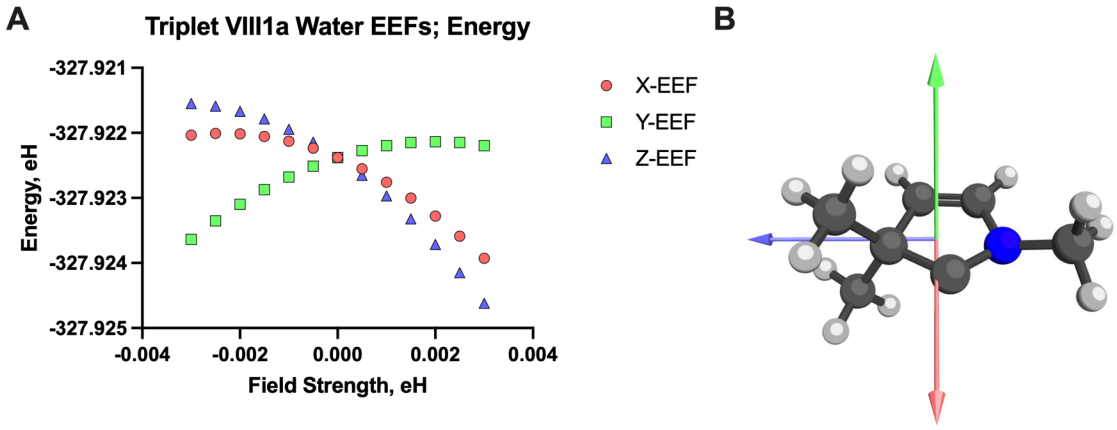


Figure S82. ^{3}VIII$_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

Table S81. IX_{1a} Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.817020	-320.818120	-320.820280
– 0.0025	-320.817120	-320.818050	-320.819820
– 0.0020	-320.817240	-320.817990	-320.819390
– 0.0015	-320.817380	-320.817950	-320.818980
– 0.0010	-320.817530	-320.817920	-320.818600
– 0.0005	-320.817700	-320.817900	-320.818240
+ 0.0000	-320.817890	-320.817890	-320.817890
+ 0.0005	-320.818100	-320.817900	-320.817570
+ 0.0010	-320.818330	-320.817920	-320.817280
+ 0.0015	-320.818570	-320.817950	-320.817000
+ 0.0020	-320.818830	-320.817990	-320.816750
+ 0.0025	-320.819110	-320.818050	-320.816520
+ 0.0030	-320.819410	-320.818120	-320.816310

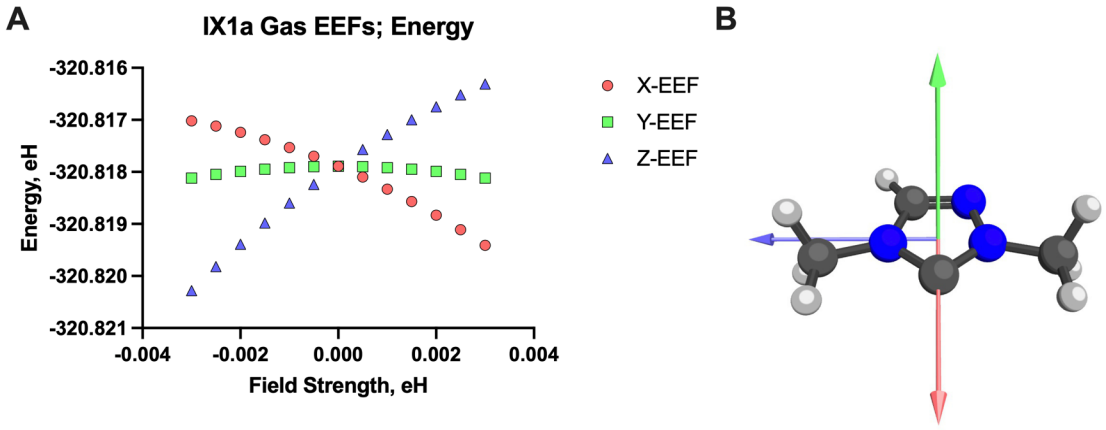


Figure S83. IX_{1a} Energy under EEFs in Gas. Axis definitions given in (B).

Table S82. IX_{1a} Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.834909	-320.836315	-320.838881
– 0.0025	-320.835047	-320.836235	-320.838346
– 0.0020	-320.835207	-320.836170	-320.837837
– 0.0015	-320.835387	-320.836119	-320.837353
– 0.0010	-320.835589	-320.836083	-320.836895
– 0.0005	-320.835811	-320.836061	-320.836462
+ 0.0000	-320.836054	-320.836054	-320.836054
+ 0.0005	-320.836318	-320.836061	-320.835672
+ 0.0010	-320.836603	-320.836083	-320.835315
+ 0.0015	-320.836909	-320.836119	-320.834983
+ 0.0020	-320.837236	-320.836170	-320.834677
+ 0.0025	-320.837584	-320.836235	-320.834396
+ 0.0030	-320.837953	-320.836315	-320.834141

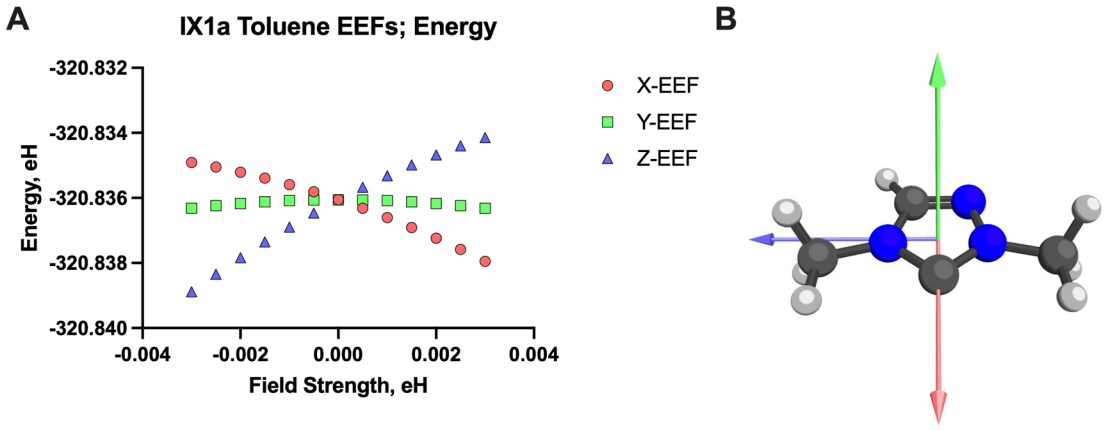


Figure S84. IX_{1a} Energy under EEFs in Toluene. Axis definitions given in (B).

Table S83. IX_{1a} Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.839211	-320.840990	-320.843916
– 0.0025	-320.839396	-320.840898	-320.843308
– 0.0020	-320.839606	-320.840822	-320.842728
– 0.0015	-320.839840	-320.840763	-320.842176
– 0.0010	-320.840098	-320.840721	-320.841652
– 0.0005	-320.840381	-320.840696	-320.841156
+ 0.0000	-320.840688	-320.840688	-320.840688
+ 0.0005	-320.841019	-320.840696	-320.840247
+ 0.0010	-320.841375	-320.840721	-320.839835
+ 0.0015	-320.841755	-320.840763	-320.839451
+ 0.0020	-320.842159	-320.840822	-320.839095
+ 0.0025	-320.842588	-320.840897	-320.838766
+ 0.0030	-320.843042	-320.840989	-320.838466

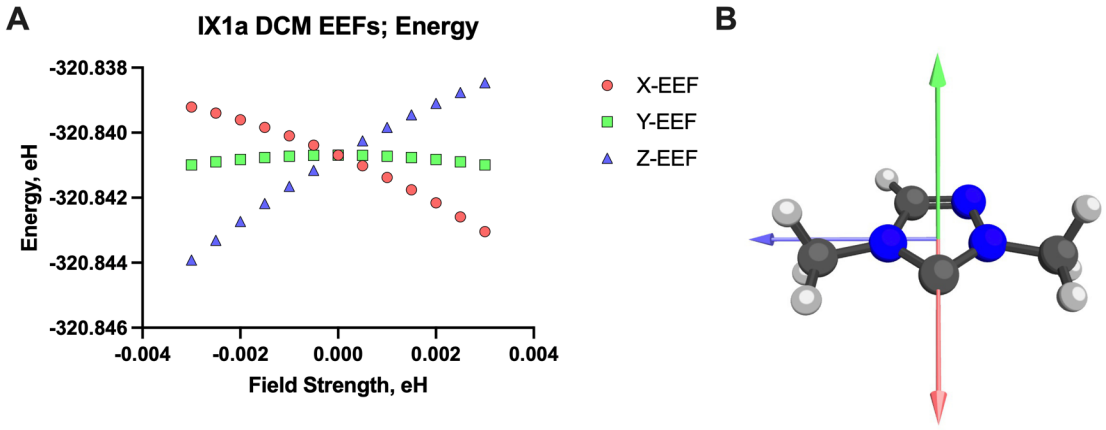


Figure S85. IX_{1a} Energy under EEFs in DCM. Axis definitions given in (B).

Table S84. IX_{1a} Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.839550	-320.841494	-320.844549
– 0.0025	-320.839757	-320.841396	-320.843914
– 0.0020	-320.839988	-320.841315	-320.843308
– 0.0015	-320.840246	-320.841253	-320.842731
– 0.0010	-320.840529	-320.841208	-320.842183
– 0.0005	-320.840838	-320.841182	-320.841663
+ 0.0000	-320.841173	-320.841173	-320.841173
+ 0.0005	-320.841533	-320.841182	-320.840711
+ 0.0010	-320.841919	-320.841208	-320.840278
+ 0.0015	-320.842331	-320.841253	-320.839874
+ 0.0020	-320.842769	-320.841315	-320.839499
+ 0.0025	-320.843233	-320.841395	-320.839153
+ 0.0030	-320.843723	-320.841493	-320.838836

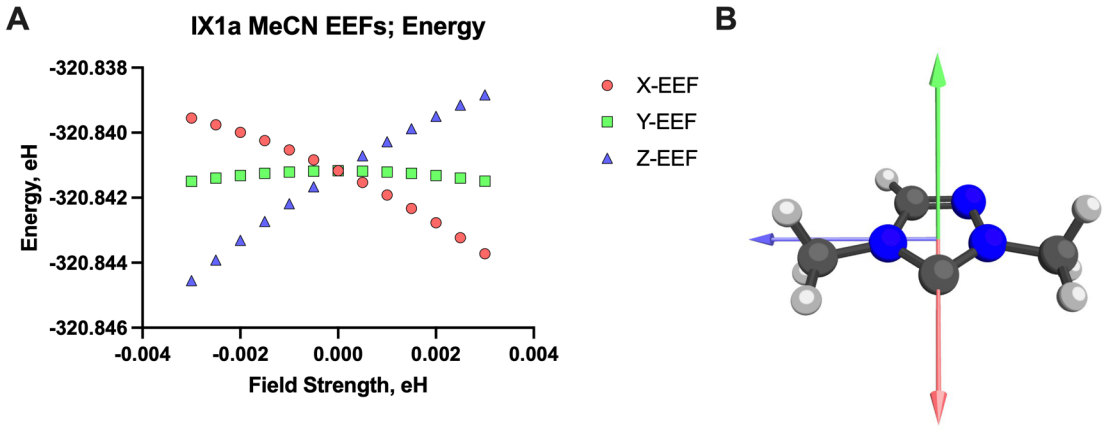


Figure S86. IX_{1a} Energy under EEFs in MeCN. Axis definitions given in (B).

Table S85. IX_{1a} Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.825461	-320.827439	-320.830519
– 0.0025	-320.825671	-320.827339	-320.829879
– 0.0020	-320.825908	-320.827258	-320.829268
– 0.0015	-320.826170	-320.827195	-320.828686
– 0.0010	-320.826458	-320.827150	-320.828132
– 0.0005	-320.826773	-320.827122	-320.827608
+ 0.0000	-320.827113	-320.827113	-320.827113
+ 0.0005	-320.827480	-320.827122	-320.826647
+ 0.0010	-320.827873	-320.827149	-320.826210
+ 0.0015	-320.828291	-320.827194	-320.825803
+ 0.0020	-320.828736	-320.827258	-320.825424
+ 0.0025	-320.829207	-320.827339	-320.825074
+ 0.0030	-320.829705	-320.827438	-320.824753

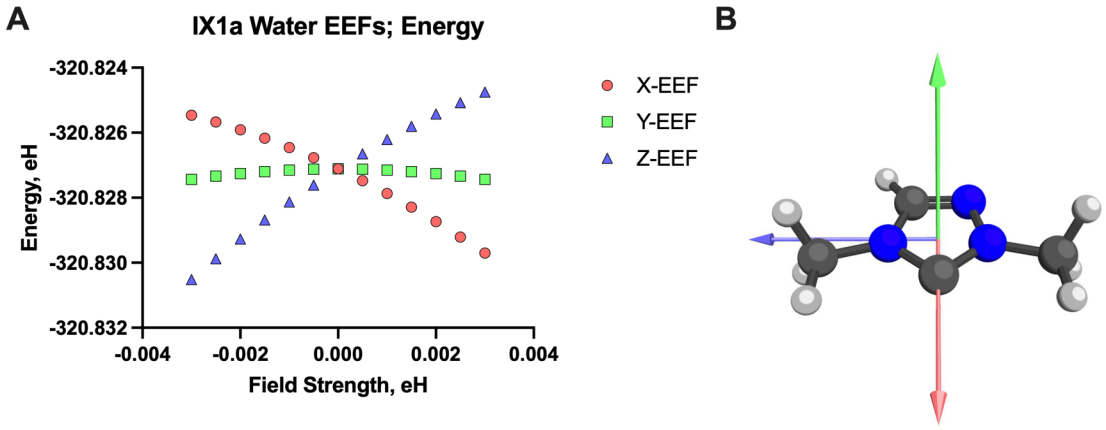


Figure S87. IX_{1a} Energy under EEFs in Water. Axis definitions given in (B).

Table S86. $^3IX_{1a}$ Under EEFs in Gas. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.679890	-320.678510	-320.681760
– 0.0025	-320.679650	-320.678510	-320.681190
– 0.0020	-320.679420	-320.678520	-320.680650
– 0.0015	-320.679220	-320.678550	-320.680130
– 0.0010	-320.679030	-320.678590	-320.679640
– 0.0005	-320.678870	-320.678650	-320.679170
+ 0.0000	-320.678720	-320.678720	-320.678720
+ 0.0005	-320.678590	-320.678810	-320.678290
+ 0.0010	-320.678480	-320.678910	-320.677890
+ 0.0015	-320.678380	-320.679030	-320.677520
+ 0.0020	-320.678310	-320.679160	-320.677160
+ 0.0025	-320.678250	-320.679310	-320.676840
+ 0.0030	-320.678210	-320.679470	-320.676530

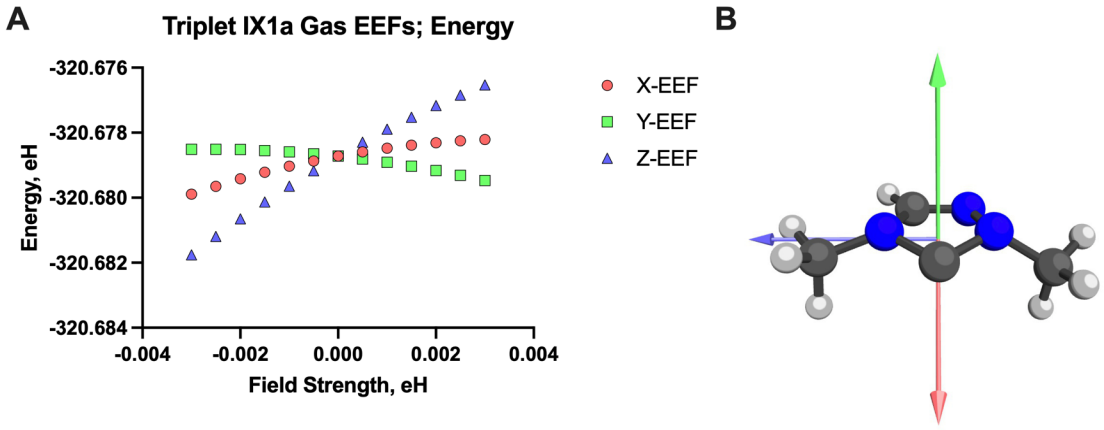


Figure S88. $^3IX_{1a}$ Energy under EEFs in Gas. Axis definitions given in (B).

Table S87. $^{3}IX_{1a}$ Under EEFs in SMD Toluene. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.694880	-320.693259	-320.697148
– 0.0025	-320.694599	-320.693256	-320.696475
– 0.0020	-320.694339	-320.693272	-320.695829
– 0.0015	-320.694101	-320.693306	-320.695210
– 0.0010	-320.693884	-320.693358	-320.694618
– 0.0005	-320.693689	-320.693428	-320.694053
+ 0.0000	-320.693516	-320.693516	-320.693516
+ 0.0005	-320.693364	-320.693621	-320.693005
+ 0.0010	-320.693235	-320.693744	-320.692522
+ 0.0015	-320.693127	-320.693885	-320.692065
+ 0.0020	-320.693042	-320.694042	-320.691636
+ 0.0025	-320.692979	-320.694217	-320.691233
+ 0.0030	-320.692938	-320.694410	-320.690858

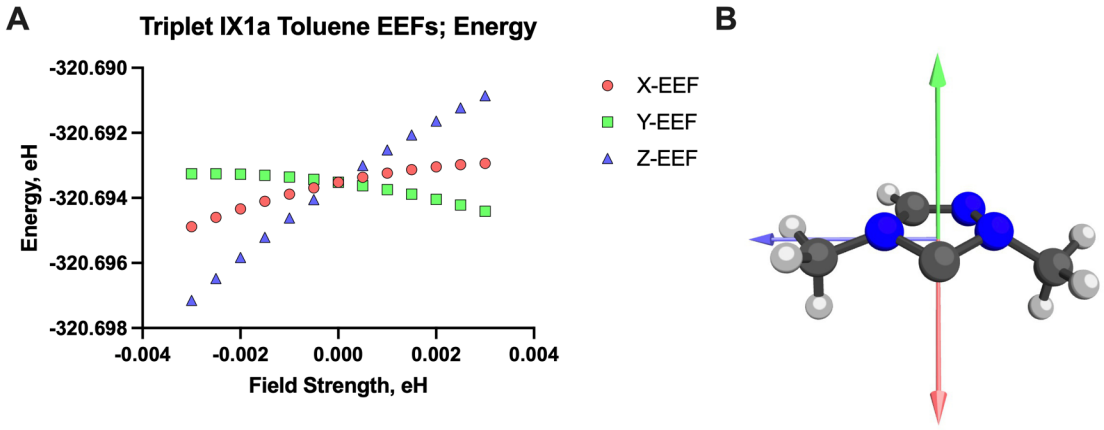


Figure S89. $^{3}IX_{1a}$ Energy under EEFs in Toluene. Axis definitions given in (B).

Table S88. $^3IX_{1a}$ Under EEFs in SMD Dichloromethane. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.698132	-320.696295	-320.700754
– 0.0025	-320.697812	-320.696291	-320.699985
– 0.0020	-320.697517	-320.696308	-320.699246
– 0.0015	-320.697247	-320.696346	-320.698537
– 0.0010	-320.697003	-320.696406	-320.697858
– 0.0005	-320.696783	-320.696488	-320.697209
+ 0.0000	-320.696590	-320.696590	-320.696590
+ 0.0005	-320.696421	-320.696712	-320.696000
+ 0.0010	-320.696278	-320.696856	-320.695440
+ 0.0015	-320.696161	-320.697020	-320.694910
+ 0.0020	-320.696070	-320.697204	-320.694411
+ 0.0025	-320.696004	-320.697409	-320.693941
+ 0.0030	-320.695965	-320.697634	-320.693501

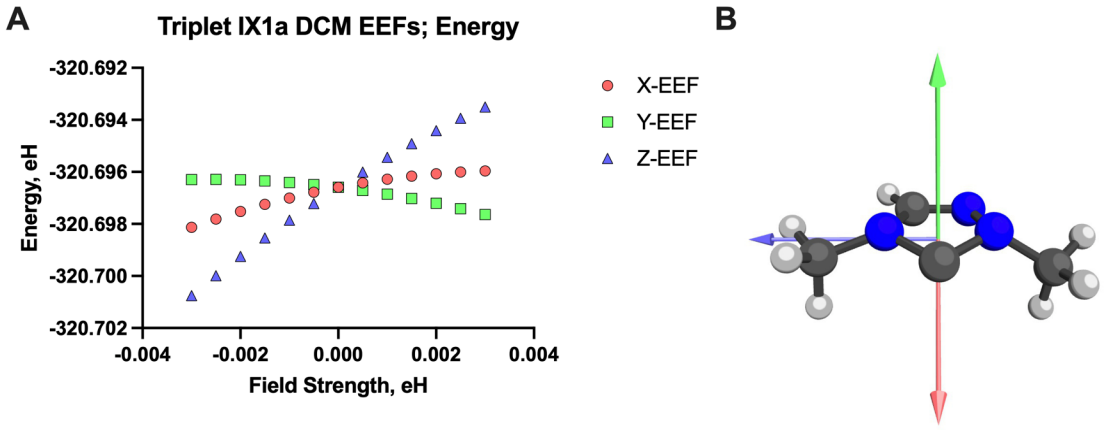


Figure S90. $^3IX_{1a}$ Energy under EEFs in DCM. Axis definitions given in (B).

Table S89. $^{3}IX_{1a}$ Under EEFs in SMD Acetonitrile. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.698078	-320.696165	-320.700830
– 0.0025	-320.697743	-320.696158	-320.700026
– 0.0020	-320.697435	-320.696175	-320.699253
– 0.0015	-320.697153	-320.696214	-320.698510
– 0.0010	-320.696898	-320.696276	-320.697799
– 0.0005	-320.696670	-320.696361	-320.697118
+ 0.0000	-320.696469	-320.696469	-320.696469
+ 0.0005	-320.696294	-320.696599	-320.695850
+ 0.0010	-320.696147	-320.696750	-320.695262
+ 0.0015	-320.696027	-320.696924	-320.694705
+ 0.0020	-320.695935	-320.697120	-320.694179
+ 0.0025	-320.695870	-320.697337	-320.693684
+ 0.0030	-320.695832	-320.697576	-320.693219

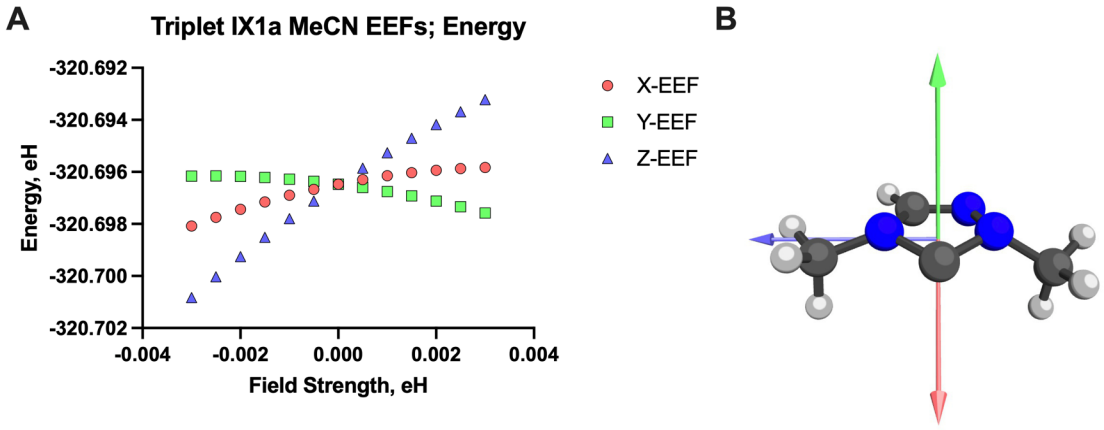


Figure S91. $^{3}IX_{1a}$ Energy under EEFs in MeCN. Axis definitions given in (B).

Table 90. $^3IX_{1a}$ Under EEFs in SMD Water. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-320.686313	-320.684385	-320.689090
– 0.0025	-320.685975	-320.684378	-320.688279
– 0.0020	-320.685664	-320.684394	-320.687499
– 0.0015	-320.685380	-320.684433	-320.686751
– 0.0010	-320.685123	-320.684496	-320.686033
– 0.0005	-320.684893	-320.684582	-320.685346
+ 0.0000	-320.684690	-320.684690	-320.684690
+ 0.0005	-320.684515	-320.684822	-320.684066
+ 0.0010	-320.684367	-320.684975	-320.683472
+ 0.0015	-320.684246	-320.685151	-320.682910
+ 0.0020	-320.684154	-320.685349	-320.682378
+ 0.0025	-320.684089	-320.685569	-320.681878
+ 0.0030	-320.684052	-320.685811	-320.681409

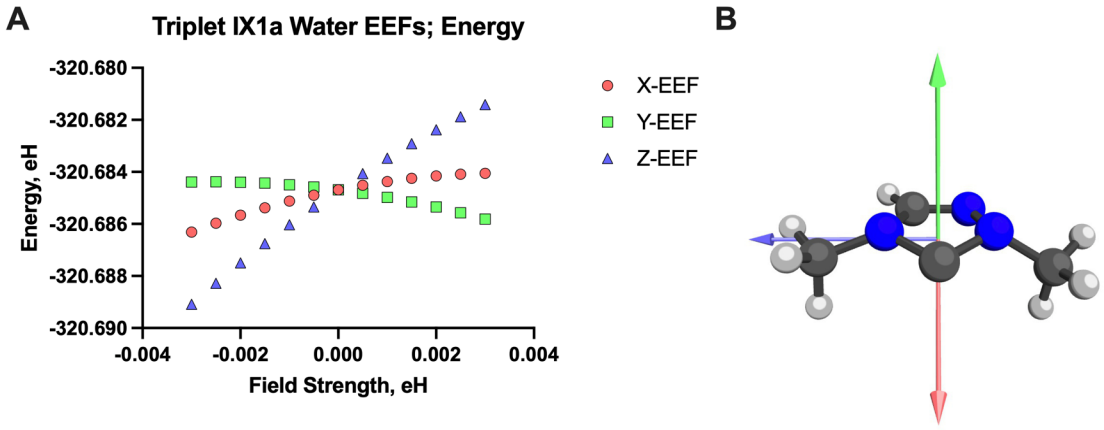


Figure S92. $^3IX_{1a}$ Energy under EEFs in Water. Axis definitions given in (B).

S4. Electronic Singlet-Triplet Gaps of NHCs in Test Set under EEFs Across Different Solvents

Table S91. ΔE_{ST} I_{1a} Under EEFs in Gas. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-354.521265	-359.509715	-359.798520
– 0.0025	-355.335170	-359.483460	-359.719755
– 0.0020	-356.122820	-359.483460	-359.640990
– 0.0015	-356.884215	-359.430950	-359.562225
– 0.0010	-357.698120	-359.404695	-359.457205
– 0.0005	-358.485770	-359.325930	-359.378440
+ 0.0000	-359.273420	-359.273420	-359.273420
+ 0.0005	-360.087325	-359.194655	-359.194655
+ 0.0010	-360.874975	-359.142145	-359.115890
+ 0.0015	-361.662625	-359.010870	-359.010870
+ 0.0020	-362.476530	-358.932105	-358.905850
+ 0.0025	-363.290435	-358.800830	-358.800830
+ 0.0030	-364.051830	-358.669555	-358.695810

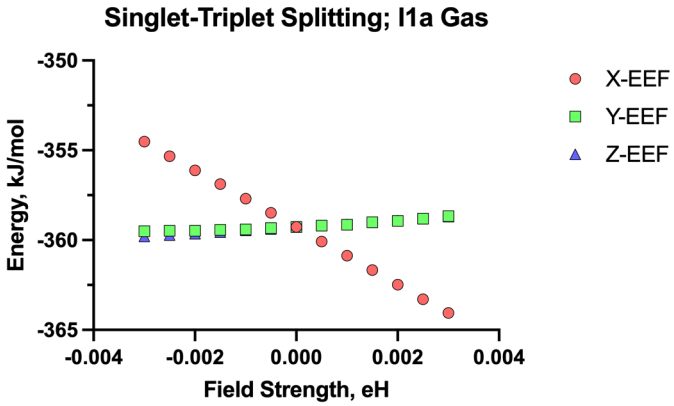


Figure S93. I_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S92. ΔE_{ST} I_{1a} Under EEFs in Toluene. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-365.100476	-371.239493	-371.545755
– 0.0025	-366.070454	-371.224562	-371.454889
– 0.0020	-367.043204	-371.196963	-371.361317
– 0.0015	-368.018722	-371.156819	-371.265155
– 0.0010	-368.996996	-371.104212	-371.166473
– 0.0005	-369.978009	-371.039191	-371.065333
+ 0.0000	-370.961752	-370.961752	-370.961752
+ 0.0005	-371.948205	-370.871855	-370.855742
+ 0.0010	-372.937341	-370.769413	-370.747280
+ 0.0015	-373.929145	-370.654306	-370.636321
+ 0.0020	-374.923584	-370.526355	-370.522805
+ 0.0025	-375.920631	-370.385345	-370.406630
+ 0.0030	-376.920251	-370.230999	-370.287666

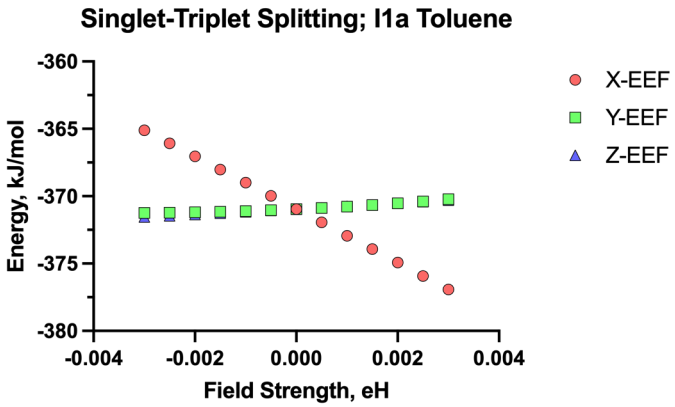


Figure S94. I_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S93. ΔE_{ST} I_{1a} Under EEFs in DCM. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-370.458533	-377.942941	-378.233689
– 0.0025	-371.637343	-377.921572	-378.135789
– 0.0020	-372.820176	-377.885196	-378.034127
– 0.0015	-374.007030	-377.833951	-377.928803
– 0.0010	-375.197891	-377.767930	-377.819905
– 0.0005	-376.392749	-377.687149	-377.707489
+ 0.0000	-377.591583	-377.591583	-377.591583
+ 0.0005	-378.794372	-377.481139	-377.472194
+ 0.0010	-380.001089	-377.355669	-377.349307
+ 0.0015	-381.211702	-377.214966	-377.222882
+ 0.0020	-382.426166	-377.058749	-377.092851
+ 0.0025	-383.644445	-376.886676	-376.959121
+ 0.0030	-384.866476	-376.698320	-376.821566

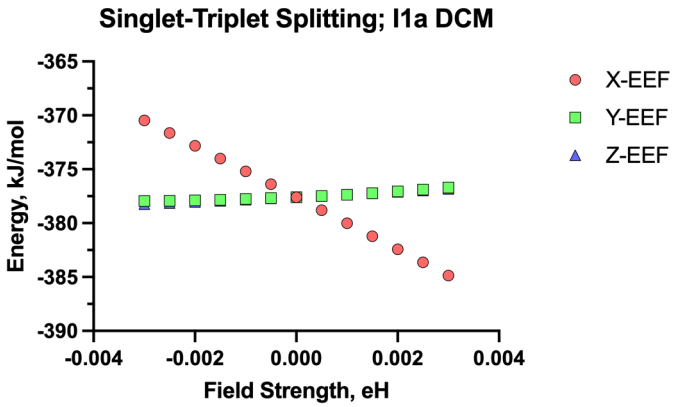


Figure S95. I_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S94. ΔE_{ST} I_{1a} Under EEFs in MeCN. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-372.724993	-380.786132	-381.062649
– 0.0025	-373.992509	-380.761893	-380.962371
– 0.0020	-375.264637	-380.721424	-380.857850
– 0.0015	-376.541378	-380.664868	-380.749201
– 0.0010	-377.822725	-380.592312	-380.636504
– 0.0005	-379.108663	-380.503767	-380.519819
+ 0.0000	-380.399180	-380.399180	-380.399180
+ 0.0005	-381.694245	-380.278426	-380.274587
+ 0.0010	-382.993836	-380.141311	-380.146032
+ 0.0015	-384.297909	-379.987567	-380.013471
+ 0.0020	-385.606421	-379.816852	-379.876842
+ 0.0025	-386.919315	-379.628732	-379.736050
+ 0.0030	-388.236529	-379.422681	-379.590970

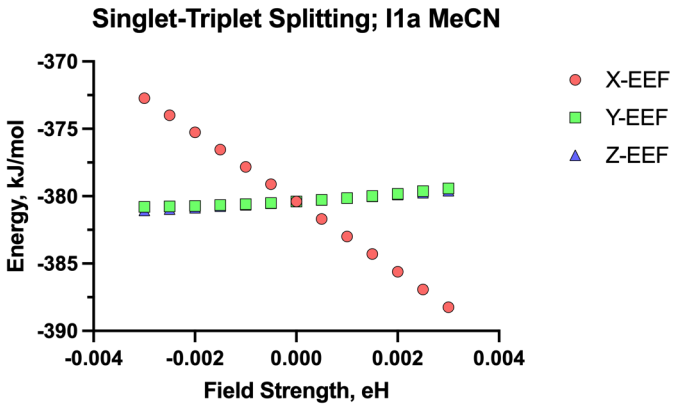


Figure S96. I_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S95. ΔE_{ST} I_{1a} Under EEFs in Water. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-363.143966	-371.325901	-371.598995
– 0.0025	-364.430002	-371.301085	-371.498247
– 0.0020	-365.720784	-371.259752	-371.393159
– 0.0015	-367.016306	-371.202054	-371.283843
– 0.0010	-368.316564	-371.128072	-371.170382
– 0.0005	-369.621542	-371.037818	-371.052833
+ 0.0000	-370.931228	-370.931228	-370.931228
+ 0.0005	-372.245598	-370.808174	-370.805577
+ 0.0010	-373.564618	-370.668444	-370.675861
+ 0.0015	-374.888253	-370.511765	-370.542042
+ 0.0020	-376.216452	-370.337771	-370.404062
+ 0.0025	-377.549161	-370.146007	-370.261818
+ 0.0030	-378.886309	-369.935922	-370.115189

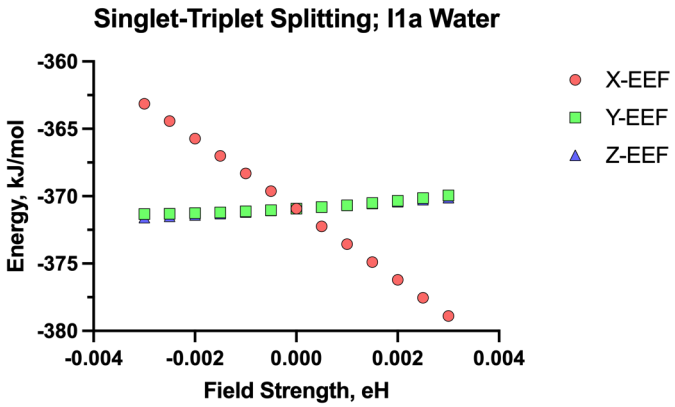


Figure S97. I_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S96. ΔE_{ST} II_{1a} Under EEFs in Gas. Energy given in kJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-159.767246	-177.591154	-177.582290
– 0.0025	-162.738091	-177.627008	-177.620772
– 0.0020	-165.716527	-177.656172	-177.652100
– 0.0015	-168.702621	-177.678730	-177.676359
– 0.0010	-171.696421	-177.694748	-177.693622
– 0.0005	-174.697971	-177.704268	-177.703932
+ 0.0000	-177.707325	-177.707325	-177.707325
+ 0.0005	-180.724512	-177.703919	-177.703801
+ 0.0010	-183.749582	-177.694047	-177.693357
+ 0.0015	-186.782570	-177.677677	-177.675966
+ 0.0020	-189.823524	-177.654767	-177.651572
+ 0.0025	-192.872488	-177.625251	-177.620113
+ 0.0030	-195.929515	-177.589048	-177.581497

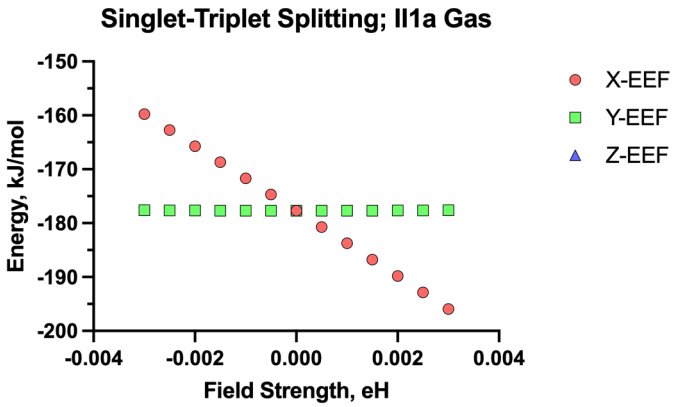


Figure S98. II_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S97. ΔE_{ST} II_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-186.018292	-207.896728	-207.852349
– 0.0025	-189.666325	-207.940112	-207.909205
– 0.0020	-193.322916	-207.975391	-207.955513
– 0.0015	-196.988198	-208.002675	-207.991396
– 0.0010	-200.662284	-208.022043	-208.016937
– 0.0005	-204.345269	-208.033556	-208.032209
+ 0.0000	-208.037245	-208.037245	-208.037245
+ 0.0005	-211.738286	-208.033123	-208.032057
+ 0.0010	-215.448464	-208.021180	-208.016635
+ 0.0015	-219.167850	-208.001378	-207.990939
+ 0.0020	-222.896504	-207.973661	-207.954907
+ 0.0025	-226.634489	-207.937951	-207.908446
+ 0.0030	-230.381865	-207.894134	-207.851438

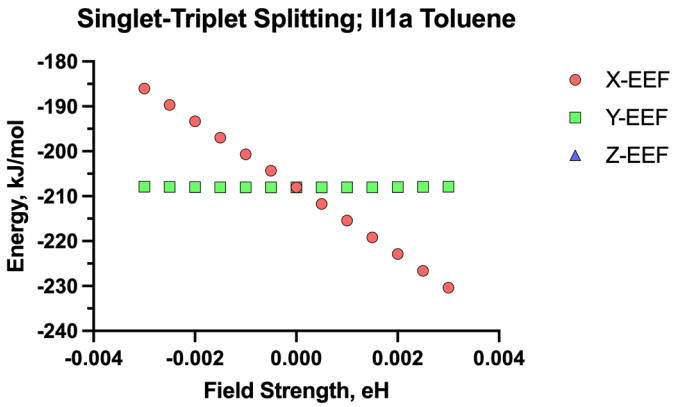


Figure S99. II_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S98. ΔE_{ST} II_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-209.954390	-235.992713	-235.909637
– 0.0025	-214.295749	-236.044112	-235.986291
– 0.0020	-218.647316	-236.085884	-236.048752
– 0.0015	-223.009277	-236.118173	-236.097166
– 0.0010	-227.381800	-236.141088	-236.131641
– 0.0005	-231.765025	-236.154709	-236.152265
+ 0.0000	-236.159078	-236.159078	-236.159078
+ 0.0005	-240.564066	-236.154210	-236.152097
+ 0.0010	-244.980088	-236.140093	-236.131305
+ 0.0015	-249.407233	-236.116679	-236.096659
+ 0.0020	-253.845575	-236.083894	-236.048080
+ 0.0025	-258.295188	-236.041623	-235.985448
+ 0.0030	-262.756133	-235.989725	-235.908626

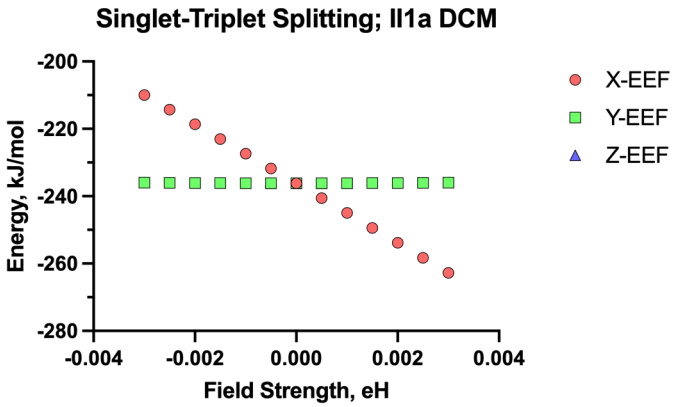


Figure S100. II_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S99. ΔE_{ST} II_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-219.325417	-247.051130	-246.953005
– 0.0025	-223.947791	-247.106263	-247.037950
– 0.0020	-228.581231	-247.151049	-247.107177
– 0.0015	-233.225948	-247.185653	-247.160839
– 0.0010	-237.882128	-247.210209	-247.199061
– 0.0005	-242.549926	-247.224802	-247.221929
+ 0.0000	-247.229485	-247.229485	-247.229485
+ 0.0005	-251.920926	-247.224282	-247.221756
+ 0.0010	-256.624346	-247.209167	-247.198717
+ 0.0015	-261.339844	-247.184091	-247.160325
+ 0.0020	-266.067493	-247.148967	-247.106489
+ 0.0025	-270.807358	-247.103661	-247.037091
+ 0.0030	-275.559497	-247.048006	-246.951975

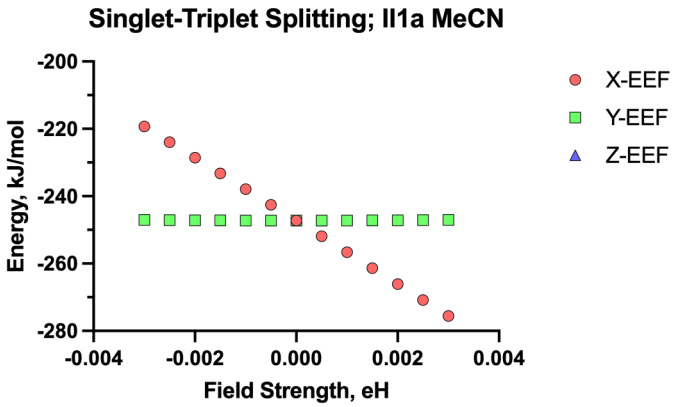


Figure S101. II_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S100. ΔE_{ST} II_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-217.896557	-245.970183	-245.869091
– 0.0025	-222.576870	-246.026145	-245.955761
– 0.0020	-227.268439	-246.071601	-246.026395
– 0.0015	-231.971479	-246.106719	-246.081152
– 0.0010	-236.686184	-246.131638	-246.120151
– 0.0005	-241.412711	-246.146446	-246.143487
+ 0.0000	-246.151201	-246.151201	-246.151201
+ 0.0005	-250.901778	-246.145921	-246.143314
+ 0.0010	-255.664545	-246.130588	-246.119807
+ 0.0015	-260.439597	-246.105144	-246.080635
+ 0.0020	-265.227004	-246.069500	-246.025707
+ 0.0025	-270.026839	-246.023520	-245.954902
+ 0.0030	-274.839146	-245.967030	-245.868061

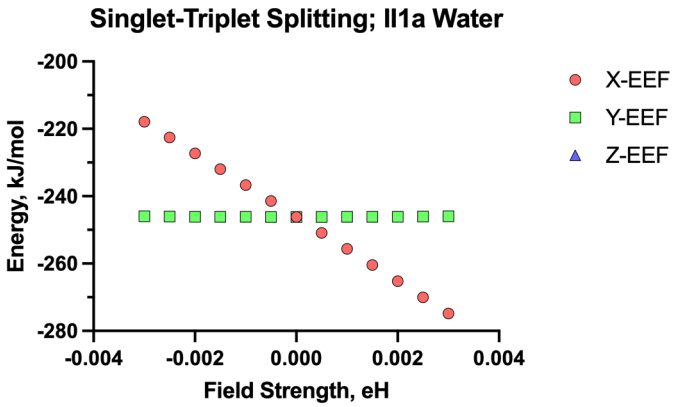


Figure S102. II_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S101. ΔE_{ST} III_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-252.25804	-266.461995	-273.47208
– 0.0025	-255.014815	-266.85582	-272.68443
– 0.0020	-257.745335	-267.249645	-271.89678
– 0.0015	-260.475855	-267.617215	-271.082875
– 0.0010	-263.206375	-267.984785	-270.32148
– 0.0005	-265.96315	-268.352355	-269.48132
+ 0.0000	-268.69367	-268.69367	-268.69367
+ 0.0005	-271.42419	-269.06124	-267.879765
+ 0.0010	-274.15471	-269.3763	-267.092115
+ 0.0015	-276.88523	-269.717615	-266.251955
+ 0.0020	-279.61575	-270.032675	-265.464305
+ 0.0025	-282.320015	-270.347735	-264.6504
+ 0.0030	-285.050535	-270.662795	-263.836495

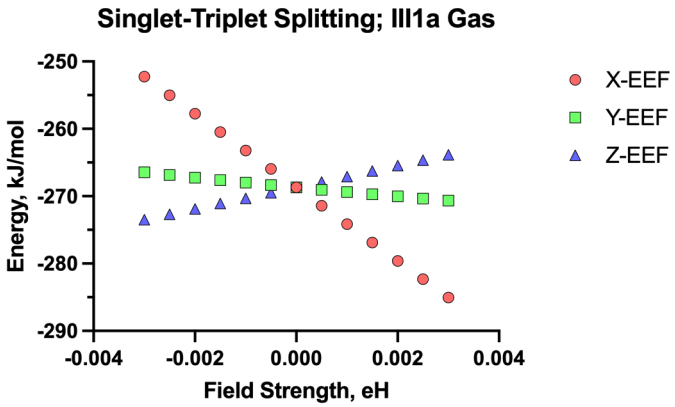


Figure S103. III_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S102. ΔE_{ST} III_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-271.060545	-288.442227	-297.042325
– 0.0025	-274.423401	-288.922628	-296.074721
– 0.0020	-277.782392	-289.393036	-295.103168
– 0.0015	-281.137456	-289.853640	-294.127708
– 0.0010	-284.488505	-290.304591	-293.148354
– 0.0005	-287.835408	-290.746016	-292.165120
+ 0.0000	-291.178006	-291.178006	-291.178006
+ 0.0005	-294.516087	-291.600625	-290.186998
+ 0.0010	-297.849406	-292.013915	-289.192067
+ 0.0015	-301.177669	-292.417882	-288.193188
+ 0.0020	-304.500530	-292.812516	-287.190310
+ 0.0025	-307.817590	-293.197771	-286.183373
+ 0.0030	-311.128385	-293.573572	-285.172314

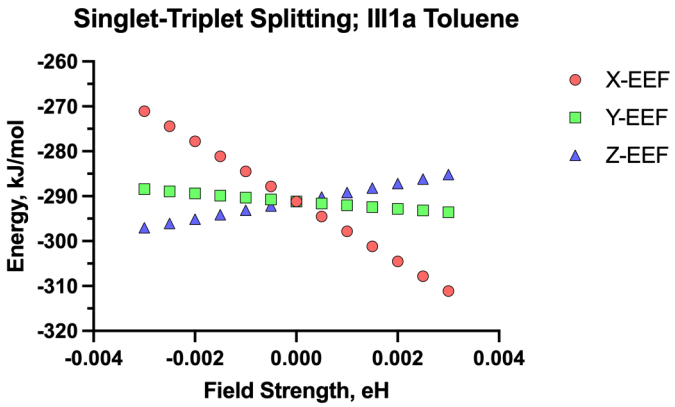


Figure S104. III_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S103. ΔE_{ST} III_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-287.353978	-308.041479	-318.403871
– 0.0025	-291.384262	-308.639613	-317.256611
– 0.0020	-295.408203	-309.224430	-316.103754
– 0.0015	-299.425675	-309.796290	-314.945342
– 0.0010	-303.436484	-310.355498	-313.781395
– 0.0005	-307.440355	-310.902303	-312.611926
+ 0.0000	-311.436926	-311.436926	-311.436926
+ 0.0005	-315.425743	-311.959529	-310.256377
+ 0.0010	-319.406245	-312.470246	-309.070245
+ 0.0015	-323.377749	-312.969165	-307.878483
+ 0.0020	-327.339432	-313.456342	-306.681029
+ 0.0025	-331.290308	-313.931791	-305.477812
+ 0.0030	-335.229191	-314.395491	-304.268738

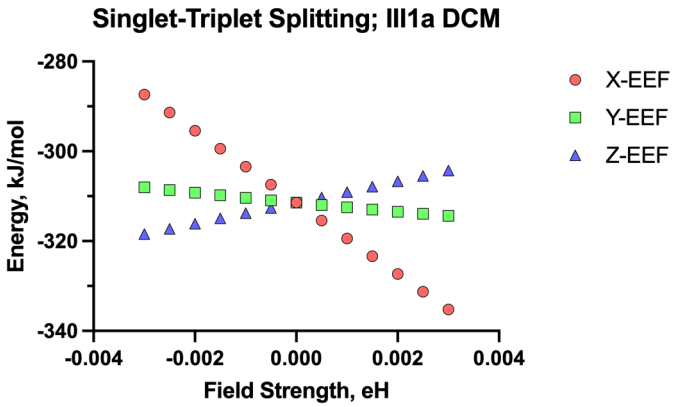


Figure S105. III_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S104. ΔE_{ST} III_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-293.799518	-315.819006	-326.953426
– 0.0025	-298.110350	-316.477324	-325.734813
– 0.0020	-302.413647	-317.120277	-324.509860
– 0.0015	-306.709266	-317.748347	-323.278600
– 0.0010	-310.996965	-318.361952	-322.041055
– 0.0005	-315.276402	-318.961440	-320.797229
+ 0.0000	-319.547111	-319.547111	-319.547111
+ 0.0005	-323.808507	-320.119207	-318.290678
+ 0.0010	-328.059843	-320.677924	-317.027883
+ 0.0015	-332.300201	-321.223409	-315.758672
+ 0.0020	-336.528454	-321.755760	-314.482973
+ 0.0025	-340.743213	-322.275045	-313.200694
+ 0.0030	-344.942787	-322.781270	-311.911739

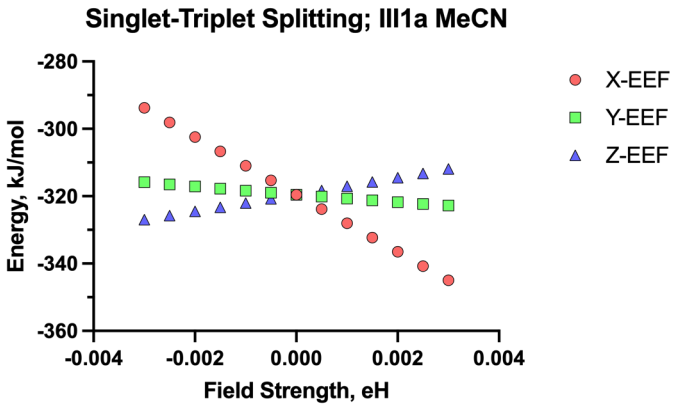


Figure S106. III_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S105. ΔE_{ST} III_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-290.153969	-312.445931	-323.745052
– 0.0025	-294.523360	-313.117873	-322.511867
– 0.0020	-298.884959	-313.773954	-321.272177
– 0.0015	-303.238615	-314.414678	-320.026020
– 0.0010	-307.584080	-315.040503	-318.773421
– 0.0005	-311.920994	-315.651796	-317.514378
+ 0.0000	-316.248879	-316.248879	-316.248879
+ 0.0005	-320.567107	-316.832013	-314.976895
+ 0.0010	-324.874896	-317.401408	-313.698384
+ 0.0015	-329.171270	-317.957231	-312.413289
+ 0.0020	-333.455028	-318.499591	-311.121527
+ 0.0025	-337.724687	-319.028564	-309.823015
+ 0.0030	-341.978424	-319.544168	-308.517637

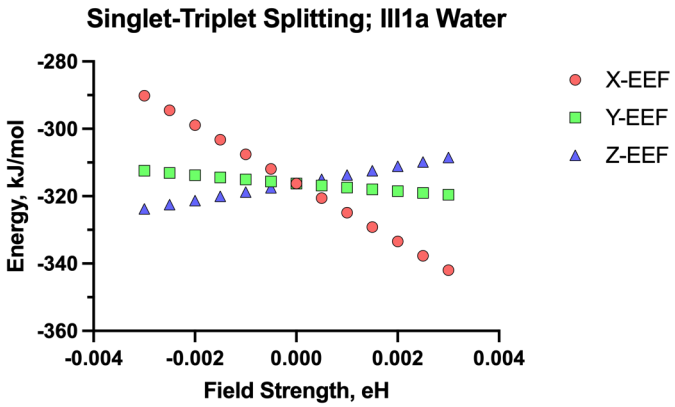


Figure S107. III_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S106. ΔE_{ST} IV_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-327.636145	-330.077860	-328.843875
– 0.0025	-328.476305	-330.576705	-329.500250
– 0.0020	-329.316465	-330.996785	-330.156625
– 0.0015	-330.156625	-331.443120	-330.813000
– 0.0010	-331.049295	-331.863200	-331.469375
– 0.0005	-331.889455	-332.335790	-332.099495
+ 0.0000	-332.729615	-332.729615	-332.729615
+ 0.0005	-333.622285	-333.175950	-333.412245
+ 0.0010	-334.462445	-333.569775	-334.042365
+ 0.0015	-335.328860	-334.016110	-334.698740
+ 0.0020	-336.221530	-334.409935	-335.355115
+ 0.0025	-337.087945	-334.830015	-335.985235
+ 0.0030	-337.980615	-335.197585	-336.641610

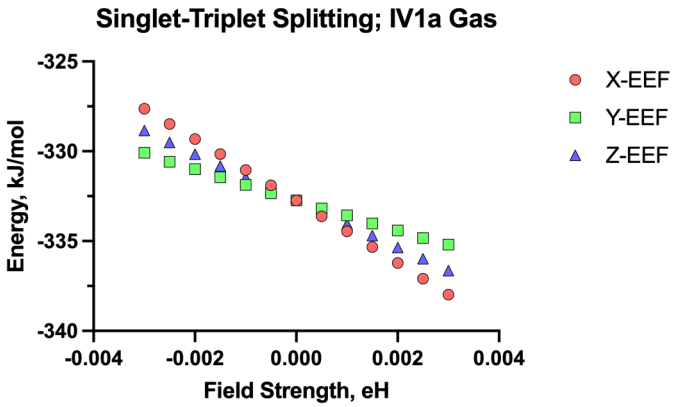


Figure S108. IV_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S107. ΔE_{ST} IV_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-337.094876	-340.072902	-338.659233
– 0.0025	-338.106975	-340.611621	-339.420179
– 0.0020	-339.122366	-341.144455	-340.180469
– 0.0015	-340.141023	-341.671385	-340.940170
– 0.0010	-341.162923	-342.192371	-341.699342
– 0.0005	-342.188031	-342.707368	-342.458046
+ 0.0000	-343.216319	-343.216319	-343.216319
+ 0.0005	-344.247757	-343.719157	-343.974211
+ 0.0010	-345.282306	-344.215805	-344.731755
+ 0.0015	-346.319928	-344.706169	-345.488983
+ 0.0020	-347.360581	-345.190149	-346.245925
+ 0.0025	-348.404223	-345.667620	-347.002608
+ 0.0030	-349.450802	-346.138453	-347.759051

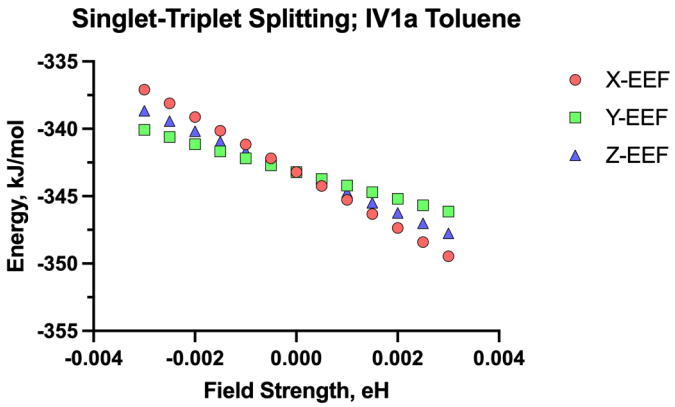


Figure S109. IV_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S108. ΔE_{ST} IV_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-344.189794	-347.758980	-346.230679
– 0.0025	-345.380891	-348.382788	-347.094644
– 0.0020	-346.576195	-348.999741	-347.957468
– 0.0015	-347.775668	-349.609837	-348.819222
– 0.0010	-348.979273	-350.213053	-349.679974
– 0.0005	-350.186966	-350.809357	-350.539781
+ 0.0000	-351.398695	-351.398695	-351.398695
+ 0.0005	-352.614406	-351.981012	-352.256763
+ 0.0010	-353.834038	-352.556225	-353.114029
+ 0.0015	-355.057518	-353.124250	-353.970524
+ 0.0020	-356.284777	-353.684964	-354.826282
+ 0.0025	-357.515729	-354.238252	-355.681337
+ 0.0030	-358.750273	-354.783957	-356.535704

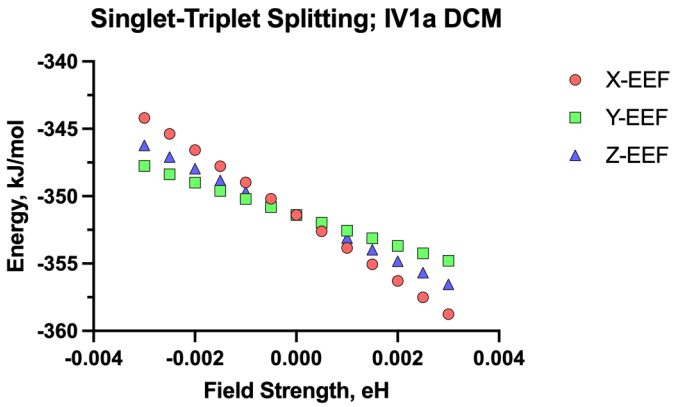


Figure S110. IV_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S109. ΔE_{ST} IV_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-346.753516	-350.535013	-348.987362
– 0.0025	-348.013386	-351.194384	-349.889523
– 0.0020	-349.277850	-351.846395	-350.790285
– 0.0015	-350.546864	-352.491052	-351.689721
– 0.0010	-351.820387	-353.128348	-352.587902
– 0.0005	-353.098365	-353.758258	-353.484888
+ 0.0000	-354.380735	-354.380735	-354.380735
+ 0.0005	-355.667430	-354.995722	-355.275487
+ 0.0010	-356.958380	-355.603142	-356.169194
+ 0.0015	-358.253497	-356.202908	-357.061890
+ 0.0020	-359.552687	-356.794903	-357.953610
+ 0.0025	-360.855840	-357.378996	-358.844387
+ 0.0030	-362.162841	-357.955036	-359.734243

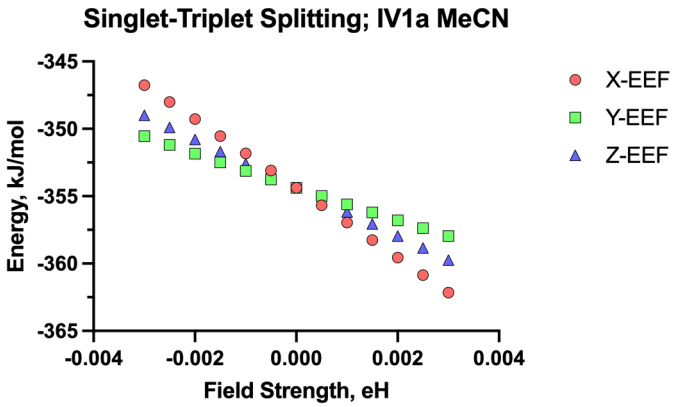


Figure S111. IV_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S110. ΔE_{ST} IV_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-340.993930	-344.852165	-343.360057
– 0.0025	-342.273255	-345.517864	-344.259926
– 0.0020	-343.557282	-346.176447	-345.158380
– 0.0015	-344.845972	-346.827915	-346.055498
– 0.0010	-346.139275	-347.472262	-346.951347
– 0.0005	-347.437138	-348.109474	-347.845997
+ 0.0000	-348.739504	-348.739504	-348.739504
+ 0.0005	-350.046297	-349.362305	-349.631920
+ 0.0010	-351.357451	-349.977803	-350.523290
+ 0.0015	-352.672866	-350.585916	-351.413663
+ 0.0020	-353.992447	-351.186544	-352.303069
+ 0.0025	-355.316085	-351.779555	-353.191549
+ 0.0030	-356.643654	-352.364816	-354.079133

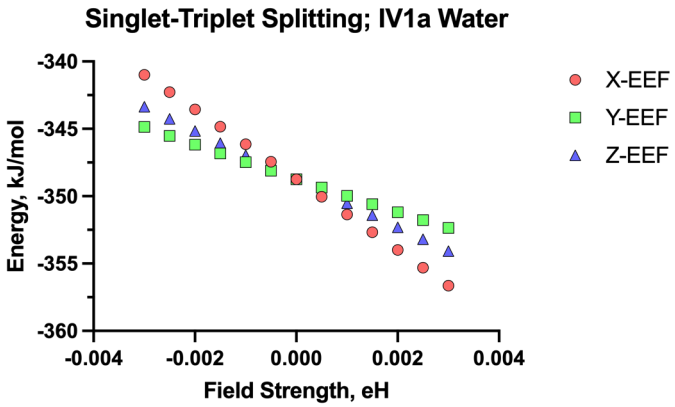


Figure S112. IV_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S111. ΔE_{ST} V_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-276.832720	-281.479855	-283.107665
– 0.0025	-277.856665	-281.716150	-283.081410
– 0.0020	-278.880610	-281.978700	-283.081410
– 0.0015	-279.878300	-282.214995	-283.028900
– 0.0010	-280.902245	-282.477545	-283.002645
– 0.0005	-281.926190	-282.713840	-282.976390
+ 0.0000	-282.950135	-282.950135	-282.950135
+ 0.0005	-283.947825	-283.186430	-282.897625
+ 0.0010	-284.998025	-283.396470	-282.871370
+ 0.0015	-286.021970	-283.632765	-282.792605
+ 0.0020	-287.045915	-283.842805	-282.766350
+ 0.0025	-288.069860	-284.052845	-282.713840
+ 0.0030	-289.093805	-284.262885	-282.661330

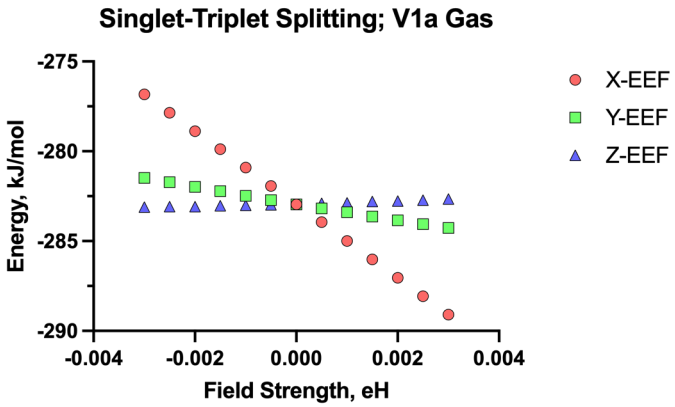


Figure S113. V_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S112. ΔE_{ST} V_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-282.272184	-287.927561	-289.947085
– 0.0025	-283.508280	-288.237115	-289.918876
– 0.0020	-284.746287	-288.542169	-289.886514
– 0.0015	-285.986169	-288.842694	-289.850062
– 0.0010	-287.227888	-289.138649	-289.809574
– 0.0005	-288.471404	-289.429992	-289.765095
+ 0.0000	-289.716668	-289.716671	-289.716671
+ 0.0005	-290.963636	-289.998626	-289.664326
+ 0.0010	-292.212258	-290.275795	-289.608104
+ 0.0015	-293.462479	-290.548114	-289.548022
+ 0.0020	-294.714247	-290.815492	-289.484099
+ 0.0025	-295.967495	-291.077848	-289.416353
+ 0.0030	-297.222161	-291.335087	-289.344795

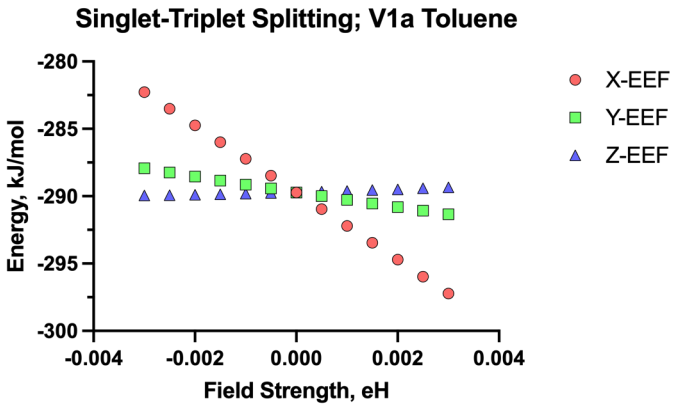


Figure S114. V_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S113. ΔE_{ST} V_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-287.053253	-293.877075	-296.189744
– 0.0025	-288.528845	-294.235826	-296.160556
– 0.0020	-290.007009	-294.588945	-296.126603
– 0.0015	-291.487697	-294.936406	-296.087958
– 0.0010	-292.970860	-295.278160	-296.044667
– 0.0005	-294.456433	-295.614163	-295.996785
+ 0.0000	-295.944351	-295.944351	-295.944351
+ 0.0005	-297.434549	-296.268664	-295.887407
+ 0.0010	-298.926938	-296.587011	-295.825973
+ 0.0015	-300.421433	-296.899314	-295.760070
+ 0.0020	-301.917939	-297.205468	-295.689725
+ 0.0025	-303.416349	-297.505361	-295.614938
+ 0.0030	-304.916541	-297.798868	-295.535716

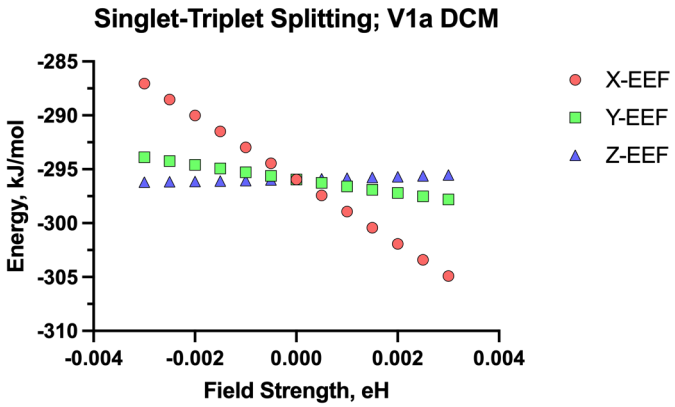


Figure S115. V_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S114. ΔE_{ST} V_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-288.964864	-296.287221	-298.689737
– 0.0025	-290.538927	-296.663489	-298.662245
– 0.0020	-292.115876	-297.033587	-298.629779
– 0.0015	-293.695661	-297.397474	-298.592405
– 0.0010	-295.278218	-297.755106	-298.550176
– 0.0005	-296.863479	-298.106424	-298.503151
+ 0.0000	-298.451365	-298.451365	-298.451365
+ 0.0005	-300.041791	-298.789850	-298.394857
+ 0.0010	-301.634658	-299.121787	-298.333654
+ 0.0015	-303.229859	-299.447076	-298.267772
+ 0.0020	-304.827269	-299.765601	-298.197233
+ 0.0025	-306.426755	-300.077232	-298.122041
+ 0.0030	-308.028163	-300.381825	-298.042197

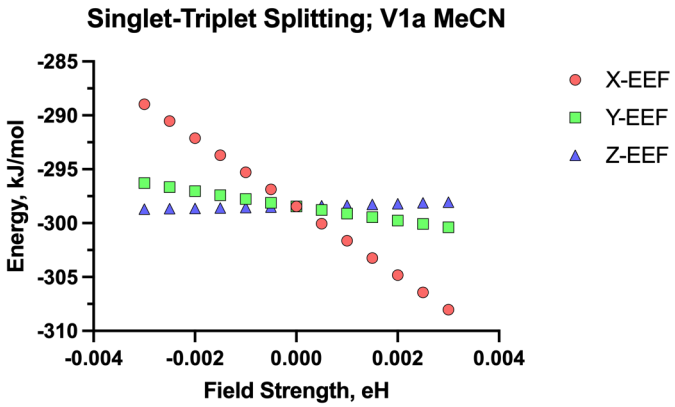


Figure S116. V_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S115. ΔE_{ST} V_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-287.333276	-294.759931	-297.178875
– 0.0025	-288.927679	-295.139630	-297.151871
– 0.0020	-290.525041	-295.513037	-297.119853
– 0.0015	-292.125304	-295.880111	-297.082886
– 0.0010	-293.728403	-296.240810	-297.041025
– 0.0005	-295.334275	-296.595069	-296.994326
+ 0.0000	-296.942827	-296.942827	-296.942827
+ 0.0005	-298.553978	-297.284000	-296.886565
+ 0.0010	-300.167623	-297.618494	-296.825566
+ 0.0015	-301.783653	-297.946206	-296.759850
+ 0.0020	-303.401929	-298.267016	-296.689434
+ 0.0025	-305.022320	-298.580787	-296.614324
+ 0.0030	-306.644658	-298.887372	-296.534522

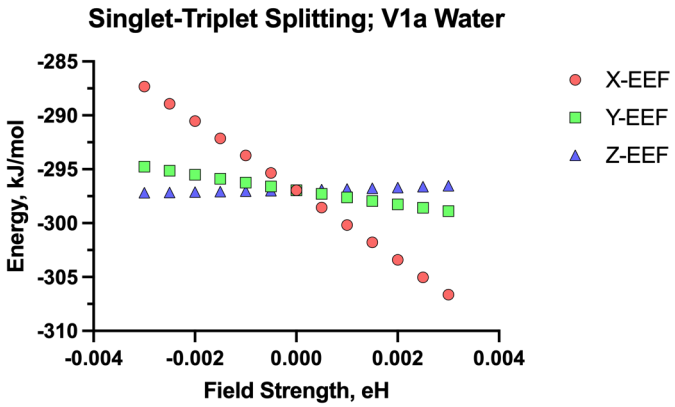


Figure S117. V_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S116. ΔE_{ST} VI_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-293.389806	-298.252211	-297.949774
– 0.0025	-294.205294	-298.285095	-297.997419
– 0.0020	-295.022494	-298.308470	-298.049800
– 0.0015	-295.841353	-298.322380	-298.106957
– 0.0010	-296.661827	-298.326848	-298.168935
– 0.0005	-297.483861	-298.321865	-298.235743
+ 0.0000	-298.307409	-298.307409	-298.307409
+ 0.0005	-299.132420	-298.283425	-298.383921
+ 0.0010	-299.958849	-298.249840	-298.465288
+ 0.0015	-300.786648	-298.206553	-298.551481
+ 0.0020	-301.615762	-298.153442	-298.642483
+ 0.0025	-302.446150	-298.090356	-298.738251
+ 0.0030	-303.277762	-298.017115	-298.838742

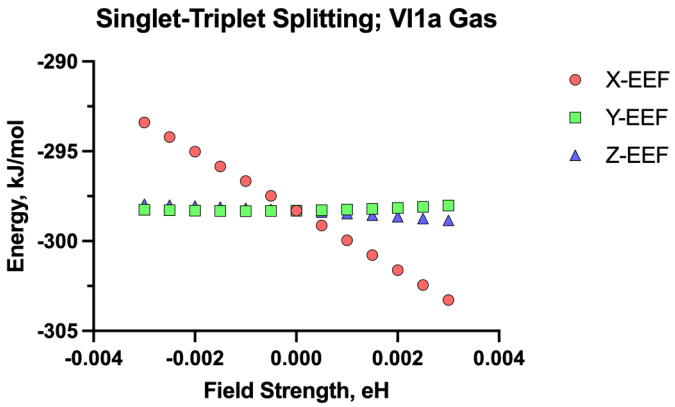


Figure S118. VI_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S117. ΔE_{ST} VI_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-303.015645	-308.947636	-308.650283
– 0.0025	-304.017667	-308.994034	-308.702840
– 0.0020	-305.021627	-309.029024	-308.761341
– 0.0015	-306.027453	-309.052659	-308.825832
– 0.0010	-307.035083	-309.064957	-308.896339
– 0.0005	-308.044449	-309.065910	-308.972889
+ 0.0000	-309.055484	-309.055484	-309.055484
+ 0.0005	-310.068116	-309.033606	-309.144121
+ 0.0010	-311.082286	-309.000191	-309.238791
+ 0.0015	-312.097919	-308.955106	-309.339474
+ 0.0020	-313.114946	-308.898201	-309.446127
+ 0.0025	-314.133296	-308.829287	-309.558714
+ 0.0030	-315.152901	-308.748133	-309.677171

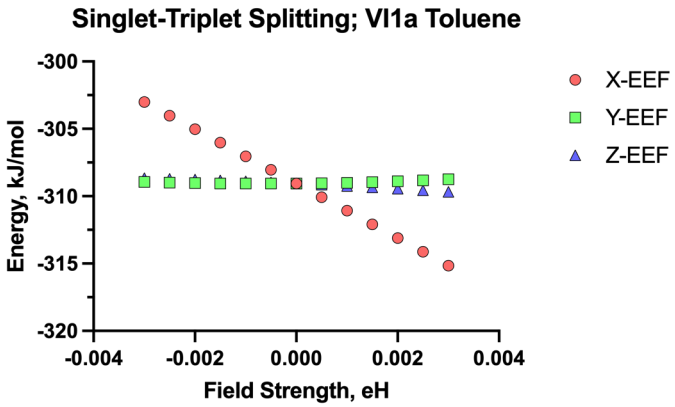


Figure S119. VI_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S118. ΔE_{ST} VI_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-306.620561	-313.736333	-313.421431
– 0.0025	-307.825805	-313.794425	-313.480940
– 0.0020	-309.033196	-313.838990	-313.547342
– 0.0015	-310.242646	-313.870084	-313.620683
– 0.0010	-311.454081	-313.887725	-313.700986
– 0.0005	-312.667400	-313.891889	-313.788266
+ 0.0000	-313.882518	-313.882518	-313.882518
+ 0.0005	-315.099351	-313.859524	-313.983745
+ 0.0010	-316.317798	-313.822773	-314.091918
+ 0.0015	-317.537774	-313.772092	-314.207012
+ 0.0020	-318.759175	-313.707272	-314.328985
+ 0.0025	-319.981907	-313.628060	-314.457789
+ 0.0030	-321.205873	-313.534151	-314.593352

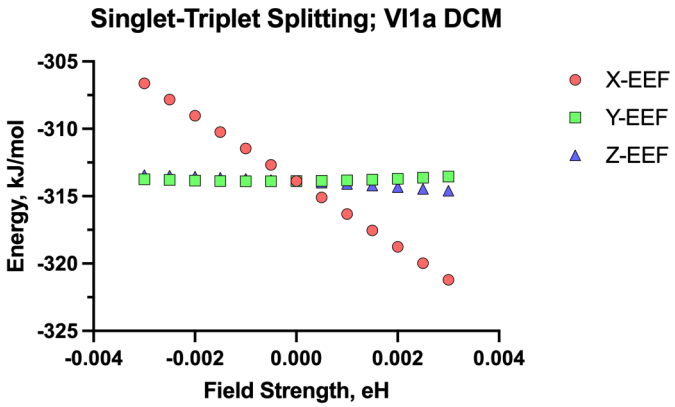


Figure S120. VI_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S119. ΔE_{ST} VI_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-308.583364	-316.197382	-315.866963
– 0.0025	-309.872981	-316.259473	-315.929815
– 0.0020	-311.164829	-316.307047	-315.999866
– 0.0015	-312.458815	-316.340160	-316.077155
– 0.0010	-313.754840	-316.358816	-316.161707
– 0.0005	-315.052809	-316.362996	-316.253529
+ 0.0000	-316.352626	-316.352626	-316.352626
+ 0.0005	-317.654186	-316.327594	-316.458979
+ 0.0010	-318.957387	-316.287744	-316.572577
+ 0.0015	-320.262124	-316.232879	-316.693381
+ 0.0020	-321.568289	-316.162749	-316.821351
+ 0.0025	-322.875775	-316.077064	-316.956430
+ 0.0030	-324.184458	-315.975472	-317.098556

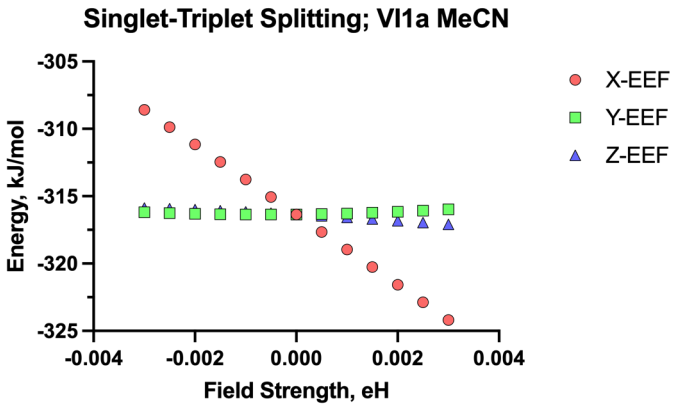


Figure S121. VI_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S120. ΔE_{ST} VI_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-293.898798	-301.616584	-301.282258
– 0.0025	-295.205893	-301.679446	-301.345840
– 0.0020	-296.515235	-301.727569	-301.416679
– 0.0015	-297.826730	-301.761010	-301.494811
– 0.0010	-299.140278	-301.779777	-301.580260
– 0.0005	-300.455782	-301.783847	-301.673035
+ 0.0000	-301.773140	-301.773140	-301.773140
+ 0.0005	-303.092246	-301.747539	-301.880557
+ 0.0010	-304.412999	-301.706886	-301.995268
+ 0.0015	-305.735287	-301.650976	-302.117241
+ 0.0020	-307.059007	-301.579551	-302.246431
+ 0.0025	-308.384036	-301.492306	-302.382786
+ 0.0030	-309.710258	-301.388880	-302.526238

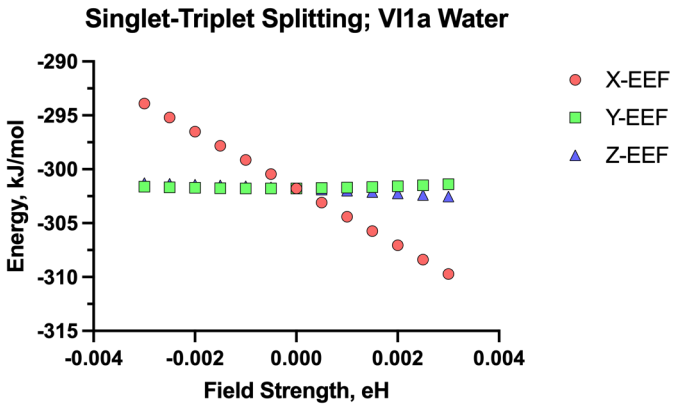


Figure S122. VI_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S121. ΔE_{ST} VII_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-248.753462	-253.118114	-256.156921
– 0.0025	-249.986174	-253.645202	-256.151748
– 0.0020	-251.218213	-254.163189	-256.147450
– 0.0015	-252.449575	-254.671849	-256.144048
– 0.0010	-253.680247	-255.170946	-256.141564
– 0.0005	-254.910205	-255.660223	-256.140012
+ 0.0000	-256.139398	-256.139398	-256.139398
+ 0.0005	-257.367785	-256.608184	-256.139731
+ 0.0010	-258.595291	-257.066249	-256.140997
+ 0.0015	-259.821848	-257.513246	-256.143197
+ 0.0020	-261.047363	-257.948801	-256.146314
+ 0.0025	-262.271734	-258.372501	-256.150325
+ 0.0030	-263.494849	-258.783901	-256.155211

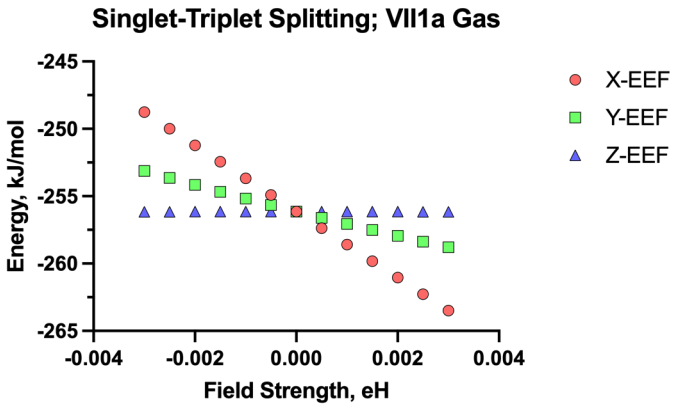


Figure S123. VII_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S122. ΔE_{ST} VII_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-257.558833	-262.711728	-266.665660
– 0.0025	-259.074641	-263.394534	-266.657306
– 0.0020	-260.589408	-264.066305	-266.650385
– 0.0015	-262.103122	-264.726792	-266.644932
– 0.0010	-263.615753	-265.375710	-266.640973
– 0.0005	-265.127267	-266.012754	-266.638526
+ 0.0000	-266.637599	-266.637599	-266.637599
+ 0.0005	-268.146681	-267.249894	-266.638203
+ 0.0010	-269.654427	-267.849254	-266.640327
+ 0.0015	-271.160732	-268.435263	-266.643963
+ 0.0020	-272.665477	-269.007465	-266.649091
+ 0.0025	-274.168531	-269.565378	-266.655691
+ 0.0030	-275.669744	-270.108463	-266.663717

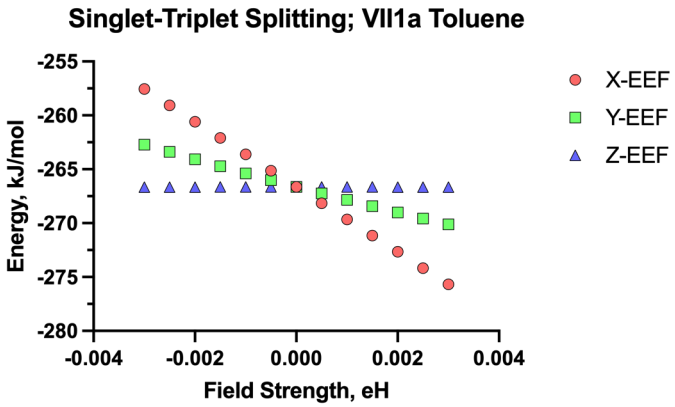


Figure S124. VII_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S123. ΔE_{ST} VII_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-260.875262	-266.825509	-271.893133
– 0.0025	-262.710904	-267.698023	-271.881392
– 0.0020	-264.544227	-268.557191	-271.871678
– 0.0015	-266.375227	-269.402707	-271.864037
– 0.0010	-268.203870	-270.234237	-271.858505
– 0.0005	-270.030105	-271.051416	-271.855105
+ 0.0000	-271.853850	-271.853850	-271.853850
+ 0.0005	-273.675018	-272.641109	-271.854746
+ 0.0010	-275.493492	-273.412723	-271.857789
+ 0.0015	-277.309133	-274.168179	-271.862961
+ 0.0020	-279.121791	-274.906924	-271.870241
+ 0.0025	-280.931286	-275.628356	-271.879599
+ 0.0030	-282.737417	-276.331814	-271.890983

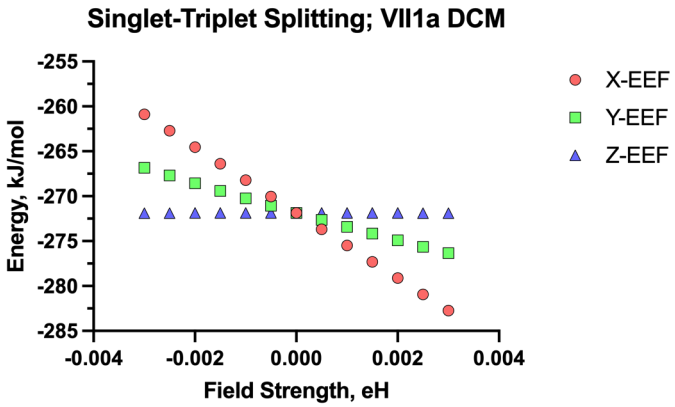


Figure S125. VII_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S124. ΔE_{ST} VII_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-262.639144	-268.904692	-274.484840
– 0.0025	-264.614231	-269.864795	-274.471647
– 0.0020	-266.586095	-270.810401	-274.460736
– 0.0015	-268.554721	-271.741177	-274.452158
– 0.0010	-270.520083	-272.656765	-274.445949
– 0.0005	-272.482117	-273.556766	-274.442142
+ 0.0000	-274.440745	-274.440745	-274.440745
+ 0.0005	-276.395860	-275.308229	-274.441766
+ 0.0010	-278.347334	-276.158704	-274.445203
+ 0.0015	-280.295017	-276.991602	-274.451037
+ 0.0020	-282.238730	-277.806318	-274.459244
+ 0.0025	-284.178273	-278.602173	-274.469781
+ 0.0030	-286.113419	-279.378449	-274.482601

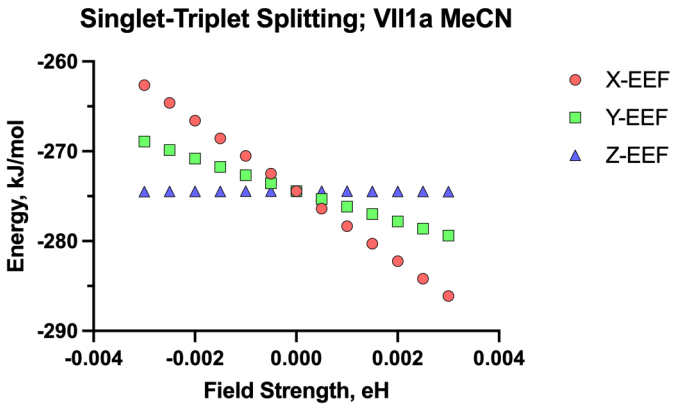


Figure S126. VII_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S125. ΔE_{ST} VII_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-250.065653	-256.395264	-262.086255
– 0.0025	-252.070290	-257.374347	-262.072750
– 0.0020	-254.071470	-258.338669	-262.061586
– 0.0015	-256.069192	-259.287898	-262.052809
– 0.0010	-258.063420	-260.221659	-262.046461
– 0.0005	-260.054097	-261.139555	-262.042562
+ 0.0000	-262.041136	-262.041136	-262.041136
+ 0.0005	-264.024434	-262.925927	-262.042186
+ 0.0010	-266.003858	-263.793395	-262.045710
+ 0.0015	-267.979253	-264.642962	-262.051683
+ 0.0020	-269.950434	-265.474004	-262.060084
+ 0.0025	-271.917199	-266.285837	-262.070873
+ 0.0030	-273.879311	-267.077719	-262.084000

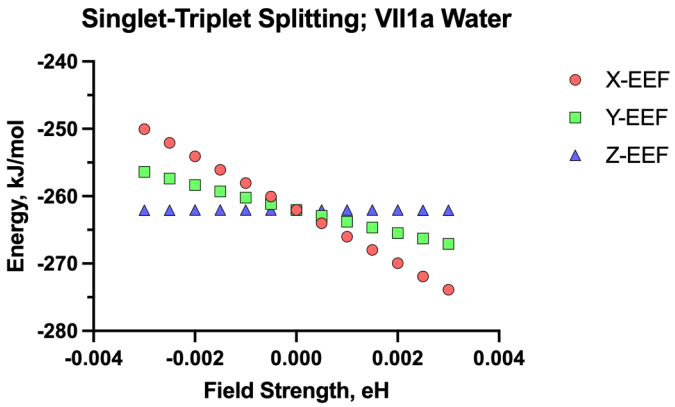


Figure S127. VII_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S126. ΔE_{ST} $VIII_{1a}$ Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-189.783669	-194.786234	-195.983338
– 0.0025	-190.840026	-195.016364	-196.012006
– 0.0020	-191.896640	-195.243793	-196.038749
– 0.0015	-192.953519	-195.468499	-196.063545
– 0.0010	-194.010690	-195.690461	-196.086371
– 0.0005	-195.068168	-195.909633	-196.107194
+ 0.0000	-196.125974	-196.125974	-196.125974
+ 0.0005	-197.184129	-196.339424	-196.142675
+ 0.0010	-198.242654	-196.549918	-196.157243
+ 0.0015	-199.301579	-196.757383	-196.169631
+ 0.0020	-200.360918	-196.961731	-196.179778
+ 0.0025	-201.420704	-197.162870	-196.187607
+ 0.0030	-202.480957	-197.360686	-196.193055

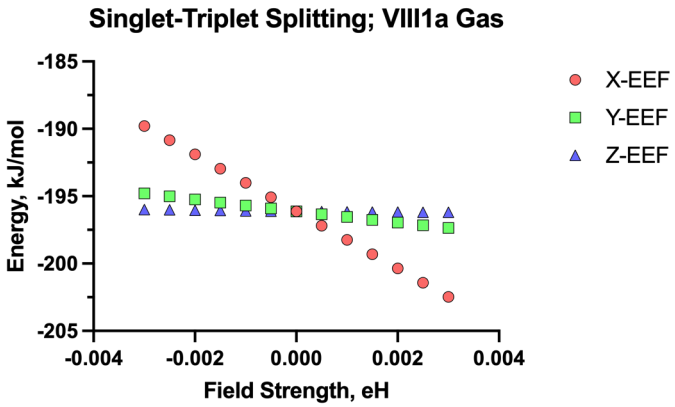


Figure S128. $VIII_{1a}$ Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S127. ΔE_{ST} $VIII_{1a}$ Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-198.120422	-204.335424	-205.670467
– 0.0025	-199.421168	-204.609198	-205.718779
– 0.0020	-200.722037	-204.879653	-205.764953
– 0.0015	-202.023075	-205.146764	-205.808965
– 0.0010	-203.324328	-205.410503	-205.850778
– 0.0005	-204.625844	-205.670821	-205.890363
+ 0.0000	-205.927664	-205.927664	-205.927664
+ 0.0005	-207.229838	-206.180964	-205.962633
+ 0.0010	-208.532414	-206.430641	-205.995210
+ 0.0015	-209.835437	-206.676606	-206.025330
+ 0.0020	-211.138956	-206.918745	-206.052913
+ 0.0025	-212.443015	-207.156941	-206.077876
+ 0.0030	-213.747663	-207.391062	-206.100122

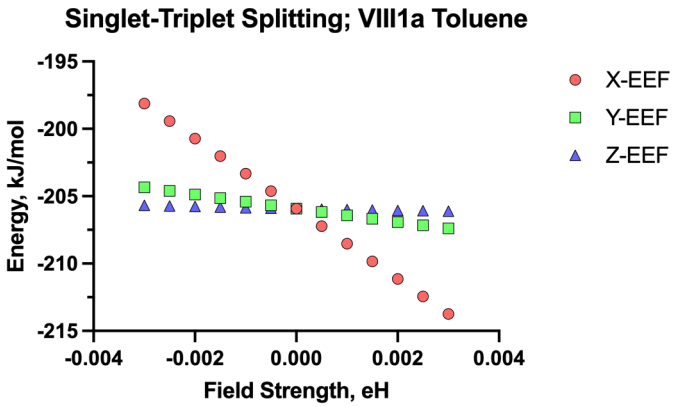


Figure S129. $VIII_{1a}$ Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S128. ΔE_{ST} $VIII_{1a}$ Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-205.039536	-212.667411	-214.111738
– 0.0025	-206.619346	-212.986759	-214.185588
– 0.0020	-208.199186	-213.301976	-214.257215
– 0.0015	-209.779149	-213.613032	-214.326586
– 0.0010	-211.359337	-213.919890	-214.393664
– 0.0005	-212.939841	-214.222490	-214.458409
+ 0.0000	-214.520760	-214.520760	-214.520760
+ 0.0005	-216.102190	-214.814616	-214.580663
+ 0.0010	-217.684217	-215.103952	-214.638036
+ 0.0015	-219.266936	-215.388637	-214.692809
+ 0.0020	-220.850436	-215.668544	-214.744885
+ 0.0025	-222.434807	-215.943505	-214.794171
+ 0.0030	-224.020139	-216.213343	-214.840543

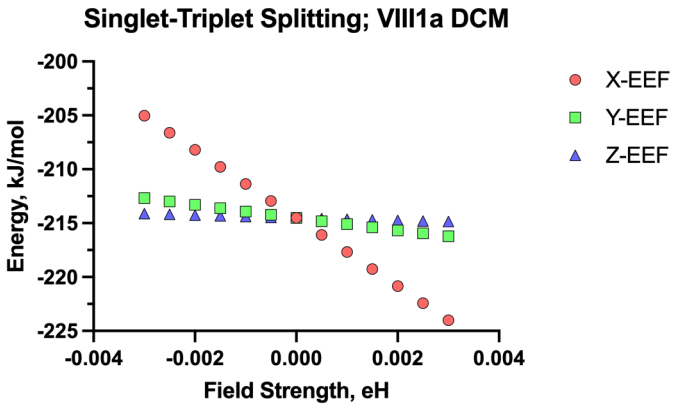


Figure S130. $VIII_{1a}$ Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S129. ΔE_{ST} $VIII_{1a}$ Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-207.684779	-215.932270	-217.416319
– 0.0025	-209.386001	-216.270949	-217.501758
– 0.0020	-211.087236	-216.605057	-217.584981
– 0.0015	-212.788620	-216.934563	-217.665951
– 0.0010	-214.490280	-217.259419	-217.744627
– 0.0005	-216.192337	-217.579564	-217.820969
+ 0.0000	-217.894913	-217.894913	-217.894913
+ 0.0005	-219.598138	-218.205365	-217.966398
+ 0.0010	-221.302122	-218.510806	-218.035341
+ 0.0015	-223.006987	-218.811084	-218.101669
+ 0.0020	-224.712851	-219.106043	-218.165274
+ 0.0025	-226.419822	-219.395502	-218.226060
+ 0.0030	-228.128020	-219.679250	-218.283899

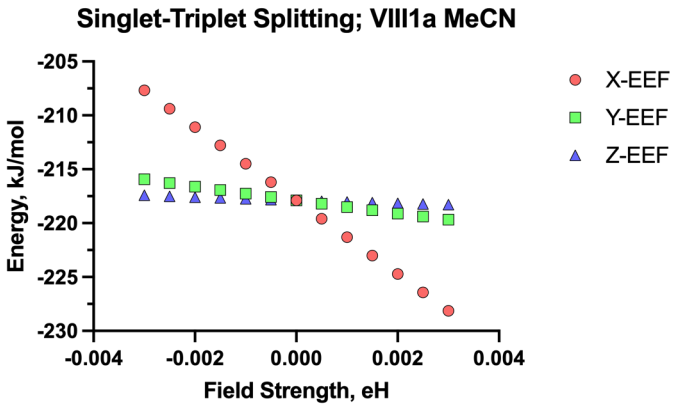


Figure S131. $VIII_{1a}$ Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S130. ΔE_{ST} $VIII_{1a}$ Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-206.558387	-214.936873	-216.429086
– 0.0025	-208.285242	-215.279642	-216.516985
– 0.0020	-210.012117	-215.617736	-216.602671
– 0.0015	-211.739147	-215.951124	-216.686107
– 0.0010	-213.466464	-216.279763	-216.767258
– 0.0005	-215.194203	-216.603582	-216.846073
+ 0.0000	-216.922494	-216.922494	-216.922494
+ 0.0005	-218.651461	-217.236396	-216.996454
+ 0.0010	-220.381238	-217.545168	-217.067878
+ 0.0015	-222.111939	-217.848662	-217.136682
+ 0.0020	-223.843692	-218.146712	-217.202766
+ 0.0025	-225.576614	-218.439129	-217.266027
+ 0.0030	-227.310825	-218.725697	-217.326337

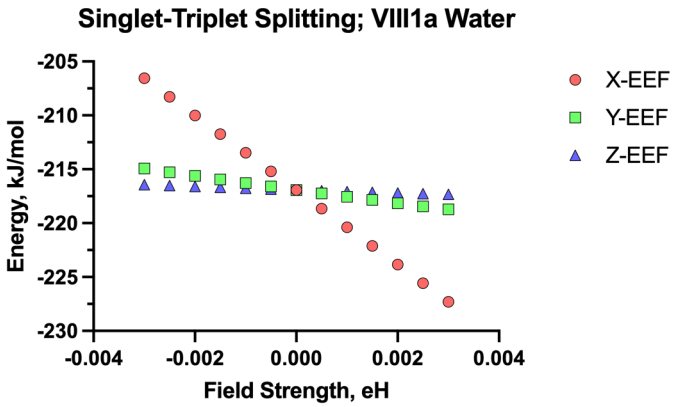


Figure S132. $VIII_{1a}$ Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

Table S131. ΔE_{ST} IX_{1a} Under EEFs in Gas. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-360.034815	-366.546055	-363.684260
– 0.0025	-360.927485	-366.362270	-363.973065
– 0.0020	-361.846410	-366.178485	-364.261870
– 0.0015	-362.739080	-365.994700	-364.550675
– 0.0010	-363.631750	-365.810915	-364.839480
– 0.0005	-364.498165	-365.600875	-365.128285
+ 0.0000	-365.390835	-365.390835	-365.390835
+ 0.0005	-366.283505	-365.180795	-365.679640
+ 0.0010	-367.176175	-364.970755	-365.968445
+ 0.0015	-368.068845	-364.734460	-366.204740
+ 0.0020	-368.935260	-364.498165	-366.493545
+ 0.0025	-369.827930	-364.261870	-366.729840
+ 0.0030	-370.720600	-364.025575	-366.992390

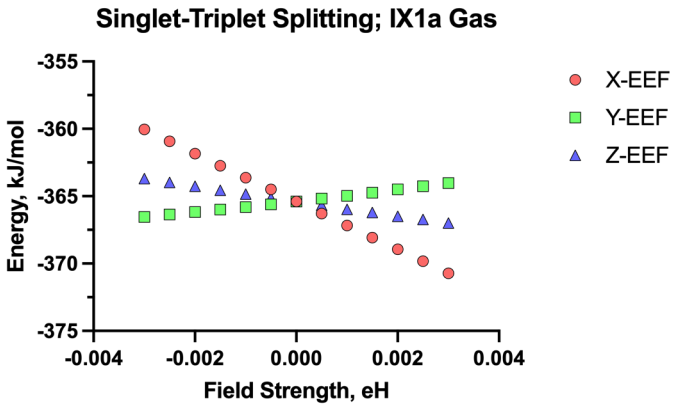


Figure S133. IX_{1a} Singlet Triplet Splitting under EEFs in Gas. Axis definitions given in S2.

Table S132. ΔE_{ST} IX_{1a} Under EEFs in Toluene. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-367.644002	-375.594736	-372.119873
– 0.0025	-368.747227	-375.392068	-372.483426
– 0.0020	-369.848687	-375.179240	-372.842498
– 0.0015	-370.948262	-374.956692	-373.197124
– 0.0010	-372.045842	-374.724813	-373.547331
– 0.0005	-373.141303	-374.483976	-373.893128
+ 0.0000	-374.234506	-374.234506	-374.234506
+ 0.0005	-375.325312	-373.976706	-374.571450
+ 0.0010	-376.413579	-373.710850	-374.903933
+ 0.0015	-377.499142	-373.437202	-375.231907
+ 0.0020	-378.581830	-373.155993	-375.555324
+ 0.0025	-379.661470	-372.867437	-375.874110
+ 0.0030	-380.737862	-372.571738	-376.188185

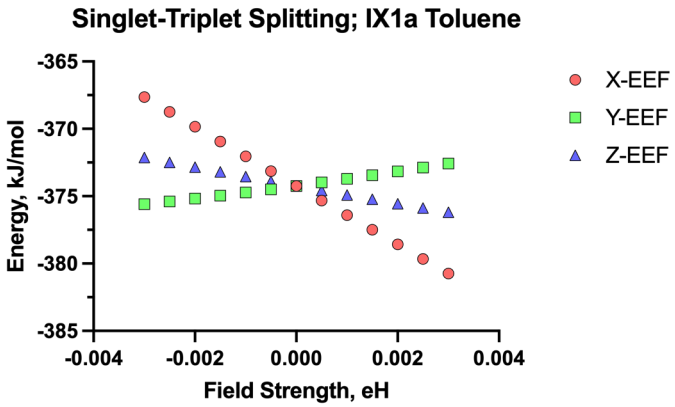


Figure S134. IX_{1a} Singlet Triplet Splitting under EEFs in Toluene. Axis definitions given in S2.

Table S133. ΔE_{ST} IX_{1a} Under EEFs in DCM. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-370.401531	-379.896654	-375.872401
– 0.0025	-371.728587	-379.666049	-376.294479
– 0.0020	-373.053577	-379.422486	-376.711492
– 0.0015	-374.376346	-379.166558	-377.123496
– 0.0010	-375.696736	-378.898796	-377.530517
– 0.0005	-377.014572	-378.619685	-377.932573
+ 0.0000	-378.329664	-378.329664	-378.329664
+ 0.0005	-379.641805	-378.029133	-378.721774
+ 0.0010	-380.950782	-377.718466	-379.108878
+ 0.0015	-382.256354	-377.397992	-379.490938
+ 0.0020	-383.558266	-377.068025	-379.867900
+ 0.0025	-384.856245	-376.728847	-380.239694
+ 0.0030	-386.149989	-376.380713	-380.606240

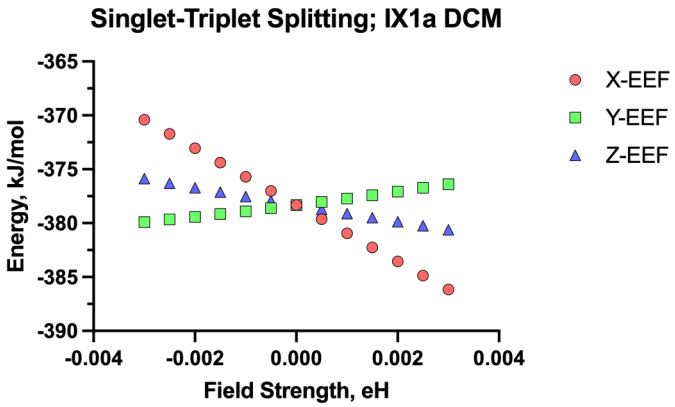


Figure S135. IX_{1a} Singlet Triplet Splitting under EEFs in DCM. Axis definitions given in S2.

Table S134. ΔE_{ST} IX_{1a} Under EEFs in MeCN. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-371.435203	-381.560893	-377.336078
– 0.0025	-372.855410	-381.321434	-377.779756
– 0.0020	-374.273413	-381.067509	-378.218159
– 0.0015	-375.689052	-380.799797	-378.651340
– 0.0010	-377.102127	-380.518916	-379.079333
– 0.0005	-378.512454	-380.225417	-379.502154
+ 0.0000	-379.919809	-379.919809	-379.919809
+ 0.0005	-381.323957	-379.602556	-380.332288
+ 0.0010	-382.724641	-379.274072	-380.739558
+ 0.0015	-384.121580	-378.934747	-381.141588
+ 0.0020	-385.514479	-378.584933	-381.538322
+ 0.0025	-386.903006	-378.224949	-381.929692
+ 0.0030	-388.286804	-377.855086	-382.315622

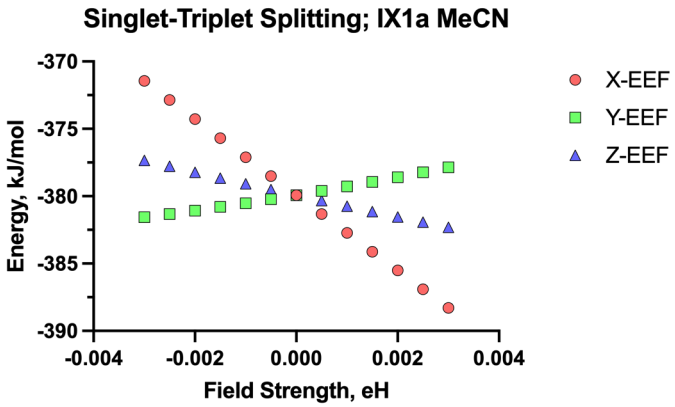


Figure S136. IX_{1a} Singlet Triplet Splitting under EEFs in MeCN. Axis definitions given in S2.

Table S135. ΔE_{ST} IX_{1a} Under EEFs in Water. Energy given in KJ/mol.

Field	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-365.331428	-375.586935	-371.322409
– 0.0025	-366.770945	-375.345862	-371.770398
– 0.0020	-368.208235	-375.089981	-372.213073
– 0.0015	-369.643118	-374.819987	-372.650479
– 0.0010	-371.075413	-374.536517	-373.082657
– 0.0005	-372.504908	-374.240143	-373.509627
+ 0.0000	-373.931384	-373.931384	-373.931384
+ 0.0005	-375.354600	-373.610724	-374.347928
+ 0.0010	-376.774284	-373.278588	-374.759225
+ 0.0015	-378.190153	-372.935375	-375.165241
+ 0.0020	-379.601897	-372.581447	-375.565918
+ 0.0025	-381.009170	-372.217135	-375.961198
+ 0.0030	-382.411605	-371.842741	-376.350995

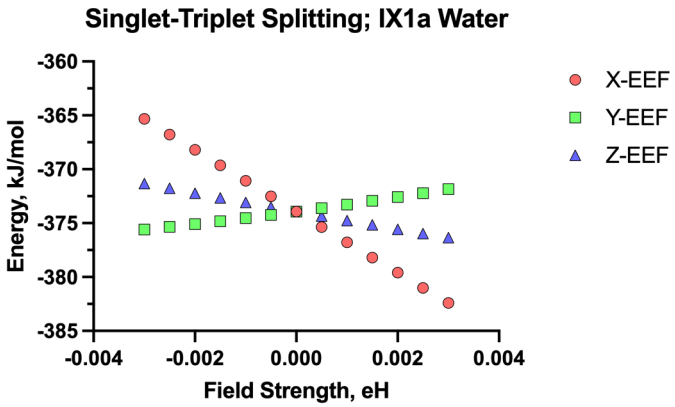


Figure S137. IX_{1a} Singlet Triplet Splitting under EEFs in Water. Axis definitions given in S2.

S5. Benchmark: Effect of Geometry Optimisation versus Single-Points of I_{1a} under EEFs

Energy of structure optimised under electric field, measured relative to energy of structure optimised without external electric field. In the worst case, the maximum change relative to the optimisation without external field is only 5 kJ/mol in the triplet state, and 0.63 kJ/mol in the singlet state.

Table S136. Change in Energy of I_{1a} due to Optimisation under EEFs in Gas. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.774663	-304.777589	-304.777699	-0.033339	-0.233446	-0.050215
– 0.0025	-304.775044	-304.777485	-304.777561	-0.009339	-0.170104	-0.029652
– 0.0020	-304.775444	-304.777400	-304.777449	-0.011657	-0.103833	-0.022422
– 0.0015	-304.775865	-304.777333	-304.777361	-0.014015	-0.061271	-0.002240
– 0.0010	-304.776306	-304.777284	-304.777298	0.010064	-0.011613	0.005427
– 0.0005	-304.776767	-304.777257	-304.777261	0.008320	-0.018914	-0.001392
+ 0.0000	-304.777248	-304.777248	-304.777248	0.005658	0.005658	0.005658
+ 0.0005	-304.777749	-304.777257	-304.777261	0.002731	-0.018791	-0.001405
+ 0.0010	-304.778270	-304.777284	-304.777298	-0.000289	-0.011366	0.005395
+ 0.0015	-304.778811	-304.777333	-304.777361	-0.002980	-0.060360	-0.002316
+ 0.0020	-304.779372	-304.777399	-304.777449	-0.005766	-0.102607	-0.022522
+ 0.0025	-304.779953	-304.777484	-304.777561	-0.008680	-0.168554	-0.029778
+ 0.0030	-304.780554	-304.777588	-304.777699	-0.038015	-0.231590	-0.050368

Table S137. Change in Energy of $^3I_{1a}$ due to Optimisation under EEFs in Gas. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.639710	-304.641438	-304.641446	-0.236765	-2.280241	-2.115896
– 0.0025	-304.639780	-304.641192	-304.641167	-0.209867	-1.816402	-1.645852
– 0.0020	-304.639867	-304.640972	-304.640928	-0.176951	-1.395697	-1.229010
– 0.0015	-304.639969	-304.640780	-304.640731	-0.103148	-0.971380	-0.841785
– 0.0010	-304.640093	-304.640619	-304.640576	-0.061156	-0.600875	-0.487471
– 0.0005	-304.640252	-304.640492	-304.640466	-0.056912	-0.266633	-0.225601
+ 0.0000	-304.640410	-304.640410	-304.640410	-0.000158	-0.000158	-0.000158
+ 0.0005	-304.640604	-304.640453	-304.640464	-0.010872	-0.033843	-0.035927
+ 0.0010	-304.640821	-304.640542	-304.640571	-0.001856	-0.135282	-0.133360
+ 0.0015	-304.641059	-304.640664	-304.640723	0.002400	-0.247451	-0.270581
+ 0.0020	-304.641316	-304.640818	-304.640918	-0.015068	-0.440102	-0.467171
+ 0.0025	-304.641592	-304.641000	-304.641154	-0.032708	-0.629797	-0.693040
+ 0.0030	-304.641889	-304.641210	-304.641430	-0.023737	-0.839892	-0.972435

Table S138. Change in Energy of I_{1a} due to Optimisation under EEFs in Toluene. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.790591	-304.794242	-304.794347	-0.223721	-0.614609	-0.343867
– 0.0025	-304.791070	-304.794114	-304.794186	-0.226641	-0.508625	-0.318660
– 0.0020	-304.791573	-304.794010	-304.794056	-0.231430	-0.422674	-0.300596
– 0.0015	-304.792100	-304.793928	-304.793954	-0.238051	-0.356146	-0.286565
– 0.0010	-304.792650	-304.793871	-304.793881	-0.246471	-0.309019	-0.276560
– 0.0005	-304.793225	-304.793836	-304.793838	-0.256664	-0.279692	-0.270568
+ 0.0000	-304.793823	-304.793823	-304.793823	-0.268594	-0.268594	-0.268594
+ 0.0005	-304.794446	-304.793835	-304.793838	-0.282236	-0.279490	-0.270626
+ 0.0010	-304.795092	-304.793870	-304.793881	-0.297572	-0.308268	-0.276673
+ 0.0015	-304.795762	-304.793928	-304.793954	-0.314582	-0.355028	-0.286739
+ 0.0020	-304.796457	-304.794009	-304.794056	-0.336739	-0.421170	-0.300825
+ 0.0025	-304.797175	-304.794113	-304.794186	-0.357396	-0.506764	-0.318948
+ 0.0030	-304.797917	-304.794241	-304.794347	-0.379739	-0.612369	-0.344221

Table S139. Change in Energy of $^3I_{1a}$ due to Optimisation under EEFs in Toluene. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.651540	-304.653993	-304.653984	-0.246789	-3.629134	-3.365421
– 0.0025	-304.651643	-304.653652	-304.653607	-0.230201	-2.949224	-2.683621
– 0.0020	-304.651768	-304.653351	-304.653283	-0.217651	-2.321415	-2.062837
– 0.0015	-304.651918	-304.653085	-304.653009	-0.209137	-1.729207	-1.501439
– 0.0010	-304.652091	-304.652855	-304.652788	-0.204566	-1.175765	-1.001500
– 0.0005	-304.652288	-304.652661	-304.652620	-0.204046	-0.664291	-0.567922
+ 0.0000	-304.652508	-304.652508	-304.652508	-0.207454	-0.207454	-0.207454
+ 0.0005	-304.652752	-304.652610	-304.652613	-0.214952	-0.364089	-0.339603
+ 0.0010	-304.653020	-304.652757	-304.652775	-0.226607	-0.583278	-0.549727
+ 0.0015	-304.653312	-304.652941	-304.652993	-0.242394	-0.848433	-0.828747
+ 0.0020	-304.653628	-304.653162	-304.653264	-0.262461	-1.153141	-1.174074
+ 0.0025	-304.653967	-304.653417	-304.653588	-0.286839	-1.494863	-1.585492
+ 0.0030	-304.654331	-304.653708	-304.653965	-0.315848	-1.871661	-2.059062

Table S140. Change in Energy of I_{1a} due to Optimisation under EEFs in DCM. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.794822	-304.799299	-304.799349	-0.558034	-1.152240	-0.723472
– 0.0025	-304.795409	-304.799135	-304.799170	-0.564863	-0.992323	-0.696311
– 0.0020	-304.796024	-304.799001	-304.799024	-0.574115	-0.862369	-0.674118
– 0.0015	-304.796667	-304.798898	-304.798911	-0.585760	-0.762267	-0.656884
– 0.0010	-304.797339	-304.798824	-304.798830	-0.599769	-0.691604	-0.644594
– 0.0005	-304.798038	-304.798780	-304.798781	-0.616126	-0.649381	-0.637235
+ 0.0000	-304.798765	-304.798765	-304.798765	-0.634807	-0.634807	-0.634807
+ 0.0005	-304.799521	-304.798779	-304.798781	-0.655792	-0.646472	-0.637303
+ 0.0010	-304.800304	-304.798824	-304.798830	-0.679067	-0.690685	-0.644731
+ 0.0015	-304.801116	-304.798897	-304.798911	-0.704616	-0.760838	-0.657092
+ 0.0020	-304.801956	-304.799001	-304.799025	-0.732430	-0.860466	-0.674394
+ 0.0025	-304.802824	-304.799134	-304.799170	-0.762492	-0.989913	-0.696655
+ 0.0030	-304.803721	-304.799298	-304.799349	-0.794802	-1.149431	-0.723884

Table S141. Change in Energy of $^3I_{1a}$ due to Optimisation under EEFs in DCM. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.653651	-304.656830	-304.656727	-0.372075	-5.042454	-4.502882
– 0.0025	-304.653780	-304.656390	-304.656257	-0.354939	-4.137646	-3.611927
– 0.0020	-304.653937	-304.656001	-304.655849	-0.344962	-3.299198	-2.799817
– 0.0015	-304.654123	-304.655644	-304.655504	-0.341971	-2.482479	-2.070490
– 0.0010	-304.654337	-304.655340	-304.655220	-0.345794	-1.742699	-1.416281
– 0.0005	-304.654579	-304.654751	-304.654772	-0.356448	-0.187689	-0.248118
+ 0.0000	-304.654849	-304.654849	-304.654849	-0.373845	-0.373845	-0.373845
+ 0.0005	-304.655148	-304.655007	-304.654995	-0.398378	-0.655309	-0.598391
+ 0.0010	-304.655475	-304.655215	-304.655208	-0.430151	-1.002476	-0.913309
+ 0.0015	-304.655831	-304.655470	-304.655487	-0.469308	-1.406906	-1.319424
+ 0.0020	-304.656215	-304.655769	-304.655832	-0.516179	-1.864113	-1.814620
+ 0.0025	-304.656629	-304.656111	-304.656240	-0.571989	-2.370462	-2.391179
+ 0.0030	-304.657073	-304.656496	-304.656708	-0.636673	-2.921410	-3.042527

Table S142. Change in Energy of I_{1a} due to Optimisation under EEFs in MeCN. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.794963	-304.799805	-304.799818	-0.730002	-1.441877	-0.925161
– 0.0025	-304.795597	-304.799624	-304.799633	-0.740260	-1.253626	-0.896272
– 0.0020	-304.796261	-304.799476	-304.799482	-0.753180	-1.101087	-0.872674
– 0.0015	-304.796954	-304.799360	-304.799364	-0.768725	-0.982060	-0.854346
– 0.0010	-304.797677	-304.799278	-304.799280	-0.786873	-0.898275	-0.841278
– 0.0005	-304.798430	-304.799229	-304.799230	-0.807596	-0.848194	-0.833454
+ 0.0000	-304.799213	-304.799213	-304.799213	-0.830871	-0.830871	-0.830871
+ 0.0005	-304.800025	-304.799229	-304.799230	-0.856680	-0.847703	-0.833525
+ 0.0010	-304.800868	-304.799278	-304.799280	-0.885004	-0.897283	-0.841423
+ 0.0015	-304.801741	-304.799360	-304.799364	-0.915827	-0.980519	-0.854566
+ 0.0020	-304.802643	-304.799475	-304.799482	-0.949142	-1.099116	-0.872966
+ 0.0025	-304.803576	-304.799623	-304.799633	-0.984935	-1.251069	-0.896640
+ 0.0030	-304.804539	-304.799804	-304.799818	-1.023199	-1.438813	-0.925602

Table S143. Change in Energy of $^3I_{1a}$ due to Optimisation under EEFs in MeCN. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.652914	-304.656455	-304.656273	-0.503495	-5.861739	-5.112655
– 0.0025	-304.653054	-304.655965	-304.655761	-0.484623	-4.840837	-4.124248
– 0.0020	-304.653224	-304.655514	-304.655316	-0.475163	-3.850802	-3.222746
– 0.0015	-304.653425	-304.655119	-304.654937	-0.474549	-2.940660	-2.409542
– 0.0010	-304.653656	-304.654769	-304.654105	-0.482478	-2.080234	-0.320230
– 0.0005	-304.653918	-304.654084	-304.654118	-0.498950	-0.274023	-0.362432
+ 0.0000	-304.654210	-304.654210	-304.654210	-0.524494	-0.524494	-0.524494
+ 0.0005	-304.654532	-304.654397	-304.654375	-0.558806	-0.869933	-0.791538
+ 0.0010	-304.654886	-304.654639	-304.654612	-0.602471	-1.288798	-1.160870
+ 0.0015	-304.655270	-304.654932	-304.654921	-0.656102	-1.772034	-1.631922
+ 0.0020	-304.655686	-304.655273	-304.655299	-0.720490	-2.313202	-2.197801
+ 0.0025	-304.656134	-304.655661	-304.655743	-0.796650	-2.907463	-2.850642
+ 0.0030	-304.656615	-304.656094	-304.656252	-0.886243	-3.550563	-3.585212

Table S144. Change in Energy of I_{1a} due to Optimisation under EEFs in Water. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.780028	-304.784929	-304.784932	-0.572661	-1.265236	-0.726177
– 0.0025	-304.780668	-304.784744	-304.784746	-0.575297	-1.070926	-0.696587
– 0.0020	-304.781339	-304.784592	-304.784594	-0.580719	-0.911996	-0.672417
– 0.0015	-304.782040	-304.784474	-304.784475	-0.588889	-0.788404	-0.653642
– 0.0010	-304.782770	-304.784390	-304.784390	-0.599777	-0.700528	-0.640252
– 0.0005	-304.783531	-304.784340	-304.784340	-0.613354	-0.647713	-0.632236
+ 0.0000	-304.784323	-304.784323	-304.784323	-0.629590	-0.629590	-0.629590
+ 0.0005	-304.785144	-304.784338	-304.784340	-0.648464	-0.644085	-0.632310
+ 0.0010	-304.785996	-304.784390	-304.784390	-0.669957	-0.699525	-0.640399
+ 0.0015	-304.786878	-304.784474	-304.784475	-0.694048	-0.786904	-0.653865
+ 0.0020	-304.787791	-304.784592	-304.784594	-0.720726	-0.909988	-0.672711
+ 0.0025	-304.788734	-304.784743	-304.784746	-0.749977	-1.068418	-0.696957
+ 0.0030	-304.789708	-304.784928	-304.784932	-0.781793	-1.262188	-0.726620

Table S145. Change in Energy of $^3I_{1a}$ due to Optimisation under EEFs in Water. Energy given in Hartree, changes in energy given in KJ/mol.

Field	E, X-EEF	E, Y-EEF	E, Z-EEF	ΔE, X-EEF	ΔE, Y-EEF	ΔE, Z-EEF
– 0.0030	-304.641824	-304.645156	-304.644948	-0.862876	-5.616837	-4.795702
– 0.0025	-304.641981	-304.644715	-304.644505	-0.881399	-4.727029	-3.991926
– 0.0020	-304.642167	-304.644319	-304.644120	-0.904886	-3.885388	-3.251918
– 0.0015	-304.642382	-304.643968	-304.643797	-0.933347	-3.090647	-2.587071
– 0.0010	-304.642626	-304.643662	-304.643465	-0.966759	-2.345643	-1.812259
– 0.0005	-304.642899	-304.643403	-304.643134	-1.005144	-1.655866	-0.949835
+ 0.0000	-304.643202	-304.643202	-304.643202	-1.048551	-1.048551	-1.048551
+ 0.0005	-304.643534	-304.643342	-304.643334	-1.097057	-1.265139	-1.227610
+ 0.0010	-304.643896	-304.643533	-304.643528	-1.150835	-1.547661	-1.481764
+ 0.0015	-304.644288	-304.643772	-304.643783	-1.210038	-1.886829	-1.809642
+ 0.0020	-304.644709	-304.644059	-304.644100	-1.274880	-2.279183	-2.212084
+ 0.0025	-304.645161	-304.644391	-304.644479	-1.345821	-2.720924	-2.688050
+ 0.0030	-304.645642	-304.644768	-304.644919	-1.423197	-3.208466	-3.235774

S6. Benchmark: Point Charges Approximately Reproduce D-LEF Electrostatic Switches

When the charged D-LEFs are replaced by simple point charges at the heavy-atom position (N/B) in the optimised structure of **I_{1a}**, we observe that a negative charge raises the nucleophilicity, while a positive charge lowers it, and vice-versa.

We note that the effects of the positive charge upon the GEI values are unrealistically large in magnitude; we ascribe this to the lack of polarisation on the point charge, especially considering the already highly polarisable nature of the LUMO and its unfavourable interaction with a bare charge. To be specific, when the point charge is replaced by the corresponding cation, the latter can polarise to accommodate the unfavourable electrostatic interactions, reducing its impact on the measured quantities, while the former cannot. That reasonable results are seen for the corresponding anion is because the interactions between it and the LUMO are favourable and balanced.

Table S146. Point Charge Benchmarks. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	GEI	N	ΔGEI	ΔN
I_{1a} No Charge	-7.430886	-0.159459	0.990406	3.492582		
I_{1a} Positive Charge	-12.112334	-9.120442	18.835519	-1.188866	17.845	-4.68
I_{1a} Negative Charge	-3.919801	1.973370	0.080360	7.003668	-0.910	3.51
I_{2a} No Charge	-7.491840	-0.181228	1.006687	3.431628		
I_{2a} Positive Charge	-12.386353	-9.545483	21.164537	-1.462884	20.158	-4.89
I_{2a} Negative Charge	-3.826738	1.923845	0.078709	7.096731	-0.912	3.67

S7. Benchmark: Comparison of CCSD(T) and DFT Energies of I_{1a} under EEFs

The relative changes in energy of the singlet I_{1a} at the M06-2X and CCSD(T) levels of theory compare favourably, being in the X-axis 15.46 kJ/mol and 15.65 kJ/mol in each case, and negligible along the other axes. For the triplet, these values along the X-axis are 5.94 kJ/mol and 6.08 kJ/mol, respectively, and negligible along the other axes.

Table S147. Energy of I_{1a} Under EEFs in Gas at CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.280532	-304.283405	-304.283584
– 0.0020	-304.281328	-304.283267	-304.283346
– 0.0010	-304.282202	-304.283184	-304.283204
+ 0.0000	-304.283156	-304.283156	-304.283156
+ 0.0010	-304.284189	-304.283184	-304.283204
+ 0.0020	-304.285301	-304.283267	-304.283346
+ 0.0030	-304.286493	-304.283405	-304.283584

Table S148. Energy of $^3I_{1a}$ Under EEFs in Gas at CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ. Energy given in Hartree.

Field	Energy, X-EEF	Energy, Y-EEF	Energy, Z-EEF
– 0.0030	-304.143339	-304.144318	-304.144397
– 0.0020	-304.143535	-304.144190	-304.144218
– 0.0010	-304.143807	-304.144135	-304.144137
+ 0.0000	-304.144155	-304.144155	-304.144155
+ 0.0010	-304.144579	-304.144248	-304.144271
+ 0.0020	-304.145079	-304.144416	-304.144486
+ 0.0030	-304.145656	-304.144658	-304.144799

S8. Benchmark: Investigation of Spin-State Switching of Simple Carbenes Under EEFs

We selected several carbenes, given below, to assess whether it was feasible to switch the spin state of simple carbenes under EEFs. Broadly, we found that it was not feasible under the field strengths we investigated. These field strengths were chosen to be physically reasonable, with reference to our previous STM experiments, in the range of +/- 0.003 a.u. Calculations were performed at the M06-2X/def2-TZVP level of theory.

Of all the species given below, we only observe electrostatic switching of spin states with A12 and A21.

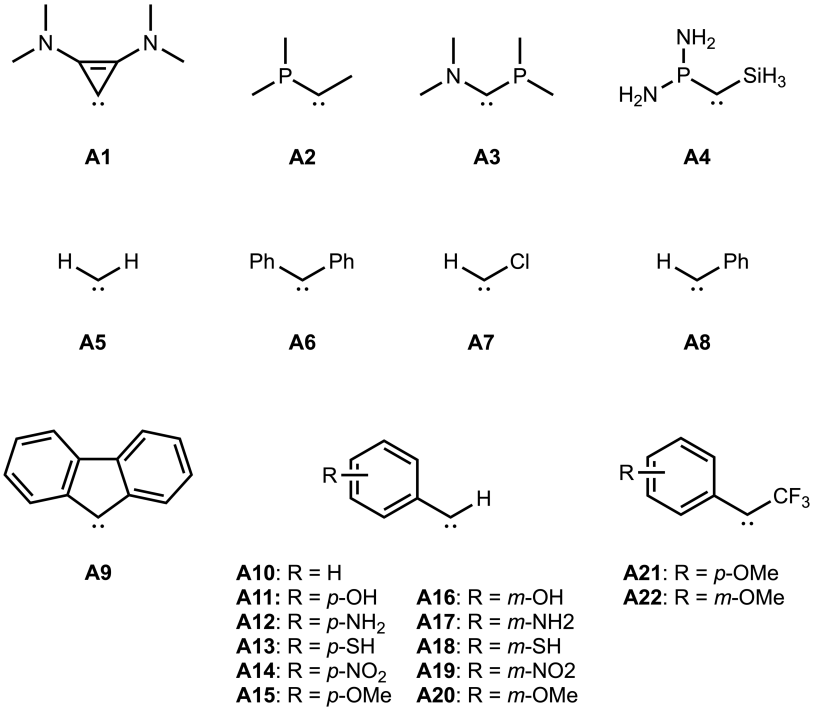


Figure S138. Species Selected for Possible Spin Switching Under EEFs.

Table S149. Energy of A1 and ^{3}A1 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A1, X-EEF	Energy A1, Y-EEF	Energy A1, Z-EEF	Energy ^{3}A1, X-EEF	Energy ^{3}A1, Y-EEF	Energy ^{3}A1, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-383.303884	-383.308712	-383.309583	-383.195103	-383.199942	-383.200131	-285.61	-285.58	-287.37
– 0.0025	-383.304673	-383.308713	-383.309400	-383.195562	-383.199602	-383.199732	-286.47	-286.47	-287.93
– 0.0020	-383.305487	-383.308732	-383.309251	-383.196046	-383.199285	-383.199366	-287.34	-287.35	-288.50
– 0.0015	-383.306324	-383.308769	-383.309134	-383.196556	-383.198989	-383.199034	-288.20	-288.23	-289.07
– 0.0010	-383.307187	-383.308823	-383.309051	-383.197090	-383.198716	-383.198735	-289.06	-289.09	-289.63
– 0.0005	-383.308073	-383.308895	-383.309001	-383.197650	-383.198465	-383.198469	-289.91	-289.93	-290.20
+ 0.0000	-383.308984	-383.308984	-383.308984	-383.198236	-383.198236	-383.198236	-290.77	-290.77	-290.77
+ 0.0005	-383.309919	-383.309091	-383.309001	-383.198847	-383.198029	-383.198036	-291.62	-291.59	-291.34
+ 0.0010	-383.310879	-383.309216	-383.309051	-383.199483	-383.197844	-383.197870	-292.47	-292.41	-291.90
+ 0.0015	-383.311863	-383.309358	-383.309134	-383.200144	-383.197681	-383.197737	-293.32	-293.21	-292.47
+ 0.0020	-383.312872	-383.309517	-383.309250	-383.200831	-383.197539	-383.197637	-294.16	-294.00	-293.04
+ 0.0025	-383.313905	-383.309694	-383.309400	-383.201544	-383.197420	-383.197571	-295.00	-294.78	-293.61
+ 0.0030	-383.314962	-383.309889	-383.309583	-383.202281	-383.197323	-383.197538	-295.84	-295.54	-294.17

Table S150. Energy of A2 and ^{3}A2 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A2, X-EEF	Energy A2, Y-EEF	Energy A2, Z-EEF	Energy ^{3}A2, X-EEF	Energy ^{3}A2, Y-EEF	Energy ^{3}A2, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-499.055716	-499.058211	-499.061321	-499.044275	-499.043858	-499.043805	-30.04	-37.68	-45.99
– 0.0025	-499.056043	-499.058137	-499.060699	-499.044103	-499.043751	-499.043693	-31.35	-37.77	-44.65
– 0.0020	-499.056390	-499.058076	-499.060102	-499.043948	-499.043662	-499.043606	-32.67	-37.84	-43.31
– 0.0015	-499.056756	-499.058029	-499.059531	-499.043808	-499.043592	-499.043541	-33.99	-37.91	-41.98
– 0.0010	-499.057141	-499.057996	-499.058985	-499.043685	-499.043539	-499.043500	-35.33	-37.96	-40.66
– 0.0005	-499.057545	-499.057975	-499.058464	-499.043578	-499.043504	-499.043482	-36.67	-38.00	-39.34
+ 0.0000	-499.057969	-499.057969	-499.057969	-499.043487	-499.043487	-499.043487	-38.02	-38.02	-38.02
+ 0.0005	-499.058412	-499.057976	-499.057499	-499.043412	-499.043488	-499.043515	-39.38	-38.04	-36.71
+ 0.0010	-499.058874	-499.057997	-499.057054	-499.043353	-499.043507	-499.043567	-40.75	-38.04	-35.41
+ 0.0015	-499.059356	-499.058031	-499.056634	-499.043311	-499.043544	-499.043641	-42.13	-38.03	-34.11
+ 0.0020	-499.059857	-499.058078	-499.056240	-499.043284	-499.043599	-499.043739	-43.51	-38.02	-32.82
+ 0.0025	-499.060378	-499.058139	-499.055871	-499.043274	-499.043672	-499.043861	-44.90	-37.98	-31.53
+ 0.0030	-499.060917	-499.058214	-499.055527	-499.043280	-499.043763	-499.044005	-46.31	-37.94	-30.25

Table S151. Energy of A3 and ^{3}A3 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A3, X-EEF	Energy A3, Y-EEF	Energy A3, Z-EEF	Energy ^{3}A3, X-EEF	Energy ^{3}A3, Y-EEF	Energy ^{3}A3, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-593.742181	-593.743284	-593.747248	-593.696529	-593.696100	-593.698251	-119.86	-123.88	-128.64
– 0.0025	-593.742470	-593.743399	-593.746674	-593.696425	-593.696065	-593.697834	-120.89	-124.28	-128.23
– 0.0020	-593.742783	-593.743534	-593.746132	-593.696343	-593.696052	-593.697448	-121.93	-124.66	-127.82
– 0.0015	-593.743119	-593.743689	-593.745620	-593.696282	-593.696062	-593.697095	-122.97	-125.04	-127.40
– 0.0010	-593.743480	-593.743863	-593.745139	-593.696243	-593.696095	-593.696774	-124.02	-125.41	-126.98
– 0.0005	-593.743863	-593.744057	-593.744689	-593.696225	-593.696150	-593.696485	-125.08	-125.78	-126.56
+ 0.0000	-593.744270	-593.744270	-593.744270	-593.696228	-593.696228	-593.696228	-126.14	-126.14	-126.14
+ 0.0005	-593.744701	-593.744504	-593.743883	-593.696253	-593.696328	-593.696003	-127.20	-126.48	-125.71
+ 0.0010	-593.745156	-593.744757	-593.743526	-593.696299	-593.696451	-593.695811	-128.27	-126.83	-125.27
+ 0.0015	-593.745634	-593.745029	-593.743199	-593.696367	-593.696597	-593.695650	-129.35	-127.16	-124.84
+ 0.0020	-593.746135	-593.745321	-593.742904	-593.696456	-593.696765	-593.695522	-130.43	-127.48	-124.40
+ 0.0025	-593.746660	-593.745633	-593.742640	-593.696567	-593.696956	-593.695426	-131.52	-127.80	-123.96
+ 0.0030	-593.747209	-593.745964	-593.742407	-593.696699	-593.697169	-593.695362	-132.61	-128.11	-123.52

Table S152. Energy of A4 and ^{3}A4 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A4, X-EEF	Energy A4, Y-EEF	Energy A4, Z-EEF	Energy ^{3}A4, X-EEF	Energy ^{3}A4, Y-EEF	Energy ^{3}A4, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-782.573527	-782.575738	-782.581885	-782.546026	-782.545414	-782.545889	-72.20	-79.61	-94.51
– 0.0025	-782.573805	-782.575659	-782.580747	-782.545672	-782.545158	-782.545532	-73.86	-80.08	-92.46
– 0.0020	-782.574103	-782.575594	-782.579638	-782.545334	-782.544919	-782.545201	-75.53	-80.54	-90.41
– 0.0015	-782.574418	-782.575543	-782.578556	-782.545013	-782.544699	-782.544898	-77.20	-80.98	-88.37
– 0.0010	-782.574753	-782.575507	-782.577502	-782.544709	-782.544498	-782.544622	-78.88	-81.42	-86.33
– 0.0005	-782.575106	-782.575485	-782.576476	-782.544421	-782.544314	-782.544372	-80.56	-81.84	-84.29
+ 0.0000	-782.575477	-782.575477	-782.575477	-782.544149	-782.544149	-782.544149	-82.25	-82.25	-82.25
+ 0.0005	-782.575867	-782.575483	-782.574506	-782.543894	-782.544003	-782.543953	-83.94	-82.65	-80.22
+ 0.0010	-782.576276	-782.575504	-782.573564	-782.543656	-782.543875	-782.543784	-85.64	-83.04	-78.19
+ 0.0015	-782.576703	-782.575539	-782.572648	-782.543434	-782.543765	-782.543642	-87.35	-83.42	-76.16
+ 0.0020	-782.577149	-782.575588	-782.571761	-782.543229	-782.543673	-782.543526	-89.06	-83.79	-74.13
+ 0.0025	-782.577613	-782.575651	-782.570901	-782.543041	-782.543600	-782.543437	-90.77	-84.15	-72.11
+ 0.0030	-782.578096	-782.575729	-782.570070	-782.542869	-782.543545	-782.543374	-92.49	-84.50	-70.09

Table S153. Energy of A5 and ^{3}A5 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A5, X-EEF	Energy A5, Y-EEF	Energy A5, Z-EEF	Energy ^{3}A5, X-EEF	Energy ^{3}A5, Y-EEF	Energy ^{3}A5, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-39.120717	-39.122949	-39.122974	-39.143871	-39.144625	-39.144639	60.79	56.91	56.88
– 0.0025	-39.121073	-39.122935	-39.122952	-39.143982	-39.144610	-39.144620	60.15	56.91	56.89
– 0.0020	-39.121431	-39.122923	-39.122934	-39.144096	-39.144598	-39.144605	59.51	56.91	56.90
– 0.0015	-39.121794	-39.122914	-39.122920	-39.144213	-39.144589	-39.144593	58.86	56.91	56.90
– 0.0010	-39.122160	-39.122907	-39.122910	-39.144332	-39.144583	-39.144584	58.21	56.91	56.91
– 0.0005	-39.122529	-39.122903	-39.122904	-39.144453	-39.144579	-39.144579	57.56	56.91	56.91
+ 0.0000	-39.122902	-39.122902	-39.122902	-39.144577	-39.144577	-39.144577	56.91	56.91	56.91
+ 0.0005	-39.123279	-39.122903	-39.122904	-39.144704	-39.144579	-39.144579	56.25	56.91	56.91
+ 0.0010	-39.123659	-39.122907	-39.122910	-39.144833	-39.144583	-39.144584	55.59	56.91	56.91
+ 0.0015	-39.124042	-39.122914	-39.122920	-39.144965	-39.144589	-39.144593	54.93	56.91	56.90
+ 0.0020	-39.124429	-39.122923	-39.122934	-39.145100	-39.144598	-39.144605	54.27	56.91	56.90
+ 0.0025	-39.124820	-39.122935	-39.122952	-39.145237	-39.144610	-39.144620	53.60	56.91	56.89
+ 0.0030	-39.125214	-39.122949	-39.122974	-39.145376	-39.144625	-39.144639	52.94	56.91	56.88

Table S154. Energy of A6 and ^{3}A6 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A6, X-EEF	Energy A6, Y-EEF	Energy A6, Z-EEF	Energy ^{3}A6, X-EEF	Energy ^{3}A6, Y-EEF	Energy ^{3}A6, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-501.246528	-501.249412	-501.250147	-501.259118	-501.259599	-501.260361	33.05	26.75	26.82
– 0.0025	-501.246848	-501.249275	-501.249785	-501.259046	-501.259479	-501.260008	32.02	26.79	26.84
– 0.0020	-501.247203	-501.249163	-501.249489	-501.259009	-501.259380	-501.259719	31.00	26.83	26.86
– 0.0015	-501.247592	-501.249076	-501.249259	-501.259006	-501.259304	-501.259494	29.97	26.85	26.87
– 0.0010	-501.248015	-501.249013	-501.249095	-501.259038	-501.259249	-501.259334	28.94	26.87	26.88
– 0.0005	-501.248472	-501.248976	-501.248996	-501.259104	-501.259216	-501.259238	27.92	26.89	26.89
+ 0.0000	-501.248964	-501.248964	-501.248964	-501.259206	-501.259206	-501.259206	26.89	26.89	26.89
+ 0.0005	-501.249489	-501.248976	-501.248996	-501.259341	-501.259216	-501.259238	25.87	26.89	26.89
+ 0.0010	-501.250050	-501.249013	-501.249095	-501.259512	-501.259249	-501.259334	24.84	26.87	26.88
+ 0.0015	-501.250644	-501.249076	-501.249259	-501.259717	-501.259304	-501.259494	23.82	26.85	26.87
+ 0.0020	-501.251273	-501.249163	-501.249489	-501.259956	-501.259380	-501.259719	22.80	26.83	26.86
+ 0.0025	-501.251936	-501.249275	-501.249785	-501.260230	-501.259479	-501.260008	21.78	26.79	26.84
+ 0.0030	-501.252633	-501.249412	-501.250147	-501.260539	-501.259599	-501.260361	20.76	26.75	26.82

Table S155. Energy of A7 and ^{3}A7 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A7, X-EEF	Energy A7, Y-EEF	Energy A7, Z-EEF	Energy ^{3}A7, X-EEF	Energy ^{3}A7, Y-EEF	Energy ^{3}A7, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-498.758577	-498.760447	-498.760330	-498.755339	-498.755954	-498.755276	-8.50	-11.80	-13.27
– 0.0025	-498.758861	-498.760422	-498.760316	-498.755417	-498.755931	-498.755357	-9.04	-11.79	-13.02
– 0.0020	-498.759151	-498.760402	-498.760310	-498.755500	-498.755912	-498.755445	-9.59	-11.79	-12.77
– 0.0015	-498.759446	-498.760386	-498.760312	-498.755588	-498.755898	-498.755542	-10.13	-11.78	-12.52
– 0.0010	-498.759747	-498.760375	-498.760322	-498.755680	-498.755887	-498.755647	-10.68	-11.78	-12.27
– 0.0005	-498.760054	-498.760368	-498.760340	-498.755777	-498.755881	-498.755759	-11.23	-11.78	-12.03
+ 0.0000	-498.760366	-498.760366	-498.760366	-498.755879	-498.755879	-498.755879	-11.78	-11.78	-11.78
+ 0.0005	-498.760684	-498.760368	-498.760400	-498.755985	-498.755881	-498.756007	-12.34	-11.78	-11.53
+ 0.0010	-498.761007	-498.760375	-498.760442	-498.756097	-498.755887	-498.756142	-12.89	-11.78	-11.29
+ 0.0015	-498.761336	-498.760386	-498.760493	-498.756212	-498.755898	-498.756286	-13.45	-11.78	-11.05
+ 0.0020	-498.761670	-498.760402	-498.760551	-498.756333	-498.755912	-498.756437	-14.01	-11.79	-10.80
+ 0.0025	-498.762011	-498.760422	-498.760617	-498.756458	-498.755931	-498.756595	-14.58	-11.79	-10.56
+ 0.0030	-498.762356	-498.760447	-498.760692	-498.756588	-498.755954	-498.756762	-15.14	-11.80	-10.32

Table S156. Energy of A8 and ^{3}A8 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A8, X-EEF	Energy A8, Y-EEF	Energy A8, Z-EEF	Energy ^{3}A8, X-EEF	Energy ^{3}A8, Y-EEF	Energy ^{3}A8, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-270.187722	-270.190979	-270.194457	-270.202620	-270.203178	-270.203640	39.12	32.03	24.11
– 0.0025	-270.188174	-270.190916	-270.193776	-270.202627	-270.203117	-270.203461	37.95	32.03	25.43
– 0.0020	-270.188649	-270.190865	-270.193122	-270.202656	-270.203067	-270.203310	36.77	32.04	26.75
– 0.0015	-270.189147	-270.190826	-270.192494	-270.202705	-270.203029	-270.203187	35.60	32.04	28.07
– 0.0010	-270.189667	-270.190797	-270.191894	-270.202775	-270.203001	-270.203090	34.42	32.04	29.39
– 0.0005	-270.190209	-270.190780	-270.191321	-270.202866	-270.202984	-270.203021	33.23	32.04	30.72
+ 0.0000	-270.190775	-270.190775	-270.190775	-270.202979	-270.202979	-270.202979	32.04	32.04	32.04
+ 0.0005	-270.191363	-270.190780	-270.190255	-270.203112	-270.202984	-270.202964	30.85	32.04	33.37
+ 0.0010	-270.191973	-270.190798	-270.189763	-270.203266	-270.203001	-270.202976	29.65	32.04	34.69
+ 0.0015	-270.192606	-270.190826	-270.189297	-270.203442	-270.203029	-270.203015	28.45	32.04	36.02
+ 0.0020	-270.193262	-270.190866	-270.188857	-270.203639	-270.203067	-270.203081	27.24	32.04	37.35
+ 0.0025	-270.193940	-270.190917	-270.188445	-270.203856	-270.203117	-270.203175	26.03	32.03	38.67
+ 0.0030	-270.194641	-270.190979	-270.188059	-270.204095	-270.203178	-270.203296	24.82	32.03	40.00

Table S157. Energy of A9 and ^{3}A9 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A9, X-EEF	Energy A9, Y-EEF	Energy A9, Z-EEF	Energy ^{3}A9, X-EEF	Energy ^{3}A9, Y-EEF	Energy ^{3}A9, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-500.045394	-500.049182	-500.049909	-500.060090	-500.060581	-500.061315	38.59	29.93	29.95
– 0.0025	-500.045875	-500.049080	-500.049584	-500.060027	-500.060482	-500.060992	37.15	29.94	29.95
– 0.0020	-500.046395	-500.048996	-500.049319	-500.059999	-500.060400	-500.060727	35.72	29.94	29.95
– 0.0015	-500.046951	-500.048931	-500.049113	-500.060009	-500.060337	-500.060521	34.28	29.95	29.95
– 0.0010	-500.047546	-500.048885	-500.048966	-500.060055	-500.060292	-500.060374	32.84	29.95	29.95
– 0.0005	-500.048178	-500.048857	-500.048877	-500.060137	-500.060265	-500.060286	31.40	29.95	29.95
+ 0.0000	-500.048848	-500.048848	-500.048848	-500.060256	-500.060256	-500.060256	29.95	29.95	29.95
+ 0.0005	-500.049555	-500.048857	-500.048877	-500.060412	-500.060265	-500.060286	28.50	29.95	29.95
+ 0.0010	-500.050300	-500.048885	-500.048966	-500.060604	-500.060292	-500.060374	27.05	29.95	29.95
+ 0.0015	-500.051083	-500.048931	-500.049113	-500.060833	-500.060337	-500.060521	25.60	29.95	29.95
+ 0.0020	-500.051904	-500.048996	-500.049319	-500.061098	-500.060400	-500.060727	24.14	29.94	29.95
+ 0.0025	-500.052762	-500.049080	-500.049584	-500.061400	-500.060482	-500.060992	22.68	29.94	29.95
+ 0.0030	-500.053658	-500.049182	-500.049909	-500.061739	-500.060581	-500.061315	21.22	29.93	29.95

Table S158. Energy of A10 and ^{3}A10 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A10, X-EEF	Energy A10, Y-EEF	Energy A10, Z-EEF	Energy ^{3}A10, X-EEF	Energy ^{3}A10, Y-EEF	Energy ^{3}A10, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-270.187722	-270.190979	-270.194457	-270.202620	-270.203178	-270.203640	39.12	32.03	24.11
– 0.0025	-270.188174	-270.190917	-270.193776	-270.202627	-270.203117	-270.203461	37.95	32.03	25.43
– 0.0020	-270.188649	-270.190866	-270.193122	-270.202656	-270.203067	-270.203310	36.77	32.04	26.75
– 0.0015	-270.189147	-270.190826	-270.192495	-270.202705	-270.203028	-270.203187	35.60	32.04	28.07
– 0.0010	-270.189667	-270.190797	-270.191894	-270.202775	-270.203001	-270.203090	34.42	32.04	29.39
– 0.0005	-270.190209	-270.190780	-270.191321	-270.202866	-270.202984	-270.203021	33.23	32.04	30.72
+ 0.0000	-270.190775	-270.190775	-270.190775	-270.202979	-270.202979	-270.202979	32.04	32.04	32.04
+ 0.0005	-270.191363	-270.190780	-270.190255	-270.203112	-270.202984	-270.202964	30.85	32.04	33.37
+ 0.0010	-270.191973	-270.190797	-270.189762	-270.203266	-270.203001	-270.202976	29.65	32.04	34.69
+ 0.0015	-270.192606	-270.190826	-270.189296	-270.203442	-270.203029	-270.203015	28.45	32.04	36.02
+ 0.0020	-270.193262	-270.190866	-270.188857	-270.203638	-270.203067	-270.203081	27.24	32.04	37.35
+ 0.0025	-270.193940	-270.190917	-270.188444	-270.203856	-270.203117	-270.203175	26.03	32.03	38.67
+ 0.0030	-270.194641	-270.190979	-270.188058	-270.204095	-270.203178	-270.203295	24.82	32.03	40.00

Table S159. Energy of A11 and ^{3}A11 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A11, X-EEF	Energy A11, Y-EEF	Energy A11, Z-EEF	Energy ^{3}A11, X-EEF	Energy ^{3}A11, Y-EEF	Energy ^{3}A11, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-345.428062	-345.430325	-345.435448	-345.436692	-345.435864	-345.437259	22.66	14.54	4.76
– 0.0025	-345.428345	-345.430260	-345.434479	-345.436465	-345.435801	-345.436914	21.32	14.55	6.39
– 0.0020	-345.428650	-345.430206	-345.433542	-345.436260	-345.435749	-345.436601	19.98	14.55	8.03
– 0.0015	-345.428980	-345.430164	-345.432637	-345.436076	-345.435709	-345.436318	18.63	14.56	9.67
– 0.0010	-345.429333	-345.430134	-345.431763	-345.435915	-345.435680	-345.436067	17.28	14.56	11.30
– 0.0005	-345.429709	-345.430116	-345.430921	-345.435775	-345.435663	-345.435846	15.93	14.56	12.93
+ 0.0000	-345.430109	-345.430109	-345.430109	-345.435657	-345.435657	-345.435657	14.56	14.56	14.56
+ 0.0005	-345.430533	-345.430115	-345.429329	-345.435561	-345.435663	-345.435498	13.20	14.57	16.20
+ 0.0010	-345.430981	-345.430132	-345.428580	-345.435486	-345.435680	-345.435370	11.83	14.57	17.83
+ 0.0015	-345.431452	-345.430161	-345.427862	-345.435433	-345.435709	-345.435272	10.45	14.57	19.46
+ 0.0020	-345.431946	-345.430202	-345.427175	-345.435402	-345.435750	-345.435206	9.07	14.56	21.08
+ 0.0025	-345.432465	-345.430255	-345.426519	-345.435393	-345.435802	-345.435169	7.69	14.56	22.71
+ 0.0030	-345.433007	-345.430320	-345.425893	-345.435406	-345.435866	-345.435163	6.30	14.56	24.34

Table S160. Energy of A12 and ^{3}A12 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A12, X-EEF	Energy A12, Y-EEF	Energy A12, Z-EEF	Energy ^{3}A12, X-EEF	Energy ^{3}A12, Y-EEF	Energy ^{3}A12, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-325.557123	-325.562247	-325.569432	-325.563014	-325.565368	-325.566888	15.47	8.19	-6.68
– 0.0025	-325.557879	-325.562182	-325.568112	-325.563129	-325.565117	-325.566328	13.78	7.71	-4.68
– 0.0020	-325.558661	-325.562129	-325.566828	-325.563267	-325.564879	-325.565803	12.09	7.22	-2.69
– 0.0015	-325.559469	-325.562090	-325.565579	-325.563428	-325.564654	-325.565313	10.40	6.73	-0.70
– 0.0010	-325.560302	-325.562062	-325.564366	-325.563613	-325.564440	-325.564857	8.69	6.24	1.29
– 0.0005	-325.561161	-325.562047	-325.563188	-325.563820	-325.564239	-325.564437	6.98	5.76	3.28
+ 0.0000	-325.562045	-325.562045	-325.562045	-325.564051	-325.564051	-325.564051	5.27	5.27	5.27
+ 0.0005	-325.562955	-325.562055	-325.560938	-325.564305	-325.563875	-325.563699	3.54	4.78	7.25
+ 0.0010	-325.563891	-325.562078	-325.559865	-325.564582	-325.563711	-325.563382	1.81	4.29	9.23
+ 0.0015	-325.564853	-325.562113	-325.558827	-325.564882	-325.563560	-325.563099	0.08	3.80	11.22
+ 0.0020	-325.565840	-325.562161	-325.557824	-325.565205	-325.563421	-325.562851	-1.67	3.31	13.20
+ 0.0025	-325.566853	-325.562222	-325.556856	-325.565552	-325.563294	-325.562636	-3.42	2.82	15.18
+ 0.0030	-325.567892	-325.562295	-325.555922	-325.565922	-325.563180	-325.562455	-5.17	2.33	17.15

Table S161. Energy of A13 and ^{3}A13 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A13, X-EEF	Energy A13, Y-EEF	Energy A13, Z-EEF	Energy ^{3}A13, X-EEF	Energy ^{3}A13, Y-EEF	Energy ^{3}A13, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-668.380894	-668.383377	-668.387706	-668.391409	-668.392626	-668.392331	27.61	24.28	12.14
– 0.0025	-668.381197	-668.383300	-668.386841	-668.391504	-668.392547	-668.392236	27.06	24.28	14.16
– 0.0020	-668.381527	-668.383238	-668.386017	-668.391624	-668.392482	-668.392180	26.51	24.27	16.18
– 0.0015	-668.381885	-668.383189	-668.385234	-668.391770	-668.392431	-668.392165	25.95	24.26	18.20
– 0.0010	-668.382271	-668.383154	-668.384491	-668.391940	-668.392393	-668.392189	25.39	24.26	20.21
– 0.0005	-668.382685	-668.383133	-668.383789	-668.392136	-668.392368	-668.392253	24.82	24.25	22.22
+ 0.0000	-668.383126	-668.383126	-668.383126	-668.392358	-668.392358	-668.392358	24.24	24.24	24.24
+ 0.0005	-668.383595	-668.383133	-668.382504	-668.392604	-668.392360	-668.392501	23.65	24.23	26.25
+ 0.0010	-668.384093	-668.383154	-668.381921	-668.392875	-668.392377	-668.392684	23.06	24.22	28.26
+ 0.0015	-668.384618	-668.383188	-668.381378	-668.393172	-668.392407	-668.392906	22.46	24.20	30.27
+ 0.0020	-668.385171	-668.383237	-668.380874	-668.393494	-668.392451	-668.393168	21.85	24.19	32.28
+ 0.0025	-668.385752	-668.383299	-668.380410	-668.393841	-668.392508	-668.393469	21.24	24.18	34.29
+ 0.0030	-668.386361	-668.383375	-668.379985	-668.394214	-668.392579	-668.393808	20.62	24.16	36.29

Table S162. Energy of A14 and ^{3}A14 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A14, X-EEF	Energy A14, Y-EEF	Energy A14, Z-EEF	Energy ^{3}A14, X-EEF	Energy ^{3}A14, Y-EEF	Energy ^{3}A14, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-474.700432	-474.701017	-474.699637	-474.722205	-474.720601	-474.715286	57.16	51.42	41.09
– 0.0025	-474.700424	-474.700948	-474.699745	-474.721837	-474.720534	-474.716043	56.22	51.42	42.79
– 0.0020	-474.700442	-474.700891	-474.699886	-474.721495	-474.720479	-474.716837	55.27	51.43	44.50
– 0.0015	-474.700488	-474.700846	-474.700062	-474.721178	-474.720436	-474.717668	54.32	51.43	46.23
– 0.0010	-474.700561	-474.700814	-474.700271	-474.720887	-474.720406	-474.718536	53.37	51.44	47.95
– 0.0005	-474.700661	-474.700795	-474.700513	-474.720621	-474.720387	-474.719440	52.40	51.44	49.69
+ 0.0000	-474.700789	-474.700789	-474.700789	-474.720381	-474.720381	-474.720381	51.44	51.44	51.44
+ 0.0005	-474.700944	-474.700795	-474.701098	-474.720167	-474.720387	-474.721360	50.47	51.44	53.20
+ 0.0010	-474.701126	-474.700814	-474.701441	-474.719979	-474.720406	-474.722375	49.50	51.44	54.96
+ 0.0015	-474.701336	-474.700846	-474.701817	-474.719816	-474.720437	-474.723428	48.52	51.44	56.74
+ 0.0020	-474.701573	-474.700890	-474.702226	-474.719678	-474.720480	-474.724518	47.54	51.43	58.53
+ 0.0025	-474.701837	-474.700947	-474.702669	-474.719567	-474.720535	-474.725646	46.55	51.43	60.33
+ 0.0030	-474.702129	-474.701016	-474.703144	-474.719481	-474.720602	-474.726812	45.56	51.42	62.14

Table S163. Energy of A15 and ^{3}A15 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A15, X-EEF	Energy A15, Y-EEF	Energy A15, Z-EEF	Energy ^{3}A15, X-EEF	Energy ^{3}A15, Y-EEF	Energy ^{3}A15, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-384.721365	-384.724044	-384.730060	-384.729897	-384.729469	-384.731478	22.40	14.24	3.72
– 0.0025	-384.721704	-384.723965	-384.728920	-384.729723	-384.729390	-384.731007	21.05	14.25	5.48
– 0.0020	-384.722069	-384.723900	-384.727817	-384.729574	-384.729327	-384.730574	19.70	14.25	7.24
– 0.0015	-384.722459	-384.723849	-384.726752	-384.729448	-384.729277	-384.730178	18.35	14.25	8.99
– 0.0010	-384.722875	-384.723813	-384.725725	-384.729346	-384.729241	-384.729819	16.99	14.25	10.75
– 0.0005	-384.723317	-384.723792	-384.724736	-384.729267	-384.729220	-384.729497	15.62	14.25	12.50
+ 0.0000	-384.723784	-384.723784	-384.723784	-384.729213	-384.729213	-384.729213	14.25	14.25	14.25
+ 0.0005	-384.724277	-384.723791	-384.722870	-384.729181	-384.729219	-384.728965	12.88	14.25	16.00
+ 0.0010	-384.724796	-384.723813	-384.721994	-384.729174	-384.729241	-384.728754	11.50	14.25	17.75
+ 0.0015	-384.725340	-384.723849	-384.721155	-384.729190	-384.729276	-384.728580	10.11	14.25	19.49
+ 0.0020	-384.725909	-384.723899	-384.720353	-384.729230	-384.729325	-384.728442	8.72	14.25	21.24
+ 0.0025	-384.726505	-384.723964	-384.719588	-384.729294	-384.729389	-384.728341	7.32	14.24	22.98
+ 0.0030	-384.727126	-384.724043	-384.718860	-384.729381	-384.729467	-384.728277	5.92	14.24	24.72

Table S164. Energy of A16 and ^{3}A16 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A16, X-EEF	Energy A16, Y-EEF	Energy A16, Z-EEF	Energy ^{3}A16, X-EEF	Energy ^{3}A16, Y-EEF	Energy ^{3}A16, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-345.421649	-345.423545	-345.426177	-345.436561	-345.435987	-345.435403	39.15	32.66	24.22
– 0.0025	-345.421869	-345.423480	-345.425630	-345.436373	-345.435922	-345.435393	38.08	32.67	25.63
– 0.0020	-345.422113	-345.423427	-345.425113	-345.436208	-345.435870	-345.435412	37.01	32.67	27.04
– 0.0015	-345.422381	-345.423385	-345.424624	-345.436066	-345.435829	-345.435459	35.93	32.67	28.45
– 0.0010	-345.422674	-345.423356	-345.424165	-345.435946	-345.435800	-345.435536	34.85	32.67	29.86
– 0.0005	-345.422990	-345.423338	-345.423734	-345.435849	-345.435782	-345.435641	33.76	32.67	31.26
+ 0.0000	-345.423332	-345.423332	-345.423332	-345.435776	-345.435776	-345.435776	32.67	32.67	32.67
+ 0.0005	-345.423697	-345.423338	-345.422958	-345.435724	-345.435781	-345.435938	31.58	32.67	34.08
+ 0.0010	-345.424087	-345.423355	-345.422614	-345.435696	-345.435798	-345.436130	30.48	32.67	35.49
+ 0.0015	-345.424501	-345.423385	-345.422297	-345.435690	-345.435826	-345.436351	29.38	32.67	36.90
+ 0.0020	-345.424940	-345.423426	-345.422010	-345.435708	-345.435866	-345.436600	28.27	32.66	38.31
+ 0.0025	-345.425403	-345.423479	-345.421751	-345.435748	-345.435918	-345.436878	27.16	32.66	39.72
+ 0.0030	-345.425890	-345.423544	-345.421520	-345.435811	-345.435981	-345.437184	26.05	32.65	41.13

Table S165. Energy of A17 and ^{3}A17 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A17, X-EEF	Energy A17, Y-EEF	Energy A17, Z-EEF	Energy ^{3}A17, X-EEF	Energy ^{3}A17, Y-EEF	Energy ^{3}A17, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-325.548912	-325.550129	-325.556096	-325.563779	-325.562307	-325.565085	39.04	31.97	23.60
– 0.0025	-325.549198	-325.550245	-325.555170	-325.563628	-325.562429	-325.564697	37.88	31.99	25.02
– 0.0020	-325.549510	-325.550373	-325.554275	-325.563500	-325.562565	-325.564341	36.73	32.01	26.43
– 0.0015	-325.549848	-325.550514	-325.553412	-325.563397	-325.562712	-325.564017	35.57	32.03	27.84
– 0.0010	-325.550211	-325.550667	-325.552581	-325.563317	-325.562872	-325.563723	34.41	32.04	29.25
– 0.0005	-325.550599	-325.550833	-325.551781	-325.563261	-325.563045	-325.563461	33.25	32.06	30.67
+ 0.0000	-325.551012	-325.551012	-325.551012	-325.563230	-325.563230	-325.563230	32.08	32.08	32.08
+ 0.0005	-325.551451	-325.551204	-325.550275	-325.563222	-325.563427	-325.563030	30.90	32.09	33.49
+ 0.0010	-325.551915	-325.551408	-325.549569	-325.563239	-325.563637	-325.562861	29.73	32.11	34.90
+ 0.0015	-325.552405	-325.551625	-325.548894	-325.563279	-325.563859	-325.562723	28.55	32.12	36.31
+ 0.0020	-325.552920	-325.551854	-325.548250	-325.563343	-325.564093	-325.562616	27.37	32.13	37.72
+ 0.0025	-325.553460	-325.552096	-325.547637	-325.563432	-325.564340	-325.562540	26.18	32.15	39.13
+ 0.0030	-325.554026	-325.552351	-325.547055	-325.563544	-325.564599	-325.562496	24.99	32.16	40.54

Table S166. Energy of A18 and ^{3}A18 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A18, X-EEF	Energy A18, Y-EEF	Energy A18, Z-EEF	Energy ^{3}A18, X-EEF	Energy ^{3}A18, Y-EEF	Energy ^{3}A18, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-668.375988	-668.378638	-668.381059	-668.389741	-668.391611	-668.391899	36.11	34.06	28.46
– 0.0025	-668.376328	-668.378570	-668.380533	-668.389934	-668.391524	-668.391710	35.72	34.01	29.35
– 0.0020	-668.376696	-668.378517	-668.380043	-668.390154	-668.391452	-668.391557	35.33	33.96	30.23
– 0.0015	-668.377091	-668.378477	-668.379589	-668.390400	-668.391393	-668.391439	34.94	33.91	31.11
– 0.0010	-668.377513	-668.378451	-668.379171	-668.390673	-668.391347	-668.391357	34.55	33.86	31.99
– 0.0005	-668.377963	-668.378439	-668.378788	-668.390972	-668.391315	-668.391309	34.15	33.81	32.87
+ 0.0000	-668.378441	-668.378441	-668.378441	-668.391297	-668.391297	-668.391297	33.75	33.75	33.75
+ 0.0005	-668.378946	-668.378457	-668.378129	-668.391649	-668.391293	-668.391320	33.35	33.70	34.63
+ 0.0010	-668.379479	-668.378486	-668.377852	-668.392028	-668.391302	-668.391379	32.95	33.65	35.51
+ 0.0015	-668.380039	-668.378530	-668.377611	-668.392433	-668.391324	-668.391472	32.54	33.59	36.39
+ 0.0020	-668.380627	-668.378587	-668.377405	-668.392864	-668.391361	-668.391601	32.13	33.54	37.27
+ 0.0025	-668.381242	-668.378659	-668.377234	-668.393322	-668.391411	-668.391764	31.72	33.48	38.15
+ 0.0030	-668.381885	-668.378744	-668.377098	-668.393806	-668.391474	-668.391963	31.30	33.42	39.03

Table S167. Energy of A19 and ^{3}A19 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A19, X-EEF	Energy A19, Y-EEF	Energy A19, Z-EEF	Energy ^{3}A19, X-EEF	Energy ^{3}A19, Y-EEF	Energy ^{3}A19, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-474.696778	-474.702498	-474.701204	-474.714438	-474.718299	-474.714406	46.37	41.49	34.66
– 0.0025	-474.697626	-474.702429	-474.701299	-474.714979	-474.718232	-474.714935	45.56	41.49	35.80
– 0.0020	-474.698501	-474.702372	-474.701427	-474.715547	-474.718177	-474.715498	44.75	41.50	36.94
– 0.0015	-474.699403	-474.702328	-474.701588	-474.716141	-474.718134	-474.716093	43.95	41.50	38.08
– 0.0010	-474.700332	-474.702296	-474.701782	-474.716761	-474.718104	-474.716722	43.13	41.50	39.22
– 0.0005	-474.701288	-474.702277	-474.702010	-474.717407	-474.718085	-474.717384	42.32	41.50	40.37
+ 0.0000	-474.702271	-474.702271	-474.702271	-474.718079	-474.718079	-474.718079	41.51	41.51	41.51
+ 0.0005	-474.703280	-474.702277	-474.702565	-474.718777	-474.718086	-474.718808	40.69	41.51	42.65
+ 0.0010	-474.704317	-474.702296	-474.702892	-474.719502	-474.718104	-474.719569	39.87	41.51	43.79
+ 0.0015	-474.705380	-474.702327	-474.703252	-474.720252	-474.718135	-474.720364	39.05	41.50	44.93
+ 0.0020	-474.706470	-474.702371	-474.703645	-474.721028	-474.718178	-474.721191	38.22	41.50	46.07
+ 0.0025	-474.707587	-474.702428	-474.704072	-474.721831	-474.718234	-474.722052	37.40	41.50	47.21
+ 0.0030	-474.708730	-474.702497	-474.704531	-474.722659	-474.718301	-474.722946	36.57	41.49	48.35

Table S168. Energy of A20 and ^{3}A20 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A20, X-EEF	Energy A20, Y-EEF	Energy A20, Z-EEF	Energy ^{3}A20, X-EEF	Energy ^{3}A20, Y-EEF	Energy ^{3}A20, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-384.715863	-384.717516	-384.720816	-384.730450	-384.729581	-384.729616	38.30	31.68	23.10
– 0.0025	-384.716025	-384.717436	-384.720141	-384.730196	-384.729504	-384.729489	37.21	31.68	24.54
– 0.0020	-384.716215	-384.717371	-384.719499	-384.729969	-384.729440	-384.729393	36.11	31.69	25.98
– 0.0015	-384.716432	-384.717320	-384.718889	-384.729769	-384.729391	-384.729329	35.01	31.69	27.41
– 0.0010	-384.716678	-384.717283	-384.718311	-384.729595	-384.729357	-384.729297	33.91	31.70	28.84
– 0.0005	-384.716951	-384.717261	-384.717766	-384.729449	-384.729336	-384.729298	32.81	31.70	30.28
+ 0.0000	-384.717253	-384.717253	-384.717253	-384.729330	-384.729330	-384.729330	31.71	31.71	31.71
+ 0.0005	-384.717583	-384.717260	-384.716772	-384.729237	-384.729337	-384.729393	30.60	31.71	33.14
+ 0.0010	-384.717940	-384.717281	-384.716324	-384.729172	-384.729359	-384.729489	29.49	31.71	34.57
+ 0.0015	-384.718326	-384.717316	-384.715907	-384.729133	-384.729395	-384.729616	28.37	31.71	35.99
+ 0.0020	-384.718740	-384.717366	-384.715523	-384.729122	-384.729445	-384.729776	27.26	31.72	37.42
+ 0.0025	-384.719182	-384.717430	-384.715170	-384.729137	-384.729510	-384.729966	26.14	31.72	38.85
+ 0.0030	-384.719651	-384.717508	-384.714850	-384.729179	-384.729588	-384.730189	25.02	31.72	40.27

Table S169. Energy of A21 and ^{3}A21 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A21, X-EEF	Energy A21, Y-EEF	Energy A21, Z-EEF	Energy ^{3}A21, X-EEF	Energy ^{3}A21, Y-EEF	Energy ^{3}A21, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-721.819741	-721.821838	-721.813228	-721.824420	-721.823633	-721.818560	12.28	4.71	14.00
– 0.0025	-721.819971	-721.821744	-721.814502	-721.824173	-721.823541	-721.819248	11.03	4.72	12.46
– 0.0020	-721.820228	-721.821668	-721.815820	-721.823952	-721.823465	-721.819979	9.78	4.72	10.92
– 0.0015	-721.820512	-721.821608	-721.817181	-721.823757	-721.823406	-721.820753	8.52	4.72	9.38
– 0.0010	-721.820825	-721.821566	-721.818587	-721.823588	-721.823364	-721.821569	7.26	4.72	7.83
– 0.0005	-721.821164	-721.821540	-721.820037	-721.823446	-721.823339	-721.822428	5.99	4.72	6.28
+ 0.0000	-721.821532	-721.821532	-721.821532	-721.823330	-721.823330	-721.823330	4.72	4.72	4.72
+ 0.0005	-721.821926	-721.821540	-721.823070	-721.823240	-721.823339	-721.824275	3.45	4.72	3.16
+ 0.0010	-721.822349	-721.821566	-721.824654	-721.823177	-721.823364	-721.825264	2.17	4.72	1.60
+ 0.0015	-721.822799	-721.821608	-721.826281	-721.823140	-721.823406	-721.826296	0.90	4.72	0.04
+ 0.0020	-721.823276	-721.821668	-721.827954	-721.823129	-721.823465	-721.827371	-0.39	4.72	-1.53
+ 0.0025	-721.823781	-721.821744	-721.829671	-721.823145	-721.823541	-721.828490	-1.67	4.72	-3.10
+ 0.0030	-721.824314	-721.821838	-721.831434	-721.823186	-721.823633	-721.829653	-2.96	4.71	-4.67

Table S170. Energy of A22 and ^{3}A22 Under EEFs in Gas. Energy given in Hartree, changes in energy given in kJ/mol.

Field	Energy A22, X-EEF	Energy A22, Y-EEF	Energy A22, Z-EEF	Energy ^{3}A22, X-EEF	Energy ^{3}A22, Y-EEF	Energy ^{3}A22, Z-EEF	ΔE_{ST}, X-EEF	ΔE_{ST}, Y-EEF	ΔE_{ST}, Z-EEF
– 0.0030	-721.807502	-721.810669	-721.803586	-721.820654	-721.821491	-721.816889	34.53	28.41	34.93
– 0.0025	-721.807909	-721.810575	-721.804614	-721.820676	-721.821399	-721.817505	33.52	28.42	33.85
– 0.0020	-721.808344	-721.810498	-721.805683	-721.820725	-721.821323	-721.818162	32.51	28.42	32.76
– 0.0015	-721.808807	-721.810439	-721.806792	-721.820800	-721.821264	-721.818859	31.49	28.42	31.68
– 0.0010	-721.809297	-721.810396	-721.807941	-721.820903	-721.821222	-721.819595	30.47	28.42	30.60
– 0.0005	-721.809816	-721.810370	-721.809131	-721.821032	-721.821197	-721.820372	29.45	28.42	29.51
+ 0.0000	-721.810362	-721.810362	-721.810362	-721.821188	-721.821188	-721.821188	28.43	28.43	28.43
+ 0.0005	-721.810936	-721.810370	-721.811633	-721.821371	-721.821197	-721.822045	27.40	28.42	27.34
+ 0.0010	-721.811538	-721.810396	-721.812945	-721.821581	-721.821222	-721.822942	26.37	28.42	26.25
+ 0.0015	-721.812167	-721.810439	-721.814298	-721.821817	-721.821264	-721.823879	25.34	28.42	25.15
+ 0.0020	-721.812825	-721.810498	-721.815691	-721.822081	-721.821323	-721.824856	24.30	28.42	24.06
+ 0.0025	-721.813510	-721.810575	-721.817126	-721.822371	-721.821399	-721.825874	23.26	28.42	22.97
+ 0.0030	-721.814223	-721.810669	-721.818601	-721.822688	-721.821491	-721.826931	22.22	28.41	21.87

S9. Natural Resonance Theory Calculation Results

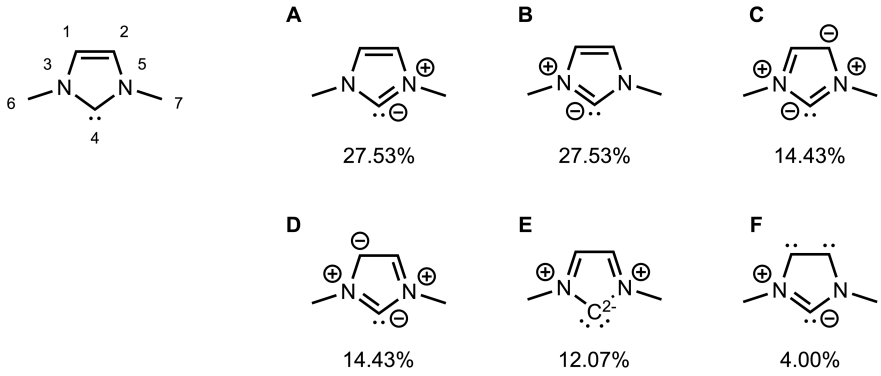


Figure S139. The NRT results for $\mathbf{I_{1a}}$, demonstrating that in the Natural Bonding Orbital basis, the carbenic structure is ylidic, and not formally carbenic, in the gas phase.

S10. Gibbs Free Energies and Components, Frontier Orbital Energies, Nucleophilicity and Electrophilicity Parameters of Unsubstituted NHCs in Test Set Across Different Solvents

Table S171. Reference Species. Entropy given in J/mol.K and frontier orbital energy given in eV. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	E(HOMO)
TCE, Gas	-447.521116	0.047645	0.010036	394.029200	0.044746	-447.463434	-447.508180	-10.923
TCE, TOL[a]	-447.524835	0.047476	0.010157	396.712900	0.045050	-447.467202	-447.509233	-10.640
TCE, DCM[a]	-447.532845	0.047581	0.010133	396.356700	0.045010	-447.475130	-447.517121	-10.407
TCE, MeCN[a]	-447.534565	0.047652	0.010109	395.968900	0.044966	-447.476803	-447.518750	-10.321
TCE, Water[a]	-447.527489	0.047403	0.010098	395.664100	0.044931	-447.469988	-447.511900	-10.294

[a] The Gibbs free energies for these species are phase-corrected via the Direct method to account for solvation

Table S172. Unsubstituted NHCs in Test Set in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G
I_{1a}	-304.777248	0.127783	0.007878	341.729700	0.038807	-304.641587	-304.680394
$^3I_{1a}$	-304.640405	0.125222	0.008220	354.795100	0.040290	-304.506962	-304.547253
II_{1a}	-383.326623	0.182763	0.011173	404.772100	0.045966	-383.132687	-383.178652
$^3II_{1a}$	-383.258939	0.180579	0.011164	405.032300	0.045995	-383.067197	-383.113192
III_{1a}	-344.060072	0.155410	0.009548	374.889500	0.042572	-343.895114	-343.937686
$^3III_{1a}$	-343.957724	0.152556	0.009969	389.966400	0.044284	-343.795199	-343.839483
IV_{1a}	-285.327785	0.086895	0.006065	303.317400	0.034444	-285.234825	-285.269270
$^3IV_{1a}$	-285.201048	0.084569	0.006585	322.646500	0.036639	-285.109894	-285.146534
V_{1a}	-608.304080	0.083758	0.006444	314.938500	0.035764	-608.213878	-608.249642
$^3V_{1a}$	-608.196307	0.081862	0.007069	336.380300	0.038199	-608.107376	-608.145575
VI_{1a}	-305.973317	0.150582	0.008534	347.482700	0.039460	-305.814201	-305.853661
$^3VI_{1a}$	-305.859700	0.149471	0.008326	356.266200	0.040457	-305.701903	-305.742360
VII_{1a}	-345.281574	0.180342	0.009263	367.321600	0.041713	-345.091970	-345.133682
$^3VII_{1a}$	-345.184027	0.179025	0.009146	372.390100	0.042288	-344.995856	-345.038145
$VIII_{1a}$	-327.997986	0.165895	0.009336	365.808900	0.041541	-327.822755	-327.864296
$^3VIII_{1a}$	-327.923282	0.164367	0.009707	382.781000	0.043468	-327.749208	-327.792676
IX_{1a}	-320.817894	0.116342	0.007686	338.829800	0.038477	-320.693866	-320.732343
$^3IX_{1a}$	-320.678717	0.113727	0.008069	353.652400	0.040160	-320.556921	-320.597081

Table S173. Orbital Energies and Philicity Parameters of Unsubstituted NHCs in Test Set. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	CHI	ETA	GEI	N
$\mathbf{I_{1a}}$	-7.440410	-0.163813	3.802111	7.276598	0.993325	3.483058
$\mathbf{^3I_{1a}}$	-4.319808	-2.359500	3.339654	1.960309	2.844779	6.603660
$\mathbf{II_{1a}}$	-5.875211	-0.542867	3.209039	5.332344	0.965610	5.048257
$\mathbf{^3II_{1a}}$	-4.239807	-1.787516	3.013661	2.452290	1.851770	6.683662
$\mathbf{III_{1a}}$	-6.449372	-0.398919	3.424145	6.050453	0.968917	4.474097
$\mathbf{^3III_{1a}}$	-4.328788	-1.837585	3.083187	2.491203	1.907922	6.594680
$\mathbf{IV_{1a}}$	-8.069266	-0.279733	4.174499	7.789533	1.118581	2.854203
$\mathbf{^3IV_{1a}}$	-5.130163	-2.695832	3.912998	2.434331	3.144920	5.793305
$\mathbf{V_{1a}}$	-7.775383	-0.267488	4.021435	7.507895	1.076996	3.148086
$\mathbf{^3V_{1a}}$	-4.708115	-2.400045	3.554080	2.308070	2.736373	6.215354
$\mathbf{VI_{1a}}$	-7.227889	-0.239188	3.733539	6.988701	0.997275	3.695579
$\mathbf{^3VI_{1a}}$	-4.593555	-2.236776	3.415166	2.356778	2.474428	6.329914
$\mathbf{VII_{1a}}$	-6.725295	-0.252522	3.488908	6.472773	0.940283	4.198173
$\mathbf{^3VII_{1a}}$	-4.722537	-1.980173	3.351355	2.742364	2.047792	6.200932
$\mathbf{VIII_{1a}}$	-7.108976	-0.215786	3.662381	6.893189	0.972919	3.814493
$\mathbf{^3VIII_{1a}}$	-5.098870	-2.126842	3.612856	2.972028	2.195930	5.824598
$\mathbf{IX_{1a}}$	-7.873616	-0.198099	4.035857	7.675517	1.061045	3.049853
$\mathbf{^3IX_{1a}}$	-4.604167	-2.714064	3.659116	1.890103	3.541904	6.319301

Table S174. Unsubstituted Singlet NHCs in Test Set in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
I_{1a}	-304.793823	0.128038	0.007860	341.802100	0.038815	-304.657926	-304.696740	-304.693721
II_{1a}	-383.347085	0.183061	0.011151	404.834200	0.045973	-383.152873	-383.198846	-383.195827
III_{1a}	-344.080315	0.155669	0.009533	374.765700	0.042558	-343.915113	-343.957671	-343.954652
IV_{1a}	-285.336113	0.087198	0.006032	302.652600	0.034369	-285.242883	-285.277252	-285.274233
V_{1a}	-608.312739	0.083961	0.006411	314.263300	0.035688	-608.222368	-608.258055	-608.255036
VI_{1a}	-305.989059	0.150721	0.008553	348.356600	0.039559	-305.829785	-305.869344	-305.866325
VII_{1a}	-345.297371	0.180456	0.009275	367.959200	0.041785	-345.107640	-345.149426	-345.146407
$VIII_{1a}$	-328.009647	0.166108	0.009289	364.973000	0.041446	-327.834251	-327.875697	-327.872678
IX_{1a}	-320.836154	0.116398	0.007655	338.072700	0.038391	-320.712101	-320.750492	-320.747473

Table S175. Unsubstituted Singlet NHCs in Test Set in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{1a}	-304.798765	0.127896	0.007882	342.638700	0.038910	-304.662986	-304.701896	-304.698877
II_{1a}	-383.361529	0.183093	0.011180	406.047500	0.046110	-383.167256	-383.213367	-383.210348
III_{1a}	-344.090936	0.155777	0.009508	374.425800	0.042520	-343.925651	-343.968171	-343.965152
IV_{1a}	-285.341627	0.087106	0.006036	302.833500	0.034390	-285.248485	-285.282875	-285.279856
V_{1a}	-608.318001	0.083973	0.006407	314.216200	0.035682	-608.227621	-608.263303	-608.260284
VI_{1a}	-305.993524	0.150640	0.008557	348.208400	0.039542	-305.834328	-305.873870	-305.870851
VII_{1a}	-345.302062	0.180246	0.009329	369.384100	0.041947	-345.112487	-345.154434	-345.151415
$VIII_{1a}$	-328.015110	0.165955	0.009277	364.766900	0.041423	-327.839879	-327.881301	-327.878282
IX_{1a}	-320.840927	0.116365	0.007655	338.118000	0.038396	-320.716907	-320.755303	-320.752284

Table S176. Unsubstituted Singlet NHCs in Test Set in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{1a}	-304.799213	0.127870	0.007882	342.646800	0.038911	-304.663460	-304.702371	-304.699352
II_{1a}	-383.364921	0.183393	0.011049	402.965300	0.045760	-383.170478	-383.216238	-383.213219
III_{1a}	-344.093313	0.155827	0.009482	373.836200	0.042453	-343.928003	-343.970456	-343.967437
IV_{1a}	-285.342796	0.087088	0.006042	303.079900	0.034418	-285.249665	-285.284083	-285.281064
V_{1a}	-608.318523	0.083963	0.006419	314.654100	0.035732	-608.228140	-608.263872	-608.260853
VI_{1a}	-305.993746	0.150606	0.008568	348.513400	0.039577	-305.834573	-305.874150	-305.871131
VII_{1a}	-345.302245	0.180197	0.009333	369.499200	0.041960	-345.112715	-345.154675	-345.151656
$VIII_{1a}$	-328.015226	0.165926	0.009267	364.550600	0.041398	-327.840033	-327.881431	-327.878412
IX_{1a}	-320.841486	0.116359	0.007655	338.138400	0.038399	-320.717473	-320.755871	-320.752852

Table S177. Unsubstituted Singlet NHCs in Test Set in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
I_{1a}	-304.784323	0.127864	0.007929	343.570000	0.039016	-304.648529	-304.687545	-304.684526
II_{1a}	-383.357607	0.183628	0.011042	402.870800	0.045750	-383.162938	-383.208687	-383.205668
III_{1a}	-344.081096	0.155912	0.009518	374.538300	0.042532	-343.915666	-343.958198	-343.955179
IV_{1a}	-285.335190	0.086797	0.006085	303.823400	0.034502	-285.242308	-285.276810	-285.273791
V_{1a}	-608.310676	0.084011	0.006434	314.931400	0.035763	-608.220231	-608.255994	-608.252975
VI_{1a}	-305.981202	0.150817	0.008514	346.637000	0.039364	-305.821871	-305.861235	-305.858216
VII_{1a}	-345.289543	0.180299	0.009414	371.435300	0.042180	-345.099830	-345.142010	-345.138991
$VIII_{1a}$	-328.005237	0.165998	0.009283	364.821500	0.041429	-327.829955	-327.871384	-327.868365
IX_{1a}	-320.827393	0.116449	0.007691	338.840400	0.038478	-320.703253	-320.741731	-320.738712

Table S178. Orbital Energies and Philicity Parameters of Unsubstituted Singlet NHCs in Test Set in SMD Toluene. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	CHI	ETA	GEI	N
I_{1a}	-7.652931	-0.043810	3.848371	7.609121	0.973171	3.270537
II_{1a}	-6.283382	-0.269665	3.276523	6.013717	0.892593	4.640086
III_{1a}	-6.795500	-0.174425	3.484963	6.621075	0.917144	4.127968
IV_{1a}	-8.223010	-0.090342	4.156676	8.132668	1.062256	2.700458
V_{1a}	-7.899739	-0.094151	3.996945	7.805587	1.023342	3.023730
VI_{1a}	-7.283673	-0.093063	3.688368	7.190610	0.945960	3.639796
VII_{1a}	-6.889924	-0.101498	3.495711	6.788425	0.900061	4.033544
$VIII_{1a}$	-7.258638	-0.072110	3.665374	7.186528	0.934733	3.664830
IX_{1a}	-8.045320	-0.048981	4.047150	7.996339	1.024183	2.878149

Table S179. Orbital Energies and Philicity Parameters of Unsubstituted Singlet NHCs in Test Set in SMD DCM. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	CHI	ETA	GEI	N
I_{1a}	-7.814023	0.021769	3.896127	7.835792	0.968620	3.109446
II_{1a}	-6.770738	-0.087076	3.428907	6.683662	0.879563	4.152730
III_{1a}	-7.200134	-0.033198	3.616666	7.166936	0.912543	3.723334
IV_{1a}	-8.413762	0.026395	4.193683	8.440157	1.041863	2.509706
V_{1a}	-8.076885	0.008436	4.034225	8.085320	1.006452	2.846584
VI_{1a}	-7.298095	-0.007075	3.652585	7.291020	0.914918	3.625373
VII_{1a}	-7.130201	-0.015783	3.572992	7.114418	0.897211	3.793268
$VIII_{1a}$	-7.464901	0.003265	3.730818	7.468166	0.931889	3.458568
IX_{1a}	-8.247772	0.021497	4.113138	8.269269	1.022938	2.675696

Table S180. Orbital Energies and Philicity Parameters of Unsubstituted Singlet NHCs in Test Set in SMD MeCN. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	CHI	ETA	GEI	N
I_{1a}	-7.837969	0.037007	3.900481	7.874976	0.965955	3.085500
II_{1a}	-6.973463	-0.037552	3.505507	6.935911	0.885866	3.950005
III_{1a}	-7.284217	0.000544	3.641836	7.284761	0.910323	3.639251
IV_{1a}	-8.408592	0.053606	4.177493	8.462198	1.031141	2.514877
V_{1a}	-8.151716	0.034286	4.058715	8.186002	1.006179	2.771752
VI_{1a}	-7.305442	0.013878	3.645782	7.319320	0.907989	3.618026
VII_{1a}	-7.234964	0.004626	3.615169	7.239590	0.902637	3.688504
$VIII_{1a}$	-7.553882	-0.022041	3.787962	7.531841	0.952533	3.369586
IX_{1a}	-8.328046	0.034558	4.146744	8.362604	1.028118	2.595422

Table S181. Orbital Energies and Philicity Parameters of Unsubstituted Singlet NHCs in Test Set in SMD Water. All quantities given in eV.

Species	E(HOMO)	E(LUMO)	CHI	ETA	GEI	N
I_{1a}	-7.842867	0.039457	3.901705	7.882323	0.965661	3.080601
II_{1a}	-7.015641	-0.029388	3.522514	6.986252	0.888037	3.907828
III_{1a}	-7.302449	0.005987	3.648231	7.308435	0.910564	3.621020
IV_{1a}	-8.453490	0.076192	4.188649	8.529682	1.028455	2.469978
V_{1a}	-8.168587	0.038368	4.065110	8.206955	1.006775	2.754881
VI_{1a}	-7.424084	0.025307	3.699388	7.449390	0.918563	3.499385
VII_{1a}	-7.258910	0.006803	3.626054	7.265713	0.904816	3.664558
$VIII_{1a}$	-7.574018	-0.025579	3.799798	7.548440	0.956388	3.349450
IX_{1a}	-8.345189	0.036463	4.154363	8.381652	1.029554	2.578279

S11. Correction Procedure for Electrostatic Switch Values

For some BF_2-substituted species used in the calculation of electrostatic switches, we observe the favourable formation of an organoboron compound via an intramolecular carbene addition, or otherwise a notable interaction. However, using the uncharged member of each D-LEF pair to calculate our electrostatic switches is not strictly necessary. In the ideal case where the effects we observe are purely electrostatic (i.e. no through-bond effects), we could simply use the unsubstituted species as a reference, provided that the difference between the measured GEI and N values obtained for the uncharged species possessing no C-B interactions are small.

To that point, we find that the maximum difference in the GEI values of the BF_2-substituted species relative to the unsubstituted carbenes is 12.00%, with an average difference of 0.029 eV regardless of position, in the gas-phase. Likewise, we find that the maximum difference in the N values of the BF_2-substituted species relative to the unsubstituted carbenes is 19.39%, with an average difference of 0.002 eV regardless of position, in the gas-phase. However, we also find that these differences increase on average with increasing solvent polarity; therefore, while we have confidence that our correction procedure is valid for low-polarity environments, the values obtained for the BF_2 to BF_3^- switches at the R_1 positions which have formed C-B interactions should in general be regarded with some caution.

S12. Gibbs Free Energies and Components, Frontier Orbital Energies, Nucleophilicity and Electrophilicity Parameters of D-LEF-Substituted NHCs in Test Set Across Different Solvents

Table S182. Energies of $I_{1b\text{-}e}$ & $I_{2b\text{-}e}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
I_{1b}[a]	-528.884820	0.128363	0.010003	391.314600	0.044437	-528.746453	-528.790891	-528.790891
I_{1c}	-628.864102	0.129903	0.011241	415.938100	0.047234	-628.722958	-628.770192	-628.770192
I_{1d}	-438.734088	0.202546	0.011189	410.023900	0.046562	-438.520353	-438.566915	-438.566915
I_{1e}	-478.416093	0.245437	0.012391	430.284800	0.048863	-478.158265	-478.207128	-478.207128
I_{2b}	-568.189054	0.156232	0.011938	430.578900	0.048896	-568.020885	-568.069781	-568.069781
I_{2c}	-668.179075	0.158056	0.012750	443.252400	0.050335	-668.008269	-668.058605	-668.058605
I_{2d}	-478.041002	0.230407	0.012916	443.445900	0.050357	-477.797680	-477.848037	-477.848037
I_{2e}	-517.719598	0.273647	0.013998	460.557000	0.052301	-517.431952	-517.484253	-517.484253

[a] Forms a weak C-B interaction

Table S183. Energies of $I_{1b\text{-}e}$ & $I_{2b\text{-}e}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
I_{1b}[a]	-528.890910	0.128116	0.010293	399.732200	0.045393	-528.752501	-528.797894	-528.794875
I_{1c}	-628.925655	0.130203	0.011205	415.695400	0.047206	-628.784247	-628.831453	-628.828434
I_{1d}	-438.752816	0.202763	0.011148	409.331300	0.046483	-438.538905	-438.585389	-438.582370
I_{1e}	-478.483721	0.245304	0.011589	414.948000	0.047121	-478.226827	-478.273949	-478.270930
I_{2b}	-568.207108	0.156283	0.011940	431.053500	0.048950	-568.038885	-568.087835	-568.084816
I_{2c}	-668.240664	0.158298	0.012756	444.217900	0.050445	-668.069609	-668.120054	-668.117035
I_{2d}	-478.059796	0.230503	0.012878	442.303400	0.050228	-477.816415	-477.866643	-477.863624
I_{2e}	-517.790690	0.275000	0.013599	450.040100	0.051106	-517.502092	-517.553198	-517.550179

[a] Forms a weak C-B interaction

Table S184. Energies of $I_{1b\text{-}e}$ & $I_{2b\text{-}e}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{1b}	-528.898025	0.127952	0.010306	400.145700	0.045440	-528.759766	-528.805206	-528.802187
I_{1c}	-628.956931	0.130109	0.011214	416.991900	0.047353	-628.815608	-628.862962	-628.859943
I_{1d}	-438.758929	0.202660	0.011137	409.254200	0.046475	-438.545133	-438.591607	-438.588588
I_{1e}	-478.514616	0.246134	0.012257	428.129700	0.048618	-478.256225	-478.304843	-478.301824
I_{2b}	-568.214484	0.156098	0.011893	429.188100	0.048738	-568.046493	-568.095231	-568.092212
I_{2c}	-668.271562	0.158256	0.012766	444.731100	0.050503	-668.100540	-668.151043	-668.148024
I_{2d}	-478.065610	0.230310	0.012895	443.081200	0.050316	-477.822405	-477.872721	-477.869702
I_{2e}	-517.824085	0.274744	0.013757	455.257500	0.051699	-517.535584	-517.587283	-517.584264

Table S185. Energies of I_{1b-e} & I_{2b-e} in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{1b}	-528.899209	0.127896	0.010310	400.285200	0.045456	-528.761003	-528.806459	-528.803440
I_{1c}	-628.965202	0.130060	0.011218	417.213100	0.047378	-628.823924	-628.871303	-628.868284
I_{1d}	-438.759213	0.202659	0.011122	408.934000	0.046438	-438.545433	-438.591871	-438.588852
I_{1e}	-478.521944	0.246285	0.012214	427.090500	0.048500	-478.263445	-478.311945	-478.308926
I_{2b}	-568.215768	0.156044	0.011898	429.440600	0.048767	-568.047826	-568.096593	-568.093574
I_{2c}	-668.279124	0.158104	0.012815	446.076800	0.050656	-668.108205	-668.158861	-668.155842
I_{2d}	-478.065664	0.230384	0.012858	442.283600	0.050225	-477.822422	-477.872647	-477.869628
I_{2e}	-517.832256	0.274704	0.013787	456.493400	0.051839	-517.543765	-517.595604	-517.592585

Table S186. Energies of I_{1b-e} & I_{2b-e} in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
I_{1b}	-528.884593	0.128038	0.010412	402.774300	0.045739	-528.746144	-528.791882	-528.788863
I_{1c}	-628.950599	0.130138	0.011232	417.436800	0.047404	-628.809229	-628.856633	-628.853614
I_{1d}	-438.747269	0.203121	0.011058	407.483600	0.046274	-438.533090	-438.579364	-438.576345
I_{1e}	-478.504559	0.246417	0.012224	427.200900	0.048513	-478.245918	-478.294431	-478.291412
I_{2b}	-568.200543	0.156087	0.011921	429.722600	0.048799	-568.032535	-568.081334	-568.078315
I_{2c}	-668.264337	0.158084	0.012858	446.839500	0.050743	-668.093394	-668.144137	-668.141118
I_{2d}	-478.051722	0.230839	0.012882	444.384400	0.050464	-477.808001	-477.858465	-477.855446
I_{2e}	-517.814468	0.274759	0.013843	457.732200	0.051980	-517.525866	-517.577845	-517.574826

Table S187. Energies of II_{1b-e} & II_{2b-e} in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
II_{1b}[a]	-607.427448	0.183541	0.013523	457.912300	0.052000	-607.230390	-607.282390	-607.282390
II_{1c}	-707.411844	0.185021	0.014292	469.763400	0.053346	-707.212530	-707.265880	-707.265880
II_{1d}	-517.279212	0.257628	0.014575	472.549000	0.053662	-517.007010	-517.060670	-517.060670
II_{1e}	-556.979326	0.301031	0.015718	490.905000	0.055747	-556.662580	-556.718320	-556.718320
II_{2b}	-607.420875	0.182995	0.013587	458.560200	0.052074	-607.224290	-607.276370	-607.276370
II_{2c}	-707.431256	0.185576	0.014287	468.749600	0.053231	-707.231390	-707.284620	-707.284620
II_{2d}	-517.284313	0.257540	0.014411	467.144500	0.053049	-517.012360	-517.065410	-517.065410
II_{2e}	-556.948936	0.299967	0.015544	485.039200	0.055081	-556.633430	-556.688510	-556.688510

[a] Forms a weak C-B interaction

Table S188. Energies of II_{1b-e} & II_{2b-e} in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
II_{1b}	-607.450576	0.183250	0.013797	465.670000	0.052881	-607.253530	-607.306410	-607.303391
II_{1c}	-707.476167	0.185595	0.014317	470.850900	0.053469	-707.276260	-707.329730	-707.326711
II_{1d}	-517.300343	0.257764	0.014637	475.238500	0.053968	-517.027940	-517.081910	-517.078891
II_{1e}	-557.039674	0.303767	0.014878	472.209100	0.053624	-556.721030	-556.774650	-556.771631
II_{2b}	-607.450576	0.183250	0.013797	465.670000	0.052881	-607.253530	-607.306410	-607.303391
II_{2c}	-707.476167	0.185595	0.014317	470.850900	0.053469	-707.276260	-707.329730	-707.326711
II_{2d}	-517.300343	0.257764	0.014637	475.238500	0.053968	-517.027940	-517.081910	-517.078891
II_{2e}	-557.039674	0.303767	0.014878	472.209100	0.053624	-556.721030	-556.774650	-556.771631

Table S189. Energies of II_{1b-e} & II_{2b-e} in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
II_{1b}	-607.465249	0.183260	0.013777	466.199700	0.052941	-607.268210	-607.321150	-607.318131
II_{1c}	-707.518839	0.185820	0.014387	473.876700	0.053813	-707.318630	-707.372450	-707.369431
II_{1d}	-517.311329	0.258319	0.014320	467.388100	0.053076	-517.038690	-517.091770	-517.088751
II_{1e}	-557.075877	0.302843	0.015122	478.276800	0.054313	-556.757910	-556.812220	-556.809201
II_{2b}	-607.459488	0.183581	0.013353	452.428900	0.051377	-607.262550	-607.313930	-607.310911
II_{2c}	-707.524518	0.185513	0.014435	473.631000	0.053785	-707.324570	-707.378360	-707.375341
II_{2d}	-517.320154	0.257607	0.014485	470.482700	0.053428	-517.048060	-517.101490	-517.098471
II_{2e}	-557.067605	0.302484	0.014989	473.276500	0.053745	-556.750130	-556.803880	-556.800861

Table S190. Energies of II_{1b-e} & II_{2b-e} in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
II_{1b}	-607.468917	0.183411	0.013697	464.326500	0.052729	-607.271810	-607.324540	-607.321521
II_{1c}	-707.530979	0.185941	0.014347	472.953000	0.053708	-707.330690	-707.384400	-707.381381
II_{1d}	-517.311329	0.258319	0.014320	467.388100	0.053076	-517.038690	-517.091770	-517.088751
II_{1e}	-557.075877	0.302843	0.015122	478.276800	0.054313	-556.757910	-556.812220	-556.809201
II_{2b}	-607.464092	0.183682	0.013315	451.918500	0.051320	-607.267100	-607.318420	-607.315401
II_{2c}	-707.533590	0.185669	0.014346	470.972400	0.053483	-707.333570	-707.387060	-707.384041
II_{2d}	-517.320154	0.257607	0.014485	470.482700	0.053428	-517.048060	-517.101490	-517.098471
II_{2e}	-557.067605	0.302484	0.014989	473.276500	0.053745	-556.750130	-556.803880	-556.800861

Table S191. Energies of II_{1b-e} & II_{2b-e} in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
II_{1b}	-607.461221	0.183570	0.013718	464.880500	0.052791	-607.263930	-607.316720	-607.313701
II_{1c}	-707.524377	0.185993	0.014409	474.614600	0.053897	-707.323970	-707.377870	-707.374851
II_{1d}	-517.310975	0.258760	0.014343	468.516500	0.053204	-517.037870	-517.091080	-517.088061
II_{1e}	-557.074399	0.302970	0.015158	478.648300	0.054355	-556.756270	-556.810630	-556.807611
II_{2b}	-607.455967	0.183758	0.013342	452.603700	0.051397	-607.258870	-607.310260	-607.307241
II_{2c}	-707.525738	0.185791	0.014362	471.381300	0.053530	-707.325590	-707.379110	-707.376091
II_{2d}	-517.315352	0.258525	0.014298	466.585800	0.052985	-517.042530	-517.095510	-517.092491
II_{2e}	-557.068061	0.302701	0.015002	473.260800	0.053743	-556.750360	-556.804100	-556.801081

Table S192. Energies of $III_{[1-4][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
III_{1b}[a]	-568.156499	0.155561	0.011957	429.548200	0.048779	-567.988980	-568.037760	-568.037760
III_{1c}	-668.152429	0.157480	0.012959	448.113600	0.050887	-667.981990	-668.032880	-668.032880
III_{1d}	-478.016039	0.230041	0.012892	441.409700	0.050126	-477.773110	-477.823230	-477.823230
III_{1e}	-517.703314	0.273344	0.013851	454.592700	0.051623	-517.416120	-517.467740	-517.467740
III_{2b}	-607.471138	0.183880	0.013507	457.009000	0.051898	-607.273750	-607.325650	-607.325650
III_{2c}	-707.477937	0.185899	0.014391	473.230800	0.053740	-707.277650	-707.331390	-707.331390
III_{2d}	-517.321881	0.258969	0.014131	461.573800	0.052416	-517.048780	-517.101200	-517.101200
III_{2e}	-556.995493	0.301446	0.015355	481.068300	0.054630	-556.678692	-556.733321	-556.733321
III_{3b}	-568.155082	0.155660	0.011933	429.091900	0.048727	-567.987490	-568.036220	-568.036220
III_{3c}	-668.163450	0.157789	0.012914	448.203600	0.050898	-667.992750	-668.043650	-668.043650
III_{3d}	-478.014071	0.229793	0.012954	443.520000	0.050366	-477.771330	-477.821690	-477.821690
III_{3e}	-517.681112	0.272883	0.013949	458.274300	0.052041	-517.394280	-517.446320	-517.446320
III_{4b}	-568.162980	0.156052	0.012085	435.193200	0.049420	-567.994840	-568.044260	-568.044260
III_{4c}	-668.140173	0.157726	0.012756	442.403000	0.050239	-667.969690	-668.019930	-668.019930
III_{4d}	-478.013434	0.230207	0.012960	444.447100	0.050471	-477.770270	-477.820740	-477.820740
III_{4e}	-517.710844	0.273835	0.014096	462.355500	0.052505	-517.422910	-517.475420	-517.475420

[a] Forms a weak C-B interaction

Table S193. Energies of $III_{[1-4][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
III_{1b}[a]	-568.176569	0.155949	0.011872	427.607800	0.048559	-568.008750	-568.057310	-568.054291
III_{1c}	-668.215132	0.158013	0.012892	447.051800	0.050767	-668.044230	-668.094990	-668.091971
III_{1d}	-478.038273	0.230222	0.012862	441.100300	0.050091	-477.795190	-477.845280	-477.842261
III_{1e}	-517.770911	0.274559	0.013725	453.653100	0.051517	-517.482630	-517.534140	-517.531121
III_{2b}	-607.491816	0.183549	0.012882	445.824800	0.050628	-607.295390	-607.346010	-607.342991
III_{2c}	-707.536149	0.186229	0.014351	472.273900	0.053631	-707.335568	-707.389199	-707.386180
III_{2d}	-517.344015	0.258614	0.014415	470.436300	0.053422	-517.070990	-517.124410	-517.121391
III_{2e}	-557.070145	0.303862	0.014752	467.810400	0.053124	-556.751530	-556.804654	-556.801635
III_{3b}	-568.176186	0.155941	0.011876	428.156100	0.048621	-568.008370	-568.056990	-568.053971
III_{3c}	-668.222125	0.158321	0.012818	445.970200	0.050644	-668.050990	-668.101630	-668.098611
III_{3d}	-478.036541	0.230240	0.012861	441.076400	0.050088	-477.793440	-477.843530	-477.840511
III_{3e}	-517.757968	0.275395	0.013377	446.057600	0.050654	-517.469200	-517.519850	-517.516831
III_{4b}	-568.182687	0.156439	0.011935	430.790000	0.048920	-568.014310	-568.063230	-568.060211
III_{4c}	-668.205829	0.158636	0.012539	437.464800	0.049678	-668.034650	-668.084330	-668.081311
III_{4d}	-478.034263	0.230425	0.012940	444.428300	0.050469	-477.790900	-477.841370	-477.838351
III_{4e}	-517.773268	0.275170	0.013701	452.928400	0.051434	-517.484400	-517.535830	-517.532811

[a] Forms a weak C-B interaction

Table S194. Energies of $III_{[1-4][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
III_{1b}[a]	-568.190648	0.155981	0.011836	426.891000	0.048477	-568.022830	-568.071310	-568.068291
III_{1c}	-668.250079	0.158113	0.012847	445.799500	0.050625	-668.079120	-668.129750	-668.126731
III_{1d}	-478.049074	0.230140	0.012848	440.987000	0.050078	-477.806090	-477.856160	-477.853141
III_{1e}	-517.805618	0.273733	0.013824	455.653000	0.051744	-517.518060	-517.569800	-517.566781
III_{2b}	-607.505779	0.184067	0.013426	455.396900	0.051715	-607.308290	-607.360000	-607.356981
III_{2c}	-707.568621	0.186076	0.013667	460.402400	0.052283	-707.368880	-707.421160	-707.418141
III_{2d}	-517.355385	0.259317	0.014017	458.900800	0.052112	-517.082050	-517.134160	-517.131141
III_{2e}	-557.111049	0.303497	0.014852	469.734100	0.053343	-556.792701	-556.846043	-556.843024
III_{3b}	-568.189312	0.155926	0.011875	428.198600	0.048626	-568.021510	-568.070140	-568.067121
III_{3c}	-668.253567	0.158144	0.012831	446.582000	0.050714	-668.082590	-668.133310	-668.130291
III_{3d}	-478.048081	0.230296	0.012825	440.253100	0.049995	-477.804960	-477.854960	-477.851941
III_{3e}	-517.799033	0.274785	0.013550	450.056900	0.051108	-517.510700	-517.561810	-517.558791
III_{4b}	-568.194183	0.156316	0.011946	431.143300	0.048960	-568.025920	-568.074880	-568.071861
III_{4c}	-668.244133	0.158217	0.012759	443.420300	0.050354	-668.073160	-668.123510	-668.120491
III_{4d}	-478.044673	0.230423	0.012890	443.057400	0.050313	-477.801360	-477.851670	-477.848651
III_{4e}	-517.808200	0.274535	0.013860	458.438800	0.052060	-517.519810	-517.571870	-517.568851

[a] Forms a weak C-B interaction

Table S195. Energies of $III_{[1-4][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
III_{1b}	-568.193646	0.155932	0.011836	426.875100	0.048476	-568.025880	-568.074350	-568.071331
III_{1c}	-668.258802	0.157953	0.012810	445.334500	0.050572	-668.088040	-668.138610	-668.135591
III_{1d}	-478.050849	0.230243	0.012781	439.147300	0.049869	-477.807820	-477.857690	-477.854671
III_{1e}	-517.814616	0.273896	0.013814	455.093700	0.051680	-517.526910	-517.578590	-517.575571
III_{2b}	-607.508919	0.183955	0.013533	459.731600	0.052207	-607.311430	-607.363640	-607.360621
III_{2c}	-707.577677	0.186175	0.014362	473.055000	0.053720	-707.377140	-707.430860	-707.427841
III_{2d}	-517.358331	0.258667	0.014348	468.844800	0.053242	-517.085320	-517.138560	-517.135541
III_{2e}	-557.121973	0.303645	0.014834	469.881000	0.053359	-556.803494	-556.856853	-556.853834
III_{3b}	-568.192761	0.155983	0.011845	427.594900	0.048557	-568.024930	-568.073490	-568.070471
III_{3c}	-668.261114	0.158000	0.012869	447.275600	0.050792	-668.090250	-668.141040	-668.138021
III_{3d}	-478.050348	0.230309	0.012817	440.212600	0.049990	-477.807220	-477.857210	-477.854191
III_{3e}	-517.810096	0.274648	0.013633	452.190800	0.051350	-517.521820	-517.573170	-517.570151
III_{4b}	-568.196919	0.156231	0.011981	432.272100	0.049088	-568.028710	-568.077800	-568.074781
III_{4c}	-668.254699	0.157946	0.012900	448.925600	0.050980	-668.083850	-668.134830	-668.131811
III_{4d}	-478.046542	0.230543	0.012821	441.074900	0.050088	-477.803180	-477.853270	-477.850251
III_{4e}	-517.816210	0.274746	0.013794	456.903300	0.051886	-517.527670	-517.579560	-517.576541

Table SX196. Energies of $III_{[1-4][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
III_{1b}	-568.181001	0.155967	0.011883	427.948900	0.048598	-568.013150	-568.061750	-568.058731
III_{1c}	-668.247378	0.158079	0.012830	445.890100	0.050635	-668.076470	-668.127100	-668.124081
III_{1d}	-478.041442	0.231045	0.012659	436.896000	0.049614	-477.797740	-477.847350	-477.844331
III_{1e}	-517.799810	0.274145	0.013836	455.596100	0.051737	-517.511830	-517.563570	-517.560551
III_{2b}	-607.498590	0.184191	0.013507	458.820300	0.052103	-607.300890	-607.353000	-607.349981
III_{2c}	-707.567435	0.186190	0.014432	474.992100	0.053940	-707.366810	-707.420750	-707.417731
III_{2d}	-517.349546	0.259089	0.014315	468.184100	0.053167	-517.076140	-517.129310	-517.126291
III_{2e}	-557.109015	0.303719	0.014876	470.665200	0.053448	-556.790420	-556.843869	-556.840850
III_{3b}	-568.179967	0.156073	0.011868	428.114200	0.048616	-568.012030	-568.060640	-568.057621
III_{3c}	-668.249178	0.158059	0.012902	447.871500	0.050860	-668.078220	-668.129080	-668.126061
III_{3d}	-478.039606	0.230973	0.012744	439.673000	0.049929	-477.795890	-477.845820	-477.842801
III_{3e}	-517.795610	0.274876	0.013630	452.061100	0.051336	-517.507100	-517.558440	-517.555421
III_{4b}	-568.184595	0.156281	0.012041	433.715800	0.049252	-568.016270	-568.065530	-568.062511
III_{4c}	-668.245190	0.158368	0.012829	446.193700	0.050669	-668.073990	-668.124660	-668.121641
III_{4d}	-478.035420	0.231166	0.012798	441.459300	0.050132	-477.791460	-477.841590	-477.838571
III_{4e}	-517.800872	0.275013	0.013762	455.814700	0.051762	-517.512100	-517.563860	-517.560841

Table S197. Energies of $IV_{[1-3][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
IV_{1b}	-509.425382	0.087288	0.008584	366.723100	0.041645	-509.329510	-509.371160	-509.371160
IV_{1c}	-609.423891	0.089154	0.009453	382.313000	0.043415	-609.325290	-609.368700	-609.368700
IV_{1d}	-419.284202	0.161543	0.009459	376.532100	0.042759	-419.113200	-419.155960	-419.155960
IV_{1e}	-458.953180	0.204277	0.010644	396.714300	0.045051	-458.738260	-458.783310	-458.783310
IV_{2b}	-548.739621	0.115363	0.010121	395.378100	0.044899	-548.614140	-548.659040	-548.659040
IV_{2c}	-648.738228	0.117343	0.010952	409.353100	0.046486	-648.609930	-648.656420	-648.656420
IV_{2d}	-458.592395	0.189583	0.011092	407.808600	0.046310	-458.391720	-458.438030	-458.438030
IV_{2e}	-498.259548	0.232672	0.012188	425.475500	0.048317	-498.014690	-498.063010	-498.063010
IV_{3b}	-548.742543	0.115066	0.010240	398.642000	0.045269	-548.617240	-548.662510	-548.662510
IV_{3c}	-648.736104	0.116742	0.011177	415.955200	0.047236	-648.608190	-648.655420	-648.655420
IV_{3d}	-458.591628	0.189306	0.011186	410.542800	0.046621	-458.391140	-458.437760	-458.437760
IV_{3e}	-498.271251	0.232516	0.012323	428.929100	0.048709	-498.026410	-498.075120	-498.075120

Table S198. Energies of $IV_{[1-3][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
IV_{1b}	-509.433208	0.087444	0.008578	367.037000	0.041680	-509.337190	-509.378870	-509.375851
IV_{1c}	-609.473649	0.089464	0.009372	380.701800	0.043232	-609.374810	-609.418050	-609.415031
IV_{1d}	-419.295649	0.161667	0.009438	375.924100	0.042690	-419.124550	-419.167230	-419.164211
IV_{1e}	-459.018466	0.205065	0.010453	391.760500	0.044488	-458.802950	-458.847440	-458.844421
IV_{2b}	-548.749877	0.115339	0.010163	396.538400	0.045031	-548.624380	-548.669410	-548.666391
IV_{2c}	-648.788733	0.117467	0.010974	410.660800	0.046634	-648.660290	-648.706930	-648.703911
IV_{2d}	-458.603142	0.189678	0.011093	408.059100	0.046339	-458.402370	-458.448710	-458.445691
IV_{2e}	-498.327323	0.234312	0.011784	416.648000	0.047314	-498.081230	-498.128540	-498.125521
IV_{3b}	-548.752857	0.115152	0.010247	399.162700	0.045329	-548.627460	-548.672790	-548.669771
IV_{3c}	-648.789839	0.117089	0.011147	415.668600	0.047203	-648.661600	-648.708810	-648.705791
IV_{3d}	-458.603478	0.189430	0.011193	410.950300	0.046667	-458.402860	-458.449520	-458.446501
IV_{3e}	-498.334698	0.233077	0.012265	426.613500	0.048446	-498.089360	-498.137800	-498.134781

Table S199. Energies of $IV_{[1-3][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
IV_{1b}	-509.440061	0.086963	0.008560	366.640600	0.041635	-509.344540	-509.386170	-509.383151
IV_{1c}	-609.502760	0.089278	0.009433	382.702600	0.043459	-609.404050	-609.447510	-609.444491
IV_{1d}	-419.302104	0.161592	0.009413	375.254300	0.042614	-419.131100	-419.173710	-419.170691
IV_{1e}	-459.052939	0.205290	0.010448	392.788100	0.044605	-458.837200	-458.881810	-458.878791
IV_{2b}	-548.757843	0.115226	0.010146	396.021400	0.044972	-548.632470	-548.677440	-548.674421
IV_{2c}	-648.818171	0.117121	0.011081	413.743100	0.046984	-648.689970	-648.736950	-648.733931
IV_{2d}	-458.609306	0.189484	0.011141	409.977500	0.046557	-458.408680	-458.455240	-458.452221
IV_{2e}	-498.364155	0.233657	0.012011	421.761200	0.047895	-498.118490	-498.166380	-498.163361
IV_{3b}	-548.760172	0.114963	0.010262	399.529800	0.045370	-548.634950	-548.680320	-548.677301
IV_{3c}	-648.820000	0.116883	0.011182	416.611900	0.047310	-648.691940	-648.739250	-648.736231
IV_{3d}	-458.610391	0.189449	0.011122	409.315600	0.046482	-458.409820	-458.456300	-458.453281
IV_{3e}	-498.369041	0.233178	0.012225	427.494700	0.048546	-498.123640	-498.172180	-498.169161

Table S200. Energies of $IV_{[1-3][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
IV_{1b}	-509.442045	0.086979	0.008560	366.626800	0.041634	-509.346510	-509.388140	-509.385121
IV_{1c}	-609.510781	0.089275	0.009434	383.069500	0.043501	-609.412070	-609.455570	-609.452551
IV_{1d}	-419.303064	0.161600	0.009402	375.064600	0.042592	-419.132060	-419.174650	-419.171631
IV_{1e}	-459.062000	0.205310	0.010459	393.161500	0.044647	-458.846230	-458.890880	-458.887861
IV_{2b}	-548.759819	0.115333	0.010070	394.203600	0.044765	-548.634420	-548.679180	-548.676161
IV_{2c}	-648.825591	0.117112	0.011077	413.610400	0.046969	-648.697400	-648.744370	-648.741351
IV_{2d}	-458.609969	0.189509	0.011124	409.768500	0.046533	-458.409340	-458.455870	-458.452851
IV_{2e}	-498.373967	0.233579	0.012114	425.042400	0.048267	-498.128270	-498.176540	-498.173521
IV_{3b}	-548.761573	0.114894	0.010273	399.813600	0.045403	-548.636410	-548.681810	-548.678791
IV_{3c}	-648.827513	0.116863	0.011174	416.436600	0.047290	-648.699480	-648.746770	-648.743751
IV_{3d}	-458.611384	0.189427	0.011118	409.238900	0.046473	-458.410840	-458.457310	-458.454291
IV_{3e}	-498.377519	0.233267	0.012209	427.265200	0.048520	-498.132040	-498.180560	-498.177541

Table S201. Energies of $IV_{[1-3][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
IV_{1b}	-509.434003	0.086659	0.008590	367.054000	0.041682	-509.338750	-509.380440	-509.377421
IV_{1c}	-609.503227	0.088869	0.009476	383.781800	0.043582	-609.404880	-609.448460	-609.445441
IV_{1d}	-419.297435	0.161825	0.009333	373.442400	0.042408	-419.126280	-419.168690	-419.165671
IV_{1e}	-459.050868	0.205202	0.010469	393.148700	0.044646	-458.835200	-458.879840	-458.876821
IV_{2b}	-548.751669	0.114973	0.010152	395.766100	0.044943	-548.626540	-548.671490	-548.668471
IV_{2c}	-648.817831	0.116834	0.011108	413.943100	0.047007	-648.689890	-648.736900	-648.733881
IV_{2d}	-458.602932	0.189787	0.011043	407.748500	0.046304	-458.402100	-458.448410	-458.445391
IV_{2e}	-498.363087	0.233485	0.012067	423.379100	0.048079	-498.117540	-498.165610	-498.162591
IV_{3b}	-548.753015	0.114659	0.010311	400.428600	0.045472	-548.628040	-548.673520	-548.670501
IV_{3c}	-648.819307	0.116696	0.011223	417.396800	0.047399	-648.691390	-648.738790	-648.735771
IV_{3d}	-458.605457	0.189682	0.011086	408.595500	0.046400	-458.404690	-458.451090	-458.448071
IV_{3e}	-498.365872	0.233007	0.012278	428.789500	0.048693	-498.120590	-498.169280	-498.166261

Table S202. Energies of $V_{[1-3][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
V_{1b}	-832.411140	0.084120	0.008551	364.352400	0.041376	-832.318470	-832.359845	-832.359845
V_{1c}	-932.399520	0.086039	0.009851	391.590200	0.044469	-932.303630	-932.348099	-932.348099
V_{1d}	-742.260949	0.158550	0.009780	384.730400	0.043690	-742.092619	-742.136309	-742.136309
V_{1e}	-781.927113	0.201158	0.010270	390.383400	0.044332	-781.715685	-781.760016	-781.760016
V_{2b}	-871.714466	0.112246	0.010423	402.258100	0.045680	-871.591797	-871.637477	-871.637477
V_{2c}	-971.713650	0.114381	0.011261	416.698500	0.047320	-971.588008	-971.635328	-971.635328
V_{2d}	-781.565118	0.186435	0.011420	415.335000	0.047165	-781.367264	-781.414429	-781.414429
V_{2e}	-821.236131	0.229695	0.012464	431.601600	0.049012	-820.993972	-821.042984	-821.042984
V_{3b}	-871.713560	0.112154	0.010677	409.049700	0.046451	-871.590729	-871.637180	-871.637180
V_{3c}	-971.708444	0.113868	0.011640	426.938400	0.048483	-971.582936	-971.631418	-971.631418
V_{3d}	-781.565593	0.186301	0.011594	419.999600	0.047695	-781.367698	-781.415393	-781.415393
V_{3e}	-821.243135	0.229495	0.012773	439.516900	0.049911	-821.000867	-821.050778	-821.050778

Table S203. Energies of $V_{[1-3][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
V_{1b}	-832.422049	0.084196	0.008499	363.228300	0.041248	-832.329355	-832.370603	-832.367584
V_{1c}	-932.449489	0.086168	0.009782	390.268800	0.044319	-932.353539	-932.397858	-932.394839
V_{1d}	-742.272669	0.158578	0.009769	384.390600	0.043651	-742.104321	-742.147972	-742.144953
V_{1e}	-781.995930	0.201901	0.010871	403.196300	0.045787	-781.783158	-781.828945	-781.825926
V_{2b}	-871.725060	0.112353	0.010394	401.996300	0.045650	-871.602313	-871.647964	-871.644945
V_{2c}	-971.763732	0.114090	0.011425	421.603200	0.047877	-971.638217	-971.686094	-971.683075
V_{2d}	-781.576968	0.186489	0.011412	415.168800	0.047146	-781.379068	-781.426214	-781.423195
V_{2e}	-821.302562	0.230993	0.012279	427.352300	0.048530	-821.059290	-821.107820	-821.104801
V_{3b}	-871.724215	0.112298	0.010637	408.011800	0.046334	-871.601280	-871.647614	-871.644595
V_{3c}	-971.761687	0.114074	0.011577	425.517000	0.048321	-971.636036	-971.684357	-971.681338
V_{3d}	-781.577892	0.186458	0.011579	419.862800	0.047679	-781.379855	-781.427534	-781.424515
V_{3e}	-821.307363	0.230570	0.012505	432.344000	0.049097	-821.064288	-821.113385	-821.110366

Table S204. Energies of $V_{[1-3][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
V_{1b}	-832.429082	0.084096	0.008484	362.851700	0.041205	-832.336502	-832.377707	-832.374688
V_{1c}	-932.478871	0.086152	0.009794	391.377900	0.044445	-932.382925	-932.427370	-932.424351
V_{1d}	-742.278831	0.158598	0.009725	383.379200	0.043536	-742.110508	-742.154044	-742.151025
V_{1e}	-782.019420	0.202349	0.010127	388.192500	0.044083	-781.806943	-781.851026	-781.848007
V_{2b}	-871.733211	0.112274	0.010408	402.817500	0.045744	-871.610530	-871.656273	-871.653254
V_{2c}	-971.792975	0.113960	0.011435	421.796600	0.047899	-971.667581	-971.715480	-971.712461
V_{2d}	-781.583606	0.186435	0.011392	414.783300	0.047102	-781.385779	-781.432881	-781.429862
V_{2e}	-821.338462	0.230271	0.012473	432.335500	0.049096	-821.095718	-821.144813	-821.141794
V_{3b}	-871.731874	0.111942	0.010658	408.441600	0.046382	-871.609274	-871.655656	-871.652637
V_{3c}	-971.791173	0.113986	0.011619	426.908400	0.048479	-971.665567	-971.714047	-971.711028
V_{3d}	-781.584629	0.186426	0.011563	419.726700	0.047664	-781.386640	-781.434304	-781.431285
V_{3e}	-821.341350	0.230167	0.012654	437.822400	0.049719	-821.098529	-821.148248	-821.145229

Table S205. Energies of $V_{[1-3][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
V_{1b}	-832.429950	0.084061	0.008482	362.768100	0.041196	-832.337408	-832.378604	-832.375585
V_{1c}	-932.486547	0.086070	0.009811	391.948700	0.044509	-932.390666	-932.435175	-932.432156
V_{1d}	-742.279134	0.158544	0.009729	383.531300	0.043554	-742.110861	-742.154414	-742.151395
V_{1e}	-782.026725	0.201942	0.010245	390.560900	0.044352	-781.814538	-781.858889	-781.855870
V_{2b}	-871.734672	0.112346	0.010315	400.095400	0.045435	-871.612012	-871.657446	-871.654427
V_{2c}	-971.800168	0.114310	0.011294	417.961600	0.047463	-971.674564	-971.722028	-971.719009
V_{2d}	-781.583813	0.186384	0.011398	414.928500	0.047119	-781.386031	-781.433150	-781.430131
V_{2e}	-821.347518	0.230368	0.012431	431.396500	0.048989	-821.104720	-821.153709	-821.150690
V_{3b}	-871.733111	0.111892	0.010660	408.450200	0.046383	-871.610559	-871.656942	-871.653923
V_{3c}	-971.798797	0.114042	0.011544	424.679100	0.048226	-971.673210	-971.721437	-971.718418
V_{3d}	-781.584892	0.186390	0.011575	420.297900	0.047729	-781.386927	-781.434656	-781.431637
V_{3e}	-821.349720	0.230302	0.012635	437.585300	0.049692	-821.106782	-821.156474	-821.153455

Table S206. Energies of $V_{[1-3][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
V_{1b}	-832.422162	0.084080	0.008496	363.055200	0.041228	-832.329586	-832.370814	-832.367795
V_{1c}	-932.478746	0.086122	0.009808	391.839800	0.044497	-932.382816	-932.427313	-932.424294
V_{1d}	-742.273250	0.159054	0.009658	382.043900	0.043385	-742.104538	-742.147923	-742.144904
V_{1e}	-782.016289	0.202022	0.010273	391.159200	0.044420	-781.803994	-781.848414	-781.845395
V_{2b}	-871.726385	0.112292	0.010367	401.115300	0.045550	-871.603726	-871.649277	-871.646258
V_{2c}	-971.792109	0.114359	0.011299	417.999600	0.047468	-971.666450	-971.713918	-971.710899
V_{2d}	-781.577177	0.186832	0.011384	414.905100	0.047116	-781.378961	-781.426077	-781.423058
V_{2e}	-821.336597	0.230715	0.012370	430.586600	0.048897	-821.093512	-821.142409	-821.139390
V_{3b}	-871.724044	0.111952	0.010670	408.579400	0.046398	-871.601422	-871.647820	-871.644801
V_{3c}	-971.789968	0.114099	0.011556	424.784000	0.048238	-971.664313	-971.712551	-971.709532
V_{3d}	-781.577897	0.186893	0.011526	419.883900	0.047682	-781.379477	-781.427159	-781.424140
V_{3e}	-821.337922	0.230511	0.012630	437.456400	0.049677	-821.094781	-821.144458	-821.141439

Table S207. Energies of $VI_{[1-2][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
VI_{1b}	-530.070341	0.150733	0.011021	412.131300	0.046801	-529.908587	-529.955388	-529.955388
VI_{1c}	-630.056583	0.152520	0.011866	426.548200	0.048438	-629.892197	-629.940636	-629.940636
VI_{1d}	-439.930684	0.225246	0.011930	423.576300	0.048101	-439.693508	-439.741609	-439.738590
VI_{1e}	-479.619242	0.268587	0.013084	442.420800	0.050241	-479.337571	-479.387812	-479.384793
VI_{2b}	-569.383205	0.178894	0.012511	442.191600	0.050215	-569.191800	-569.242015	-569.242015
VI_{2c}	-669.373398	0.180708	0.013310	454.741300	0.051640	-669.179381	-669.231021	-669.231021
VI_{2d}	-479.231997	0.253299	0.013374	451.438200	0.051265	-478.965323	-479.016588	-479.013569
VI_{2e}	-518.911985	0.297332	0.014093	456.217900	0.051808	-518.600560	-518.652368	-518.649349

Table S208. Energies of $VI_{[1-2][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
VI_{1b}	-530.088139	0.150885	0.011183	417.869500	0.047453	-529.926072	-529.973525	-529.970506
VI_{1c}	-630.118012	0.152956	0.011858	426.500800	0.048433	-629.953197	-630.001631	-629.998612
VI_{1d}	-439.948545	0.225249	0.011991	425.693800	0.048341	-439.711306	-439.759647	-439.756628
VI_{1e}	-479.685442	0.270623	0.012592	432.247000	0.049086	-479.402228	-479.451314	-479.448295
VI_{2b}	-569.400765	0.178991	0.012440	440.059800	0.049973	-569.209334	-569.259307	-569.256288
VI_{2c}	-669.433564	0.181378	0.013163	451.255100	0.051244	-669.239023	-669.290267	-669.287248
VI_{2d}	-479.250302	0.253417	0.013355	450.762200	0.051188	-478.983530	-479.034718	-479.031699
VI_{2e}	-518.980970	0.298616	0.013827	452.071500	0.051337	-518.668526	-518.719863	-518.716844

Table S209. Energies of $VI_{[1-2][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
VI_{1b}	-530.093562	0.150679	0.011191	417.783500	0.047443	-529.931692	-529.979135	-529.976116
VI_{1c}	-630.149209	0.152603	0.011980	430.171400	0.048850	-629.984626	-630.033476	-630.030457
VI_{1d}	-439.953806	0.225084	0.011966	424.795600	0.048239	-439.716756	-439.764995	-439.761976
VI_{1e}	-479.714783	0.269393	0.012811	436.351100	0.049552	-479.432578	-479.482130	-479.479111
VI_{2b}	-569.407412	0.178889	0.012508	442.378200	0.050236	-569.216015	-569.266251	-569.263232
VI_{2c}	-669.462983	0.180794	0.013322	455.351000	0.051709	-669.268867	-669.320576	-669.317557
VI_{2d}	-479.256436	0.253264	0.013360	450.863500	0.051200	-478.989812	-479.041012	-479.037993
VI_{2e}	-519.013080	0.298116	0.013990	456.057500	0.051790	-518.700975	-518.752764	-518.749745

Table S210. Energies of $VI_{[1-2][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
VI_{1b}	-530.094071	0.150648	0.011184	417.571400	0.047419	-529.932239	-529.979658	-529.976639
VI_{1c}	-630.157052	0.152633	0.011981	430.426500	0.048879	-629.992439	-630.041318	-630.038299
VI_{1d}	-439.952770	0.225399	0.011783	419.862500	0.047679	-439.715588	-439.763268	-439.760249
VI_{1e}	-479.721486	0.269241	0.012869	437.826300	0.049719	-479.439376	-479.489095	-479.486076
VI_{2b}	-569.408264	0.178749	0.012539	443.096000	0.050318	-569.216976	-569.267293	-569.264274
VI_{2c}	-669.469821	0.180603	0.013357	456.207700	0.051807	-669.275862	-669.327669	-669.324650
VI_{2d}	-479.256423	0.253161	0.013387	451.826300	0.051309	-478.989875	-479.041184	-479.038165
VI_{2e}	-519.023978	0.297788	0.014349	466.867400	0.053017	-518.711840	-518.764857	-518.761838

Table S211. Energies of $VI_{[1-2][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
VI_{1b}[a]	-530.096179	0.151495	0.010570	399.880700	0.045410	-529.934114	-529.979524	-529.976505
VI_{1c}	-630.144312	0.152833	0.011927	428.491100	0.048659	-629.979551	-630.028210	-630.025191
VI_{1d}	-439.941939	0.225943	0.011854	422.154500	0.047940	-439.704142	-439.752082	-439.749063
VI_{1e}	-479.705073	0.269234	0.012980	440.357600	0.050007	-479.422860	-479.472866	-479.469847
VI_{2b}	-569.394738	0.178874	0.012527	442.418000	0.050241	-569.203336	-569.253577	-569.250558
VI_{2c}	-669.456922	0.180901	0.013321	455.113300	0.051682	-669.262700	-669.314382	-669.311363
VI_{2d}	-479.245748	0.253860	0.013326	450.468800	0.051155	-478.978562	-479.029717	-479.026698
VI_{2e}	-519.007822	0.297931	0.014392	467.863900	0.053130	-518.695499	-518.748630	-518.745611

[a] Forms a weak C-B interaction

Table S213. Energies of VII$_{[1-3][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
VII$_{1b}$[a]	-569.407084	0.181259	0.011515	417.823500	0.047448	-569.214310	-569.261758	-569.261758
VII$_{1c}$	-669.344882	0.181291	0.012872	446.783200	0.050736	-669.150718	-669.201455	-669.201455
VII$_{1d}$	-479.232991	0.255043	0.012516	432.806300	0.049149	-478.965432	-479.014582	-479.014582
VII$_{1e}$	-518.930405	0.298566	0.013721	452.078500	0.051338	-518.618118	-518.669455	-518.669455
VII$_{2b}$	-608.689063	0.208963	0.013089	449.264000	0.051018	-608.467011	-608.518029	-608.518029
VII$_{2c}$	-708.676864	0.210534	0.014025	465.654300	0.052879	-708.452305	-708.505184	-708.505184
VII$_{2d}$	-518.537382	0.283033	0.014026	459.427000	0.052172	-518.240324	-518.292496	-518.292496
VII$_{2e}$	-558.213713	0.327007	0.014954	471.412500	0.053533	-557.871752	-557.925285	-557.925285
VII$_{3b}$	-608.690618	0.208491	0.013357	455.853400	0.051766	-608.468770	-608.520536	-608.520536
VII$_{3c}$	-708.676873	0.210306	0.014224	469.916900	0.053363	-708.452343	-708.505706	-708.505706
VII$_{3d}$	-518.541624	0.282793	0.014289	467.579000	0.053098	-518.244542	-518.297640	-518.297640
VII$_{3e}$	-558.214197	0.326314	0.015409	484.233600	0.054989	-557.872474	-557.927463	-557.927463

[a] Forms a weak C-B interaction

Table S214. Energies of VII$_{[1-3][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
VII$_{1b}$[a]	-569.424079	0.181340	0.011445	416.168100	0.047260	-569.231294	-569.278554	-569.275535
VII$_{1c}$	-669.422459	0.182996	0.012434	436.101200	0.049523	-669.227028	-669.276551	-669.273532
VII$_{1d}$	-479.252302	0.255151	0.012511	432.866100	0.049156	-478.984640	-479.033796	-479.030777
VII$_{1e}$	-518.994821	0.299392	0.013523	448.018400	0.050877	-518.681905	-518.732782	-518.729763
VII$_{2b}$	-608.706050	0.208907	0.013109	449.951900	0.051096	-608.484034	-608.535130	-608.532111
VII$_{2c}$	-708.732482	0.211093	0.013803	459.537100	0.052185	-708.507587	-708.559772	-708.556753
VII$_{2d}$	-518.553952	0.283231	0.014067	461.248100	0.052379	-518.256654	-518.309033	-518.306014
VII$_{2e}$	-558.282737	0.328525	0.014600	464.340300	0.052730	-557.939613	-557.992343	-557.989324
VII$_{3b}$	-608.707899	0.208440	0.013373	456.330200	0.051821	-608.486086	-608.537907	-608.534888
VII$_{3c}$	-708.738365	0.210457	0.014242	471.395700	0.053531	-708.513667	-708.567198	-708.564179
VII$_{3d}$	-518.559994	0.282848	0.014291	467.824900	0.053126	-518.262854	-518.315980	-518.312961
VII$_{3e}$	-558.287318	0.328149	0.015050	476.929500	0.054160	-557.944120	-557.998280	-557.995261

[a] Forms a weak C-B interaction

Table S215. Energies of $VII_{[1-3][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
VII_{1b}[a]	-569.432225	0.181032	0.011467	416.582700	0.047307	-569.239726	-569.287033	-569.284014
VII_{1c}	-669.456543	0.182455	0.012677	441.891200	0.050181	-669.261410	-669.311591	-669.308572
VII_{1d}	-479.259627	0.255148	0.012493	432.539500	0.049119	-478.991986	-479.041105	-479.038086
VII_{1e}	-519.023614	0.299110	0.013550	448.971000	0.050985	-518.710955	-518.761939	-518.758920
VII_{2b}	-608.712970	0.208628	0.013140	450.557300	0.051165	-608.491202	-608.542367	-608.539348
VII_{2c}	-708.766640	0.210651	0.014021	465.469900	0.052858	-708.541967	-708.594826	-708.591807
VII_{2d}	-518.561602	0.282959	0.013996	458.843200	0.052106	-518.264647	-518.316753	-518.313734
VII_{2e}	-558.316532	0.327466	0.015049	475.354000	0.053981	-557.974017	-558.027998	-558.024979
VII_{3b}	-608.715068	0.208141	0.013414	457.385100	0.051940	-608.493514	-608.545454	-608.542435
VII_{3c}	-708.768369	0.210160	0.014305	472.889500	0.053701	-708.543903	-708.597604	-708.594585
VII_{3d}	-518.566076	0.282663	0.014292	467.863200	0.053130	-518.269121	-518.322252	-518.319233
VII_{3e}	-558.322430	0.327509	0.015182	479.879600	0.054495	-557.979739	-558.034234	-558.031215

[a] Forms a weak C-B interaction

Table S216. Energies of $VII_{[1-3][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
VII_{1b}[a]	-569.433008	0.180901	0.011482	416.881500	0.047341	-569.240625	-569.287966	-569.284947
VII_{1c}	-669.460437	0.182094	0.012826	445.834600	0.050629	-669.265518	-669.316147	-669.313128
VII_{1d}	-479.260401	0.255106	0.012499	432.687600	0.049136	-478.992796	-479.041932	-479.038913
VII_{1e}	-519.030046	0.299211	0.013495	448.045500	0.050880	-518.717340	-518.768220	-518.765201
VII_{2b}	-608.713694	0.208560	0.013140	450.533100	0.051162	-608.491993	-608.543156	-608.540137
VII_{2c}	-708.773626	0.210507	0.014055	466.478800	0.052973	-708.549064	-708.602037	-708.599018
VII_{2d}	-518.561576	0.282943	0.013975	458.425400	0.052058	-518.264658	-518.316716	-518.313697
VII_{2e}	-558.323058	0.327720	0.014904	471.127900	0.053501	-557.980434	-558.033935	-558.030916
VII_{3b}	-608.715912	0.208056	0.013423	457.634000	0.051969	-608.494433	-608.546402	-608.543383
VII_{3c}	-708.772724	0.210135	0.014311	472.316100	0.053636	-708.548277	-708.601913	-708.598894
VII_{3d}	-518.565967	0.282623	0.014283	467.595700	0.053100	-518.269061	-518.322161	-518.319142
VII_{3e}	-558.325663	0.327918	0.015095	478.336700	0.054320	-557.982651	-558.036970	-558.033951

[a] Forms a weak C-B interaction

Table S217. Energies of VII$_{[1-3][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
VII$_{1b}$[a]	-569.423142	0.180999	0.011560	418.752400	0.047553	-569.230582	-569.278135	-569.275116
VII$_{1c}$	-669.449587	0.182195	0.012875	446.691100	0.050726	-669.254517	-669.305243	-669.302224
VII$_{1d}$	-479.249931	0.255766	0.012447	431.770700	0.049032	-478.981717	-479.030748	-479.027729
VII$_{1e}$	-519.014436	0.299358	0.013553	449.147100	0.051005	-518.701524	-518.752529	-518.749510
VII$_{2b}$	-608.700350	0.208655	0.013213	452.174500	0.051349	-608.478483	-608.529831	-608.526812
VII$_{2c}$	-708.760608	0.210607	0.014126	468.175700	0.053166	-708.535875	-708.589041	-708.586022
VII$_{2d}$	-518.550828	0.283557	0.014001	459.626500	0.052195	-518.253270	-518.305465	-518.302446
VII$_{2e}$	-558.306529	0.327961	0.014944	472.111600	0.053613	-557.963624	-558.017236	-558.014217
VII$_{3b}$	-608.702365	0.208167	0.013501	459.456100	0.052175	-608.480697	-608.532873	-608.529854
VII$_{3c}$	-708.762103	0.210118	0.014415	475.560100	0.054004	-708.537570	-708.591574	-708.588555
VII$_{3d}$	-518.553925	0.283219	0.014291	468.046300	0.053151	-518.256415	-518.309566	-518.306547
VII$_{3e}$	-558.309646	0.328112	0.015162	479.905700	0.054498	-557.966371	-558.020869	-558.017850

[a] Forms a weak C-B interaction

Table S218. Energies of VIII$_{[1-4][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
VIII$_{1b}$[a]	-552.110754	0.166580	0.011490	413.904400	0.047003	-551.932683	-551.979686	-551.979686
VIII$_{1c}$	-652.072855	0.167091	0.012150	429.845700	0.048813	-651.893614	-651.942427	-651.942427
VIII$_{1d}$	-461.948324	0.240426	0.012711	434.600500	0.049353	-461.695187	-461.744540	-461.744540
VIII$_{1e}$	-501.630443	0.283380	0.013931	454.330900	0.051593	-501.333133	-501.384726	-501.384726
VIII$_{2b}$	-591.410093	0.194369	0.013360	451.949200	0.051323	-591.202364	-591.253687	-591.253687
VIII$_{2c}$	-691.404218	0.196316	0.014177	465.749100	0.052890	-691.193724	-691.246614	-691.246614
VIII$_{2d}$	-501.262418	0.268657	0.014331	464.512300	0.052750	-500.979430	-501.032180	-501.032180
VIII$_{2e}$	-540.936232	0.311809	0.015418	480.880900	0.054608	-540.609005	-540.663614	-540.663614
VIII$_{3b}$	-591.410812	0.194535	0.013390	452.516200	0.051387	-591.202886	-591.254274	-591.254274
VIII$_{3c}$	-691.397864	0.196169	0.014281	467.058100	0.053039	-691.187414	-691.240453	-691.240453
VIII$_{3d}$	-501.261022	0.268716	0.014319	463.451300	0.052629	-500.977987	-501.030617	-501.030617
VIII$_{3e}$	-540.940021	0.312042	0.015483	482.836800	0.054831	-540.612495	-540.667326	-540.667326
VIII$_{4b}$	-552.097777	0.166203	0.011912	424.986200	0.048261	-551.919661	-551.967922	-551.967922
VIII$_{4c}$	-652.066269	0.167392	0.012880	443.161800	0.050325	-651.885996	-651.936321	-651.936321
VIII$_{4d}$	-461.945292	0.240418	0.012922	438.868100	0.049838	-461.691951	-461.741789	-461.741789
VIII$_{4e}$	-501.636373	0.284475	0.013780	449.789600	0.051078	-501.338118	-501.389196	-501.389196

[a] Forms a weak C-B interaction

Table S219. Energies of VIII$_{[1-4][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
VIII$_{1b}$[a]	-552.124212	0.166717	0.011415	412.411100	0.046833	-551.946081	-551.992914	-551.989895
VIII$_{1c}$	-652.143586	0.168514	0.012625	437.853300	0.049722	-651.962447	-652.012169	-652.009150
VIII$_{1d}$	-461.959114	0.240115	0.012843	437.531300	0.049686	-461.706155	-461.755841	-461.752822
VIII$_{1e}$	-501.695562	0.284497	0.013614	448.280200	0.050906	-501.397452	-501.448358	-501.445339
VIII$_{2b}$	-591.423369	0.194311	0.013375	452.724900	0.051411	-591.215682	-591.267093	-591.264074
VIII$_{2c}$	-691.458196	0.196861	0.014048	463.060700	0.052585	-691.247287	-691.299872	-691.296853
VIII$_{2d}$	-501.276274	0.268672	0.014325	464.736000	0.052775	-500.993276	-501.046052	-501.043033
VIII$_{2e}$	-540.998524	0.313264	0.015297	479.440200	0.054445	-540.669964	-540.724408	-540.721389
VIII$_{3b}$	-591.423907	0.194710	0.013287	450.461900	0.051154	-591.215910	-591.267064	-591.264045
VIII$_{3c}$	-691.455424	0.196280	0.014281	468.131000	0.053161	-691.244862	-691.298023	-691.295004
VIII$_{3d}$	-501.275046	0.268764	0.014316	463.573600	0.052643	-500.991966	-501.044609	-501.041590
VIII$_{3e}$	-541.005702	0.315237	0.014591	463.597100	0.052646	-540.675873	-540.728519	-540.725500
VIII$_{4b}$	-552.109772	0.166115	0.011941	426.543900	0.048438	-551.931716	-551.980154	-551.977135
VIII$_{4c}$	-652.135584	0.168482	0.012671	438.259700	0.049768	-651.954431	-652.004199	-652.001180
VIII$_{4d}$	-461.958991	0.240560	0.012872	437.931500	0.049731	-461.705560	-461.755291	-461.752272
VIII$_{4e}$	-501.693100	0.285247	0.013708	449.794000	0.051078	-501.394146	-501.445224	-501.442205

[a] Forms a weak C-B interaction

Table S220. Energies of VIII$_{[1-4][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
VIII$_{1b}$[a]	-552.131603	0.166392	0.011413	412.240600	0.046814	-551.953798	-552.000612	-551.997593
VIII$_{1c}$	-652.174601	0.168086	0.012679	439.329400	0.049890	-651.993837	-652.043727	-652.040708
VIII$_{1d}$	-461.970836	0.240225	0.012705	434.452700	0.049336	-461.717906	-461.767242	-461.764223
VIII$_{1e}$	-501.727883	0.284258	0.013706	450.131200	0.051117	-501.429919	-501.481036	-501.478017
VIII$_{2b}$	-591.431557	0.194479	0.013174	447.960200	0.050870	-591.223904	-591.274774	-591.271755
VIII$_{2c}$	-691.487974	0.196353	0.014157	465.494100	0.052861	-691.277463	-691.330324	-691.327305
VIII$_{2d}$	-501.280940	0.268299	0.014350	465.471000	0.052859	-500.998291	-501.051149	-501.048130
VIII$_{2e}$	-541.038419	0.312891	0.015192	477.400600	0.054213	-540.710336	-540.764549	-540.761530
VIII$_{3b}$	-591.431826	0.194619	0.013232	449.325600	0.051025	-591.223975	-591.275000	-591.271981
VIII$_{3c}$	-691.486845	0.196158	0.014318	469.446300	0.053310	-691.276370	-691.329680	-691.326661
VIII$_{3d}$	-501.281429	0.268461	0.014337	464.030600	0.052695	-500.998631	-501.051326	-501.048307
VIII$_{3e}$	-541.039454	0.313757	0.014969	471.798200	0.053577	-540.710727	-540.764304	-540.761285
VIII$_{4b}$	-552.116818	0.165959	0.011938	426.501700	0.048433	-551.938921	-551.987354	-551.984335
VIII$_{4c}$	-652.168594	0.167887	0.012847	442.696800	0.050272	-651.987860	-652.038132	-652.035113
VIII$_{4d}$	-461.965448	0.240339	0.012865	437.083000	0.049635	-461.712244	-461.761879	-461.758860
VIII$_{4e}$	-501.727790	0.284676	0.013742	449.762000	0.051075	-501.429372	-501.480446	-501.477427

[a] Forms a weak C-B interaction

Table S221. Energies of VIII$_{[1-4][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
VIII$_{1b}$[a]	-552.132048	0.166273	0.011415	412.217100	0.046811	-551.954360	-552.001171	-551.998152
VIII$_{1c}$	-652.178357	0.167620	0.012022	426.951800	0.048484	-651.998715	-652.047199	-652.044180
VIII$_{1d}$	-461.971298	0.240247	0.012686	434.062200	0.049292	-461.718366	-461.767657	-461.764638
VIII$_{1e}$	-501.735282	0.284240	0.013708	450.367400	0.051143	-501.437335	-501.488479	-501.485460
VIII$_{2b}$	-591.432468	0.194341	0.013183	448.136400	0.050890	-591.224943	-591.275833	-591.272814
VIII$_{2c}$	-691.496618	0.196175	0.014152	465.266800	0.052835	-691.286291	-691.339126	-691.336107
VIII$_{2d}$	-501.282125	0.268311	0.014292	463.759400	0.052664	-500.999522	-501.052186	-501.049167
VIII$_{2e}$	-541.046635	0.312838	0.015207	477.529600	0.054228	-540.718591	-540.772819	-540.769800
VIII$_{3b}$	-591.432715	0.194487	0.013251	449.653900	0.051062	-591.224977	-591.276039	-591.273020
VIII$_{3c}$	-691.494156	0.196152	0.014300	469.177100	0.053279	-691.283704	-691.336983	-691.333964
VIII$_{3d}$	-501.281261	0.268386	0.014324	463.676900	0.052655	-500.998551	-501.051206	-501.048187
VIII$_{3e}$	-541.042964	0.313273	0.015150	474.867400	0.053926	-540.714541	-540.768467	-540.765448
VIII$_{4b}$	-552.118030	0.165854	0.011904	424.897800	0.048251	-551.940273	-551.988524	-551.985505
VIII$_{4c}$	-652.176581	0.167943	0.012801	441.588200	0.050146	-651.995837	-652.045983	-652.042964
VIII$_{4d}$	-461.965789	0.240334	0.012839	436.421600	0.049560	-461.712616	-461.762176	-461.759157
VIII$_{4e}$	-501.729851	0.285387	0.013565	447.019700	0.050763	-501.430899	-501.481662	-501.478643

[a] Forms a weak C-B interaction

Table S222. Energies of VIII$_{[1-4][b-e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
VIII$_{1b}$[a]	-552.122280	0.166318	0.011433	412.536400	0.046847	-551.944529	-551.991376	-551.988357
VIII$_{1c}$	-652.172421	0.168165	0.012664	438.985600	0.049851	-651.991591	-652.041442	-652.038423
VIII$_{1d}$	-461.963742	0.240897	0.012611	432.710300	0.049138	-461.710235	-461.759373	-461.756354
VIII$_{1e}$	-501.721968	0.284459	0.013686	449.879400	0.051088	-501.423824	-501.474912	-501.471893
VIII$_{2b}$	-591.422020	0.194433	0.013191	448.210800	0.050898	-591.214397	-591.265295	-591.262276
VIII$_{2c}$	-691.484569	0.196343	0.014154	465.181100	0.052826	-691.274072	-691.326897	-691.323878
VIII$_{2d}$	-501.272476	0.268905	0.014271	463.948000	0.052686	-500.989300	-501.041986	-501.038967
VIII$_{2e}$	-541.033427	0.313027	0.015189	477.068200	0.054176	-540.705211	-540.759387	-540.756368
VIII$_{3b}$	-591.421884	0.194503	0.013289	450.354100	0.051142	-591.214092	-591.265234	-591.262215
VIII$_{3c}$	-691.482528	0.196296	0.014284	467.647900	0.053106	-691.271948	-691.325054	-691.322035
VIII$_{3d}$	-501.270395	0.269132	0.014257	463.695700	0.052657	-500.987006	-501.039663	-501.036644
VIII$_{3e}$	-541.029666	0.313420	0.015167	475.104000	0.053952	-540.701079	-540.755031	-540.752012
VIII$_{4b}$	-552.107330	0.165977	0.011958	426.928500	0.048482	-551.929395	-551.977877	-551.974858
VIII$_{4c}$	-652.167048	0.168016	0.012813	441.719500	0.050161	-651.986219	-652.036380	-652.033361
VIII$_{4d}$	-461.957173	0.241073	0.012681	433.075900	0.049180	-461.703420	-461.752599	-461.749580
VIII$_{4e}$	-501.721528	0.284974	0.013700	448.756900	0.050960	-501.422854	-501.473815	-501.470796

[a] Forms a weak C-B interaction

Table S223. Energies of $IX_{[1-2,4][b-e]}$ in Gas. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Gas)
IX_{1b}	-544.916142	0.116756	0.010145	398.144100	0.045213	-544.789241	-544.834454	-544.834454
IX_{1c}	-644.913916	0.118645	0.011022	412.739300	0.046870	-644.784250	-644.831120	-644.831120
IX_{1d}	-454.769821	0.190799	0.011029	408.302800	0.046367	-454.567992	-454.614359	-454.614359
IX_{1e}	-494.447174	0.233723	0.012207	427.351700	0.048530	-494.201244	-494.249773	-494.249773
IX_{2b}	-584.233074	0.144822	0.011793	429.569000	0.048782	-584.076460	-584.125241	-584.125241
IX_{2c}	-684.228394	0.146682	0.012516	438.611800	0.049808	-684.069195	-684.119004	-684.119004
IX_{2d}	-494.084483	0.218913	0.012739	440.449300	0.050017	-493.852831	-493.902848	-493.902848
IX_{2e}	-533.757736	0.261961	0.013956	459.852800	0.052221	-533.481819	-533.534039	-533.534039
IX_{4b}	-544.915717	0.116754	0.010187	399.999300	0.045424	-544.788776	-544.834200	-544.834200
IX_{4c}	-644.895527	0.118117	0.011121	416.614800	0.047310	-644.766288	-644.813599	-644.813599
IX_{4d}	-454.770402	0.190715	0.011139	411.378200	0.046716	-454.568548	-454.615264	-454.615264
IX_{4e}	-494.455551	0.233905	0.012242	428.663200	0.048679	-494.209404	-494.258083	-494.258083

Table S224. Energies of $IX_{[1-2,4][b-e]}$ in SMD Toluene. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Toluene)
IX_{1b}	-544.932365	0.116674	0.010149	398.768800	0.045284	-544.805543	-544.850826	-544.847807
IX_{1c}	-644.973554	0.118721	0.010972	411.392000	0.046717	-644.843861	-644.890579	-644.887560
IX_{1d}	-454.790825	0.190686	0.011042	408.461200	0.046385	-454.589097	-454.635482	-454.632463
IX_{1e}	-494.519048	0.234353	0.012054	424.735400	0.048233	-494.272640	-494.320873	-494.317854
IX_{2b}	-584.250808	0.144668	0.011825	430.880400	0.048930	-584.094316	-584.143246	-584.140227
IX_{2c}	-684.287912	0.147496	0.012321	435.380100	0.049441	-684.128095	-684.177537	-684.174518
IX_{2d}	-494.102826	0.218978	0.012721	440.033700	0.049970	-493.871126	-493.921096	-493.918077
IX_{2e}	-533.828356	0.262824	0.013767	456.609100	0.051852	-533.551765	-533.603617	-533.600598
IX_{4b}	-544.933788	0.116457	0.010133	397.832700	0.045178	-544.807198	-544.852376	-544.849357
IX_{4c}	-644.963519	0.118621	0.010249	399.653300	0.045384	-644.834650	-644.880034	-644.877015
IX_{4d}	-454.791063	0.190727	0.011093	410.037100	0.046564	-454.589242	-454.635806	-454.632787
IX_{4e}	-494.512556	0.234371	0.011581	415.645700	0.047200	-494.266604	-494.313805	-494.310786

Table S225. Energies of $IX_{[1-2,4][b-e]}$ in SMD DCM. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
IX_{1b}	-544.939520	0.116305	0.010117	397.249800	0.045111	-544.813098	-544.858210	-544.855191
IX_{1c}	-645.001452	0.118624	0.010989	412.849800	0.046883	-644.871839	-644.918722	-644.915703
IX_{1d}	-454.797947	0.190689	0.011018	407.910600	0.046322	-454.596240	-454.642562	-454.639543
IX_{1e}	-494.552483	0.234417	0.012065	424.836700	0.048244	-494.306000	-494.354245	-494.351226
IX_{2b}	-584.258190	0.144602	0.011658	424.795200	0.048239	-584.101929	-584.150169	-584.147150
IX_{2c}	-684.318658	0.146753	0.012569	441.545800	0.050142	-684.159336	-684.209478	-684.206459
IX_{2d}	-494.108622	0.218793	0.012720	440.501300	0.050023	-493.877109	-493.927132	-493.924113
IX_{2e}	-533.862894	0.263071	0.013490	449.580400	0.051054	-533.586333	-533.637387	-533.634368
IX_{4b}	-544.940307	0.116264	0.010152	398.139100	0.045212	-544.813892	-544.859104	-544.856085
IX_{4c}	-644.998180	0.118412	0.011073	415.647400	0.047201	-644.868695	-644.915896	-644.912877
IX_{4d}	-454.797718	0.190673	0.011076	409.889800	0.046547	-454.595969	-454.642516	-454.639497
IX_{4e}	-494.555151	0.234341	0.012152	426.933100	0.048482	-494.308658	-494.357140	-494.354121

Table S226. Energies of $IX_{[1-2,4][b-e]}$ in SMD MeCN. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
IX_{1b}	-544.940971	0.116268	0.010121	397.420600	0.045131	-544.814582	-544.859713	-544.856694
IX_{1c}	-645.008861	0.118500	0.011023	413.986500	0.047012	-644.879339	-644.926351	-644.923332
IX_{1d}	-454.798912	0.190766	0.010998	407.541700	0.046280	-454.597149	-454.643429	-454.640410
IX_{1e}	-494.560869	0.234602	0.012031	424.175100	0.048169	-494.314236	-494.362405	-494.359386
IX_{2b}	-584.259491	0.144542	0.011665	424.941500	0.048256	-584.103284	-584.151540	-584.148521
IX_{2c}	-684.326168	0.146646	0.012595	442.292600	0.050226	-684.166927	-684.217154	-684.214135
IX_{2d}	-494.108651	0.218819	0.012677	439.243700	0.049880	-493.877156	-493.927036	-493.924017
IX_{2e}	-533.871205	0.263237	0.013499	450.365800	0.051143	-533.594470	-533.645613	-533.642594
IX_{4b}	-544.941473	0.116258	0.010153	398.205400	0.045220	-544.815062	-544.860282	-544.857263
IX_{4c}	-645.007365	0.118182	0.010330	400.972800	0.045534	-644.878853	-644.924388	-644.921369
IX_{4d}	-454.798438	0.190630	0.011068	409.801700	0.046537	-454.596741	-454.643277	-454.640258
IX_{4e}	-494.562154	0.234431	0.012110	426.171800	0.048396	-494.315613	-494.364009	-494.360990

Table S227. Energies of $IX_{[1\text{-}2,4][b\text{-}e]}$ in SMD Water. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(Water)
IX_{1b}	-544.926678	0.116383	0.010134	397.134200	0.045098	-544.800161	-544.845259	-544.842240
IX_{1c}	-644.995529	0.118641	0.011010	413.462800	0.046953	-644.865878	-644.912831	-644.909812
IX_{1d}	-454.787900	0.191478	0.010913	405.949600	0.046099	-454.585509	-454.631608	-454.628589
IX_{1e}	-494.545289	0.235006	0.011958	422.284700	0.047954	-494.298325	-494.346279	-494.343260
IX_{2b}	-584.246910	0.144552	0.011687	425.239700	0.048290	-584.090671	-584.138961	-584.135942
IX_{2c}	-684.313866	0.146651	0.012634	443.159400	0.050325	-684.154581	-684.204906	-684.201887
IX_{2d}	-494.096968	0.219451	0.012581	437.308400	0.049660	-493.864936	-493.914596	-493.911577
IX_{2e}	-533.855564	0.263333	0.013522	450.792800	0.051192	-533.578709	-533.629900	-533.626881
IX_{4b}	-544.926239	0.116058	0.009455	384.499900	0.043664	-544.800727	-544.844390	-544.841371
IX_{4c}	-644.993313	0.118311	0.010346	401.287000	0.045570	-644.864656	-644.910226	-644.907207
IX_{4d}	-454.787540	0.191046	0.010283	394.255800	0.044771	-454.586211	-454.630982	-454.627963
IX_{4e}	-494.529775	0.234316	0.011653	417.300000	0.047388	-494.283806	-494.331194	-494.328175

Table S228. Orbital Energies and Philicity Parameters of $I_{[1-2][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
I_{1b}[a]	-8.740843	-0.448716	4.594779	8.292127	1.273015	2.182626		
I_{1c}	-4.004972	1.854728	1.075122	5.859701	0.098630	6.918496	-1.174384 (-0.8946)[b]	4.735870 (3.4354)[b]
I_{1d}	-7.426533	-0.216603	3.821568	7.209930	1.012796	3.496936		
I_{1e}	-11.395586	-3.444418	7.420002	7.951168	3.462160	-0.472118	2.449363	-3.969053
I_{2b}	-7.462179	-0.371708	3.916944	7.090472	1.081906	3.461289		
I_{2c}	-3.474895	1.978268	0.748313	5.453163	0.051344	7.448574	-1.030562	3.987285
I_{2d}	-7.300544	-0.255515	3.778029	7.045029	1.013020	3.622924		
I_{2e}	-10.707138	-3.591903	7.149521	7.115234	3.591986	0.216331	2.578966	-3.406594

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S229. Orbital Energies and Philicity Parameters of $I_{[1-2][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
I_{1b}[a]	-7.781097	-0.140139	3.960618	7.640958	1.026474	2.858829		
I_{1c}	-6.214537	0.800015	2.707261	7.014552	0.522433	4.425388	-0.504041 (-0.4507)[b]	1.566560 (1.1549)[b]
I_{1d}	-7.556059	-0.088165	3.822112	7.467894	0.978090	3.083867		
I_{1e}	-9.361262	-1.363019	5.362140	7.998244	1.797429	1.278663	0.819339	-1.805204
I_{2b}	-7.602046	-0.220684	3.911365	7.381362	1.036311	3.037880		
I_{2c}	-5.618336	0.875390	2.371473	6.493726	0.433024	5.021590	-0.603287	1.983710
I_{2d}	-7.516602	-0.111839	3.814221	7.404763	0.982359	3.123323		
I_{2e}	-8.932139	-1.430775	5.181457	7.501364	1.789508	1.707787	0.807148	-1.415537

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S230. Orbital Energies and Philicity Parameters of $I_{[1-2][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
I_{1b}	-7.866813	-0.081090	3.973951	7.785723	1.014183	2.540183		
I_{1c}	-7.278230	0.250889	3.513671	7.529119	0.819876	3.128766	-0.194307	0.588582
I_{1d}	-7.660278	-0.019320	3.839799	7.640958	0.964804	2.746718		
I_{1e}	-8.468185	-0.360551	4.414368	8.107634	1.201747	1.938812	0.236942	-0.807906
I_{2b}	-7.556875	-0.119186	3.838031	7.437689	0.990259	2.850121		
I_{2c}	-6.740533	0.242998	3.248768	6.983531	0.755670	3.666463	-0.234589	0.816342
I_{2d}	-7.629530	-0.030205	3.829867	7.599325	0.965078	2.777467		
I_{2e}	-8.276344	-0.392116	4.334230	7.884228	1.191337	2.130652	0.226259	-0.646815

Table S231. Orbital Energies and Philicity Parameters of $I_{[1-2][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
I_{1b}	-7.879058	-0.069661	3.974360	7.809397	1.011316	2.441678		
I_{1c}	-7.567760	0.052790	3.757485	7.620550	0.926357	2.752976	-0.084959	0.311298
I_{1d}	-7.689122	-0.004082	3.846602	7.685041	0.962672	2.631614		
I_{1e}	-8.210493	-0.105580	4.158036	8.104913	1.066592	2.110243	0.103920	-0.521370
I_{2b}	-7.567488	-0.098777	3.833132	7.468710	0.983631	2.753248		
I_{2c}	-7.054553	0.032654	3.510950	7.087207	0.869649	3.266183	-0.113981	0.512935
I_{2d}	-7.658374	-0.010885	3.834629	7.647489	0.961386	2.662362		
I_{2e}	-8.045864	-0.122995	4.084430	7.922868	1.052811	2.274872	0.091425	-0.387490

Table S232. Orbital Energies and Philicity Parameters of $I_{[1-2][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
I_{1b}	-7.972937	-0.037007	4.004972	7.935930	1.010581	2.320587		
I_{1c}	-7.604495	0.010612	3.796941	7.615107	0.946590	2.689030	-0.063992	0.368442
I_{1d}	-7.745994	-0.000272	3.873133	7.745722	0.968351	2.547530		
I_{1e}	-8.160696	-0.060954	4.110825	8.099742	1.043174	2.132829	0.074823	-0.414702
I_{2b}	-7.567488	-0.095240	3.831364	7.472248	0.982258	2.726037		
I_{2c}	-7.108159	-0.008980	3.558570	7.099180	0.891893	3.185365	-0.090365	0.459328
I_{2d}	-7.642047	-0.001088	3.821568	7.640958	0.955664	2.651478		
I_{2e}	-7.995251	-0.075648	4.035449	7.919603	1.028135	2.298274	0.072471	-0.353204

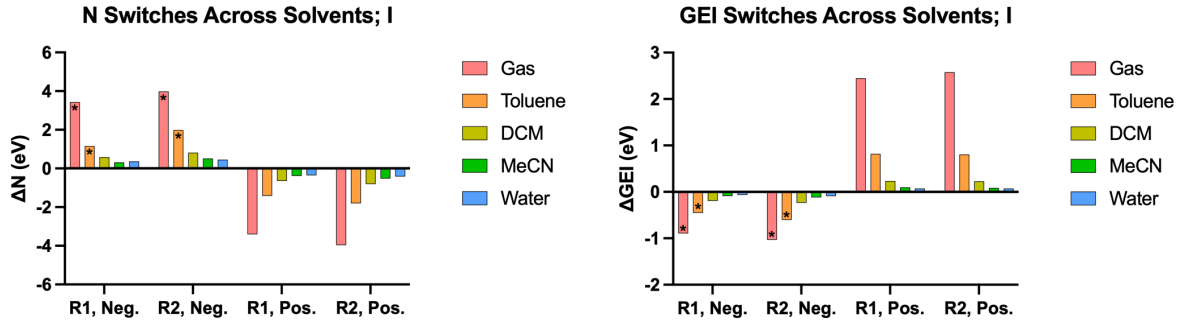


Figure S140. I Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S233. Orbital Energies and Philicity Parameters of $II_{[1-2][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
II_{1b}[a]	-6.102426	-0.585861	3.344144	5.516565	1.013611	4.821042		
II_{1c}	-2.647124	1.712413	0.467356	4.359537	0.025051	8.276344	-0.988560 (-0.9406)[b]	3.455302 (3.2281)[b]
II_{1d}	-5.936981	-0.494975	3.215978	5.442006	0.950248	4.986487		
II_{1e}	-9.852428	-3.288496	6.570462	6.563931	3.288500	1.071040	2.338251	-3.915447
II_{2b}	-6.001472	-0.627767	3.314619	5.373705	1.022265	4.921996		
II_{2c}	-2.723044	1.946703	0.388170	4.669747	0.016133	8.200425	-1.006132	3.278428
II_{2d}	-5.893443	-0.470213	3.181828	5.423230	0.933395	5.030025		
II_{2e}	-9.539769	-3.870276	6.705023	5.669493	3.964845	1.383699	3.031451	-3.646326

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S234. Orbital Energies and Philicity Parameters of $II_{[1-2][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
II_{1b}	-6.751146	-0.332795	3.541971	6.418351	0.977319	3.888780		
II_{1c}	-4.900771	0.627223	2.136774	5.527994	0.412971	5.739154	-0.564348	1.850375
II_{1d}	-6.330730	-0.248440	3.289585	6.082290	0.889580	4.309196		
II_{1e}	-7.910351	-1.374992	4.642671	6.535360	1.649060	2.729575	0.759480	-1.579621
II_{2b}	-6.355220	-0.360007	3.357613	5.995213	0.940214	4.284705		
II_{2c}	-5.028393	0.800015	2.114189	5.828408	0.383449	5.611533	-0.556765	1.326827
II_{2d}	-6.298620	-0.230208	3.264414	6.068412	0.878022	4.341305		
II_{2e}	-7.764226	-1.509960	4.637093	6.254266	1.719037	2.875700	0.841015	-1.465605

Table S235. Orbital Energies and Philicity Parameters of $II_{[1-2][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
II_{1b}	-7.021627	-0.132519	3.577073	6.889108	0.928673	3.385369		
II_{1c}	-6.308417	0.145853	3.081282	6.454270	0.735505	4.098580	-0.193168	0.713211
II_{1d}	-6.785976	-0.091974	3.438975	6.694002	0.883369	3.621020		
II_{1e}	-7.323674	-0.404089	3.863881	6.919584	1.078792	3.083323	0.195422	-0.537697
II_{2b}	-6.808290	-0.183405	3.495847	6.624885	0.922352	3.598706		
II_{2c}	-6.400391	0.195106	3.102643	6.595497	0.729770	4.006605	-0.192582	0.407899
II_{2d}	-6.789242	-0.075103	3.432173	6.714138	0.877239	3.617754		
II_{2e}	-7.279319	-0.432933	3.856126	6.846386	1.085953	3.127677	0.208714	-0.490077

Table S236. Orbital Energies and Philicity Parameters of $II_{[1-2][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
II_{1b}	-7.177276	-0.092519	3.634897	7.084758	0.932458	3.143460		
II_{1c}	-6.779446	-0.003265	3.391356	6.776180	0.848656	3.541290	-0.083802	0.397831
II_{1d}	-7.010743	-0.053062	3.531902	6.957680	0.896443	3.309993		
II_{1e}	-7.245305	-0.147758	3.696531	7.097547	0.962610	3.075431	0.066167	-0.234562
II_{2b}	-7.003395	-0.133336	3.568366	6.870060	0.926719	3.317341		
II_{2c}	-6.832508	0.006531	3.412989	6.839039	0.851618	3.488228	-0.075102	0.170888
II_{2d}	-6.994416	-0.035103	3.514759	6.959313	0.887554	3.326320		
II_{2e}	-7.229794	-0.147758	3.688776	7.082036	0.960675	3.090942	0.073121	-0.235379

Table S237. Orbital Energies and Philicity Parameters of $II_{[1-2][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
II_{1b}	-7.212107	-0.087893	3.650000	7.124214	0.935015	3.081418		
II_{1c}	-6.872237	-0.036463	3.454350	6.835773	0.872801	3.421288	-0.062215	0.339870
II_{1d}	-7.046389	-0.044627	3.545508	7.001763	0.897676	3.247135		
II_{1e}	-7.236869	-0.103948	3.670408	7.132922	0.944346	3.056655	0.046670	-0.190480
II_{2b}	-7.045845	-0.124628	3.585237	6.921217	0.928588	3.247679		
II_{2c}	-6.915503	-0.031021	3.473262	6.884482	0.876141	3.378022	-0.052448	0.130343
II_{2d}	-7.045301	-0.028300	3.536800	7.017001	0.891332	3.248224		
II_{2e}	-7.224080	-0.097145	3.660612	7.126935	0.940101	3.069445	0.048769	-0.178779

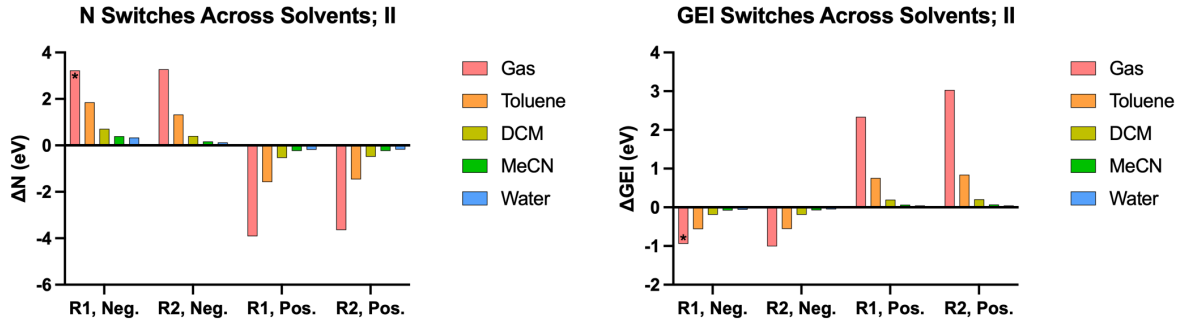


Figure S141. II Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S238. Orbital Energies and Philicity Parameters of $III_{[1-4][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
III_{1b}[a]	-8.271174	-0.692258	4.481716	7.578916	1.325109	2.652294		
III_{1c}	-3.083595	1.741801	0.670897	4.825396	0.046639	7.839874	-1.278470 (-0.9223)[b]	5.187579 (3.3656)[b]
III_{1d}	-6.462433	-0.367082	3.414757	6.095351	0.956513	4.461035		
III_{1e}	-10.429854	-3.413397	6.921625	7.016457	3.414038	0.493615	2.457524	-3.967421
III_{2b}	-6.448283	-0.571711	3.509997	5.876572	1.048237	4.475185		
III_{2c}	-3.103459	1.985343	0.559058	5.088802	0.030709	7.820009	-1.017528	3.344824
III_{2d}	-6.383792	-0.409804	3.396798	5.973989	0.965706	4.539676		
III_{2e}	-9.789842	-3.745920	6.767881	6.043922	3.789279	1.133627	2.823573	-3.406050
III_{3b}	-6.607742	-0.525996	3.566869	6.081746	1.045962	4.315726		
III_{3c}	-3.307000	2.107250	0.599875	5.414250	0.033232	7.616468	-1.012731	3.300742
III_{3d}	-6.417534	-0.404905	3.411220	6.012629	0.967665	4.505934		
III_{3e}	-9.861136	-3.760342	6.810739	6.100794	3.801650	1.062333	2.833985	-3.443601
III_{4b}	-6.954415	-0.519738	3.737076	6.434677	1.085193	3.969053		
III_{4c}	-3.114071	1.758944	0.677564	4.873016	0.047106	7.809397	-1.038088	3.840343
III_{4d}	-6.550054	-0.355381	3.452717	6.194673	0.962218	4.373415		
III_{4e}	-10.446725	-3.293939	6.870332	7.152786	3.299516	0.476744	2.337297	-3.896671

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S239. Orbital Energies and Philicity Parameters of $III_{[1-4][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
III_{1b}[a]	-8.091579	-0.317285	4.204432	7.774294	1.136904	2.548347		
III_{1c}	-5.408536	0.698244	2.355146	6.106780	0.454144	5.231390	-0.682760 (-0.4630)[b]	2.683043 (1.1034)[b]
III_{1d}	-6.800671	-0.169799	3.485235	6.630872	0.915933	3.839255		
III_{1e}	-8.454035	-1.385604	4.919819	7.068431	1.712164	2.185891	0.796231	-1.653364
III_{2b}	-6.755500	-0.332251	3.543875	6.423249	0.977625	3.884426		
III_{2c}	-5.229213	0.827770	2.200721	6.056983	0.399801	5.410713	-0.577824	1.526287
III_{2d}	-6.686927	-0.209800	3.448363	6.477127	0.917939	3.952999		
III_{2e}	-8.104913	-1.505334	4.805123	6.599578	1.749294	2.535013	0.831356	-1.417986
III_{3b}	-6.876318	-0.287897	3.582107	6.588422	0.973791	3.763607		
III_{3c}	-5.551124	0.927636	2.311744	6.478760	0.412437	5.088802	-0.561354	1.325195
III_{3d}	-6.772915	-0.183949	3.478432	6.588966	0.918163	3.867011		
III_{3e}	-8.189540	-1.515130	4.852335	6.674410	1.763838	2.450386	0.845675	-1.416625
III_{4b}	-7.121221	-0.242726	3.681973	6.878495	0.985457	3.518705		
III_{4c}	-5.292071	0.720013	2.286029	6.012085	0.434619	5.347854	-0.550839	1.829150
III_{4d}	-6.859175	-0.155377	3.507276	6.703798	0.917464	3.780751		
III_{4e}	-8.463559	-1.339617	4.901588	7.123942	1.686255	2.176367	0.768791	-1.604384

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S240. Orbital Energies and Philicity Parameters of $III_{[1-4][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
III_{1b}[a]	-7.999332	-0.113744	4.056538	7.885589	1.043391	2.407664		
III_{1c}	-6.764752	0.188575	3.288088	6.953326	0.777435	3.642245	-0.265955	1.234581
III_{1d}	-7.166664	-0.050885	3.608775	7.115778	0.915097	3.240332		
III_{1e}	-7.738375	-0.386946	4.062661	7.351429	1.122585	2.668621	0.207488	-0.571711
III_{2b}	-7.011831	-0.179867	3.595849	6.831964	0.946297	3.395165		
III_{2c}	-6.399030	0.198371	3.100330	6.597402	0.728472	4.007966	-0.217825	0.612801
III_{2d}	-7.061084	-0.069389	3.565236	6.991695	0.909001	3.345913		
III_{2e}	-7.594699	-0.427219	4.010959	7.167480	1.122277	2.812297	0.213276	-0.533615
III_{3b}	-7.239318	-0.140955	3.690137	7.098363	0.959172	3.167678		
III_{3c}	-6.792779	0.228031	3.282374	7.020811	0.767289	3.614217	-0.191884	0.446539
III_{3d}	-7.186800	-0.042178	3.614489	7.144623	0.914291	3.220196		
III_{3e}	-7.665721	-0.414974	4.040347	7.250747	1.125705	2.741275	0.211414	-0.478920
III_{4b}	-7.397688	-0.092247	3.744968	7.305442	0.959886	3.009308		
III_{4c}	-6.501617	0.215786	3.142916	6.717404	0.735248	3.905379	-0.224638	0.896071
III_{4d}	-7.243672	-0.037824	3.640748	7.205848	0.919742	3.163324		
III_{4e}	-7.791165	-0.369803	4.080484	7.421362	1.121785	2.615831	0.202043	-0.547493

[a] Forms a weak C-B interaction

Table S241. Orbital Energies and Philicity Parameters of $III_{[1-4][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
III_{1b}	-7.328027	-0.077552	3.702790	7.250475	0.945500	2.992709		
III_{1c}	-7.071152	0.018504	3.526324	7.089656	0.876979	3.249584	-0.068521	0.256876
III_{1d}	-7.246393	-0.022858	3.634625	7.223536	0.914407	3.074343		
III_{1e}	-7.557964	-0.128438	3.843201	7.429526	0.994020	2.762772	0.079613	-0.311570
III_{2b}	-7.062172	-0.136057	3.599114	6.926115	0.935129	3.258564		
III_{2c}	-6.702437	0.004082	3.349178	6.706519	0.836275	3.618299	-0.098854	0.359735
III_{2d}	-7.154147	-0.037007	3.595577	7.117139	0.908242	3.166589		
III_{2e}	-7.490207	-0.146397	3.818302	7.343810	0.992634	2.830529	0.084392	-0.336061
III_{3b}	-7.335919	-0.104492	3.720205	7.231427	0.956929	2.984817		
III_{3c}	-7.111697	0.016599	3.547549	7.128296	0.882757	3.209039	-0.074172	0.224222
III_{3d}	-7.313605	-0.009524	3.661565	7.304081	0.917778	3.007131		
III_{3e}	-7.587080	-0.130343	3.858711	7.456737	0.998403	2.733656	0.080624	-0.273474
III_{4b}	-7.442043	-0.069661	3.755852	7.372382	0.956707	2.878693		
III_{4c}	-7.034416	0.021225	3.506596	7.055641	0.871375	3.286320	-0.085333	0.407627
III_{4d}	-7.403403	-0.013061	3.708232	7.390341	0.930335	2.917333		
III_{4e}	-7.671163	-0.116465	3.893814	7.554698	1.003467	2.649573	0.073132	-0.267760

Table S242. Orbital Energies and Philicity Parameters of $III_{[1-4][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
III_{1b}	-7.342449	-0.074831	3.708640	7.267618	0.946253	2.951075		
III_{1c}	-7.134282	-0.016599	3.575441	7.117683	0.898029	3.159242	-0.048224	0.208167
III_{1d}	-7.309796	-0.014422	3.662109	7.295374	0.919147	2.983729		
III_{1e}	-7.531841	-0.084355	3.808098	7.447485	0.973591	2.761684	0.054444	-0.222045
III_{2b}	-7.090744	-0.130615	3.610679	6.960129	0.936549	3.202781		
III_{2c}	-6.768017	-0.033742	3.400880	6.734275	0.858740	3.525508	-0.077809	0.322727
III_{2d}	-7.202311	-0.030477	3.616394	7.171834	0.911782	3.091214		
III_{2e}	-7.461635	-0.100682	3.781159	7.360953	0.971149	2.831889	0.059366	-0.259325
III_{3b}	-7.350341	-0.099866	3.725103	7.250475	0.956930	2.943184		
III_{3c}	-7.172378	-0.022313	3.597346	7.150065	0.904950	3.121146	-0.051980	0.177962
III_{3d}	-7.340545	-0.004354	3.672449	7.336191	0.919202	2.952980		
III_{3e}	-7.577012	-0.080274	3.828643	7.496738	0.977659	2.716513	0.058457	-0.236467
III_{4b}	-7.457281	-0.068028	3.762655	7.389253	0.957984	2.836243		
III_{4c}	-6.857270	-0.001361	3.429315	6.855910	0.857669	3.436254	-0.100315	0.600011
III_{4d}	-7.437417	-0.005170	3.721294	7.432247	0.931618	2.856107		
III_{4e}	-7.654836	-0.071838	3.863337	7.582998	0.984134	2.638688	0.052516	-0.217419

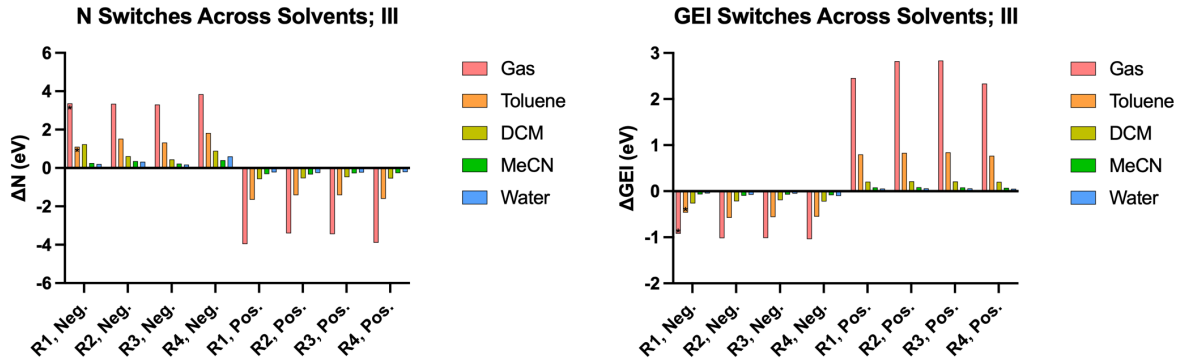


Figure S142. III Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S243. Orbital Energies and Philicity Parameters of $IV_{[1-3][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IV_{1b}	-8.769959	-0.371163	4.570561	8.398796	1.243632	2.153509		
IV_{1c}	-4.447430	2.223443	1.111993	6.670872	0.092681	6.476039	-1.150951	4.322529
IV_{1d}	-7.999877	-0.307761	4.153819	7.692116	1.121552	2.923592		
IV_{1e}	-12.108524	-3.697484	7.903004	8.411041	3.712827	-1.185056	2.591275	-4.108648
IV_{2b}	-8.048585	-0.526268	4.287427	7.522317	1.221833	2.874883		
IV_{2c}	-3.960890	2.329567	0.815661	6.290457	0.052882	6.962578	-1.168951	4.087695
IV_{2d}	-7.863547	-0.355925	4.109736	7.507623	1.124852	3.059921		
IV_{2e}	-11.418716	-3.835990	7.627353	7.582726	3.836121	-0.495247	2.711269	-3.555168
IV_{3b}	-8.053483	-0.366265	4.209874	7.687218	1.152760	2.869985		
IV_{3c}	-4.297767	1.963846	1.166960	6.261613	0.108742	6.625701	-1.044019	3.755716
IV_{3d}	-7.844227	-0.283815	4.064021	7.560413	1.092286	3.079241		
IV_{3e}	-11.416267	-3.663742	7.540004	7.752525	3.666654	-0.492798	2.574368	-3.572039

Table S244. Orbital Energies and Philicity Parameters of $IV_{[1-3][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IV_{1b}	-8.688597	-0.162452	4.425524	8.526145	1.148542	1.951329		
IV_{1c}	-6.705975	0.980426	2.862774	7.686401	0.533115	3.933951	-0.615426	1.982622
IV_{1d}	-7.924773	-0.127621	4.026197	7.797152	1.039499	2.715152		
IV_{1e}	-10.001819	-1.464517	5.733168	8.537301	1.925035	0.638107	0.885536	-2.077045
IV_{2b}	-8.172941	-0.293611	4.233276	7.879330	1.137192	2.466985		
IV_{2c}	-6.449372	0.905323	2.772024	7.354694	0.522396	4.190554	-0.614797	1.723569
IV_{2d}	-7.918787	-0.151840	4.035313	7.766947	1.048272	2.721139		
IV_{2e}	-9.552831	-1.517307	5.535069	8.035523	1.906347	1.087095	0.858074	-1.634044
IV_{3b}	-8.182465	-0.221229	4.201847	7.961236	1.108843	2.457461		
IV_{3c}	-6.409371	0.863145	2.773113	7.272516	0.528713	4.230555	-0.580129	1.773094
IV_{3d}	-7.867629	-0.125445	3.996537	7.742185	1.031512	2.772296		
IV_{3e}	-9.588205	-1.458803	5.523504	8.129403	1.876466	1.051720	0.844954	-1.720576

Table S245. Orbital Energies and Philicity Parameters of $IV_{[1-3][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IV_{1b}	-8.466552	-0.100682	4.283617	8.365870	1.096681	1.940444		
IV_{1c}	-7.772934	0.282182	3.745376	8.055116	0.870741	2.634063	-0.225940	0.693618
IV_{1d}	-7.902188	-0.020953	3.961570	7.881235	0.995659	2.504808		
IV_{1e}	-9.099761	-0.380415	4.740088	8.719346	1.288424	1.307235	0.292766	-1.197573
IV_{2b}	-8.202329	-0.148574	4.175452	8.053755	1.082377	2.204667		
IV_{2c}	-7.540004	0.243542	3.648231	7.783546	0.854982	2.866992	-0.227395	0.662325
IV_{2d}	-7.831710	-0.029388	3.930549	7.802322	0.990040	2.575286		
IV_{2e}	-8.838532	-0.407355	4.622943	8.431177	1.267415	1.568465	0.277375	-1.006821
IV_{3b}	-8.166138	-0.131703	4.148921	8.034435	1.071235	2.240858		
IV_{3c}	-7.495377	0.243814	3.625782	7.739191	0.849332	2.911619	-0.221903	0.670761
IV_{3d}	-7.777287	-0.030205	3.903746	7.747083	0.983547	2.629709		
IV_{3e}	-8.854042	-0.400824	4.627433	8.453218	1.266567	1.552954	0.283021	-1.076755

Table S246. Orbital Energies and Philicity Parameters of $IV_{[1-3][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IV_{1b}	-8.450497	-0.072654	4.261576	8.377843	1.083873	1.870239		
IV_{1c}	-8.045864	0.063675	3.991095	8.109538	0.982105	2.274872	-0.101768	0.404633
IV_{1d}	-7.894841	0.002993	3.945924	7.897834	0.985733	2.425895		
IV_{1e}	-8.820572	-0.103131	4.461852	8.717441	1.141856	1.500164	0.156123	-0.925731
IV_{2b}	-8.120695	-0.100138	4.110417	8.020557	1.053264	2.200041		
IV_{2c}	-7.828989	0.029388	3.899800	7.858377	0.967658	2.491747	-0.085606	0.291706
IV_{2d}	-7.799329	0.000544	3.899392	7.799873	0.974712	2.521407		
IV_{2e}	-8.634446	-0.120002	4.377224	8.514444	1.125152	1.686290	0.150440	-0.835118
IV_{3b}	-8.149811	-0.106941	4.128376	8.042871	1.059540	2.170925		
IV_{3c}	-7.778376	0.028300	3.875038	7.806676	0.961736	2.542360	-0.097804	0.371435
IV_{3d}	-7.785451	-0.005170	3.895310	7.780281	0.975122	2.535285		
IV_{3e}	-8.642610	-0.127349	4.384979	8.515260	1.129034	1.678126	0.153913	-0.857159

Table S247. Orbital Energies and Philicity Parameters of $IV_{[1-3][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IV_{1b}	-8.489409	-0.059321	4.274365	8.430089	1.083630	1.804115		
IV_{1c}	-8.132396	0.033198	4.049599	8.165594	1.004168	2.161129	-0.079462	0.357013
IV_{1d}	-8.010217	0.023402	3.993408	8.033619	0.992536	2.283308		
IV_{1e}	-8.791728	-0.042178	4.416953	8.749550	1.114884	1.501797	0.122349	-0.781511
IV_{2b}	-8.228180	-0.091974	4.160077	8.136206	1.063533	2.065345		
IV_{2c}	-7.936746	-0.000272	3.968509	7.936474	0.992195	2.356778	-0.071337	0.291434
IV_{2d}	-7.926134	0.023402	3.951366	7.949535	0.982025	2.367391		
IV_{2e}	-8.611316	-0.058504	4.334910	8.552812	1.098554	1.682208	0.116528	-0.685183
IV_{3b}	-8.188451	-0.088709	4.138580	8.099742	1.057308	2.105073		
IV_{3c}	-7.886949	0.000272	3.943339	7.887221	0.985767	2.406575	-0.071542	0.301502
IV_{3d}	-7.934569	0.013334	3.960618	7.947903	0.986832	2.358955		
IV_{3e}	-8.611861	-0.067484	4.339672	8.544376	1.102056	1.681664	0.115223	-0.677291

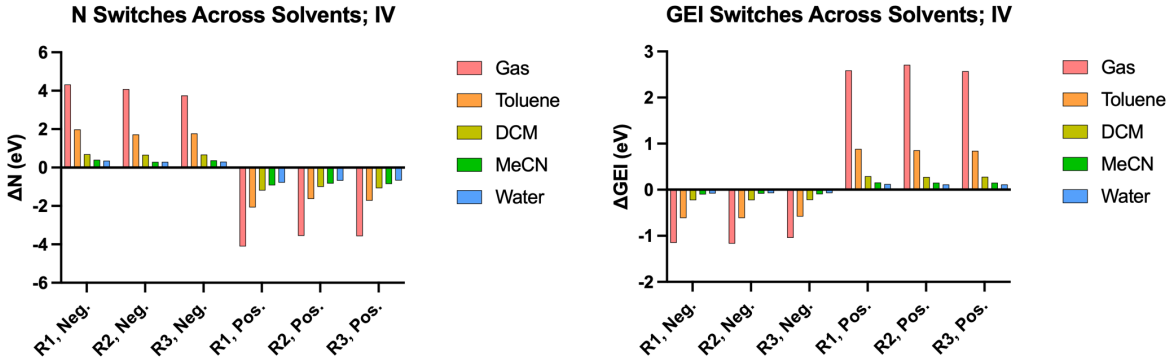


Figure S143. IV Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S248. Orbital Energies and Philicity Parameters of $V_{[1-3][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
V_{1b}[a]	-9.320990	-0.706680	5.013835	8.614310	1.459115	1.602479		
V_{1c}	-4.236813	2.183442	1.026686	6.420255	0.082090	6.686655	-1.377025 (-0.9949)[b]	5.084176 (3.5386)[b]
V_{1d}	-7.640142	-0.294971	3.967557	7.345171	1.071555	3.283326		
V_{1e}	-11.707701	-3.596802	7.652251	8.110899	3.609769	-0.784232	2.538214	-4.067559
V_{2b}	-7.772389	-0.460689	4.116539	7.311700	1.158820	3.151079		
V_{2c}	-3.961162	2.330656	0.815253	6.291818	0.052818	6.962306	-1.106003	3.811227
V_{2d}	-7.571025	-0.373612	3.972319	7.197413	1.096180	3.352443		
V_{2e}	-10.999932	-3.818574	7.409253	7.181358	3.822190	-0.076464	2.726011	-3.428907
V_{3b}	-7.772389	-0.375245	4.073817	7.397144	1.121783	3.151079		
V_{3c}	-4.333958	2.016092	1.158933	6.350050	0.105757	6.589510	-1.016026	3.438431
V_{3d}	-7.586808	-0.320006	3.953407	7.266802	1.075399	3.336661		
V_{3e}	-11.036396	-3.759254	7.397825	7.277142	3.760254	-0.112927	2.684855	-3.449588

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S249. Orbital Energies and Philicity Parameters of $V_{[1-3][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
V_{1b}[a]	-9.196633	-0.543684	4.870159	8.652950	1.370541	1.443292		
V_{1c}	-6.391139	0.941786	2.724676	7.332925	0.506201	4.248786	-0.864340 (-0.5003)[b]	2.805494 (1.2251)[b]
V_{1d}	-7.667898	-0.134696	3.901297	7.533201	1.010203	2.972028		
V_{1e}	-9.628206	-1.460163	5.544185	8.168043	1.881600	1.011719	0.871398	-1.960309
V_{2b}	-7.862731	-0.259052	4.060892	7.603679	1.084399	2.777194		
V_{2c}	-6.456447	0.924099	2.766174	7.380545	0.518371	4.183479	-0.566028	1.406285
V_{2d}	-7.705994	-0.174697	3.940345	7.531296	1.030787	2.933932		
V_{2e}	-9.162891	-1.523021	5.342956	7.639870	1.868303	1.477034	0.837516	-1.456898
V_{3b}	-7.868718	-0.233202	4.050960	7.635516	1.074601	2.771208		
V_{3c}	-6.420255	0.890629	2.764813	7.310884	0.522795	4.219670	-0.551806	1.448462
V_{3d}	-7.724497	-0.148302	3.936400	7.576195	1.022627	2.915428		
V_{3e}	-9.213232	-1.523294	5.368263	7.689939	1.873763	1.426693	0.851136	-1.488735

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S250. Orbital Energies and Philicity Parameters of $V_{[1-3][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
V_{1b}[a]	-9.034454	-0.446267	4.740360	8.588187	1.308251	1.372543		
V_{1c}	-7.555787	0.263950	3.645918	7.819737	0.849947	2.851209	-0.458305	1.478667
V_{1d}	-7.724225	-0.040001	3.882113	7.684224	0.980633	2.682771		
V_{1e}	-8.559071	-0.398919	4.478995	8.160152	1.229229	1.847925	0.248597	-0.834845
V_{2b}	-8.026272	-0.138234	4.082253	7.888038	1.056333	2.380725		
V_{2c}	-7.519596	0.236467	3.641564	7.756062	0.854879	2.887401	-0.201454	0.506676
V_{2d}	-7.796880	-0.059049	3.927964	7.737831	0.996979	2.610117		
V_{2e}	-8.437436	-0.422321	4.429878	8.015115	1.224176	1.969560	0.227197	-0.640556
V_{3b}	-8.032258	-0.126261	4.079259	7.905997	1.052388	2.374738		
V_{3c}	-7.515786	0.235651	3.640068	7.751437	0.854686	2.891210	-0.197702	0.516472
V_{3d}	-7.780281	-0.045715	3.912998	7.734565	0.989813	2.626715		
V_{3e}	-8.485328	-0.455247	4.470287	8.030081	1.244288	1.921668	0.254475	-0.705047

[a] Forms a weak C-B interaction

Table S251. Orbital Energies and Philicity Parameters of $V_{[1-3][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
V_{1b}[a]	-8.977038	-0.418783	4.697910	8.558254	1.289420	1.343698		
V_{1c}	-7.903004	0.050613	3.926195	7.953617	0.969057	2.417732	-0.320363	1.074034
V_{1d}	-7.743817	-0.017415	3.880616	7.726402	0.974528	2.576919		
V_{1e}	-8.316345	-0.130070	4.223208	8.186275	1.089353	2.004391	0.114825	-0.572528
V_{2b}	-8.082871	-0.108029	4.095450	7.974842	1.051602	2.237865		
V_{2c}	-7.496738	0.037007	3.729865	7.533745	0.923305	2.823998	-0.128296	0.586133
V_{2d}	-7.792254	-0.029388	3.910821	7.762865	0.985108	2.528482		
V_{2e}	-8.279610	-0.136057	4.207833	8.143553	1.087109	2.041126	0.102001	-0.487356
V_{3b}	-8.101103	-0.099322	4.100212	8.001781	1.050500	2.219633		
V_{3c}	-7.631979	0.032926	3.799526	7.664904	0.941721	2.688757	-0.108779	0.469124
V_{3d}	-7.782458	-0.021225	3.901841	7.761233	0.980796	2.538278		
V_{3e}	-8.326141	-0.173609	4.249875	8.152532	1.107719	1.994595	0.126924	-0.543684

[a] Forms a weak C-B interaction

Table S252. Orbital Energies and Philicity Parameters of $V_{[1-3][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
V_{1b}[a]	-8.971595	-0.414429	4.693012	8.557166	1.286896	1.321929		
V_{1c}	-7.968856	0.008980	3.979938	7.977835	0.992745	2.324669	-0.294151	1.002740
V_{1d}	-7.825452	-0.011973	3.918712	7.813479	0.982680	2.468073		
V_{1e}	-8.273623	-0.083267	4.178445	8.190356	1.065851	2.019901	0.083171	-0.448172
V_{2b}	-8.086409	-0.102587	4.094498	7.983822	1.049930	2.207116		
V_{2c}	-7.552249	-0.004898	3.778574	7.547351	0.945870	2.741275	-0.104061	0.534160
V_{2d}	-7.922868	-0.023130	3.972999	7.899739	0.999066	2.370656		
V_{2e}	-8.253759	-0.086260	4.170009	8.167499	1.064523	2.039766	0.065457	-0.330891
V_{3b}	-8.116341	-0.094424	4.105382	8.021918	1.050507	2.177183		
V_{3c}	-7.684497	-0.006531	3.845514	7.677966	0.963014	2.609028	-0.087493	0.431845
V_{3d}	-7.878242	-0.011973	3.945107	7.866269	0.989279	2.415283		
V_{3e}	-8.299746	-0.119186	4.209466	8.180560	1.083031	1.993779	0.093752	-0.421504

[a] Forms a weak C-B interaction

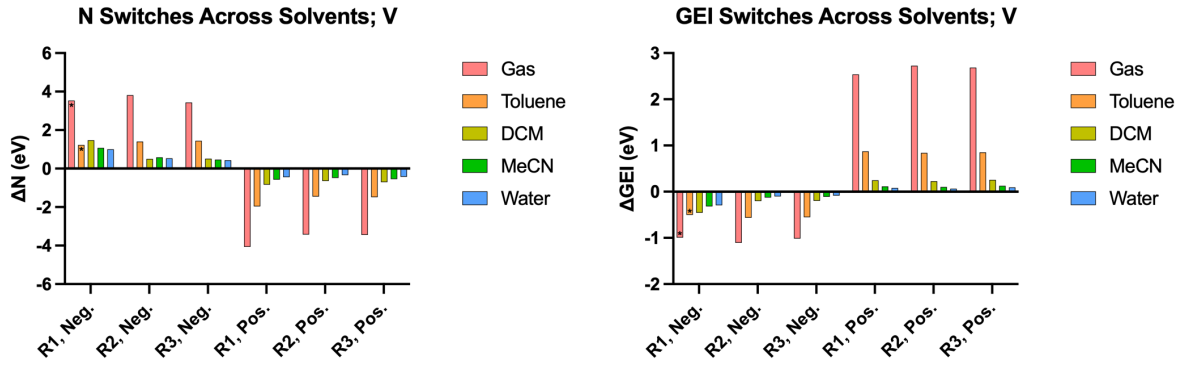


Figure S144. V Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S253. Orbital Energies and Philicity Parameters of $VI_{[1-2][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VI_{1b}	-7.446669	-0.309666	3.878167	7.137003	1.053676	3.476799		
VI_{1c}	-3.741022	1.914593	0.913214	5.655615	0.073729	7.182446	-0.979948	3.705647
VI_{1d}	-7.270339	-0.223950	3.747144	7.046389	0.996332	3.653129		
VI_{1e}	-11.141704	-3.381015	7.261359	7.760688	3.397079	-0.218235	2.400746	-3.871364
VI_{2b}	-7.326123	-0.360823	3.843473	6.965299	1.060420	3.597346		
VI_{2c}	-3.967965	2.055548	0.956208	6.023513	0.075897	6.955503	-0.984523	3.358158
VI_{2d}	-7.170473	-0.264223	3.717348	6.906251	1.000447	3.752995		
VI_{2e}	-10.748499	-3.538569	7.143534	7.209930	3.538875	0.174969	2.538428	-3.578026

Table S254. Orbital Energies and Philicity Parameters of $VI_{[1-2][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VI_{1b}	-7.547351	-0.162996	3.855174	7.384355	1.006341	3.092574		
VI_{1c}	-5.719290	0.805457	2.456916	6.524747	0.462580	4.920636	-0.543761	1.828061
VI_{1d}	-7.379185	-0.093607	3.736396	7.285578	0.958102	3.260741		
VI_{1e}	-9.118537	-1.341794	5.230165	7.776743	1.758746	1.521389	0.800644	-1.739352
VI_{2b}	-7.394695	-0.202997	3.798846	7.191698	1.003326	3.245230		
VI_{2c}	-5.961199	0.901241	2.529979	6.862440	0.466364	4.678726	-0.536961	1.433496
VI_{2d}	-7.247754	-0.108573	3.678164	7.139180	0.947510	3.392172		
VI_{2e}	-8.728870	-1.408189	5.068530	7.320680	1.754618	1.911056	0.807108	-1.481116

Table S255. Orbital Energies and Philicity Parameters of $VI_{[1-2][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VI_{1b}	-7.466261	-0.068028	3.767145	7.398233	0.959106	2.940735		
VI_{1c}	-6.711145	0.235379	3.237883	6.946524	0.754614	3.695851	-0.204492	0.755116
VI_{1d}	-7.409934	-0.026939	3.718436	7.382994	0.936393	2.997062		
VI_{1e}	-8.242330	-0.367082	4.304706	7.875248	1.176502	2.164666	0.240109	-0.832396
VI_{2b}	-7.298095	-0.124900	3.711498	7.173195	0.960187	3.108901		
VI_{2c}	-6.918496	0.247624	3.335436	7.166120	0.776231	3.488500	-0.183955	0.379599
VI_{2d}	-7.313061	-0.034014	3.673538	7.279047	0.926967	3.093935		
VI_{2e}	-7.786539	-0.386130	4.086334	7.400410	1.128190	2.620457	0.201222	-0.473478

Table S256. Orbital Energies and Philicity Parameters of $VI_{[1-2][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VI_{1b}	-7.451295	-0.056055	3.753675	7.395239	0.952645	2.869441		
VI_{1c}	-6.970470	0.042994	3.463738	7.013464	0.855318	3.350266	-0.097327	0.480825
VI_{1d}	-7.363130	-0.012517	3.687824	7.350613	0.925096	2.957606		
VI_{1e}	-7.963141	-0.115921	4.039531	7.847221	1.039719	2.357595	0.114623	-0.600011
VI_{2b}	-7.284761	-0.099049	3.691905	7.185712	0.948421	3.035975		
VI_{2c}	-7.171018	0.039457	3.565781	7.210474	0.881689	3.149718	-0.066732	0.113744
VI_{2d}	-7.331565	-0.011973	3.671769	7.319592	0.920945	2.989171		
VI_{2e}	-7.554970	-0.133608	3.844289	7.421362	0.995677	2.765766	0.074732	-0.223406

Table S257. Orbital Energies and Philicity Parameters of $VI_{[1-2][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VI_{1b}[a]	-7.989536	-0.050613	4.020075	7.938923	1.017833	2.303988		
VI_{1c}	-7.148704	0.007891	3.570406	7.156596	0.890633	3.144820	-0.127200	0.840832
VI_{1d}	-7.270611	-0.020136	3.645374	7.250475	0.916406	3.022913		
VI_{1e}	-7.891575	-0.072927	3.982251	7.818649	1.014134	2.401949	0.097729	-0.620964
VI_{2b}	-7.401770	-0.093879	3.747825	7.307891	0.961029	2.891754		
VI_{2c}	-7.310612	0.003537	3.653537	7.314150	0.912501	2.982913	-0.048528	0.091158
VI_{2d}	-7.383811	0.005714	3.689048	7.389525	0.920836	2.909714		
VI_{2e}	-7.605856	-0.080001	3.842929	7.525854	0.981158	2.687669	0.060322	-0.222045

[a] Forms a weak C-B interaction

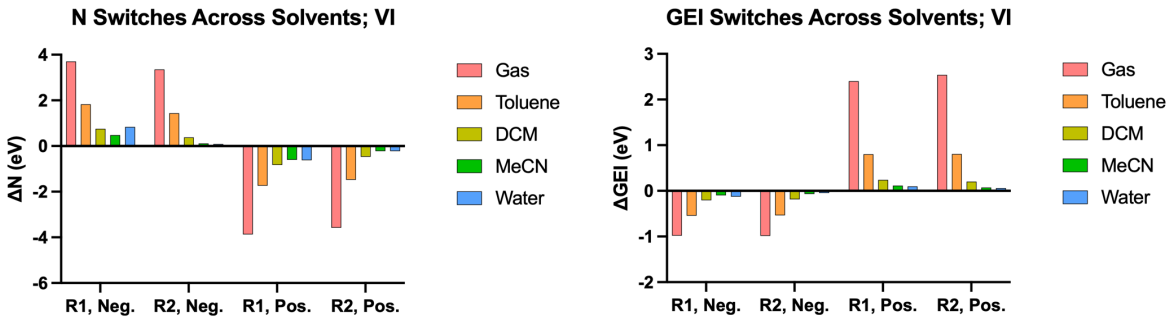


Figure S145. VI Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S258. Orbital Energies and Philicity Parameters of $VII_{[1-3][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VII_{1b}[a]	-8.332400	-0.546677	4.439538	7.785723	1.265746	2.591069		
VII_{1c}	-3.034070	1.726835	0.653618	4.760905	0.044867	7.889398	-1.220879 (-0.8954)[b]	5.298330 (3.6912)[b]
VII_{1d}	-6.708152	-0.266400	3.487276	6.441752	0.943927	4.215316		
VII_{1e}	-10.624415	-3.318701	6.971558	7.305714	3.326343	0.299053	2.382416	-3.916263
VII_{2b}	-6.819174	-0.315108	3.567141	6.504066	0.978195	4.104294		
VII_{2c}	-3.650408	1.871872	0.889268	5.522279	0.071601	7.273060	-0.906595	3.168766
VII_{2d}	-6.594136	-0.289529	3.441833	6.304607	0.939489	4.329332		
VII_{2e}	-9.907939	-3.449316	6.678628	6.458623	3.453063	1.015529	2.513574	-3.313803
VII_{3b}	-6.869788	-0.386130	3.627959	6.483658	1.015020	4.053681		
VII_{3c}	-3.796533	2.004391	0.896071	5.800924	0.069208	7.126935	-0.945812	3.073254
VII_{3d}	-6.700533	-0.284631	3.492582	6.415902	0.950617	4.222936		
VII_{3e}	-9.649975	-3.641700	6.645838	6.008275	3.675528	1.273493	2.724911	-2.949443

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S259. Orbital Energies and Philicity Parameters of $VII_{[1-3][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VII_{1b}[a]	-8.090218	-0.250617	4.170418	7.839601	1.109265	2.549707		
VII_{1c}	-5.400645	0.752395	2.324125	6.153040	0.438934	5.239281	-0.670331 (-0.4611)[b]	2.689574 (1.2057)[b]
VII_{1d}	-6.868971	-0.112111	3.490541	6.756860	0.901593	3.770954		
VII_{1e}	-8.599888	-1.315126	4.957507	7.284761	1.686869	2.040038	0.785276	-1.730917
VII_{2b}	-6.911965	-0.178235	3.545100	6.733731	0.933192	3.727960		
VII_{2c}	-5.632758	0.801648	2.415555	6.434405	0.453415	5.007168	-0.479778	1.279207
VII_{2d}	-6.814821	-0.099049	3.456935	6.715771	0.889727	3.825105		
VII_{2e}	-8.077429	-1.377441	4.727435	6.699988	1.667812	2.562497	0.778085	-1.262608
VII_{3b}	-6.978089	-0.214970	3.596529	6.763119	0.956291	3.661837		
VII_{3c}	-5.815346	0.817430	2.498958	6.632776	0.470752	4.824579	-0.485539	1.162743
VII_{3d}	-6.888563	-0.124900	3.506732	6.763663	0.909061	3.751362		
VII_{3e}	-8.046680	-1.456081	4.751381	6.590599	1.712714	2.593245	0.803653	-1.158117

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S260. Orbital Energies and Philicity Parameters of $VII_{[1-3][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VII_{1b}[a]	-7.946542	-0.093607	4.020075	7.852935	1.028978	2.460454		
VII_{1c}	-6.628422	0.212521	3.207951	6.840943	0.752159	3.778574	-0.276820	1.318120
VII_{1d}	-7.122037	-0.024490	3.573264	7.097547	0.899481	3.284959		
VII_{1e}	-7.748171	-0.360823	4.054497	7.387348	1.112642	2.658825	0.213161	-0.626134
VII_{2b}	-7.099996	-0.104764	3.602380	6.995232	0.927570	3.307000		
VII_{2c}	-6.685294	0.222317	3.231489	6.907611	0.755870	3.721702	-0.171700	0.414702
VII_{2d}	-7.048022	-0.035103	3.541562	7.012919	0.894254	3.358974		
VII_{2e}	-7.387076	-0.399463	3.893270	6.987613	1.084601	3.019920	0.190347	-0.339054
VII_{3b}	-7.183535	-0.121363	3.652449	7.062172	0.944496	3.223461		
VII_{3c}	-6.839855	0.219052	3.310402	7.058907	0.776236	3.567141	-0.168259	0.343680
VII_{3d}	-7.144623	-0.041906	3.593264	7.102717	0.908916	3.262374		
VII_{3e}	-7.493745	-0.410076	3.951910	7.083669	1.102366	2.913251	0.193450	-0.349122

[a] Forms a weak C-B interaction

Table S261. Orbital Energies and Philicity Parameters of $VII_{[1-3][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VII_{1b}[a]	-7.902188	-0.069117	3.985652	7.833071	1.013997	2.418548		
VII_{1c}	-6.953326	0.030477	3.461425	6.983803	0.857804	3.367410	-0.156194	0.948861
VII_{1d}	-7.236869	-0.004626	3.620748	7.232243	0.906345	3.083867		
VII_{1e}	-7.547351	-0.117009	3.832180	7.430342	0.988219	2.773385	0.081874	-0.310482
VII_{2b}	-7.186256	-0.083539	3.634897	7.102717	0.930100	3.134480		
VII_{2c}	-6.987613	0.029933	3.478840	7.017545	0.862291	3.333123	-0.067810	0.198643
VII_{2d}	-7.157412	-0.013878	3.585645	7.143534	0.899894	3.163324		
VII_{2e}	-7.258366	-0.125445	3.691905	7.132922	0.955441	3.062370	0.055546	-0.100954
VII_{3b}	-7.276598	-0.096600	3.686599	7.179997	0.946450	3.044138		
VII_{3c}	-7.126663	0.018232	3.554216	7.144895	0.884019	3.194073	-0.062430	0.149935
VII_{3d}	-7.250203	-0.022858	3.636530	7.227345	0.914883	3.070533		
VII_{3e}	-7.379457	-0.144765	3.762111	7.234692	0.978167	2.941279	0.063284	-0.129254

[a] Forms a weak C-B interaction

Table S262. Orbital Energies and Philicity Parameters of VII[1-3][b-e] in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VII$_{1b}$[a]	-7.899194	-0.066940	3.983067	7.832254	1.012788	2.394330		
VII$_{1c}$	-6.967476	-0.015238	3.491357	6.952238	0.876666	3.326048	-0.136122	0.931718
VII$_{1d}$	-7.262992	0.000816	3.631088	7.263808	0.907568	3.030533		
VII$_{1e}$	-7.505446	-0.074287	3.789866	7.431158	0.966410	2.788079	0.058842	-0.242453
VII$_{2b}$	-7.213739	-0.079729	3.646734	7.134010	0.932061	3.079785		
VII$_{2c}$	-7.052104	-0.008436	3.530270	7.043668	0.884681	3.241421	-0.047380	0.161636
VII$_{2d}$	-7.206120	-0.017143	3.611632	7.188977	0.907214	3.087404		
VII$_{2e}$	-7.227073	-0.081634	3.654354	7.145439	0.934463	3.066452	0.027249	-0.020953
VII$_{3b}$	-7.297823	-0.091974	3.694899	7.205848	0.947305	2.995702		
VII$_{3c}$	-7.196596	-0.014422	3.605509	7.182174	0.904997	3.096928	-0.042308	0.101226
VII$_{3d}$	-7.276870	-0.019048	3.647959	7.257822	0.916777	3.016655		
VII$_{3e}$	-7.363946	-0.098777	3.731362	7.265169	0.958206	2.929578	0.041430	-0.087076

[a] Forms a weak C-B interaction

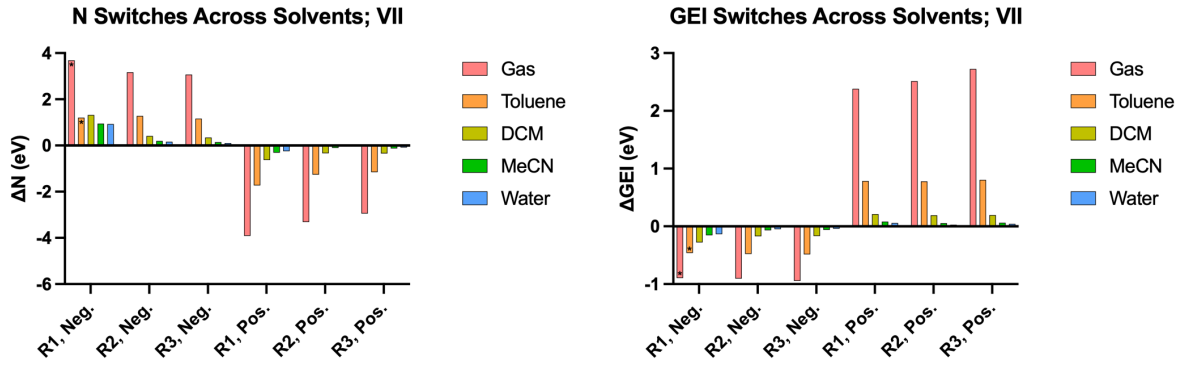


Figure S146. VII Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S263. Orbital Energies and Philicity Parameters of $VIII_{[1-4][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
$VIII_{1b}$[a]	-8.925064	-0.950494	4.937779	7.974570	1.528713	1.998404		
$VIII_{1c}$	-3.402512	1.826428	0.788042	5.228941	0.059382	7.520956	-1.469331 (-0.9135)[b]	5.522552 (3.7065)[b]
$VIII_{1d}$	-7.108431	-0.242453	3.675442	6.865978	0.983755	3.815037		
$VIII_{1e}$	-11.053811	-3.681701	7.367756	7.372110	3.681702	-0.130343	2.697948	-3.945379
$VIII_{2b}$	-7.139452	-0.394021	3.766737	6.745431	1.051697	3.784016		
$VIII_{2c}$	-3.782655	1.991057	0.895799	5.773713	0.069492	7.140813	-0.982205	3.356797
$VIII_{2d}$	-6.939449	-0.293067	3.616258	6.646382	0.983792	3.984020		
$VIII_{2e}$	-10.257606	-3.763879	7.010743	6.493726	3.784461	0.665863	2.800669	-3.318157
$VIII_{3b}$	-7.166936	-0.334700	3.750818	6.832236	1.029578	3.756532		
$VIII_{3c}$	-3.827010	1.846293	0.990359	5.673303	0.086441	7.096458	-0.943137	3.339926
$VIII_{3d}$	-6.973463	-0.272114	3.622788	6.701349	0.979250	3.950005		
$VIII_{3e}$	-10.275293	-3.828643	7.051968	6.446650	3.857061	0.648175	2.877811	-3.301830
$VIII_{4b}$	-7.312517	-0.273202	3.792860	7.039314	1.021817	3.610951		
$VIII_{4c}$	-3.668095	1.728467	0.969814	5.396563	0.087142	7.255373	-0.934675	3.644421
$VIII_{4d}$	-7.055097	-0.223406	3.639251	6.831692	0.969317	3.868371		
$VIII_{4e}$	-10.847004	-3.600611	7.223808	7.246393	3.600646	0.076464	2.631329	-3.791907

[a] Forms a weak C-B interaction; [b] A corrected switch, calculated relative to the unsubstituted molecule, see S10.

Table S264. Orbital Energies and Philicity Parameters of $VIII_{[1-4][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
$VIII_{1b}$[a]	-8.852409	-0.754028	4.803219	8.098382	1.424415	1.787516		
$VIII_{1c}$	-5.763372	0.823417	2.469978	6.586789	0.463108	4.876553	-0.961307 (-0.4716)[b]	3.089037 (1.2117)[b]
$VIII_{1d}$	-7.049111	-0.102859	3.575985	6.946252	0.920473	3.590815		
$VIII_{1e}$	-9.016222	-1.538532	5.277377	7.477690	1.862253	1.623704	0.941781	-1.967111
$VIII_{2b}$	-7.248570	-0.218235	3.733403	7.030335	0.991297	3.391356		
$VIII_{2c}$	-5.864871	0.853893	2.505489	6.718764	0.467160	4.775055	-0.524137	1.383699
$VIII_{2d}$	-7.123398	-0.127077	3.625237	6.996320	0.939233	3.516528		
$VIII_{2e}$	-8.452674	-1.495266	4.973970	6.957408	1.777988	2.187252	0.838755	-1.329276
$VIII_{3b}$	-7.246121	-0.183949	3.715035	7.062172	0.977142	3.393805		
$VIII_{3c}$	-5.856707	0.842193	2.507257	6.698900	0.469207	4.783218	-0.507935	1.389414
$VIII_{3d}$	-7.132922	-0.118370	3.625646	7.014552	0.937003	3.507004		
$VIII_{3e}$	-8.484784	-1.563022	5.023903	6.921761	1.823206	2.155142	0.886204	-1.351862
$VIII_{4b}$	-7.384355	-0.144220	3.764288	7.240135	0.978563	3.255571		
$VIII_{4c}$	-5.898341	0.740966	2.578687	6.639307	0.500777	4.741585	-0.477786	1.486014
$VIII_{4d}$	-7.183263	-0.083267	3.633265	7.099996	0.929621	3.456663		
$VIII_{4e}$	-8.750095	-1.408189	5.079142	7.341905	1.756879	1.889831	0.827258	-1.566832

[a] Forms a weak C-B interaction

Table S265. Orbital Energies and Philicity Parameters of $VIII_{[1-4][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
$VIII_{1b}$[a]	-8.685331	-0.644910	4.665121	8.040422	1.353371	1.721665		
$VIII_{1c}$	-6.942170	0.241909	3.350130	7.184079	0.781128	3.464826	-0.572243	1.743162
$VIII_{1d}$	-7.508983	-0.070750	3.789866	7.438233	0.965490	2.898013		
$VIII_{1e}$	-8.152260	-0.593480	4.372870	7.558780	1.264886	2.254736	0.299396	-0.643277
$VIII_{2b}$	-7.425444	-0.129798	3.777621	7.295646	0.978010	2.981552		
$VIII_{2c}$	-6.984892	0.229936	3.377478	7.214828	0.790549	3.422104	-0.187460	0.440552
$VIII_{2d}$	-7.374287	-0.056055	3.715171	7.318231	0.943021	3.032709		
$VIII_{2e}$	-7.808853	-0.564908	4.186881	7.243944	1.209974	2.598144	0.266953	-0.434566
$VIII_{3b}$	-7.424900	-0.108846	3.766873	7.316054	0.969739	2.982096		
$VIII_{3c}$	-6.958225	0.227487	3.365369	7.185712	0.788071	3.448772	-0.181668	0.466675
$VIII_{3d}$	-7.346531	-0.030749	3.688640	7.315782	0.929912	3.060465		
$VIII_{3e}$	-7.829261	-0.541507	4.185384	7.287754	1.201841	2.577735	0.271929	-0.482730
$VIII_{4b}$	-7.532929	-0.084900	3.808914	7.448030	0.973937	2.874067		
$VIII_{4c}$	-7.030879	0.225855	3.402512	7.256733	0.797679	3.376117	-0.176258	0.502050
$VIII_{4d}$	-7.342177	-0.026123	3.684150	7.316054	0.927615	3.064819		
$VIII_{4e}$	-8.012394	-0.439464	4.225929	7.572930	1.179099	2.394602	0.251485	-0.670217

[a] Forms a weak C-B interaction

Table S266. Orbital Energies and Philicity Parameters of $VIII_{[1-4][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
$VIII_{1b}$[a]	-8.630092	-0.612801	4.621446	8.017292	1.331981	1.690644		
$VIII_{1c}$	-7.230883	0.040273	3.595305	7.271156	0.888870	3.089853	-0.443112	1.399210
$VIII_{1d}$	-7.614291	-0.111839	3.863065	7.502452	0.994560	2.706445		
$VIII_{1e}$	-7.950896	-0.357013	4.153955	7.593883	1.136134	2.369840	0.141575	-0.336605
$VIII_{2b}$	-7.510616	-0.112111	3.811363	7.398505	0.981718	2.810120		
$VIII_{2c}$	-7.319864	0.023130	3.648367	7.342994	0.906346	3.000872	-0.075372	0.190752
$VIII_{2d}$	-7.456465	-0.043538	3.750002	7.412927	0.948513	2.864271		
$VIII_{2e}$	-7.671707	-0.324632	3.998170	7.347075	1.087872	2.649029	0.139359	-0.215242
$VIII_{3b}$	-7.507895	-0.091702	3.799798	7.416192	0.973442	2.812841		
$VIII_{3c}$	-7.274693	0.023130	3.625782	7.297823	0.900700	3.046043	-0.072743	0.233202
$VIII_{3d}$	-7.426805	-0.008163	3.717484	7.418641	0.931416	2.893931		
$VIII_{3e}$	-7.674973	-0.243542	3.959257	7.431431	1.054690	2.645763	0.123274	-0.248168
$VIII_{4b}$	-7.602862	-0.122451	3.862657	7.480411	0.997279	2.717874		
$VIII_{4c}$	-7.358504	0.045171	3.656667	7.403675	0.903012	2.962232	-0.094268	0.244358
$VIII_{4d}$	-7.421362	-0.024490	3.722926	7.396872	0.936895	2.899374		
$VIII_{4e}$	-7.844772	-0.247896	4.046334	7.596876	1.077602	2.475964	0.140707	-0.423409

[a] Forms a weak C-B interaction

Table S267. Orbital Energies and Philicity Parameters of VIII$_{[1-4][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
VIII$_{1b}$[a]	-8.622201	-0.602732	4.612467	8.019469	1.326450	1.671324		
VIII$_{1c}$	-7.375919	0.003810	3.686055	7.379729	0.920562	2.917605	-0.405888	1.246282
VIII$_{1d}$	-7.646673	-0.109934	3.878303	7.536739	0.997861	2.646852		
VIII$_{1e}$	-7.916065	-0.310210	4.113138	7.605856	1.112163	2.377459	0.114302	-0.269393
VIII$_{2b}$	-7.530208	-0.110478	3.820343	7.419730	0.983528	2.763317		
VIII$_{2c}$	-7.379457	-0.011429	3.695443	7.368028	0.926727	2.914068	-0.056801	0.150751
VIII$_{2d}$	-7.510888	-0.035375	3.773131	7.475513	0.952210	2.782637		
VIII$_{2e}$	-7.651299	-0.281366	3.966332	7.369933	1.067295	2.642226	0.115085	-0.140411
VIII$_{3b}$	-7.526398	-0.088437	3.807418	7.437961	0.974489	2.767126		
VIII$_{3c}$	-7.347620	-0.005442	3.676531	7.342177	0.920495	2.945905	-0.053994	0.178779
VIII$_{3d}$	-7.485037	-0.029933	3.757485	7.455105	0.946914	2.808488		
VIII$_{3e}$	-7.653203	-0.200004	3.926604	7.453200	1.034335	2.640321	0.087421	-0.168166
VIII$_{4b}$	-7.619189	-0.075376	3.847282	7.543814	0.981041	2.674335		
VIII$_{4c}$	-7.420818	0.007347	3.706736	7.428165	0.924851	2.872706	-0.056190	0.198371
VIII$_{4d}$	-7.518507	-0.031565	3.775036	7.486942	0.951717	2.775018		
VIII$_{4e}$	-7.791437	-0.162452	3.976945	7.628985	1.036579	2.502087	0.084862	-0.272930

[a] Forms a weak C-B interaction

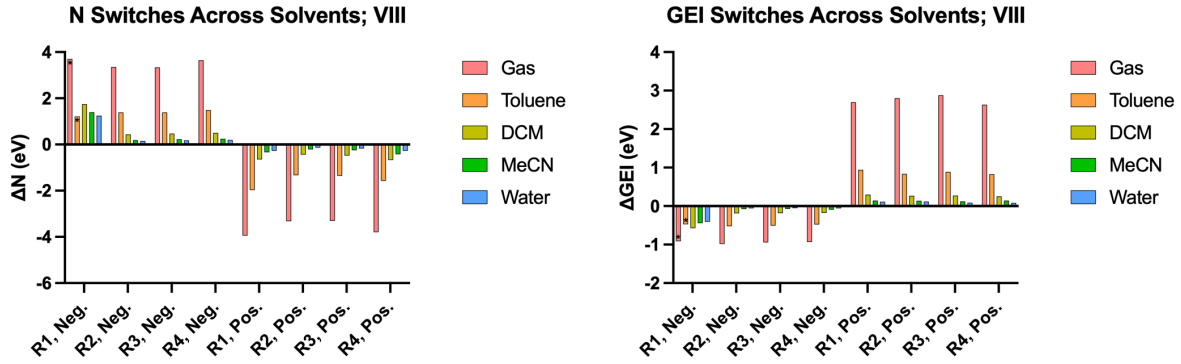


Figure S147. VIII Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

Table S268. Orbital Energies and Philicity Parameters of $IX_{[1-2,4][b-e]}$ in Gas. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IX_{1b}	-8.559615	-0.269937	4.414776	8.289678	1.175573	2.363853		
IX_{1c}	-4.397905	2.000854	1.198526	6.398758	0.112246	6.525563	-1.063328	4.161710
IX_{1d}	-7.815655	-0.240821	4.028238	7.574835	1.071093	3.107813		
IX_{1e}	-11.806478	-3.616394	7.711436	8.190084	3.630380	-0.883010	2.559288	-3.990822
IX_{2b}	-7.956066	-0.383681	4.169873	7.572386	1.148109	2.967402		
IX_{2c}	-4.405796	2.052555	1.176621	6.458351	0.107182	6.517672	-1.040927	3.550270
IX_{2d}	-7.667898	-0.268304	3.968101	7.399593	1.063966	3.255571		
IX_{2e}	-11.040477	-3.656394	7.348436	7.384083	3.656481	-0.117009	2.592515	-3.372580
IX_{4b}	-8.464919	-0.316741	4.390830	8.148179	1.183049	2.458549		
IX_{4c}	-4.266202	1.777448	1.244377	6.043650	0.128108	6.657267	-1.054941	4.198717
IX_{4d}	-7.786539	-0.202453	3.994496	7.584087	1.051939	3.136929		
IX_{4e}	-11.816546	-3.387002	7.601774	8.429544	3.427645	-0.893078	2.375705	-4.030007

Table S269. Orbital Energies and Philicity Parameters of $IX_{[1-2,4][b-e]}$ in SMD Toluene. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IX_{1b}	-8.463559	-0.126805	4.295182	8.336754	1.106461	2.176367		
IX_{1c}	-6.611279	0.900153	2.855563	7.511432	0.542789	4.028646	-0.563672	1.852279
IX_{1d}	-7.881779	-0.081362	3.981571	7.800417	1.016157	2.758146		
IX_{1e}	-9.738956	-1.433768	5.586362	8.305188	1.878792	0.900969	0.862635	-1.857177
IX_{2b}	-8.057020	-0.205446	4.131233	7.851574	1.086858	2.582905		
IX_{2c}	-6.571006	0.922466	2.824270	7.493473	0.532230	4.068919	-0.554628	1.486014
IX_{2d}	-7.825996	-0.111839	3.968917	7.714157	1.021000	2.813930		
IX_{2e}	-9.286975	-1.486558	5.386767	7.800417	1.859981	1.352950	0.838981	-1.460980
IX_{4b}	-8.180560	-0.108301	4.144431	8.072259	1.063910	2.459365		
IX_{4c}	-6.515223	0.764640	2.875292	7.279863	0.567820	4.124702	-0.496090	1.665337
IX_{4d}	-7.766403	-0.058777	3.912590	7.707626	0.993066	2.873523		
IX_{4e}	-9.659227	-1.351046	5.505136	8.308182	1.823896	0.980698	0.830831	-1.892824

Table S270. Orbital Energies and Philicity Parameters of $IX_{[1-2,4][b-e]}$ in SMD DCM. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IX_{1b}	-8.326957	-0.090342	4.208650	8.236616	1.075243	2.080039		
IX_{1c}	-7.781369	0.264767	3.758301	8.046136	0.877740	2.625627	-0.197504	0.545588
IX_{1d}	-7.892664	-0.003810	3.948237	7.888854	0.988012	2.514332		
IX_{1e}	-8.875811	-0.378238	4.627025	8.497573	1.259734	1.531185	0.271721	-0.983148
IX_{2b}	-8.187907	-0.123812	4.155860	8.064095	1.070868	2.219089		
IX_{2c}	-7.689122	0.249801	3.719661	7.938923	0.871395	2.717874	-0.199473	0.498785
IX_{2d}	-7.838785	-0.034014	3.936400	7.804771	0.992678	2.568211		
IX_{2e}	-8.624650	-0.400007	4.512329	8.224643	1.237811	1.782346	0.245134	-0.785865
IX_{4b}	-8.326413	-0.066940	4.196677	8.259473	1.066175	2.080583		
IX_{4c}	-7.742729	0.245719	3.748505	7.988448	0.879476	2.664267	-0.186700	0.583684
IX_{4d}	-7.852935	0.004354	3.924291	7.857289	0.979985	2.554061		
IX_{4e}	-8.902750	-0.353476	4.628113	8.549275	1.252705	1.504246	0.272719	-1.049815

Table S271. Orbital Energies and Philicity Parameters of $IX_{[1-2,4][b-e]}$ in SMD MeCN. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IX_{1b}	-8.391721	-0.072927	4.232324	8.318794	1.076632	1.929015		
IX_{1c}	-8.120967	0.049797	4.035585	8.170764	0.996599	2.199769	-0.080033	0.270753
IX_{1d}	-7.897834	0.009524	3.944155	7.907358	0.983663	2.422902		
IX_{1e}	-8.671726	-0.112655	4.392190	8.559071	1.126953	1.649010	0.143289	-0.773892
IX_{2b}	-8.270358	-0.105308	4.187833	8.165050	1.073964	2.050378		
IX_{2c}	-8.010217	0.031837	3.989190	8.042054	0.989401	2.310519	-0.084563	0.260141
IX_{2d}	-7.828173	-0.018504	3.923338	7.809669	0.985482	2.492563		
IX_{2e}	-8.476892	-0.131703	4.304298	8.345189	1.110039	1.843844	0.124557	-0.648720
IX_{4b}	-8.392265	-0.065035	4.228650	8.327230	1.073675	1.928471		
IX_{4c}	-8.095389	0.053879	4.020755	8.149267	0.991897	2.225347	-0.081778	0.296876
IX_{4d}	-7.891575	0.014422	3.938577	7.905997	0.981052	2.429161		
IX_{4e}	-8.693223	-0.107485	4.400354	8.585738	1.127633	1.627513	0.146581	-0.801648

Table S272. Orbital Energies and Philicity Parameters of $IX_{[1-2,4][b-e]}$ in SMD Water. All quantities given in eV.

Species	HOMO	LUMO	CHI	ETA	GEI	N	ΔGEI	ΔN
IX_{1b}	-8.397163	-0.077008	4.237086	8.320155	1.078880	1.896362		
IX_{1c}	-8.181104	0.007891	4.086607	8.188996	1.019683	2.112420	-0.059197	0.216058
IX_{1d}	-8.064368	0.016055	4.024156	8.080422	1.002041	2.229157		
IX_{1e}	-8.632813	-0.066668	4.349741	8.566146	1.104362	1.660711	0.102320	-0.568446
IX_{2b}	-8.287773	-0.102043	4.194908	8.185730	1.074874	2.005752		
IX_{2c}	-8.063551	-0.010612	4.037082	8.052939	1.011931	2.229973	-0.062943	0.224222
IX_{2d}	-7.957699	-0.013334	3.985516	7.944365	0.999724	2.335826		
IX_{2e}	-8.452402	-0.085988	4.269195	8.366414	1.089238	1.841123	0.089514	-0.494703
IX_{4b}	-8.400428	-0.066124	4.233276	8.334305	1.075112	1.893096		
IX_{4c}	-8.153621	0.010885	4.071368	8.164505	1.015128	2.139904	-0.059984	0.246807
IX_{4d}	-8.031442	0.013334	4.009054	8.044775	0.998941	2.262083		
IX_{4e}	-8.609140	-0.068028	4.338584	8.541111	1.101924	1.684385	0.102983	-0.577698

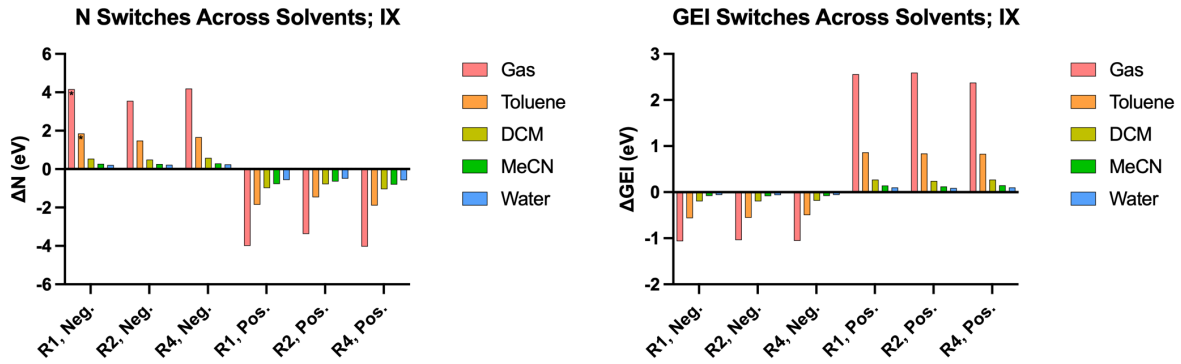


Figure S148. IX Nucleophilicity and Electrophilicity Switches Induced by Incorporation of D-LEFs.

S13. Gibbs Free Energy Surfaces & Components for D-LEF-Substituted and Unsubstituted Benzoin Condensations Across Different Solvents

Table S273. Energies of Model Benzoin Reaction in SMD Toluene, Uncharged. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(TOL)
I_{1a}	-304.705053	0.127653	0.007850	340.587200	0.038677	-304.569550	-304.608226	-304.605207
A	-345.469638	0.110744	0.007230	332.524600	0.037761	-345.351665	-345.389426	-345.386407
TS1	-650.167389	0.240537	0.014164	471.935500	0.053593	-649.912688	-649.966281	-649.963262
B	-650.179357	0.242247	0.014102	468.448900	0.053197	-649.923008	-649.976205	-649.973186
TS2	-765.849026	0.292365	0.017626	534.862700	0.060739	-765.539035	-765.599774	-765.596755
C	-650.189680	0.242021	0.014518	473.107400	0.053726	-649.933141	-649.986867	-649.983848
TS3	-995.669486	0.355755	0.019878	571.439900	0.064892	-995.293852	-995.358744	-995.355725
D	-995.678515	0.357885	0.020229	579.647100	0.065824	-995.300401	-995.366225	-995.363206
TS4	-995.667608	0.356312	0.020460	585.981600	0.066544	-995.290836	-995.357380	-995.354361
E	-690.965686	0.226323	0.013641	463.532600	0.052638	-690.725722	-690.778360	-690.775341
Methanol	-115.670411	0.051294	0.004281	238.059600	0.027034	-115.614836	-115.641870	-115.638851

Table S274. Model Benzoin Reaction Gibbs Free Energy Surface in SMD Toluene. Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1111.0168737	-1110.9885212	-1110.9984452	-1110.9831628	-1111.0091072	-1110.9945768	-1111.0020578	-1110.9932128	-1111.0194002
Rel. Energy	0.00	74.44	48.38	88.51	20.39	58.54	38.90	62.12	-6.63

Table S275. Energies of Model Benzoin Reaction in SMD Toluene, I_{1c} (Anionic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(TOL)
I_{1c}	-628.706663	0.130244	0.011205	415.973200	0.047238	-628.565215	-628.612452	-628.609433
TS1	-974.172100	0.242677	0.017642	539.267900	0.061239	-973.911781	-973.973019	-973.970000
B	-974.198396	0.246054	0.017087	524.661700	0.059580	-973.935255	-973.994835	-973.991816
TS2	-1089.866859	0.294538	0.021097	602.190200	0.068384	-1089.551223	-1089.619608	-1089.616589
C	-974.197461	0.244172	0.017979	541.487500	0.061491	-973.935310	-973.996801	-973.993782
TS3	-1319.685272	0.358774	0.022215	611.246800	0.069413	-1319.304283	-1319.373695	-1319.370676
D	-1319.695822	0.360404	0.023697	646.436100	0.073409	-1319.311721	-1319.385129	-1319.382110
TS4	-1319.676363	0.358937	0.023868	649.858800	0.073797	-1319.293558	-1319.367356	-1319.364337

Table S276. Model Benzoin Reaction Gibbs Free Energy Surface in SMD Toluene, I_{1c} (Anionic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1435.021100	-1434.995259	-1435.017075	-1435.002997	-1435.019041	-1435.009528	-1435.020962	-1435.003189	-1435.023626
Rel. Energy	0.00	67.84	10.57	47.53	5.40	30.38	0.36	47.02	-6.63

Table S277. Energies of Model Benzoin Reaction in SMD Toluene, I_{2c} (Anionic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(TOL)
I_{2c}	-668.008859	0.158104	0.012740	442.979600	0.050304	-667.838014	-667.888318	-667.885299
TS1	-1013.475881	0.270908	0.019086	564.796100	0.064138	-1013.185887	-1013.250025	-1013.247006
B	-1013.496304	0.273236	0.018865	557.199800	0.063275	-1013.204204	-1013.267479	-1013.264460
TS2	-1129.166345	0.322744	0.022610	627.403300	0.071247	-1128.820991	-1128.892239	-1128.889220
C	-1013.497918	0.272367	0.019433	566.227500	0.064300	-1013.206117	-1013.270418	-1013.267399
TS3	-1358.983601	0.386203	0.024977	663.040900	0.075294	-1358.572421	-1358.647716	-1358.644697
D	-1358.995128	0.388756	0.025042	667.386300	0.075788	-1358.581330	-1358.657118	-1358.654099
TS4	-1358.975687	0.386528	0.025543	679.526600	0.077167	-1358.563616	-1358.640783	-1358.637764

Table S278. Model Benzoin Reaction Gibbs Free Energy Surface in SMD Toluene, I_{2c} (Anionic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1474.296966	-1474.272265	-1474.289719	-1474.275628	-1474.292658	-1474.283549	-1474.292951	-1474.276616	-1474.299492
Rel. Energy	0.00	64.85	19.03	56.02	11.31	35.23	10.54	53.43	-6.63

Table S279. Energies of Model Benzoin Reaction in SMD Toluene, I_{1e} (Cationic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(TOL)
I_{1e}	-478.341450	0.244814	0.012518	433.277900	0.049203	-478.084118	-478.133321	-478.130302
TS1	-823.808147	0.359217	0.018215	541.302000	0.061470	-823.430715	-823.492185	-823.489166
B	-823.820830	0.361872	0.018007	533.448200	0.060578	-823.440951	-823.491529	-823.488510
TS2	-939.478948	0.411056	0.021680	604.993400	0.068703	-939.046212	-939.114915	-939.111896
C	-823.828108	0.359499	0.018979	550.241300	0.062485	-823.449630	-823.512115	-823.509096
TS3	-1169.291588	0.475120	0.024073	640.733600	0.072761	-1168.792395	-1168.865156	-1168.862137
D	-1169.312809	0.477266	0.024470	648.946300	0.073694	-1168.811073	-1168.884767	-1168.881748
TS4	-1169.307998	0.474643	0.024702	655.719400	0.074463	-1168.808653	-1168.883116	-1168.880097

Table S280. Model Benzoin Reaction Gibbs Free Energy Surface in SMD Toluene, I_{1e} (Cationic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1284.541969	-1284.514425	-1284.513769	-1284.498304	-1284.534355	-1284.500989	-1284.520600	-1284.518949	-1284.544495
Rel. Energy	0.00	72.32	74.04	114.64	19.99	107.59	56.10	60.44	-6.63

Table S281. Energies of Model Benzoin Reaction in SMD Toluene, I_{2e} (Cationic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(TOL)
I_{2e}	-517.635458	0.273552	0.013697	451.407300	0.051261	-517.348210	-517.399471	-517.396452
TS1	-863.097740	0.388747	0.019379	559.913000	0.063583	-862.689613	-862.753196	-862.750177
B	-863.099465	0.389779	0.019612	563.358400	0.063975	-862.690075	-862.754049	-862.751030
TS2	-978.769316	0.440511	0.022789	619.807500	0.070385	-978.306015	-978.376400	-978.373381
C	-863.123535	0.389644	0.020193	573.111700	0.065082	-862.713698	-862.778780	-862.775761
TS3	-1208.587316	0.507535	0.024664	651.768900	0.074014	-1208.055117	-1208.129131	-1208.126112
D	-1208.601090	0.506810	0.025561	668.472800	0.075911	-1208.068720	-1208.144631	-1208.141612
TS4	-1208.591226	0.503773	0.025815	673.735700	0.076509	-1208.061638	-1208.138147	-1208.135128

Table S282. Model Benzoin Reaction Gibbs Free Energy Surface in SMD Toluene, I_{2e} (Cationic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1323.808119	-1323.775436	-1323.776289	-1323.759789	-1323.801020	-1323.764964	-1323.780464	-1323.773980	-1323.810645
Rel. Energy	0.00	85.81	83.57	126.89	18.64	113.30	72.61	89.63	-6.63

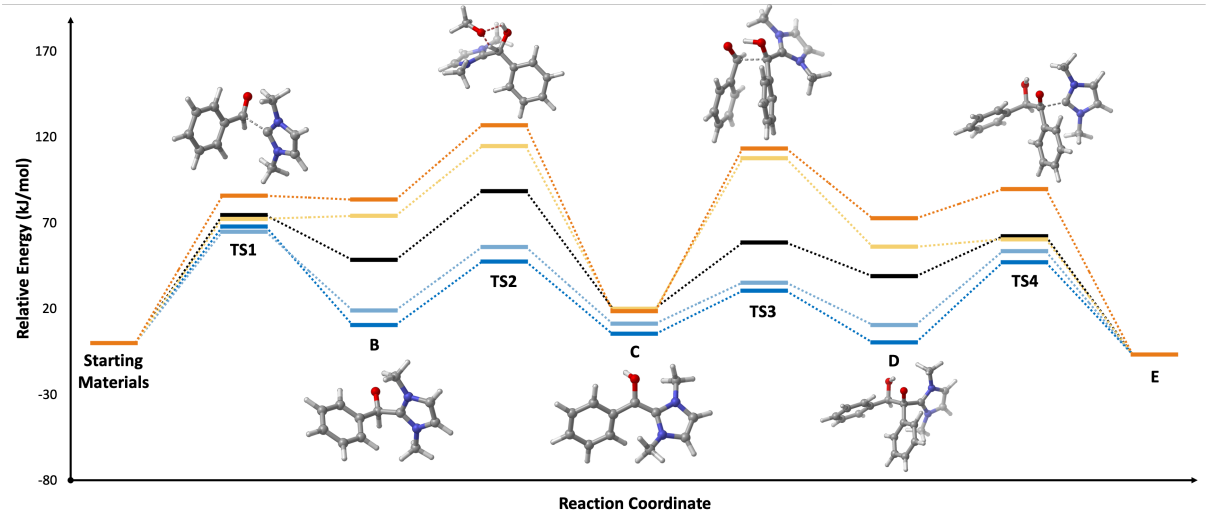


Figure S149. Gibbs Free Energy (kJ/mol) at 298.15 K of the benzoin condensation catalysed by I1a (black), I1b (dark blue), I1c (light blue), I1d (yellow), and I1e (orange) at the SMD//M06-2X/cc-pVDZ level of theory in SMD Toluene.

Table S283. Energies of Model Benzoin Reaction in SMD DCM, Uncharged. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{1a}	-304.709700	0.127492	0.007901	342.529900	0.038897	-304.574307	-304.613204	-304.610185
A	-345.471814	0.110671	0.007232	332.557500	0.037765	-345.353911	-345.391676	-345.388657
TS1	-650.174361	0.240323	0.014207	472.721700	0.053682	-649.919831	-649.973513	-649.970494
B	-650.191020	0.242238	0.014098	468.158400	0.053164	-649.934684	-649.987847	-649.984828
TS2	-765.859645	0.291767	0.017762	537.609500	0.061051	-765.550117	-765.611167	-765.608148
C	-650.195757	0.241736	0.014516	473.108700	0.053726	-649.939505	-649.993230	-649.990211
TS3	-995.678824	0.355139	0.020057	574.278600	0.065215	-995.303628	-995.368843	-995.365824
D	-995.690525	0.357785	0.020195	579.178900	0.065771	-995.312546	-995.378317	-995.375298
TS4	-995.675293	0.356019	0.020539	587.949800	0.066767	-995.298736	-995.365503	-995.362484
E	-690.969987	0.225935	0.013713	464.819100	0.052785	-690.730338	-690.783123	-690.780104
Methanol	-115.672326	0.051276	0.004262	237.773600	0.027001	-115.616788	-115.643790	-115.640771

Table S284. Model Benzoin Reaction Gibbs Free Energy Surface in SMD DCM. Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1111.028272	-1110.999923	-1111.014257	-1110.996806	-1111.019640	-1111.006596	-1111.016070	-1111.003256	-1111.031061
Rel. Energy	0.00	74.43	36.79	82.61	22.66	56.91	32.04	65.68	-7.32

Table S285. Energies of Model Benzoin Reaction in SMD DCM, I_{1c} (Anionic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{1c}	-628.737890	0.130142	0.011207	415.956000	0.047236	-628.596541	-628.643777	-628.640758
TS1	-974.203696	0.242551	0.017649	539.273700	0.061240	-973.943497	-974.004736	-974.001717
B	-974.228192	0.244811	0.017461	533.708200	0.060607	-973.965919	-974.026527	-974.023508
TS2	-1089.896519	0.294074	0.021220	604.600800	0.068658	-1089.581225	-1089.649883	-1089.646864
C	-974.226373	0.243825	0.018027	542.821000	0.061642	-973.964521	-974.026163	-974.023144
TS3	-1319.712659	0.357479	0.023706	641.997100	0.072905	-1319.331474	-1319.404378	-1319.401359
D	-1319.725935	0.359975	0.023747	647.297200	0.073507	-1319.342213	-1319.415720	-1319.412701
TS4	-1319.706314	0.358387	0.024005	653.569100	0.074219	-1319.323922	-1319.398141	-1319.395122

Table S286. Model Benzoin Reaction Gibbs Free Energy Surface in SMD DCM, I_{1c} (Anionic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1435.058845	-1435.031146	-1435.052937	-1435.035522	-1435.052573	-1435.042131	-1435.053473	-1435.035894	-1435.061634
Rel. Energy	0.00	72.72	15.51	61.23	16.47	43.88	14.10	60.26	-7.32

Table S287. Energies of Model Benzoin Reaction in SMD DCM, I_{2c} (Anionic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{2c}	-668.039313	0.157687	0.012923	448.684900	0.050952	-667.868703	-667.919655	-667.916636
TS1	-1013.506483	0.270622	0.019161	566.426300	0.064323	-1013.216700	-1013.281023	-1013.278004
B	-1013.527051	0.272838	0.019013	560.798000	0.063684	-1013.235200	-1013.298884	-1013.295865
TS2	-1129.195948	0.321886	0.022820	632.455700	0.071821	-1128.851242	-1128.923063	-1128.920044
C	-1013.527436	0.272049	0.019477	567.017000	0.064390	-1013.235910	-1013.300300	-1013.297281
TS3	-1359.012708	0.385655	0.025047	664.046500	0.075409	-1358.602007	-1358.677415	-1358.674396
D	-1359.026050	0.388241	0.025114	669.044700	0.075976	-1358.612694	-1358.688670	-1358.685651
TS4	-1359.006284	0.385928	0.025651	682.016600	0.077449	-1358.594705	-1358.672155	-1358.669136

Table S288. Model Benzoin Reaction Gibbs Free Energy Surface in SMD DCM, I_{2c} (Anionic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1474.334723	-1474.307433	-1474.325294	-1474.308702	-1474.326710	-1474.315168	-1474.326423	-1474.309908	-1474.337512
Rel. Energy	0.00	71.65	24.75	68.32	21.04	51.34	21.79	65.15	-7.32

Table S289. Energies of Model Benzoin Reaction in SMD DCM, I_{1e} (Cationic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{1e}	-478.371792	0.244849	0.012396	430.461100	0.048883	-478.114547	-478.163429	-478.160410
TS1	-823.837684	0.358602	0.018395	545.246100	0.061918	-823.460687	-823.522605	-823.519586
B	-823.854003	0.361392	0.018050	535.117200	0.060768	-823.474561	-823.535328	-823.532309
TS2	-939.512758	0.409670	0.022101	614.356200	0.069766	-939.080987	-939.150753	-939.147734
C	-823.858456	0.359321	0.018942	549.771600	0.062432	-823.480193	-823.542625	-823.539606
TS3	-1169.324543	0.473260	0.024581	651.951800	0.074035	-1168.826702	-1168.900737	-1168.897718
D	-1169.347359	0.475511	0.024905	658.200500	0.074745	-1168.846943	-1168.921688	-1168.918669
TS4	-1169.340006	0.473468	0.025018	662.918600	0.075281	-1168.841521	-1168.916801	-1168.913782

Table S290. Model Benzoin Reaction Gibbs Free Energy Surface in SMD DCM, I_{1e} (Cationic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1284.578497	-1284.549015	-1284.561738	-1284.536392	-1284.569035	-1284.538490	-1284.559441	-1284.554554	-1284.581286
Rel. Energy	0.00	77.40	44.00	110.55	24.84	105.04	50.03	62.86	-7.32

Table S291. Energies of Model Benzoin Reaction in SMD DCM, I_{2e} (Cationic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(DCM)
I_{2e}	-517.668136	0.273361	0.013885	457.146700	0.051913	-517.380891	-517.432804	-517.429785
TS1	-863.131513	0.386710	0.020051	575.392900	0.065341	-862.724752	-862.790094	-862.787075
B	-863.144328	0.388996	0.019778	567.237600	0.064415	-862.735554	-862.799969	-862.796950
TS2	-978.813110	0.438392	0.023494	635.111400	0.072123	-978.351224	-978.423347	-978.420328
C	-863.156114	0.387546	0.020491	577.632700	0.065596	-862.748077	-862.813673	-862.810654
TS3	-1208.630372	0.500674	0.026097	678.477000	0.077047	-1208.103600	-1208.180648	-1208.177629
D	-1208.643397	0.503970	0.026079	678.140300	0.077009	-1208.113348	-1208.190357	-1208.187338
TS4	-1208.630307	0.502055	0.026512	689.778300	0.078331	-1208.101740	-1208.180070	-1208.177051

Table S292. Model Benzoin Reaction Gibbs Free Energy Surface in SMD DCM, I_{2e} (Cationic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1323.847872	-1323.816504	-1323.826379	-1323.808986	-1323.840083	-1323.818401	-1323.828110	-1323.817823	-1323.850661
Rel. Energy	0.00	82.36	56.43	102.09	20.45	77.38	51.88	78.89	-7.32

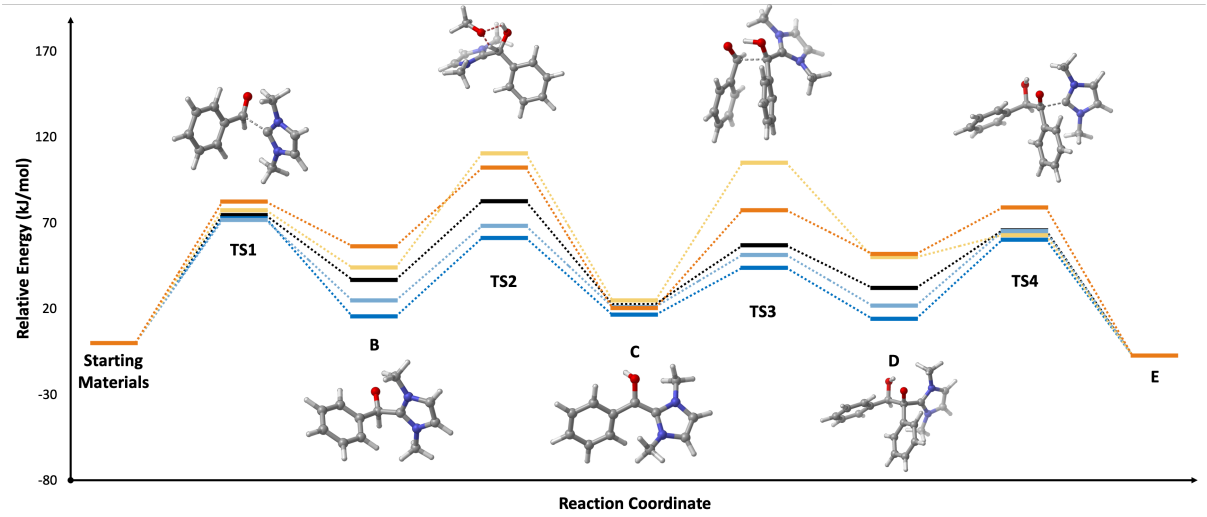


Figure S150. Gibbs Free Energy (kJ/mol) at 298.15 K of the benzoin condensation catalysed by I1a (black), I1b (dark blue), I1c (light blue), I1d (yellow), and I1e (orange) at the SMD//M06-2X/cc-pVDZ level of theory in SMD DCM.

Table S293. Energies of Model Benzoin Reaction in SMD MeCN, Uncharged. Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{1a}	-304.709991	0.127447	0.007916	343.203200	0.038974	-304.574628	-304.613602	-304.610583
A	-345.471303	0.110620	0.007243	332.845100	0.037798	-345.353439	-345.391237	-345.388218
TS1	-650.174102	0.240211	0.014216	472.801500	0.053691	-649.919675	-649.973366	-649.970347
B	-650.191700	0.242146	0.014113	468.501800	0.053203	-649.935441	-649.988643	-649.985624
TS2	-765.859695	0.291427	0.017887	541.735700	0.061519	-765.550381	-765.611900	-765.608881
C	-650.195019	0.241553	0.014541	473.576800	0.053779	-649.938925	-649.992704	-649.989685
TS3	-995.678986	0.354996	0.020141	576.410300	0.065457	-995.303849	-995.369306	-995.366287
D	-995.691075	0.357616	0.020202	579.564100	0.065815	-995.313257	-995.379071	-995.376052
TS4	-995.674404	0.355911	0.020529	587.572000	0.066724	-995.297964	-995.364689	-995.361670
E	-690.969336	0.226358	0.013607	462.369800	0.052506	-690.729371	-690.781877	-690.778858
Methanol	-115.672411	0.051266	0.004290	238.267300	0.027057	-115.616855	-115.643912	-115.640893

Table S294. Model Benzoin Reaction Gibbs Free Energy Surface in SMD MeCN. Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1111.027914	-1110.999459	-1111.014736	-1110.997100	-1111.018797	-1111.007181	-1111.016946	-1111.002564	-1111.030335
Rel. Energy	0.00	74.71	34.60	80.90	23.94	54.43	28.80	66.56	-6.36

Table S295. Energies of Model Benzoin Reaction in SMD MeCN, I_{1c} (Anionic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{1c}	-628.745741	0.129964	0.011216	416.245200	0.047268	-628.604561	-628.651829	-628.648810
TS1	-974.210957	0.242539	0.017684	540.372400	0.061364	-973.950735	-974.012099	-974.009080
B	-974.233789	0.244722	0.017458	533.624600	0.060598	-973.971608	-974.032206	-974.029187
TS2	-1089.902520	0.293981	0.021210	604.259400	0.068619	-1089.587329	-1089.655948	-1089.652929
C	-974.232030	0.243694	0.018042	543.201700	0.061686	-973.970294	-974.031979	-974.028960
TS3	-1319.718485	0.357483	0.023686	642.067300	0.072913	-1319.337316	-1319.410229	-1319.407210
D	-1319.732238	0.359954	0.023737	646.138000	0.073375	-1319.348547	-1319.421922	-1319.418903
TS4	-1319.711732	0.357958	0.024120	656.434000	0.074544	-1319.329654	-1319.404198	-1319.401179

Table S296. Model Benzoin Reaction Gibbs Free Energy Surface in SMD MeCN, I_{1c} (Anionic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1435.066141	-1435.038192	-1435.058299	-1435.041148	-1435.058072	-1435.048104	-1435.059797	-1435.042073	-1435.068562
Rel. Energy	0.00	73.38	20.59	65.62	21.18	47.36	16.66	63.19	-6.36

Table S297. Energies of Model Benzoin Reaction in SMD MeCN, I_{2c} (Anionic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{2c}	-668.046662	0.157565	0.012951	449.445400	0.051039	-667.876147	-667.927186	-667.924167
TS1	-1013.512964	0.270566	0.019166	566.489900	0.064330	-1013.223232	-1013.287562	-1013.284543
B	-1013.532725	0.272674	0.019075	562.726800	0.063903	-1013.240976	-1013.304879	-1013.301860
TS2	-1129.201632	0.321693	0.022880	634.236400	0.072023	-1128.857059	-1128.929083	-1128.926064
C	-1013.533134	0.271878	0.019505	567.722700	0.064470	-1013.241751	-1013.306221	-1013.303202
TS3	-1359.018502	0.385260	0.025199	668.201800	0.075880	-1358.608043	-1358.683923	-1358.680904
D	-1359.031621	0.388099	0.025125	669.462800	0.076024	-1358.618396	-1358.694420	-1358.691401
TS4	-1359.011755	0.385804	0.025637	681.615800	0.077404	-1358.600314	-1358.677717	-1358.674698

Table S298. Model Benzoin Reaction Gibbs Free Energy Surface in SMD MeCN, I_{2c} (Anionic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1474.341498	-1474.313655	-1474.330972	-1474.314283	-1474.332314	-1474.321798	-1474.332295	-1474.315592	-1474.343919
Rel. Energy	0.00	73.10	27.63	71.45	24.11	51.72	24.16	68.02	-6.36

Table S299. Energies of Model Benzoin Reaction in SMD MeCN, I_{1e} (Cationic Charge, Position 1). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{1e}	-478.378885	0.244989	0.012362	429.669200	0.048793	-478.121535	-478.170328	-478.167309
TS1	-823.843390	0.358326	0.018475	547.146800	0.062134	-823.466589	-823.528722	-823.525703
B	-823.860594	0.360667	0.018327	542.415100	0.061596	-823.481600	-823.543197	-823.540178
TS2	-939.519627	0.408718	0.022327	619.405800	0.070339	-939.088582	-939.158922	-939.155903
C	-823.864363	0.359180	0.018921	549.682000	0.062421	-823.486261	-823.548683	-823.545664
TS3	-1169.331428	0.472764	0.024742	655.642400	0.074454	-1168.833921	-1168.908376	-1168.905357
D	-1169.354885	0.475060	0.025014	661.573500	0.075128	-1168.854811	-1168.929939	-1168.926920
TS4	-1169.345705	0.473313	0.025091	664.221600	0.075429	-1168.847302	-1168.922730	-1168.919711

Table S300. Model Benzoin Reaction Gibbs Free Energy Surface in SMD MeCN, I_{1e} (Cationic Charge, Position 1). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1284.584640	-1284.554815	-1284.569290	-1284.544122	-1284.574776	-1284.546251	-1284.567814	-1284.560605	-1284.587061
Rel. Energy	0.00	78.30	40.30	106.38	25.90	100.79	44.18	63.10	-6.36

Table S301. Energies of Model Benzoin Reaction in SMD MeCN, I_{2e} (Cationic Charge, Position 2). Entropy given in J/mol.K. All other quantities given in Hartree.

Species	DFT Energy	ZPVE	TC	S	TS	H	G	G(MeCN)
I_{2e}	-517.675981	0.273321	0.013923	458.624300	0.052081	-517.388737	-517.440818	-517.437799
TS1	-863.138760	0.386288	0.020190	578.576800	0.065703	-862.732283	-862.797985	-862.794966
B	-863.154478	0.388568	0.019928	569.976000	0.064726	-862.745983	-862.810709	-862.807690
TS2	-978.823167	0.438024	0.023613	638.039500	0.072455	-978.361530	-978.433985	-978.430966
C	-863.162805	0.387357	0.020517	578.161400	0.065656	-862.754931	-862.820587	-862.817568
TS3	-1208.640059	0.501181	0.026038	677.162800	0.076898	-1208.112840	-1208.189738	-1208.186719
D	-1208.652644	0.503836	0.026148	679.964500	0.077216	-1208.122661	-1208.199877	-1208.196858
TS4	-1208.637955	0.501775	0.026644	693.061500	0.078704	-1208.109536	-1208.188240	-1208.185221

Table S302. Model Benzoin Reaction Gibbs Free Energy Surface in SMD MeCN, I_{2e} (Cationic Charge, Position 2). Energies given in Hartree, Relative energies given in kJ/mol.

	Starting Materials	TS1	B	TS2	C	TS3	D	TS4	E
Energy	-1323.855130	-1323.824078	-1323.836802	-1323.819185	-1323.846680	-1323.827613	-1323.837752	-1323.826115	-1323.857551
Rel. Energy	0.00	81.53	48.12	94.37	22.18	72.25	45.63	76.18	-6.36

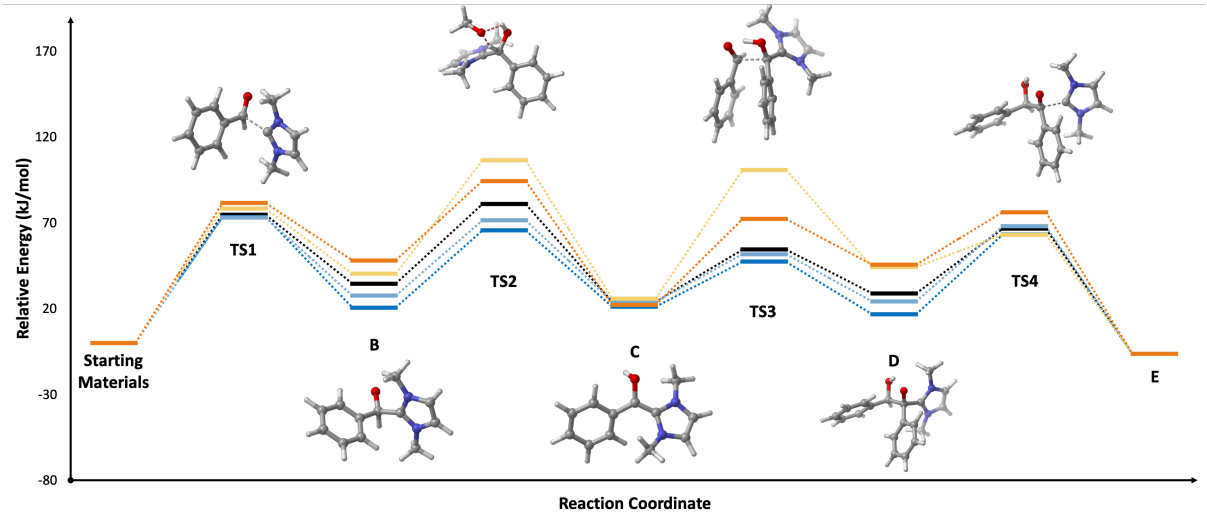


Figure S151. Gibbs Free Energy (kJ/mol) at 298.15 K of the benzoin condensation catalysed by I1a (black), I1b (dark blue), I1c (light blue), I1d (yellow), and I1e (orange) at the SMD//M06-2X/cc-pVDZ level of theory in SMD MeCN.

S14. PhotoNHC Switching Results

We investigated whether the wavelength of light required to activate photochemically active NHC-adducts could be substantially shifted via the incorporation of D-LEFs, in line with previous work by some of us [Blyth, Noble, Russell, and Coote, 2019; Hill and Coote 2018].

We found that for the system below, taken from 10.1002/angie.201914456, we could lower the absorption energy of the photoactive I1a adduct by 0.1644 eV with an anionic D-LEF, and raise it by 0.057 eV in MeCN. We note that these results are smaller than reported in our previous works, above, but consistent with the understanding that these effects are electrostatic, and now operating further from the reactive centre (being now attached to the NHC, rather than directly attached to the reacting substrate). Future work in this area is likely warranted.

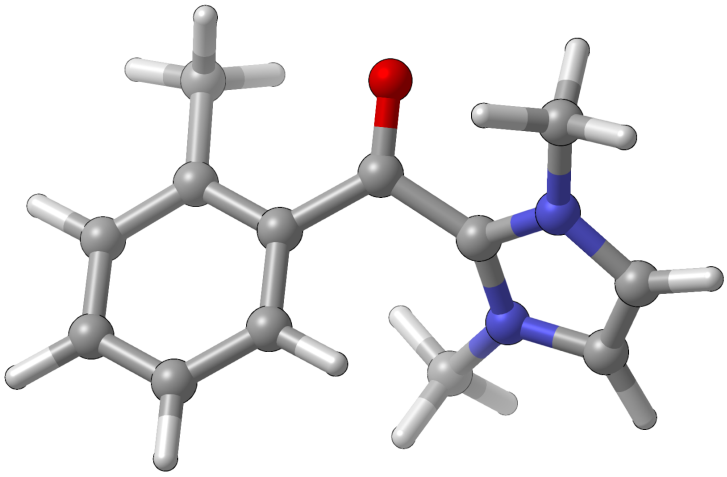


Figure S152. The PhotoNHC Used. To investigate the possible role of D-LEF-substituted NHCs in photo-reactivity.

Table S303. TD-DFT Results. For PhotoNHC with $I_{1a.}$

State Name	Energy (eV)	Wavelength (nm)	f-value	Character	Notes
T1	3.176	390.440	0.000	nπ*	
T2	3.572	347.090	0.000	ππ*	ISC
S1	3.654	339.310	0.002	nπ*	
T3	3.982	311.340	0.000	ππ*	
T4	4.125	300.590	0.000	ππ*	
S2	4.534	273.440	0.113	ππ*	Absorption
T5	4.702	263.710	0.000	ππ*	
S3	4.893	253.390	0.307	ππ*	
S4	5.144	241.030	0.099	ππ*	
T6	5.220	237.530	0.000	ππ*	

Table S304. TD-DFT Results. For PhotoNHC with $I_{1b.}$

State Name	Energy (eV)	Wavelength (nm)	f-value	Character	Notes
T1	3.170	391.100	0.000	nπ*	
T2	3.567	347.560	0.000	ππ*	ISC
S1	3.653	339.400	0.003	nπ*	
T3	3.923	316.060	0.000	ππ*	
T4	4.030	307.670	0.000	ππ*	
S2	4.543	272.920	0.158	ππ*	Absorption
T5	4.703	263.610	0.000	ππ*	
S3	4.800	258.320	0.292	ππ*	
S4	5.046	245.720	0.105	ππ*	
T6	5.183	239.220	0.000	ππ*	

Table S305. TD-DFT Results. For PhotoNHC with $I_{1c.}$

State Name	Energy (eV)	Wavelength (nm)	f-value	Character	Notes
T1	3.098	400.240	0.000	nπ*	
T2	3.456	358.720	0.000	nπ*	
S1	3.658	338.920	0.002	nπ*	
T3	3.799	326.330	0.000	ππ*	ISC
T4	4.180	296.640	0.000	ππ*	
S2	4.379	283.170	0.290	ππ*	Absorption
S3	4.635	267.490	0.055	ππ*	
T5	4.672	265.410	0.000	ππ*	
S4	4.956	250.160	0.110	ππ*	
T6	4.962	249.860	0.000	π*	

Table S306. TD-DFT Results. For PhotoNHC with $I_{1d.}$

State Name	Energy (eV)	Wavelength (nm)	f-value	Character	Notes
T1	3.165	391.690	0.000	nπ*	
T2	3.576	346.720	0.000	ππ*	ISC
S1	3.646	340.080	0.003	nπ*	
T3	3.942	314.490	0.000	ππ*	
T4	4.045	306.480	0.000	ππ*	
S2	4.536	273.320	0.142	ππ*	Absorption
T5	4.700	263.830	0.000	ππ*	
T6	4.735	261.840	0.000	ππ*	
S3	4.744	261.340	0.018	ππ*	
S4	4.829	256.750	0.286	ππ*	

Table S307. TD-DFT Results. For PhotoNHC with $I_{1e.}$

State Name	Energy (eV)	Wavelength (nm)	f-value	Character	Notes
T1	3.173	390.740	0.000	nπ*	
T2	3.518	352.430	0.000	ππ*	ISC
S1	3.647	339.930	0.002	nπ*	
T3	3.931	315.430	0.000	ππ*	
T4	4.258	291.170	0.000	ππ*	
S2	4.479	276.820	0.112	ππ*	Absorption
T5	4.698	263.890	0.000	ππ*	
S3	4.880	254.090	0.340	ππ*	
T6	5.206	238.160	0.000	ππ*	
S4	5.219	237.560	0.125	ππ*	

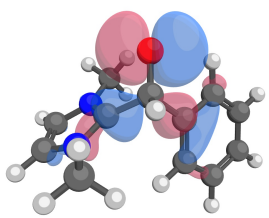
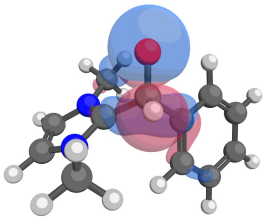
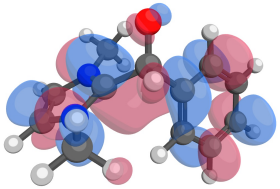
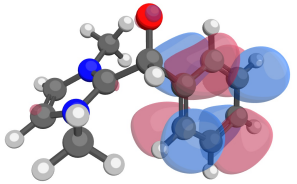
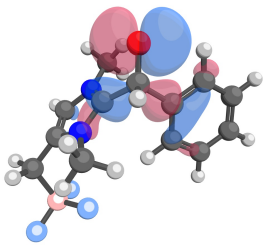
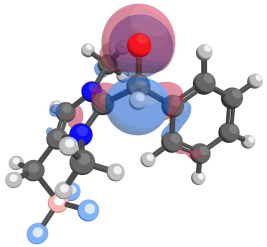
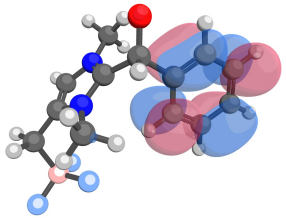
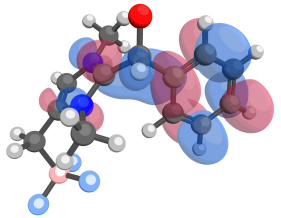
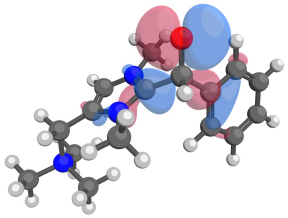
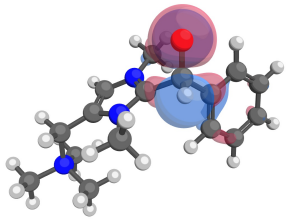
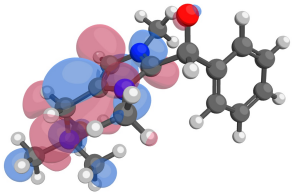
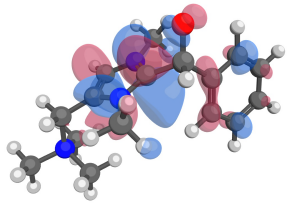
S15. Additional Analysis of Benzoin Condensation

Table S308. Changes in Mulliken Charges. Condensed Mulliken charges of relevant atoms in **B**, **TS1**, and **TS2**.

Atom	TS1	B	TS2
Carbene-C	-0.0118	0.1954	0.2305
Carbene-N1	-0.2036	-0.2230	-0.1963
Carbene-N2	-0.1993	-0.2098	-0.2222
Backbone1	0.0801	0.1010	0.1175
Backbone2	0.0918	0.1134	0.1106
Adduct-C	0.2034	0.1771	0.1387
Adduct-O	-0.3669	-0.5291	-0.1342

From the above, we observe that the carbene carbon goes from being effectively neutral to partially cationic. It is this change in electronic population that is stabilised by anionic D-LEFs or destabilised by cationic D-LEFs.

Chart S1. The frontier molecular orbitals (HOMO-1, HOMO, LUMO, and LUMO+1) of **B** in the benzoin condensation catalysed by each of $\mathbf{I_{2a}}$, $\mathbf{I_{2c}}$, and $\mathbf{I_{2e}}$.

Species	HOMO-1	HOMO	LUMO	LUMO+1
$\mathbf{I_{2a}}$				
$\mathbf{I_{2c}}$				
$\mathbf{I_{2e}}$				

S16. Investigation of Quadrupoles

Table S309. Field-Independent Quadrupole Moments of Various Species.

Component	I_{2a}	Methylated	I_{2b}	I_{2c}	Δ Anionic Charge	I_{2d}	I_{2e}	Δ Cationic Charge
Q_{XX}	-32.0786	-41.5178	-77.3187	-108.9982	-31.6795	-66.5061	-43.272	23.2341
YY	-45.2261	-50.6733	-57.1005	-76.8657	-19.7652	-67.3374	-58.6727	8.6647
ZZ	-44.8778	-51.2832	-63.446	-78.101	-14.655	-69.7324	-68.1082	1.6242
XY	0	5.4524	8.5209	13.2137	4.6928	-8.4003	6.1876	14.5879
XZ	0	0	0.0007	1.0867	1.086	-1.5725	2.0433	3.6158
YZ	0	0	0.0031	0.6016	0.5985	-1.5257	-0.7705	0.7552
Magnitude $\hat{Q}_l^2$	2072.70	2663.76	4141.93	6389.28		4912.96	4706.97	

Relative to I_{2a}, the magnitude of the field-independent quadrupole moment of I_{2b} and I_{2d} is significantly increased (from 2072.70 Debye-Angstrom to 4141.93 Debye-Angstrom and 4912.96 Debye-Angstrom, respectively). In each case, the effect manifests predominately in the XX component (where the D-LEF is predominately aligned along the X-coordinate), which is in line with the uncharged D-LEF enhancing the quadrupole moment. Upon introducing charges, the magnitude increases for I_{2c} to 6389.28 Debye-Angstrom, and decreases only slightly for I_{2e} to 4706.97 Debye-Angstrom. However, the differences once again manifest themselves predominately along the XX component, while their opposite sign and approximately-equal magnitude lend credence to the suggestion that these changes have an electrostatic origin. As an aside, it is possible that the small change in quadrupole magnitude from the cationic D-LEF arises because the cationic charge opposes the increased quadrupole caused by the remainder of the substituent in the non-XX components. Placing a methyl group at the 2-position, we also observe only a small increase in the magnitude of the quadrupole moment, to 2663.76 Debye-Angstrom, which also manifests along the XX-component.

The magnitude of the quadrupole moment is calculated according to the following equation from "Theory of Molecular Fluids Volume 1: Fundamentals" C. G. Gray and K. E. Gubbins, Oxford University Press, New York, 1984.

$$\hat{Q}_l^2 = \frac{4\pi}{2l+l}\sum_m |Q_{lm}|^2$$

Where, in the case of the quadrupole, l = 2, m = 0, 1, 2, and

$$Q_{20} = \sqrt{\frac{5}{4\pi}}(Q_{zz})$$

$$Q_{21} = -\sqrt{\frac{5}{4\pi}}\sqrt{\frac{2}{3}}(Q_{xz} + iQ_{yz})$$

$$Q_{22} = -\sqrt{\frac{5}{4\pi}}\sqrt{\frac{1}{6}}(Q_{xx} - Q_{yy} + 2iQ_{xy})$$

S17. Gaussian Log Files for Every Species

Gaussian log files for every species reported in this article are stored at https://github.com/Ecaloota/CarbenesElectricFields

If you encounter any issues accessing these files, please contact the corresponding author via the provided email, or the first author via mitchell.blyth@anu.edu.au