Electronic Supplementary Information

Substituent effect in theoretical ROA spectra

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Table of contents

Substituents and substituent constants 4
Spectral parameters of selected modes 5
Correlations of spectral parameters of selected modes with substituent constants 27
ν(C*H) in IND 27
ν(C*H) in IIN 30
ν(CN) in IND 33
ν(CN) in IIN 37
ν_s(HC=CH) in IND 42
ν(NH) in IIN 47
ν(C=C)$_1$ in IND 52
ν(C=C)$_2$ in IND 57
ν(C=C)$_3$ in IND 62
ν(C=C)$_4$ in IIN 67
ν(C=C)$_5$ in IIN 72
Gaussian 09 input headings 77
Full Gaussian 09 citation 77
Method dependence test 78
Correlations of ROA robustness parameters with substituents volume 105
Coordinates and energies of CN-IND 108
Coordinates and energies of CN-IIN 141

Tables

Table S1 Substituents used in the study along with their σ_p and *pEDA(I)* values. 4
Table S2 Spectral parameters of ν(C*H) mode in IND. 5
Table S3 Spectral parameters of ν(CN) mode in IND. 7
Table S4 Spectral parameters of ν_s(HC=CH) mode in IND 9
Table S5 Spectral parameters of ν(C=C)$_1$ mode in IND 11
Table S6 Spectral parameters of ν(C=C)$_2$ mode in IND 13
Table S7 Spectral parameters of ν(C=C)$_3$ mode in IND 15
Table S8 Spectral parameters of ν(C*H) mode in IIIN 17
Table S9 Spectral parameters of ν(CN) mode in IIN 19
Table S10 Spectral parameters of ν(NH) mode in IIN 21
Table S11 Spectral parameters of ν(C=C)$_4$ mode in IIN 23
Table S12 Spectral parameters of ν(C=C)$_5$ mode in IIN 25
Table S13 Method dependence of spectral parameters of ν(C*H) mode in IND 79
Table S14 Method dependence of spectral parameters of ν(CN) mode in IND 80
Table S15 Method dependence of spectral parameters of ν_s(HC=CH) mode in IND 82
Table S17 Method dependence of spectral parameters of ν(C=C)$_1$ mode in IND 83
Table S18 Method dependence of spectral parameters of ν(C=C)$_2$ mode in IND 85
Table S19 Method dependence of spectral parameters of ν(C=C)$_3$ mode in IND 86
Table S20 Method dependence of spectral parameters of ν(C*H) mode in IIN 88
Table S21 Method dependence of spectral parameters of ν(CN) mode in IIN 89
Table S22 Method dependence of spectral parameters of ν(NH) mode in IIN 90
Table S23 Method dependence of spectral parameters of ν(C=C)$_4$ mode in IIN 92
Table S24 Method dependence of spectral parameters of ν(C=C)$_5$ mode in IIN 93
Table S25 ROA intensity correlations with *pEDA(I)* descriptor in IND 95
Table S26 ROA intensity correlations with σ_p descriptor in IND 96
Table S27 Proportionality of $\alpha G'$ and $\beta(G')^2$ invariants in IND 98
Table S28 ROA intensity correlations with *pEDA(I)* descriptor in IIN 99
Table S29 ROA intensity correlations with σ_p descriptor in IIN 101
Table S30 Proportionality of $\alpha G'$ and $\beta(G')^2$ invariants in IIN 102

Figures

Figure S1. Correlations of frequencies and IR intensities of *ν*(C*H) in IND with σ_p. 27
Figure S2. Correlations of $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(C*H) in IND with *pEDA(I)*. 28
Figure S3. $\boldsymbol{\beta A2}$ invariant of *ν*(C*H) in IND plotted against σ_p and *pEDA(I)*. 29
Figure S4. Correlations of frequencies and IR intensities of *ν*(C*H) in IIN with σ_p. 30
Figure S5. Correlations of $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(C*H) in IIN with *pEDA(I)*. 31
Figure S6. $\boldsymbol{\beta A2}$ invariant of *ν*(C*H) in IIN plotted against σ_p and *pEDA(I)*. 32
Figure S7. Correlations of frequencies and IR intensities of *ν*(CN) in IND with σ_p. 33
Figure S8. Correlations of $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(CN) in IND with σ_p. 34
Figure S9. Mutual proportionality of $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(CN) in IND. 35
Figure S10. $\boldsymbol{\beta A2}$ invariant of *ν*(CN) in IND plotted against σ_p and *pEDA(I)*. 36
Figure S11. Correlations of frequencies and IR intensities of *ν*(CN) in IIN with σ_p. 37
Figure S12. ROA intensities of *ν*(CN) in IIN plotted against σ_p and *pEDA(I)*. 38
Figure S13. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(CN) in IIN. 39
Figure S14. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G'2}$ invariants of *ν*(CN) in IIN plotted against σ_p. 40

Figure S15. $\boldsymbol{\beta A 2}$ invariant of ν(CN) in IIN plotted against σ_p and *pEDA(I)*. 41
Figure S16. Correlations of frequencies and IR intensities of ν_s(HC=CH) in IND with σ_p. 42
Figure S17. ROA intensities of ν_s(HC=CH) in IND plotted against σ_p and *pEDA(I)*. 43
Figure S18. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of ν_s(HC=CH) in IND. 44
Figure S19. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of ν_s(HC=CH) in IND plotted against σ_p. 45
Figure S20. $\boldsymbol{\beta A 2}$ invariant of ν_s(HC=CH) in IND plotted against σ_p and *pEDA(I)*. 46
Figure S21. Correlations of frequencies and IR intensities of ν(NH) in IIN with σ_p. 47
Figure S22. ROA intensities of ν(NH) in IIN plotted against σ_p and *pEDA(I)*. 48
Figure S23. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of ν(NH) in IIN. 49
Figure S24. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of ν(NH) in IIN plotted against *pEDA(I)*. 50
Figure S25. $\boldsymbol{\beta A 2}$ invariant of ν(NH) in IIN plotted against σ_p and *pEDA(I)*. 51
Figure S26. Frequencies and IR intensities of $\nu(C=C)_1$ in IND plotted against *pEDA(I)*. 52
Figure S27. ROA intensities of $\nu(C=C)_1$ in IND plotted against σ_p and *pEDA(I)*. 53
Figure S28. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_1$ in IND. 54
Figure S29. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_1$ in IND plotted against *pEDA(I)*. 55
Figure S30. $\boldsymbol{\beta A 2}$ invariant of $\nu(C=C)_1$ in IND plotted against σ_p and *pEDA(I)*. 56
Figure S31. Frequencies and IR intensities of $\nu(C=C)_2$ in IND plotted against *pEDA(I)*. 57
Figure S32. ROA intensities of $\nu(C=C)_2$ in IND plotted against σ_p and *pEDA(I)*. 58
Figure S33. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_2$ in IND. 59
Figure S34. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_2$ in IND plotted against *pEDA(I)*. 60
Figure S35. $\boldsymbol{\beta A 2}$ invariant of $\nu(C=C)_2$ in IND plotted against σ_p and *pEDA(I)*. 61
Figure S36. Frequencies and IR intensities of $\nu(C=C)_3$ in IND plotted against *pEDA(I)*. 62
Figure S37. ROA intensities of $\nu(C=C)_3$ in IND plotted against σ_p and *pEDA(I)*. 63
Figure S38. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_3$ in IND. 64
Figure S39. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_3$ in IND plotted against *pEDA(I)*. 65
Figure S40. $\boldsymbol{\beta A 2}$ invariant of $\nu(C=C)_3$ in IND plotted against σ_p and *pEDA(I)*. 66
Figure S41. Frequencies and IR intensities of $\nu(C=C)_4$ in IIN plotted against *pEDA(I)*. 67
Figure S42. ROA intensities of $\nu(C=C)_4$ in IIN plotted against σ_p and *pEDA(I)*. 68
Figure S43. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_4$ in IIN. 69
Figure S44. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_4$ in IIN plotted against *pEDA(I)*. 70
Figure S45. $\boldsymbol{\beta A 2}$ invariant of $\nu(C=C)_4$ in IIN plotted against σ_p and *pEDA(I)*. 71
Figure S46. Frequencies and IR intensities of $\nu(C=C)_5$ in IIN plotted against *pEDA(I)*. 72
Figure S47. ROA intensities of $\nu(C=C)_5$ in IIN plotted against σ_p and *pEDA(I)*. 73
Figure S48. Relationship between $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_5$ in IIN. 74
Figure S49. $\boldsymbol{\alpha G'}$ and $\boldsymbol{\beta G' 2}$ invariants of $\nu(C=C)_5$ in IIN plotted against *pEDA(I)*. 75
Figure S50. $\boldsymbol{\beta A 2}$ invariant of $\nu(C=C)_5$ in IIN plotted against σ_p and *pEDA(I)*. 76
Figure S51. Correlation of *cos φ* with substituents volume, IND, ν(CN) mode. 105
Figure S52. Correlation of *cos φ* with substituents volume, IIN, ν(CN) mode. 106
Figure S53. Correlation of *cos φ* with substituents volume, IND, ν_s(CH=CH) mode. 106

Substituents and substituent constants

Table S1 Substituents used in the study along with their σ_p and *pEDA(I)* values.

substituent	σ_p	*pEDA(I) [e]*
BF_2	0.48	-0.078
Br	0.23	0.057
CHO	0.42	-0.088
Cl	0.23	0.064
$COCH_3$	0.50	-0.071
$CONH_2$	0.36	-0.044
$COOCH_3$	0.45	-0.062
COOH	0.45	-0.069
Et	-0.15	0.011
F	0.06	0.068
H	0.00	0.000
iPr	-0.15	0.007
Me	-0.17	0.016
MeS	0.01	0.108
$MeSO_2$	0.72	-0.016
NH_2	-0.66	0.141
$NHNH_2$	-0.55	0.133
NMe_2	-0.83	0.177
NO	0.91	-0.132
NO_2	0.78	-0.069
OCF_3	0.35	0.040
OH	-0.37	0.114
OMe	-0.27	0.120
SH	0.15	0.096
SiH_3	0.10	-0.012
$SiMe_3$	-0.07	-0.011
tBu	-0.20	0.008
Vin	-0.04	-0.009

σ_p are taken from: Hansch, C.; Leo, A.; Taft, R. W. *Chem. Rev.* **1991**, *91*, 165.

pEDA(I) values were calculated at B3LYP/aug-cc-pvDZ level according to the methodology published in: Ozimiński, W. P.; Dobrowolski, J. Cz. *J. Phys. Org. Chem.* **2009**, *22*, 769.

Spectral parameters of selected modes

Table S2 Spectral parameters of ν(C*H) mode in IND.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	48	3010.7	-1860.30	-533.09	-1860.30	-3.15	-20.80	4.25	-0.43
Br-CN-IND-A-8.out	42	3010.8	-1505.49	-442.75	-1505.49	-2.90	-17.07	4.15	-0.41
CHO-CN-IND-A-16.out	48	3010.2	-1536.71	-426.84	-1536.71	-2.44	-16.90	2.67	-0.43
CHO-CN-IND-A-17.out	48	3010.5	-2119.01	-592.54	-2119.01	-3.38	-23.38	3.92	-0.44
Cl-CN-IND-A-19.out	42	3010.8	-1468.37	-433.05	-1468.37	-2.81	-16.67	4.12	-0.41
COCH3-CN-IND-A-77.out	54	3010.7	-1745.67	-492.51	-1745.67	-2.97	-19.35	3.51	-0.43
COCH3-CN-IND-A-78.out	54	3010.1	-1814.65	-504.92	-1814.65	-3.02	-19.97	3.20	-0.43
CONH2-CN-IND-A-24.out	52	3012.4	-1615.98	-450.51	-1615.98	-2.96	-17.80	2.91	-0.42
CONH2-CN-IND-A-25.out	52	3009.6	-1841.72	-510.78	-1841.72	-3.24	-20.23	3.15	-0.43
COOCH3-CN-IND-A-71.out	57	3010.8	-1773.39	-492.72	-1773.39	-3.00	-19.50	3.09	-0.43
COOCH3-CN-IND-A-73.out	57	3009.4	-1388.79	-434.71	-1388.79	-2.72	-16.29	5.47	-0.42
COOCH3-CN-IND-A-75.out	57	3010.3	-1859.80	-518.16	-1859.80	-3.18	-20.48	3.33	-0.43
COOCH3-CN-IND-A-76.out	57	3012.2	-1875.42	-571.39	-1875.42	-3.34	-21.67	6.41	-0.42
COOH-CN-IND-A-26.out	50	3010.7	-1860.35	-525.23	-1860.35	-3.17	-20.63	3.76	-0.43
COOH-CN-IND-A-29.out	50	3010.5	-1806.81	-505.96	-1806.81	-2.99	-19.95	3.39	-0.43
COOH-CN-IND-A-30.out	50	3010.3	-1807.34	-504.11	-1807.34	-3.18	-19.92	3.27	-0.43
Et-CN-IND-A-109.out	55	3010.3	-1340.70	-383.38	-1340.70	-2.60	-14.97	3.01	-0.42
Et-CN-IND-A-110.out	55	3010.2	-1463.54	-436.96	-1463.54	-3.13	-16.73	4.44	-0.44
Et-CN-IND-A-111.out	55	3010.4	-1653.09	-500.11	-1653.09	-2.87	-19.03	5.43	-0.39
F-CN-IND-A-33.out	42	3011.0	-1323.33	-400.91	-1323.33	-2.67	-15.24	4.38	-0.41
H-CN-IND-A-35.out	41	3011.2	-1570.64	-475.65	-1570.64	-2.99	-18.09	5.19	-0.42
iPr-CN-IND-A-112.out	62	3010.2	-1721.55	-507.89	-1721.55	-3.09	-19.55	4.84	-0.41
iPr-CN-IND-A-114.out	62	3010.3	-1309.04	-386.29	-1309.04	-2.46	-14.87	3.69	-0.40
Me-CN-IND-A-41.out	48	3010.2	-1425.61	-423.43	-1425.61	-2.60	-16.25	4.19	-0.41
MeS-CN-IND-A-45.out	51	3008.2	-1605.64	-481.71	-1605.64	-2.64	-18.40	5.02	-0.40

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IND-A-46.out	51	3008.8	-25.48	-57.49	-25.48	-0.54	-1.33	3.19	-0.38
MeSO2-CN-IND-A-83.out	57	3009.6	-1710.57	-487.64	-1710.57	-3.41	-19.07	3.75	-0.43
MeSO2-CN-IND-A-84.out	57	3013.2	-1997.15	-582.98	-1997.15	-3.68	-22.55	5.23	-0.41
NH2-CN-IND-A-47.out	46	3005.8	-530.14	-174.51	-530.14	-0.60	-6.40	2.62	-0.38
NHNH2-CN-IND-A-115.out	51	3006.2	-624.33	-184.33	-624.33	-0.70	-7.09	1.77	-0.39
NHNH2-CN-IND-A-116.out	51	3006.6	-211.59	-71.32	-211.59	-0.13	-2.59	1.15	-0.37
NMe2-CN-IND-A-50.out	62	3004.5	830.62	212.91	830.62	1.20	8.76	-0.33	-0.37
NMe2-CN-IND-A-51.out	62	3004.6	139.11	-0.50	139.11	0.58	0.71	2.20	-0.35
NO2-CN-IND-A-86.out	48	3011.0	-1802.36	-497.58	-1802.36	-2.97	-19.75	2.94	-0.44
NO2-CN-IND-A-87.out	48	3011.0	-1802.36	-497.58	-1802.36	-2.97	-19.75	2.94	-0.44
NO-CN-IND-A-52.out	45	3009.4	-2344.39	-645.91	-2344.39	-3.17	-25.67	3.74	-0.46
NO-CN-IND-A-53.out	45	3010.2	-1086.29	-294.05	-1086.29	-1.05	-11.78	1.41	-0.43
OCF3-CN-IND-A-97.out	54	3011.3	-1084.78	-322.31	-1084.78	-2.30	-12.36	3.19	-0.40
OCF3-CN-IND-A-98.out	54	3011.1	-1662.59	-491.15	-1662.59	-3.22	-18.89	4.72	-0.42
OCF3-CN-IND-A-99.out	54	3011.9	-1661.21	-504.21	-1661.21	-3.29	-19.16	5.56	-0.41
OH-CN-IND-A-54.out	44	3008.6	-1166.56	-345.28	-1166.56	-2.05	-13.27	3.35	-0.40
OH-CN-IND-A-55.out	44	3009.0	-881.16	-267.60	-881.16	-1.68	-10.16	2.96	-0.39
OMe-CN-IND-A-88.out	51	3008.8	-1066.10	-403.00	-1066.10	-0.45	-13.95	8.53	-0.08
OMe-CN-IND-A-90.out	51	3008.3	-1232.04	-373.78	-1232.04	-2.49	-14.20	4.11	-0.38
SH-CN-IND-A-58.out	45	3008.9	-1227.99	-372.66	-1227.99	-2.13	-14.16	4.10	-0.41
SH-CN-IND-A-59.out	45	3009.3	-933.73	-296.22	-933.73	-1.79	-11.03	3.92	-0.40
SiH3-CN-IND-A-62.out	51	3010.8	-1681.72	-483.53	-1681.72	-3.03	-18.83	3.94	-0.41
SiMe3-CN-IND-A-65.out	69	3010.5	-1623.88	-463.93	-1623.88	-3.01	-18.12	3.62	-0.40
tBu-CN-IND-A-66.out	69	3010.3	-1477.92	-431.09	-1477.92	-2.79	-16.68	3.85	-0.40
tBu-CN-IND-A-67.out	69	3010.3	-1468.09	-427.17	-1468.09	-2.77	-16.55	3.76	-0.40
tBu-CN-IND-A-68.out	69	3010.4	-1473.62	-429.05	-1473.62	-2.77	-16.61	3.79	-0.40
Vin-CN-IND-A-69.out	51	3009.0	-56.49	-26.74	-56.49	-0.45	-0.85	0.79	-0.39
Vin-CN-IND-A-70.out	51	3008.9	-2395.24	-671.04	-2395.24	-3.65	-26.46	4.51	-0.43

Table S3 Spectral parameters of ν(CN) mode in IND.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	47	2341.1	849.27	196.82	849.27	1.54	8.52	0.97	-0.26
Br-CN-IND-A-8.out	41	2340.4	920.79	215.74	920.79	1.67	9.29	0.90	-0.26
CHO-CN-IND-A-16.out	46	2341.3	731.67	162.86	731.67	1.42	7.20	1.25	-0.25
CHO-CN-IND-A-17.out	46	2341.7	1074.34	249.01	1074.34	1.82	10.78	1.22	-0.26
Cl-CN-IND-A-19.out	41	2340.3	908.68	213.97	908.68	1.64	9.19	0.83	-0.26
COCH3-CN-IND-A-77.out	53	2340.8	989.18	227.93	989.18	1.71	9.90	1.21	-0.25
COCH3-CN-IND-A-78.out	53	2340.3	924.14	211.53	924.14	1.65	9.22	1.22	-0.25
CONH2-CN-IND-A-24.out	51	2340.5	909.18	214.86	909.18	1.58	9.21	0.78	-0.26
CONH2-CN-IND-A-25.out	51	2340.3	958.54	223.74	958.54	1.75	9.65	0.99	-0.26
COOCH3-CN-IND-A-71.out	56	2340.6	881.36	201.04	881.36	1.64	8.78	1.21	-0.25
COOCH3-CN-IND-A-73.out	56	2341.5	1013.95	242.05	1013.95	1.74	10.32	0.72	-0.26
COOCH3-CN-IND-A-75.out	56	2340.3	964.00	224.35	964.00	1.67	9.69	1.04	-0.25
COOCH3-CN-IND-A-76.out	56	2340.5	709.41	160.17	709.41	1.39	7.03	1.07	-0.26
COOH-CN-IND-A-26.out	49	2341.1	949.70	221.28	949.70	1.68	9.56	1.01	-0.26
COOH-CN-IND-A-29.out	49	2340.9	824.42	187.77	824.42	1.54	8.21	1.15	-0.26
COOH-CN-IND-A-30.out	49	2341.8	782.85	176.46	782.85	1.49	7.75	1.20	-0.26
Et-CN-IND-A-109.out	54	2337.9	1180.46	288.84	1180.46	1.99	12.17	0.39	-0.25
Et-CN-IND-A-110.out	54	2337.1	852.58	207.37	852.58	1.71	8.76	0.36	-0.26
Et-CN-IND-A-111.out	54	2337.9	746.42	172.03	746.42	1.45	7.47	0.91	-0.26
F-CN-IND-A-33.out	41	2339.8	900.46	216.65	900.46	1.59	9.20	0.53	-0.27
H-CN-IND-A-35.out	40	2338.8	920.41	220.19	920.41	1.59	9.38	0.62	-0.26
iPr-CN-IND-A-112.out	61	2337.8	1020.06	250.86	1020.06	1.86	10.54	0.26	-0.25
iPr-CN-IND-A-114.out	61	2337.7	837.82	196.22	837.82	1.59	8.45	0.83	-0.25
Me-CN-IND-A-41.out	47	2337.9	951.82	226.76	951.82	1.67	9.68	0.70	-0.26
MeS-CN-IND-A-45.out	50	2337.9	1400.90	336.92	1400.90	2.52	14.32	0.83	-0.25
MeS-CN-IND-A-46.out	50	2338.2	700.49	154.39	700.49	1.71	6.86	1.30	-0.25
MeSO2-CN-IND-A-83.out	56	2342.7	945.09	225.34	945.09	1.78	9.62	0.68	-0.25
MeSO2-CN-IND-A-84.out	56	2341.8	641.35	143.53	641.35	1.27	6.33	1.05	-0.26
NH2-CN-IND-A-47.out	45	2336.1	1007.96	242.55	1007.96	2.13	10.30	0.59	-0.26

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
NHNH2-CN-IND-A-115.out	50	2335.8	1211.23	298.37	1211.23	2.44	12.52	0.28	-0.26
NHNH2-CN-IND-A-116.out	50	2335.3	939.53	216.23	939.53	2.00	9.40	1.17	-0.25
NMe2-CN-IND-A-50.out	59	2334.9	1260.02	299.23	1260.02	2.83	12.80	0.99	-0.24
NMe2-CN-IND-A-51.out	59	2334.9	1070.27	249.77	1070.27	2.51	10.78	1.11	-0.24
NO2-CN-IND-A-86.out	47	2343.1	840.58	193.61	840.58	1.62	8.41	1.03	-0.26
NO2-CN-IND-A-87.out	47	2343.1	840.58	193.61	840.58	1.62	8.41	1.03	-0.26
NO-CN-IND-A-52.out	44	2342.5	1120.82	251.12	1120.82	2.72	11.07	1.82	-0.25
NO-CN-IND-A-53.out	44	2342.4	203.63	33.44	203.63	0.52	1.76	1.09	-0.25
OCF3-CN-IND-A-97.out	53	2340.4	756.08	174.26	756.08	1.47	7.57	0.92	-0.26
OCF3-CN-IND-A-98.out	53	2340.5	1006.46	243.45	1006.46	1.82	10.31	0.51	-0.27
OCF3-CN-IND-A-99.out	53	2341.2	708.11	162.51	708.11	1.24	7.07	0.91	-0.27
OH-CN-IND-A-54.out	43	2337.6	996.61	238.98	996.61	1.87	10.17	0.64	-0.26
OH-CN-IND-A-55.out	43	2337.9	952.87	229.18	952.87	1.78	9.74	0.57	-0.26
OMe-CN-IND-A-88.out	50	2337.4	819.52	187.58	819.52	1.69	8.18	1.08	-0.25
OMe-CN-IND-A-90.out	50	2337.0	1166.41	286.15	1166.41	2.18	12.04	0.34	-0.26
SH-CN-IND-A-58.out	43	2338.8	1042.29	251.07	1042.29	2.02	10.66	0.59	-0.26
SH-CN-IND-A-59.out	43	2338.9	888.70	213.07	888.70	1.77	9.07	0.57	-0.25
SiH3-CN-IND-A-62.out	50	2339.3	912.33	211.16	912.33	1.63	9.15	1.06	-0.25
SiMe3-CN-IND-A-65.out	68	2338.2	921.32	213.17	921.32	1.70	9.24	1.07	-0.24
tBu-CN-IND-A-66.out	68	2337.6	959.08	227.46	959.08	1.71	9.73	0.77	-0.25
tBu-CN-IND-A-67.out	68	2337.6	959.61	227.20	959.61	1.74	9.73	0.79	-0.25
tBu-CN-IND-A-68.out	68	2337.6	945.24	224.59	945.24	1.73	9.60	0.73	-0.25
Vin-CN-IND-A-69.out	50	2338.6	516.78	106.58	516.78	1.11	4.91	1.41	-0.24
Vin-CN-IND-A-70.out	50	2338.6	1517.17	365.68	1517.17	2.76	15.52	0.85	-0.25

Table S4 Spectral parameters of ν_s(HC=CH) mode in IND

symmetric vibration of HC=CH in the five-membered ring of IND

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	53	3240.3	-369.09	3.88	-369.09	-1.28	-1.84	-6.01	-0.37
Br-CN-IND-A-8.out	47	3239.7	-408.53	-2.05	-408.53	-1.35	-2.17	-6.26	-0.37
CHO-CN-IND-A-16.out	53	3240.0	-367.94	9.94	-367.94	-1.30	-1.71	-6.37	-0.37
CHO-CN-IND-A-17.out	53	3240.7	-388.69	-0.32	-388.69	-1.32	-2.03	-6.05	-0.36
Cl-CN-IND-A-19.out	47	3239.6	-380.12	2.66	-380.12	-1.34	-1.92	-6.11	-0.38
COCH3-CN-IND-A-77.out	62	3239.7	-393.15	-0.38	-393.15	-1.30	-2.06	-6.12	-0.35
COCH3-CN-IND-A-78.out	62	3239.9	-393.50	4.52	-393.50	-1.32	-1.96	-6.43	-0.37
CONH2-CN-IND-A-24.out	57	3239.6	-340.24	-1.39	-340.24	-1.20	-1.80	-5.23	-0.35
CONH2-CN-IND-A-25.out	57	3239.9	-389.78	-1.21	-389.78	-1.33	-2.06	-6.01	-0.37
COOCH3-CN-IND-A-71.out	65	3239.5	-396.82	4.28	-396.82	-1.30	-1.98	-6.47	-0.36
COOCH3-CN-IND-A-73.out	65	3240.1	-480.59	6.47	-480.59	-1.73	-2.37	-7.91	-0.36
COOCH3-CN-IND-A-75.out	65	3240.0	-390.15	5.79	-390.15	-1.34	-1.91	-6.46	-0.36
COOCH3-CN-IND-A-76.out	65	3240.3	-236.80	39.49	-236.80	-1.20	-0.41	-6.17	-0.37
COOH-CN-IND-A-26.out	55	3240.2	-379.20	4.42	-379.20	-1.30	-1.88	-6.20	-0.37
COOH-CN-IND-A-29.out	55	3240.4	-376.84	6.45	-376.84	-1.29	-1.83	-6.29	-0.37
COOH-CN-IND-A-30.out	55	3241.0	-366.30	1.97	-366.30	-1.27	-1.87	-5.85	-0.38
Et-CN-IND-A-109.out	65	3237.8	-497.52	-10.23	-497.52	-1.73	-2.80	-7.13	-0.35
Et-CN-IND-A-110.out	65	3236.8	-353.95	-3.52	-353.95	-1.57	-1.92	-5.31	-0.32
Et-CN-IND-A-111.out	65	3237.4	-226.10	19.01	-226.10	-0.98	-0.78	-4.72	-0.36
F-CN-IND-A-33.out	47	3239.5	-335.80	7.56	-335.80	-1.30	-1.59	-5.72	-0.40
H-CN-IND-A-35.out	47	3238.4	-316.02	10.42	-316.02	-1.31	-1.43	-5.59	-0.38
iPr-CN-IND-A-112.out	74	3237.8	-387.06	-1.77	-387.06	-1.37	-2.05	-5.94	-0.35
iPr-CN-IND-A-114.out	74	3237.3	-368.52	3.89	-368.52	-1.33	-1.84	-6.00	-0.35
Me-CN-IND-A-41.out	56	3237.6	-349.70	6.52	-349.70	-1.33	-1.69	-5.87	-0.36
MeS-CN-IND-A-45.out	59	3238.0	-426.65	-4.74	-426.65	-1.43	-2.32	-6.37	-0.34
MeS-CN-IND-A-46.out	59	3237.6	-419.11	-0.70	-419.11	-1.31	-2.20	-6.50	-0.35
MeSO2-CN-IND-A-83.out	65	3241.1	-547.64	-19.26	-547.64	-1.68	-3.25	-7.35	-0.37

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeSO2-CN-IND-A-84.out	65	3241.1	-267.37	12.90	-267.37	-0.98	-1.12	-4.98	-0.37
NH2-CN-IND-A-47.out	51	3236.6	-349.20	9.20	-349.20	-1.33	-1.63	-6.03	-0.36
NHNH2-CN-IND-A-115.out	56	3236.2	-385.31	9.00	-385.31	-1.49	-1.82	-6.58	-0.35
NHNH2-CN-IND-A-116.out	56	3236.0	-291.36	13.85	-291.36	-1.13	-1.23	-5.42	-0.36
NMe2-CN-IND-A-50.out	71	3235.8	-497.05	-15.67	-497.05	-1.61	-2.92	-6.79	-0.32
NMe2-CN-IND-A-51.out	71	3235.8	-344.83	1.47	-344.83	-1.16	-1.77	-5.48	-0.32
NO2-CN-IND-A-86.out	53	3241.9	-382.90	4.49	-382.90	-1.28	-1.90	-6.26	-0.38
NO2-CN-IND-A-87.out	53	3241.9	-382.90	4.49	-382.90	-1.28	-1.90	-6.26	-0.38
NO-CN-IND-A-52.out	50	3241.8	-378.40	7.89	-378.40	-1.34	-1.81	-6.41	-0.37
NO-CN-IND-A-53.out	50	3240.4	-383.95	8.80	-383.95	-1.23	-1.82	-6.55	-0.37
OCF3-CN-IND-A-97.out	59	3239.9	-347.94	9.67	-347.94	-1.29	-1.61	-6.04	-0.39
OCF3-CN-IND-A-98.out	58	3239.7	-371.46	1.00	-371.46	-1.30	-1.91	-5.87	-0.38
OCF3-CN-IND-A-99.out	59	3240.4	-192.28	26.60	-192.28	-1.01	-0.45	-4.67	-0.39
OH-CN-IND-A-54.out	49	3237.8	-355.76	4.55	-355.76	-1.32	-1.76	-5.84	-0.38
OH-CN-IND-A-55.out	49	3238.0	-347.56	4.68	-347.56	-1.31	-1.71	-5.72	-0.37
OMe-CN-IND-A-88.out	59	3237.3	-362.95	6.03	-362.95	-1.30	-1.76	-6.05	-0.36
OMe-CN-IND-A-90.out	59	3237.3	-385.09	0.84	-385.09	-1.37	-1.99	-6.07	-0.37
SH-CN-IND-A-58.out	50	3238.6	-406.28	-2.14	-406.28	-1.37	-2.16	-6.21	-0.36
SH-CN-IND-A-59.out	50	3238.5	-410.21	-2.16	-410.21	-1.35	-2.18	-6.27	-0.35
SiH3-CN-IND-A-62.out	56	3238.6	-391.31	-0.83	-391.31	-1.34	-2.06	-6.06	-0.35
SiMe3-CN-IND-A-65.out	83	3237.6	-435.48	-11.46	-435.48	-1.34	-2.51	-6.09	-0.33
tBu-CN-IND-A-66.out	83	3237.4	-421.82	-10.77	-421.82	-1.36	-2.42	-5.92	-0.33
tBu-CN-IND-A-67.out	83	3237.4	-401.39	-6.51	-401.39	-1.33	-2.23	-5.86	-0.33
tBu-CN-IND-A-68.out	83	3237.3	-408.60	-6.81	-408.60	-1.33	-2.27	-5.96	-0.33
Vin-CN-IND-A-69.out	58	3237.6	-398.73	8.44	-398.73	-1.31	-1.90	-6.76	-0.34
Vin-CN-IND-A-70.out	58	3238.8	-426.13	-3.62	-426.13	-1.43	-2.29	-6.43	-0.34

Table S5 Spectral parameters of $\nu(C=C)_1$ mode in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) parallel to C-R

NO_2 substituent not included due to very strong coupling to NO_2 stretching mode.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** $ICP_u/SCP_u(180)$ [10^4 * K]	**ROA2** $ICP_d/SCP_d(90)$ [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	$\alpha G'$ [10^4 * A^5/AMU]	$\beta(G')^2$ [10^4 * A^5/AMU]	$\beta(A)^2$ [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	44	1604.6	120.49	83.58	120.49	-0.25	2.37	-3.34	-0.15
Br-CN-IND-A-8.out	38	1594.5	-295.47	-38.08	-295.47	-0.01	-2.33	-2.24	-0.16
CHO-CN-IND-A-16.out	42	1610.4	-322.25	-1.27	-322.25	-0.27	-1.70	-4.96	-0.24
CHO-CN-IND-A-17.out	42	1602.5	-55.60	87.27	-55.60	0.15	1.53	-6.32	-0.17
Cl-CN-IND-A-19.out	38	1597.4	-285.02	-38.60	-285.02	-0.01	-2.29	-2.04	-0.18
COCH3-CN-IND-A-77.out	49	1601.2	40.46	103.99	40.46	0.01	2.38	-5.87	-0.16
COCH3-CN-IND-A-78.out	49	1608.0	-350.20	-16.08	-350.20	-0.26	-2.16	-4.47	-0.22
CONH2-CN-IND-A-24.out	46	1604.4	-181.51	-1.69	-181.51	-0.56	-0.98	-2.73	-0.21
CONH2-CN-IND-A-25.out	46	1605.1	236.19	88.34	236.19	0.37	3.07	-1.83	-0.12
COOCH3-CN-IND-A-71.out	52	1607.2	-211.70	35.04	-211.70	-0.24	-0.37	-5.50	-0.20
COOCH3-CN-IND-A-73.out	52	1604.7	118.71	197.88	118.71	0.69	4.74	-10.51	-0.16
COOCH3-CN-IND-A-75.out	52	1606.8	-191.99	20.27	-191.99	-0.19	-0.58	-4.27	-0.19
COOCH3-CN-IND-A-76.out	52	1605.3	-297.73	-50.65	-297.73	-1.62	-2.61	-1.49	-0.15
COOH-CN-IND-A-26.out	45	1607.4	-127.87	46.26	-127.87	-0.08	0.30	-4.89	-0.19
COOH-CN-IND-A-29.out	45	1607.0	-182.31	13.57	-182.31	-0.13	-0.67	-3.70	-0.21
COOH-CN-IND-A-30.out	45	1609.0	-142.36	19.25	-142.36	0.50	-0.34	-3.43	-0.21
Et-CN-IND-A-109.out	51	1606.9	722.58	166.68	722.58	0.89	7.24	0.87	-0.18
Et-CN-IND-A-110.out	51	1611.5	-233.91	-15.69	-233.91	0.09	-1.55	-2.67	-0.18
Et-CN-IND-A-111.out	51	1606.7	-868.87	-120.36	-868.87	-1.03	-7.03	-6.05	-0.18
F-CN-IND-A-33.out	38	1607.0	-260.59	-50.27	-260.59	0.12	-2.40	-0.93	-0.27
H-CN-IND-A-35.out	37	1603.4	-285.59	-42.34	-285.59	0.03	-2.37	-1.82	-0.19
iPr-CN-IND-A-112.out	58	1605.4	-30.51	33.30	-30.51	-0.12	0.53	-2.56	-0.14
iPr-CN-IND-A-114.out	58	1608.1	-199.48	2.19	-199.48	-0.19	-0.99	-3.25	-0.20
Me-CN-IND-A-41.out	44	1609.7	-142.28	-0.55	-142.28	-0.03	-0.75	-2.19	-0.20
MeS-CN-IND-A-45.out	47	1597.0	-268.23	-7.32	-268.23	0.43	-1.55	-3.73	-0.15

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IND-A-46.out	47	1594.1	-117.91	19.09	-117.91	0.24	-0.22	-3.04	-0.22
MeSO2-CN-IND-A-83.out	53	1600.7	-354.01	-84.20	-354.01	0.27	-3.60	-0.27	-0.14
MeSO2-CN-IND-A-84.out	53	1600.8	-186.82	32.17	-186.82	-0.68	-0.30	-4.93	-0.14
NH2-CN-IND-A-47.out	41	1606.8	-33.91	33.10	-33.91	0.52	0.51	-2.60	-0.30
NHNH2-CN-IND-A-115.out	46	1607.2	869.40	218.67	869.40	1.84	9.08	-0.08	-0.31
NHNH2-CN-IND-A-116.out	46	1606.3	-641.83	-175.57	-641.83	0.29	-7.00	0.94	-0.30
NMe2-CN-IND-A-50.out	56	1602.2	1083.18	274.84	1083.18	1.73	11.37	-0.25	-0.32
NMe2-CN-IND-A-51.out	56	1602.3	-662.63	-89.97	-662.63	-0.79	-5.33	-4.73	-0.31
NO-CN-IND-A-52.out	41	1618.0	117.24	-66.62	117.24	-0.11	-0.78	6.00	-0.07
NO-CN-IND-A-53.out	41	1614.9	120.74	45.67	120.74	0.36	1.58	-0.97	-0.26
OCF3-CN-IND-A-97.out	50	1609.6	-344.19	-61.32	-344.19	-0.02	-3.07	-1.55	-0.26
OCF3-CN-IND-A-98.out	50	1608.1	-255.67	-32.40	-255.67	0.08	-2.01	-1.97	-0.21
OCF3-CN-IND-A-99.out	50	1608.2	-677.17	-113.20	-677.17	-0.66	-5.89	-3.51	-0.22
OH-CN-IND-A-54.out	40	1607.1	-263.90	-47.36	-263.90	0.33	-2.36	-1.16	-0.28
OH-CN-IND-A-55.out	40	1610.3	-362.81	-77.65	-362.81	0.43	-3.51	-0.82	-0.31
OMe-CN-IND-A-88.out	47	1604.8	-74.52	-5.42	-74.52	0.31	-0.50	-0.83	-0.26
OMe-CN-IND-A-90.out	47	1606.8	-173.09	-12.12	-173.09	0.30	-1.15	-1.95	-0.21
SH-CN-IND-A-58.out	40	1596.7	-224.83	-6.08	-224.83	0.24	-1.30	-3.13	-0.18
SH-CN-IND-A-59.out	40	1596.6	-286.58	-18.73	-286.58	0.26	-1.88	-3.31	-0.19
SiH3-CN-IND-A-62.out	44	1596.3	-57.36	36.59	-57.36	-0.28	0.46	-3.18	-0.08
SiMe3-CN-IND-A-65.out	65	1596.2	-80.67	40.05	-80.67	-0.33	0.41	-3.76	-0.10
tBu-CN-IND-A-66.out	65	1608.2	-232.17	-12.34	-232.17	-0.18	-1.47	-2.86	-0.18
tBu-CN-IND-A-67.out	65	1608.3	-244.65	-14.42	-244.65	-0.16	-1.57	-2.92	-0.19
tBu-CN-IND-A-68.out	65	1608.3	-239.00	-13.08	-239.00	-0.16	-1.52	-2.92	-0.19
Vin-CN-IND-A-69.out	46	1604.4	-243.94	10.24	-243.94	-0.06	-1.06	-4.45	-0.22
Vin-CN-IND-A-70.out	46	1605.4	49.03	156.22	49.03	1.03	3.51	-9.00	-0.13

Table S6 Spectral parameters of $\nu(C{=}C)_2$ mode in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) at 120° to C-R

NO_2 substituent not included due to very strong coupling to NO_2 stretching mode.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** $ICP_u/SCP_u(180)$ [10^4 * K]	**ROA2** $ICP_d/SCP_d(90)$ [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	$\alpha G'$ [10^4 * A^5/AMU]	$\beta(G')^2$ [10^4 * A^5/AMU]	$\beta(A)^2$ [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	45	1627.7	-594.25	-115.12	-594.25	0.27	-5.49	-2.09	-0.42
Br-CN-IND-A-8.out	39	1633.2	-99.51	12.71	-99.51	0.10	-0.25	-2.35	-0.20
CHO-CN-IND-A-16.out	43	1632.3	-370.67	-53.17	-370.67	0.09	-3.04	-2.47	-0.29
CHO-CN-IND-A-17.out	43	1631.8	-424.87	-83.72	-424.87	0.26	-3.96	-1.41	-0.48
Cl-CN-IND-A-19.out	39	1635.1	-203.36	-15.81	-203.36	0.12	-1.39	-2.19	-0.36
COCH3-CN-IND-A-77.out	50	1630.4	-446.84	-81.20	-446.84	0.23	-4.02	-1.91	-0.43
COCH3-CN-IND-A-78.out	50	1630.2	-406.61	-61.99	-406.61	0.15	-3.41	-2.48	-0.33
CONH2-CN-IND-A-24.out	48	1630.7	-139.35	-11.48	-139.35	0.62	-0.96	-1.46	-0.42
CONH2-CN-IND-A-25.out	48	1631.3	-609.07	-115.92	-609.07	-0.15	-5.59	-2.27	-0.42
COOCH3-CN-IND-A-71.out	53	1631.9	-367.06	-62.55	-367.06	0.18	-3.21	-1.83	-0.44
COOCH3-CN-IND-A-73.out	53	1630.9	-695.46	-147.07	-695.46	-0.43	-6.69	-1.67	-0.41
COOCH3-CN-IND-A-75.out	53	1632.2	-531.45	-96.61	-531.45	0.27	-4.78	-2.27	-0.37
COOCH3-CN-IND-A-76.out	53	1631.3	-308.63	-22.08	-308.63	0.79	-2.07	-3.44	-0.46
COOH-CN-IND-A-26.out	46	1632.0	-352.46	-59.60	-352.46	0.15	-3.08	-1.78	-0.48
COOH-CN-IND-A-29.out	46	1632.4	-486.16	-86.12	-486.16	0.18	-4.33	-2.21	-0.39
COOH-CN-IND-A-30.out	46	1632.5	-449.30	-82.98	-449.30	-0.01	-4.07	-1.83	-0.41
Et-CN-IND-A-109.out	52	1633.0	-243.00	4.15	-243.00	-0.33	-1.18	-4.06	-0.40
Et-CN-IND-A-110.out	52	1634.5	-175.39	-11.33	-175.39	0.19	-1.15	-2.03	-0.44
Et-CN-IND-A-111.out	52	1632.7	-274.33	-67.32	-274.33	0.74	-2.83	-0.08	-0.40
F-CN-IND-A-33.out	39	1647.1	-325.79	-67.06	-325.79	0.24	-3.09	-0.90	-0.50
H-CN-IND-A-35.out	38	1639.1	-152.11	-4.36	-152.11	0.12	-0.88	-2.10	-0.21
iPr-CN-IND-A-112.out	59	1632.9	-294.03	-43.22	-294.03	0.26	-2.43	-1.89	-0.45
iPr-CN-IND-A-114.out	59	1633.7	-260.23	-29.80	-260.23	0.21	-1.98	-2.20	-0.33
Me-CN-IND-A-41.out	45	1634.2	-154.12	-7.28	-154.12	0.16	-0.95	-1.95	-0.30
MeS-CN-IND-A-45.out	48	1628.3	-386.53	-58.57	-386.53	0.20	-3.23	-2.38	-0.34

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IND-A-46.out	48	1625.7	-170.90	14.36	-170.90	0.03	-0.59	-3.57	-0.07
MeSO2-CN-IND-A-83.out	54	1635.2	-175.44	9.49	-175.44	-0.23	-0.72	-3.33	-0.35
MeSO2-CN-IND-A-84.out	54	1635.4	-333.53	-69.83	-333.53	0.46	-3.19	-0.85	-0.36
NH2-CN-IND-A-47.out	42	1635.1	-248.47	-21.19	-248.47	0.08	-1.74	-2.56	-0.24
NHNH2-CN-IND-A-115.out	47	1637.1	-460.99	-78.85	-460.99	-0.28	-4.04	-2.27	-0.23
NHNH2-CN-IND-A-116.out	47	1637.4	460.93	155.69	460.93	0.66	5.64	-2.53	-0.14
NMe2-CN-IND-A-50.out	57	1626.5	-990.40	-180.71	-990.40	-0.38	-8.92	-4.18	-0.29
NMe2-CN-IND-A-51.out	57	1626.4	-13.76	21.91	-13.76	1.55	0.38	-1.58	-0.28
NO-CN-IND-A-52.out	42	1637.1	-447.13	-92.36	-447.13	0.09	-4.25	-1.21	-0.14
NO-CN-IND-A-53.out	42	1638.3	-207.95	-60.05	-207.95	0.16	-2.33	0.50	0.34
OCF3-CN-IND-A-97.out	51	1644.4	416.12	129.72	416.12	0.00	4.87	-1.61	0.71
OCF3-CN-IND-A-98.out	51	1644.4	-342.63	-69.13	-342.63	0.23	-3.22	-1.03	-0.57
OCF3-CN-IND-A-99.out	51	1643.9	-55.50	-18.05	-55.50	0.65	-0.67	0.26	-0.42
OH-CN-IND-A-54.out	41	1646.0	-286.07	-52.88	-286.07	0.18	-2.59	-1.16	-0.50
OH-CN-IND-A-55.out	41	1645.1	521.19	153.48	521.19	0.00	5.91	-1.45	0.70
OMe-CN-IND-A-88.out	48	1633.8	215.93	94.21	215.93	0.04	3.09	-2.51	0.40
OMe-CN-IND-A-90.out	48	1637.9	-341.42	-55.05	-341.42	0.23	-2.93	-1.89	-0.56
SH-CN-IND-A-58.out	41	1629.4	-234.00	-17.94	-234.00	0.09	-1.59	-2.54	-0.30
SH-CN-IND-A-59.out	41	1628.9	-169.50	1.22	-169.50	0.00	-0.86	-2.72	-0.22
SiH3-CN-IND-A-62.out	45	1625.4	-475.99	-83.25	-475.99	0.20	-4.21	-2.23	-0.44
SiMe3-CN-IND-A-65.out	66	1624.2	-505.66	-86.94	-505.66	0.28	-4.44	-2.47	-0.39
tBu-CN-IND-A-66.out	66	1632.2	-301.99	-40.28	-301.99	0.26	-2.41	-2.20	-0.42
tBu-CN-IND-A-67.out	66	1632.4	-294.14	-39.61	-294.14	0.24	-2.36	-2.12	-0.42
tBu-CN-IND-A-68.out	66	1632.4	-292.32	-38.98	-292.32	0.23	-2.33	-2.13	-0.42
Vin-CN-IND-A-69.out	47	1629.4	-950.20	-152.73	-950.20	-0.09	-8.13	-5.30	-0.22
Vin-CN-IND-A-70.out	47	1628.1	-341.21	-52.72	-341.21	0.06	-2.88	-2.04	-0.45

Table S7 Spectral parameters of $\nu(C{=}C)_3$ mode in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) at -120° to C-R

NO_2 substituent not included due to very strong coupling to NO_2 stretching mode.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** $ICP_u/SCP_u(180)$ [10^4 * K]	**ROA2** $ICP_d/SCP_d(90)$ [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	$\alpha G'$ [10^4 * A^5/AMU]	$\beta(G')^2$ [10^4 * A^5/AMU]	$\beta(A)^2$ [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IND-A-5.out	46	1654.0	892.07	95.42	892.07	0.31	6.63	7.98	0.15
Br-CN-IND-A-8.out	40	1640.8	1015.50	147.61	1015.50	0.34	8.36	6.64	-0.14
CHO-CN-IND-A-16.out	44	1652.6	1072.64	109.87	1072.64	0.26	7.88	9.89	0.55
CHO-CN-IND-A-17.out	44	1650.9	850.01	46.82	850.01	0.04	5.40	10.36	0.58
Cl-CN-IND-A-19.out	40	1644.0	1124.71	182.00	1124.71	0.32	9.65	6.20	-0.11
COCH3-CN-IND-A-77.out	51	1650.8	833.89	59.68	833.89	0.10	5.59	9.30	0.45
COCH3-CN-IND-A-78.out	51	1652.6	1019.70	96.30	1019.70	0.24	7.32	9.91	0.49
CONH2-CN-IND-A-24.out	49	1653.8	-222.59	-137.41	-222.59	0.08	-4.02	5.11	0.19
CONH2-CN-IND-A-25.out	49	1655.3	2321.11	447.62	2321.11	0.22	21.41	8.29	0.27
COOCH3-CN-IND-A-71.out	54	1654.9	974.49	93.42	974.49	0.19	7.02	9.39	0.41
COOCH3-CN-IND-A-73.out	54	1653.8	2814.90	342.03	2814.90	0.16	21.79	22.61	0.08
COOCH3-CN-IND-A-75.out	54	1656.2	1077.71	111.95	1077.71	0.18	7.95	9.84	0.47
COOCH3-CN-IND-A-76.out	54	1655.0	-1056.73	-385.62	-1056.73	-0.41	-13.54	7.59	0.14
COOH-CN-IND-A-26.out	47	1654.3	815.74	66.71	815.74	0.18	5.64	8.58	0.32
COOH-CN-IND-A-29.out	47	1655.8	998.03	107.22	998.03	0.25	7.43	8.89	0.43
COOH-CN-IND-A-30.out	47	1654.9	2348.36	447.43	2348.36	0.29	21.55	8.73	0.27
Et-CN-IND-A-109.out	53	1657.2	676.05	213.40	676.05	0.83	7.97	-2.77	-0.01
Et-CN-IND-A-110.out	53	1660.9	1013.24	172.48	1013.24	0.34	8.87	5.05	-0.08
Et-CN-IND-A-111.out	53	1657.4	1499.14	119.60	1499.14	-0.30	10.30	15.95	-0.01
F-CN-IND-A-33.out	40	1652.2	1300.64	277.93	1300.64	0.15	12.56	2.95	0.07
H-CN-IND-A-35.out	39	1649.5	1174.61	206.50	1174.61	0.40	10.42	5.45	-0.10
iPr-CN-IND-A-112.out	60	1656.1	1029.13	147.40	1029.13	0.06	8.43	6.87	-0.05
iPr-CN-IND-A-114.out	60	1657.8	1200.19	185.51	1200.19	0.34	10.12	7.16	-0.01
Me-CN-IND-A-41.out	46	1658.9	1079.30	171.50	1079.30	0.36	9.19	6.15	-0.08
MeS-CN-IND-A-45.out	49	1650.1	1242.59	186.15	1242.59	0.19	10.35	7.78	-0.02

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IND-A-46.out	49	1645.2	1278.50	173.08	1278.50	0.27	10.26	9.16	0.12
MeSO2-CN-IND-A-83.out	55	1642.9	2048.69	499.02	2048.69	1.03	21.07	0.82	-0.10
MeSO2-CN-IND-A-84.out	55	1643.1	-47.60	-231.84	-47.60	-0.24	-5.08	13.75	-0.10
NH2-CN-IND-A-47.out	44	1662.9	1136.78	186.39	1136.78	0.07	9.80	6.11	0.15
NHNH2-CN-IND-A-115.out	48	1655.3	876.99	176.28	876.99	-0.66	8.24	2.69	-0.03
NHNH2-CN-IND-A-116.out	48	1653.7	177.56	52.12	177.56	-0.74	2.01	-0.48	-0.10
NMe2-CN-IND-A-50.out	58	1661.2	550.46	117.19	550.46	0.23	5.31	1.28	0.22
NMe2-CN-IND-A-51.out	58	1661.1	2011.61	307.56	2011.61	-0.04	16.88	12.21	0.21
NO-CN-IND-A-52.out	43	1654.7	359.89	-6.42	359.89	0.06	1.74	6.02	0.08
NO-CN-IND-A-53.out	43	1655.7	390.94	41.12	390.94	1.29	2.89	3.54	-0.50
OCF3-CN-IND-A-97.out	52	1654.1	678.42	91.19	678.42	0.39	5.43	4.90	-0.13
OCF3-CN-IND-A-98.out	52	1661.2	1147.09	208.30	1147.09	-0.08	10.31	4.90	0.03
OCF3-CN-IND-A-99.out	52	1652.9	1300.37	181.21	1300.37	-0.33	10.55	8.99	-0.04
OH-CN-IND-A-54.out	42	1660.2	1210.92	244.33	1210.92	0.12	11.40	3.65	0.03
OH-CN-IND-A-55.out	42	1656.5	646.10	95.13	646.10	0.27	5.35	4.15	-0.15
OMe-CN-IND-A-88.out	49	1654.4	879.86	132.62	879.86	0.26	7.35	5.46	-0.03
OMe-CN-IND-A-90.out	49	1661.8	1073.50	192.40	1073.50	0.05	9.60	4.75	-0.09
SH-CN-IND-A-58.out	42	1647.5	1187.24	174.20	1187.24	0.24	9.81	7.66	-0.01
SH-CN-IND-A-59.out	42	1646.1	1219.44	171.68	1219.44	0.29	9.93	8.32	0.00
SiH3-CN-IND-A-62.out	46	1646.8	1205.53	170.55	1205.53	0.49	9.83	8.18	-0.11
SiMe3-CN-IND-A-65.out	67	1646.8	1330.12	182.79	1330.12	0.42	10.74	9.36	-0.06
tBu-CN-IND-A-66.out	67	1659.5	1240.23	206.36	1240.23	0.36	10.76	6.48	-0.03
tBu-CN-IND-A-67.out	67	1659.4	1247.98	208.16	1247.98	0.34	10.84	6.49	-0.03
tBu-CN-IND-A-68.out	67	1659.5	1236.37	205.01	1236.37	0.34	10.71	6.51	-0.03
Vin-CN-IND-A-69.out	48	1656.5	1491.35	173.43	1491.35	-0.43	11.38	12.46	0.64
Vin-CN-IND-A-70.out	48	1654.0	1647.97	177.52	1647.97	0.17	12.28	14.65	0.57

Table S8 Spectral parameters of ν(C*H) mode in IIIN

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IIN-A-1.out	49	3010.7	-751.80	-187.05	-751.80	-1.99	-7.81	-0.06	-0.50
Br-CN-IIN-A-2.out	43	3011.7	-642.97	-160.58	-642.97	-1.70	-6.69	-0.01	-0.48
CHO-CN-IIN-A-3.out	49	3011.6	-995.65	-252.72	-995.65	-2.44	-10.45	0.24	-0.50
CHO-CN-IIN-A-6.out	49	3010.0	-548.98	-111.25	-548.98	-1.59	-5.18	-1.62	-0.50
Cl-CN-IIN-A-8.out	43	3011.8	-637.79	-157.91	-637.79	-1.67	-6.61	-0.10	-0.48
COCH3-CN-IIN-A-56.out	55	3009.3	-761.22	-168.97	-761.22	-1.96	-7.48	-1.33	-0.50
COCH3-CN-IIN-A-57.out	55	3011.9	-811.15	-187.64	-811.15	-2.15	-8.13	-0.95	-0.49
COCH3-CN-IIN-A-59.out	55	3011.7	-812.74	-188.43	-812.74	-2.15	-8.16	-0.92	-0.49
CONH2-CN-IIN-A-10.out	53	3011.8	-711.94	-161.62	-711.94	-1.86	-7.08	-1.02	-0.49
CONH2-CN-IIN-A-11.out	53	3009.4	-878.13	-214.49	-878.13	-2.06	-9.04	-0.32	-0.49
CONH2-CN-IIN-A-9.out	53	3012.9	-758.81	-166.76	-758.81	-1.88	-7.43	-1.43	-0.49
COOCH3-CN-IIN-A-42.out	58	3009.6	-826.89	-189.01	-826.89	-2.02	-8.24	-1.11	-0.49
COOCH3-CN-IIN-A-47.out	58	3014.1	-860.31	-208.27	-860.31	-1.85	-8.82	-0.43	-0.48
COOCH3-CN-IIN-A-49.out	58	3010.7	-786.39	-168.90	-786.39	-1.96	-7.61	-1.73	-0.49
COOCH3-CN-IIN-A-54.out	58	3010.9	-505.67	-138.62	-505.67	-1.58	-5.52	0.76	-0.49
COOH-CN-IIN-A-15.out	51	3011.0	-836.94	-200.52	-836.94	-2.14	-8.54	-0.54	-0.50
COOH-CN-IIN-A-6.out	51	3010.1	-724.04	-162.31	-724.04	-1.89	-7.15	-1.17	-0.50
Et-CN-IIN-A-79.out	56	3010.2	-709.86	-176.21	-709.86	-1.70	-7.37	-0.08	-0.48
Et-CN-IIN-A-81.out	56	3010.5	-822.46	-223.66	-822.46	-1.77	-8.94	1.13	-0.47
Et-CN-IIN-A-82.out	56	3009.1	-666.61	-152.32	-666.61	-1.48	-6.65	-0.90	-0.48
Et-CN-IIN-A-83.out	56	3010.0	-454.43	-96.40	-454.43	-1.45	-4.38	-1.08	-0.49
F-CN-IIN-A-17.out	43	3012.4	-581.16	-148.61	-581.16	-1.62	-6.12	0.21	-0.48
H-CN-IIN-A-8.out	42	3011.2	-661.92	-176.41	-661.92	-1.80	-7.12	0.68	-0.49
iPr-CN-IIN-A-86.out	63	3009.7	-819.43	-219.28	-819.43	-1.87	-8.84	0.90	-0.48
iPr-CN-IIN-A-87.out	63	3009.8	-444.17	-95.73	-444.17	-1.30	-4.31	-0.96	-0.47
Me-CN-IIN-A-9.out	49	3009.7	-722.62	-180.05	-722.62	-1.70	-7.51	-0.04	-0.48
MeS-CN-IIN-A-21.out	52	3009.3	353.57	92.17	353.57	-0.15	3.76	-0.24	-0.45
MeS-CN-IIN-A-23.out	52	3009.0	-875.49	-241.75	-875.49	-1.80	-9.60	1.43	-0.48
MeSO2-CN-IIN-A-22.out	58	3011.0	-600.78	-138.85	-600.78	-1.94	-6.02	-0.71	-0.49

file name	mode no	frequency [cm^{-1}]	ROA1 $ICP_u/SCP_u(180)$ [10^4 * K]	ROA2 $ICP_d/SCP_d(90)$ [10^4 * K]	ROA3 DCPI(180) [10^4 * K]	$\alpha G'$ [10^4 * A^5/AMU]	$\beta(G')^2$ [10^4 * A^5/AMU]	$\beta(A)^2$ [10^4 * A^5/AMU]	RC180 degree of circularity
MeSO2-CN-IIN-A-62.out	58	3013.2	-905.99	-232.79	-905.99	-2.23	-9.57	0.39	-0.48
NH2-CN-IIN-A-11.out	47	3008.0	-105.36	-15.70	-105.36	-0.44	-0.88	-0.66	-0.46
NHNH2-CN-IIN-A-91.out	52	3005.1	261.23	88.19	261.23	-0.07	3.20	-1.43	-0.45
NHNH2-CN-IIN-A-92.out	52	3008.0	-262.52	-59.82	-262.52	-0.57	-2.61	-0.36	-0.47
NMe2-CN-IIN-A-27.out	63	3005.2	81.88	40.29	81.88	0.20	1.27	-1.24	-0.43
NO2-CN-IIN-A-23.out	49	3012.0	-746.47	-175.69	-746.47	-2.24	-7.55	-0.68	-0.50
NO-CN-IIN-A-13.out	46	3011.1	-37.67	25.15	-37.67	-0.50	0.33	-2.16	-0.50
NO-CN-IIN-A-30.out	46	3009.6	-1179.62	-309.23	-1179.62	-2.82	-12.59	0.90	-0.52
OCF3-CN-IIN-A-25.out	55	3011.5	-407.72	-78.59	-407.72	-1.27	-3.76	-1.46	-0.47
OCF3-CN-IIN-A-74.out	55	3012.9	-545.52	-125.89	-545.52	-1.74	-5.46	-0.66	-0.49
OCF3-CN-IIN-A-75.out	55	3013.2	-551.12	-128.26	-551.12	-1.74	-5.54	-0.60	-0.49
OCF3-CN-IIN-A-76.out	55	3012.3	-811.29	-211.55	-811.29	-1.99	-8.63	0.55	-0.49
OCF3-CN-IIN-A-77.out	55	3011.7	-806.27	-217.29	-806.27	-2.00	-8.73	0.98	-0.48
OCF3-CN-IIN-A-78.out	55	3012.5	-804.78	-216.53	-804.78	-2.00	-8.70	0.96	-0.48
OH-CN-IIN-A-31.out	45	3010.9	-373.13	-83.17	-373.13	-1.03	-3.68	-0.63	-0.47
OMe-CN-IIN-A-24.out	52	3009.7	6.24	34.14	6.24	-0.46	0.74	-2.04	-0.45
OMe-CN-IIN-A-69.out	52	3009.5	-591.71	-164.44	-591.71	-1.66	-6.51	1.03	-0.48
SH-CN-IIN-A-32.out	46	3009.9	-524.27	-143.55	-524.27	-1.32	-5.72	0.78	-0.48
SiH3-CN-IIN-A-33.out	52	3010.0	-810.30	-200.51	-810.30	-2.00	-8.40	-0.13	-0.48
SiMe3-CN-IIN-A-34.out	70	3009.5	-865.49	-217.83	-865.49	-2.01	-9.05	0.09	-0.48
SiMe3-CN-IIN-A-35.out	70	3009.8	-656.47	-145.04	-656.47	-1.68	-6.44	-1.19	-0.47
tBu-CN-IIN-A-18.out	70	3009.0	-739.91	-187.54	-739.91	-1.80	-7.76	0.16	-0.47
tBu-CN-IIN-A-37.out	70	3009.7	-570.50	-129.93	-570.50	-1.51	-5.68	-0.79	-0.47
Vin-CN-IIN-A-38.out	52	3009.3	-1541.62	-412.31	-1541.62	-2.96	-16.62	1.68	-0.50
Vin-CN-IIN-A-40.out	52	3008.6	500.10	183.02	500.10	0.23	6.42	-3.62	-0.46

Table S9 Spectral parameters of ν(CN) mode in IIN

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IIN-A-1.out	48	2343.2	658.18	144.49	658.18	0.46	6.44	1.25	-0.32
Br-CN-IIN-A-2.out	42	2342.6	673.24	150.21	673.24	0.51	6.64	1.13	-0.31
CHO-CN-IIN-A-3.out	47	2343.7	847.00	192.44	847.00	0.64	8.42	1.21	-0.32
CHO-CN-IIN-A-6.out	47	2343.2	518.16	104.17	518.16	0.25	4.87	1.59	-0.31
Cl-CN-IIN-A-8.out	42	2342.5	654.42	145.34	654.42	0.49	6.44	1.14	-0.32
COCH3-CN-IIN-A-56.out	54	2342.4	670.25	142.30	670.25	0.44	6.46	1.58	-0.31
COCH3-CN-IIN-A-57.out	54	2343.1	717.07	155.73	717.07	0.53	6.98	1.47	-0.31
COCH3-CN-IIN-A-59.out	54	2343.1	714.88	155.18	714.88	0.53	6.96	1.47	-0.31
CONH2-CN-IIN-A-10.out	52	2343.1	646.64	140.94	646.64	0.45	6.30	1.30	-0.31
CONH2-CN-IIN-A-11.out	52	2342.1	638.36	134.71	638.36	0.42	6.13	1.56	-0.32
CONH2-CN-IIN-A-9.out	52	2342.8	637.51	139.04	637.51	0.48	6.22	1.27	-0.31
COOCH3-CN-IIN-A-42.out	57	2342.5	703.96	153.37	703.96	0.50	6.86	1.41	-0.31
COOCH3-CN-IIN-A-47.out	57	2342.9	521.27	114.16	521.27	0.33	5.09	1.01	-0.32
COOCH3-CN-IIN-A-49.out	57	2342.7	633.92	132.42	633.92	0.47	6.06	1.63	-0.31
COOCH3-CN-IIN-A-54.out	57	2343.6	703.11	158.99	703.11	0.56	6.97	1.05	-0.31
COOH-CN-IIN-A-15.out	50	2343.2	713.50	157.33	713.50	0.53	6.99	1.32	-0.32
COOH-CN-IIN-A-6.out	50	2343.0	619.83	131.54	619.83	0.42	5.97	1.46	-0.32
Et-CN-IIN-A-79.out	55	2340.3	775.90	175.28	775.90	0.65	7.69	1.17	-0.32
Et-CN-IIN-A-81.out	55	2340.6	502.60	104.62	502.60	0.31	4.80	1.31	-0.32
Et-CN-IIN-A-82.out	55	2340.4	627.81	131.38	627.81	0.49	6.01	1.60	-0.31
Et-CN-IIN-A-83.out	55	2340.5	855.35	199.44	855.35	0.75	8.61	0.90	-0.31
F-CN-IIN-A-17.out	42	2342.1	632.66	140.92	632.66	0.44	6.23	1.08	-0.33
H-CN-IIN-A-8.out	41	2341.4	661.62	146.41	661.62	0.49	6.50	1.19	-0.32
iPr-CN-IIN-A-86.out	62	2340.3	760.43	178.19	760.43	0.65	7.67	0.75	-0.32
iPr-CN-IIN-A-87.out	62	2340.3	551.27	116.46	551.27	0.41	5.30	1.33	-0.31
Me-CN-IIN-A-9.out	48	2340.5	718.33	160.24	718.33	0.58	7.08	1.21	-0.32
MeS-CN-IIN-A-21.out	51	2340.7	414.49	84.32	414.49	0.39	3.92	1.21	-0.30

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IIN-A-23.out	51	2340.3	1170.74	278.10	1170.74	1.20	11.89	0.91	-0.32
MeSO2-CN-IIN-A-22.out	57	2344.3	706.62	158.76	706.62	0.60	6.99	1.12	-0.31
MeSO2-CN-IIN-A-62.out	57	2343.7	487.36	99.68	487.36	0.22	4.62	1.39	-0.32
NH2-CN-IIN-A-11.out	46	2338.6	808.83	188.84	808.83	0.78	8.15	0.84	-0.32
NHNH2-CN-IIN-A-91.out	51	2338.1	701.63	152.65	701.63	0.75	6.83	1.42	-0.31
NHNH2-CN-IIN-A-92.out	51	2338.5	961.67	230.85	961.67	1.06	9.82	0.60	-0.32
NMe2-CN-IIN-A-27.out	60	2337.4	822.50	181.26	822.50	0.98	8.06	1.52	-0.30
NO2-CN-IIN-A-23.out	48	2344.8	664.42	145.36	664.42	0.45	6.49	1.30	-0.32
NO-CN-IIN-A-13.out	45	2344.1	267.26	42.40	267.26	-0.18	2.28	1.53	-0.31
NO-CN-IIN-A-30.out	45	2344.2	878.06	199.97	878.06	1.42	8.74	1.22	-0.32
OCF3-CN-IIN-A-25.out	54	2342.6	483.83	98.86	483.83	0.30	4.58	1.38	-0.32
OCF3-CN-IIN-A-74.out	54	2343.1	741.58	171.01	741.58	0.61	7.43	0.90	-0.32
OCF3-CN-IIN-A-75.out	54	2343.1	736.97	169.81	736.97	0.60	7.38	0.90	-0.32
OCF3-CN-IIN-A-76.out	54	2342.5	775.92	178.21	775.92	0.63	7.75	0.99	-0.33
OCF3-CN-IIN-A-77.out	54	2343.2	489.97	102.34	489.97	0.20	4.68	1.26	-0.33
OCF3-CN-IIN-A-78.out	54	2343.1	492.47	103.01	492.47	0.20	4.71	1.26	-0.33
OH-CN-IIN-A-31.out	44	2340.5	651.85	145.94	651.85	0.52	6.44	1.06	-0.32
OMe-CN-IIN-A-24.out	51	2340.1	485.61	98.19	485.61	0.38	4.57	1.45	-0.31
OMe-CN-IIN-A-69.out	51	2339.6	912.44	212.99	912.44	0.88	9.19	0.95	-0.32
SH-CN-IIN-A-32.out	44	2341.1	802.22	188.85	802.22	0.79	8.11	0.73	-0.31
SiH3-CN-IIN-A-33.out	51	2341.7	742.43	162.84	742.43	0.60	7.26	1.42	-0.31
SiMe3-CN-IIN-A-34.out	69	2340.8	764.52	170.24	764.52	0.63	7.53	1.31	-0.31
SiMe3-CN-IIN-A-35.out	69	2340.7	658.05	139.94	658.05	0.53	6.34	1.54	-0.30
tBu-CN-IIN-A-18.out	69	2340.3	720.31	161.97	720.31	0.58	7.13	1.13	-0.31
tBu-CN-IIN-A-37.out	69	2340.3	641.98	138.93	641.98	0.52	6.24	1.35	-0.31
Vin-CN-IIN-A-38.out	51	2341.1	1260.04	305.03	1260.04	1.38	12.92	0.62	-0.31
Vin-CN-IIN-A-40.out	51	2341.0	170.19	15.16	170.19	-0.13	1.20	1.71	-0.30

Table S10 Spectral parameters of ν(NH) mode in IIN

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** $ICP_u/SCP_u(180)$ [10^4 * K]	**ROA2** $ICP_d/SCP_d(90)$ [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	$\alpha G'$ [10^4 * A^5/AMU]	$\beta(G')^2$ [10^4 * A^5/AMU]	$\beta(A)^2$ [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IIN-A-1.out	53	3636.7	-388.24	-99.69	-388.24	-0.68	-4.10	0.16	-0.24
Br-CN-IIN-A-2.out	47	3636.8	-412.04	-107.18	-412.04	-0.72	-4.38	0.26	-0.23
CHO-CN-IIN-A-3.out	53	3636.5	-398.09	-100.76	-398.09	-0.72	-4.17	0.08	-0.23
CHO-CN-IIN-A-6.out	53	3636.3	-381.31	-95.06	-381.31	-0.70	-3.97	-0.02	-0.24
Cl-CN-IIN-A-8.out	47	3636.9	-388.37	-102.19	-388.37	-0.70	-4.15	0.32	-0.23
COCH3-CN-IIN-A-56.out	62	3637.4	-410.99	-104.38	-410.99	-0.72	-4.32	0.10	-0.23
COCH3-CN-IIN-A-57.out	62	3636.8	-391.41	-98.35	-391.41	-0.70	-4.09	0.03	-0.23
COCH3-CN-IIN-A-59.out	62	3636.8	-392.36	-99.20	-392.36	-0.70	-4.11	0.07	-0.23
CONH2-CN-IIN-A-10.out	58	3636.9	-379.71	-95.21	-379.71	-0.70	-3.96	0.02	-0.23
CONH2-CN-IIN-A-11.out	58	3637.5	-399.34	-98.96	-399.34	-0.70	-4.14	-0.05	-0.23
CONH2-CN-IIN-A-9.out	58	3637.0	-398.14	-100.87	-398.14	-0.72	-4.18	0.08	-0.23
COOCH3-CN-IIN-A-42.out	65	3637.7	-406.60	-103.97	-406.60	-0.73	-4.28	0.15	-0.23
COOCH3-CN-IIN-A-47.out	65	3636.2	-349.52	-93.87	-349.52	-0.74	-3.78	0.41	-0.23
COOCH3-CN-IIN-A-49.out	65	3637.7	-397.26	-101.14	-397.26	-0.70	-4.18	0.11	-0.23
COOCH3-CN-IIN-A-54.out	65	3637.0	-419.40	-99.91	-419.40	-0.71	-4.27	-0.31	-0.23
COOH-CN-IIN-A-15.out	55	3636.9	-386.77	-98.52	-386.77	-0.69	-4.07	0.11	-0.23
COOH-CN-IIN-A-6.out	55	3637.3	-387.79	-98.86	-387.79	-0.69	-4.08	0.12	-0.24
Et-CN-IIN-A-79.out	65	3638.9	-388.79	-102.40	-388.79	-0.74	-4.16	0.33	-0.23
Et-CN-IIN-A-81.out	65	3639.7	-352.46	-97.13	-352.46	-0.70	-3.86	0.56	-0.23
Et-CN-IIN-A-82.out	65	3640.4	-380.50	-101.13	-380.50	-0.69	-4.09	0.38	-0.23
Et-CN-IIN-A-83.out	65	3639.2	-409.00	-104.09	-409.00	-0.75	-4.30	0.12	-0.23
F-CN-IIN-A-17.out	47	3637.4	-346.70	-94.42	-346.70	-0.66	-3.77	0.48	-0.24
H-CN-IIN-A-8.out	47	3638.4	-353.04	-95.56	-353.04	-0.67	-3.83	0.46	-0.25
iPr-CN-IIN-A-86.out	74	3639.1	-402.45	-106.38	-402.45	-0.74	-4.31	0.36	-0.23
iPr-CN-IIN-A-87.out	74	3639.2	-395.07	-102.96	-395.07	-0.71	-4.20	0.26	-0.23
Me-CN-IIN-A-9.out	56	3639.0	-369.14	-98.11	-369.14	-0.70	-3.97	0.36	-0.23
MeS-CN-IIN-A-21.out	59	3639.5	-394.60	-107.40	-394.60	-0.68	-4.29	0.55	-0.21

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IIN-A-23.out	59	3638.2	-413.54	-111.37	-413.54	-0.78	-4.47	0.50	-0.21
MeSO2-CN-IIN-A-22.out	65	3635.6	-449.78	-115.04	-449.78	-0.75	-4.74	0.16	-0.23
MeSO2-CN-IIN-A-62.out	65	3635.6	-389.28	-97.80	-389.28	-0.73	-4.07	0.03	-0.23
NH2-CN-IIN-A-11.out	52	3639.4	-336.82	-92.41	-336.82	-0.70	-3.68	0.51	-0.22
NHNH2-CN-IIN-A-91.out	59	3641.0	-397.52	-114.17	-397.52	-0.84	-4.45	0.92	-0.21
NHNH2-CN-IIN-A-92.out	59	3639.8	-335.61	-95.14	-335.61	-0.67	-3.73	0.70	-0.21
NMe2-CN-IIN-A-27.out	71	3639.8	-361.27	-106.22	-361.27	-0.68	-4.09	0.99	-0.19
NO2-CN-IIN-A-23.out	53	3634.9	-384.52	-95.67	-384.52	-0.69	-4.00	-0.03	-0.24
NO-CN-IIN-A-13.out	50	3634.9	-398.54	-94.11	-398.54	-0.63	-4.04	-0.35	-0.24
NO-CN-IIN-A-30.out	50	3635.7	-438.16	-107.70	-438.16	-0.76	-4.53	-0.12	-0.23
OCF3-CN-IIN-A-25.out	59	3637.9	-353.37	-93.60	-353.37	-0.68	-3.79	0.33	-0.23
OCF3-CN-IIN-A-74.out	59	3636.8	-403.94	-103.01	-403.94	-0.75	-4.25	0.13	-0.24
OCF3-CN-IIN-A-75.out	59	3636.8	-408.07	-105.49	-408.07	-0.74	-4.32	0.22	-0.24
OCF3-CN-IIN-A-76.out	59	3637.7	-363.97	-96.81	-363.97	-0.73	-3.91	0.36	-0.23
OCF3-CN-IIN-A-77.out	59	3637.1	-321.71	-85.88	-321.71	-0.69	-3.46	0.34	-0.24
OCF3-CN-IIN-A-78.out	59	3637.1	-319.58	-84.51	-319.58	-0.70	-3.43	0.29	-0.24
OH-CN-IIN-A-31.out	49	3638.6	-338.24	-94.83	-338.24	-0.66	-3.74	0.64	-0.23
OMe-CN-IIN-A-24.out	59	3640.2	-348.96	-97.24	-348.96	-0.66	-3.84	0.63	-0.22
OMe-CN-IIN-A-69.out	59	3638.7	-370.53	-101.50	-370.53	-0.73	-4.04	0.55	-0.22
SH-CN-IIN-A-32.out	50	3637.9	-394.44	-105.67	-394.44	-0.73	-4.26	0.44	-0.22
SiH3-CN-IIN-A-33.out	56	3638.0	-416.07	-107.55	-416.07	-0.73	-4.41	0.22	-0.23
SiMe3-CN-IIN-A-34.out	83	3638.9	-451.04	-117.30	-451.04	-0.74	-4.79	0.28	-0.22
SiMe3-CN-IIN-A-35.out	83	3638.5	-449.50	-115.53	-449.50	-0.73	-4.75	0.20	-0.22
tBu-CN-IIN-A-18.out	83	3639.4	-418.90	-109.27	-418.90	-0.73	-4.46	0.28	-0.22
tBu-CN-IIN-A-37.out	83	3638.7	-417.85	-108.49	-417.85	-0.72	-4.44	0.25	-0.22
Vin-CN-IIN-A-38.out	59	3638.8	-423.50	-110.65	-423.50	-0.78	-4.51	0.30	-0.21
Vin-CN-IIN-A-40.out	59	3638.6	-379.90	-95.67	-379.90	-0.70	-3.97	0.04	-0.23

Table S11 Spectral parameters of ν(C=C)$_4$ mode in IIN

NO_2 substituent not included due to very strong coupling to NO_2 stretching mode.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **ICP$_u$/SCP$_u$(180)** [10^4 * K]	**ROA2** **ICP$_d$/SCP$_d$(90)** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')^2*** [10^4 * A^5/AMU]	***β(A)^2*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IIN-A-1.out	45	1623.7	183.94	60.01	183.94	-0.19	2.21	-0.88	0.14
Br-CN-IIN-A-2.out	39	1630.6	136.04	59.90	136.04	-0.09	1.96	-1.62	0.26
CHO-CN-IIN-A-3.out	43	1627.6	227.43	95.64	227.43	-0.24	3.18	-2.42	0.00
CHO-CN-IIN-A-6.out	43	1631.9	180.16	59.10	180.16	-0.11	2.17	-0.88	0.19
Cl-CN-IIN-A-8.out	39	1633.2	146.25	59.55	146.25	-0.10	2.00	-1.44	0.27
COCH3-CN-IIN-A-56.out	50	1630.6	194.74	63.63	194.74	-0.14	2.34	-0.93	0.16
COCH3-CN-IIN-A-57.out	50	1627.3	250.67	93.90	250.67	-0.21	3.26	-1.95	-0.01
COCH3-CN-IIN-A-59.out	50	1627.3	250.38	93.49	250.38	-0.20	3.25	-1.93	-0.01
CONH2-CN-IIN-A-10.out	48	1628.8	298.30	83.94	298.30	-0.07	3.30	-0.59	-0.05
CONH2-CN-IIN-A-11.out	48	1630.1	29.52	40.00	29.52	-0.33	0.99	-2.04	0.30
CONH2-CN-IIN-A-9.out	48	1628.8	148.91	50.41	148.91	-0.40	1.83	-0.82	-0.04
COOCH3-CN-IIN-A-42.out	53	1630.5	155.45	56.17	155.45	-0.12	1.98	-1.08	0.25
COOCH3-CN-IIN-A-47.out	53	1628.9	127.95	28.02	127.95	-0.42	1.25	0.25	0.16
COOCH3-CN-IIN-A-49.out	53	1630.7	218.11	78.44	218.11	-0.24	2.77	-1.49	-0.10
COOCH3-CN-IIN-A-54.out	53	1628.6	364.76	128.07	364.76	0.06	4.57	-2.31	0.15
COOH-CN-IIN-A-15.out	46	1631.0	226.64	79.36	226.64	-0.18	2.83	-1.42	-0.01
COOH-CN-IIN-A-6.out	46	1631.3	154.40	54.27	154.40	-0.10	1.93	-0.98	0.20
Et-CN-IIN-A-79.out	52	1635.2	248.81	80.69	248.81	-0.18	2.98	-1.16	0.24
Et-CN-IIN-A-81.out	52	1633.3	373.05	120.91	373.05	-0.43	4.46	-1.73	0.26
Et-CN-IIN-A-82.out	52	1632.6	322.46	88.53	322.46	-0.15	3.52	-0.49	0.39
Et-CN-IIN-A-83.out	52	1633.0	204.27	51.55	204.27	0.08	2.14	-0.03	0.27
F-CN-IIN-A-17.out	39	1648.7	108.63	47.03	108.63	-0.07	1.55	-1.24	0.52
H-CN-IIN-A-8.out	38	1640.1	147.00	60.10	147.00	-0.08	2.02	-1.46	0.54
iPr-CN-IIN-A-86.out	59	1633.0	316.32	90.42	316.32	-0.16	3.53	-0.71	0.36
iPr-CN-IIN-A-87.out	59	1633.9	241.98	78.15	241.98	-0.18	2.89	-1.10	0.18
Me-CN-IIN-A-9.out	45	1633.7	284.22	83.35	284.22	-0.16	3.22	-0.77	0.32
MeS-CN-IIN-A-21.out	48	1622.0	411.43	111.98	411.43	-0.02	4.48	-0.57	0.29

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IIN-A-23.out	48	1622.4	301.76	108.88	301.76	-0.06	3.84	-2.09	-0.10
MeSO2-CN-IIN-A-22.out	54	1633.9	-16.10	5.34	-16.10	-0.04	0.03	-0.59	0.40
MeSO2-CN-IIN-A-62.out	54	1634.0	226.75	97.69	226.75	-0.19	3.22	-2.56	0.40
NH2-CN-IIN-A-11.out	42	1633.8	307.47	76.52	307.47	-0.05	3.20	0.02	-0.13
NHNH2-CN-IIN-A-91.out	47	1635.8	195.99	66.50	195.99	0.21	2.41	-1.09	-0.10
NHNH2-CN-IIN-A-92.out	47	1635.8	411.79	108.28	411.79	0.29	4.40	-0.33	-0.12
NMe2-CN-IIN-A-27.out	57	1619.7	408.62	134.09	408.62	-0.53	4.92	-2.00	-0.30
NO-CN-IIN-A-13.out	42	1637.6	4.65	34.25	4.65	-0.40	0.74	-2.07	-0.02
NO-CN-IIN-A-30.out	42	1638.7	-49.17	-47.30	-49.17	0.12	-1.24	2.19	0.31
OCF3-CN-IIN-A-25.out	51	1646.2	417.99	100.80	417.99	-0.14	4.28	0.23	0.39
OCF3-CN-IIN-A-74.out	51	1644.0	211.17	55.10	211.17	0.09	2.25	-0.14	0.43
OCF3-CN-IIN-A-75.out	51	1644.0	212.33	55.04	212.33	0.09	2.25	-0.12	0.43
OCF3-CN-IIN-A-76.out	51	1644.6	114.09	58.57	114.09	-0.09	1.81	-1.88	0.40
OCF3-CN-IIN-A-77.out	51	1644.1	194.49	81.70	194.49	-0.33	2.72	-2.07	0.42
OCF3-CN-IIN-A-78.out	51	1644.2	192.19	81.43	192.19	-0.33	2.70	-2.09	0.42
OH-CN-IIN-A-31.out	41	1647.2	403.31	95.37	403.31	-0.11	4.09	0.34	0.33
OMe-CN-IIN-A-24.out	48	1634.3	488.29	117.57	488.29	-0.11	4.99	0.28	0.42
OMe-CN-IIN-A-69.out	48	1634.6	148.64	69.85	148.64	-0.10	2.23	-2.04	0.21
SH-CN-IIN-A-32.out	41	1626.2	288.98	95.83	288.98	-0.06	3.50	-1.47	-0.17
SiH3-CN-IIN-A-33.out	45	1621.0	229.74	71.03	229.74	-0.15	2.68	-0.85	0.36
SiMe3-CN-IIN-A-34.out	66	1620.0	246.65	80.41	246.65	-0.18	2.96	-1.17	0.34
SiMe3-CN-IIN-A-35.out	66	1620.0	188.29	62.45	188.29	-0.24	2.28	-0.96	0.18
tBu-CN-IIN-A-18.out	66	1631.9	307.16	82.28	307.16	-0.15	3.31	-0.34	0.40
tBu-CN-IIN-A-37.out	66	1633.1	225.85	74.34	225.85	-0.22	2.73	-1.12	0.16
Vin-CN-IIN-A-38.out	47	1626.5	515.72	198.22	515.72	0.04	6.82	-4.33	-0.13
Vin-CN-IIN-A-40.out	47	1625.0	301.51	87.72	301.51	-0.01	3.40	-0.77	0.70

Table S12 Spectral parameters of $\nu(C=C)_5$ mode in IIN

NO_2 substituent not included due to very strong coupling to NO_2 stretching mode.

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
BF2-CN-IIN-A-1.out	46	1661.2	86.34	-18.39	86.34	-0.02	0.07	2.50	0.69
Br-CN-IIN-A-2.out	40	1643.6	327.47	41.30	327.47	0.00	2.57	2.54	0.64
CHO-CN-IIN-A-3.out	44	1658.5	143.98	-28.07	143.98	0.07	0.17	4.00	0.48
CHO-CN-IIN-A-6.out	44	1657.9	-173.06	-90.31	-173.06	-0.32	-2.78	2.94	0.48
Cl-CN-IIN-A-8.out	40	1647.7	284.05	33.25	284.05	0.00	2.17	2.36	0.59
COCH3-CN-IIN-A-56.out	51	1658.4	-81.31	-74.58	-81.31	-0.18	-1.98	3.39	0.50
COCH3-CN-IIN-A-57.out	51	1657.2	79.64	-30.53	79.64	0.02	-0.22	3.15	0.48
COCH3-CN-IIN-A-59.out	51	1657.3	88.32	-27.73	88.32	0.02	-0.12	3.11	0.48
CONH2-CN-IIN-A-10.out	49	1661.0	233.12	-2.92	233.12	-0.06	1.15	3.83	0.60
CONH2-CN-IIN-A-11.out	49	1661.4	-469.41	-166.80	-469.41	-0.05	-5.92	3.09	0.63
CONH2-CN-IIN-A-9.out	49	1660.9	-73.79	-44.63	-73.79	0.03	-1.31	1.64	0.60
COOCH3-CN-IIN-A-42.out	54	1662.2	102.06	-32.71	102.06	-0.08	-0.15	3.64	0.52
COOCH3-CN-IIN-A-47.out	54	1660.0	-347.75	10.26	-347.75	-0.05	-1.60	-6.07	0.67
COOCH3-CN-IIN-A-49.out	54	1660.7	51.25	-35.12	51.25	-0.08	-0.46	3.00	0.52
COOCH3-CN-IIN-A-54.out	54	1659.5	664.77	-13.93	664.77	0.02	3.17	11.26	0.66
COOH-CN-IIN-A-15.out	47	1661.2	45.70	-33.13	45.70	-0.04	-0.45	2.78	0.57
COOH-CN-IIN-A-6.out	47	1662.6	45.17	-39.71	45.17	-0.09	-0.59	3.19	0.58
Et-CN-IIN-A-79.out	53	1665.9	203.41	17.99	203.41	0.01	1.43	2.05	0.60
Et-CN-IIN-A-81.out	53	1662.7	-4.06	-102.02	-4.06	-0.01	-2.15	6.31	0.71
Et-CN-IIN-A-82.out	53	1662.8	184.93	16.66	184.93	0.01	1.31	1.85	0.67
Et-CN-IIN-A-83.out	53	1662.4	403.59	130.49	403.59	0.01	4.82	-1.85	0.71
F-CN-IIN-A-17.out	40	1657.2	309.51	50.35	309.51	-0.07	2.66	1.69	0.22
H-CN-IIN-A-8.out	39	1652.9	349.72	52.64	349.72	-0.04	2.92	2.17	0.22
iPr-CN-IIN-A-86.out	60	1661.2	199.93	5.33	199.93	-0.01	1.15	2.79	0.70
iPr-CN-IIN-A-87.out	60	1662.2	217.73	28.37	217.73	0.01	1.73	1.63	0.70
Me-CN-IIN-A-9.out	46	1663.3	188.97	11.43	188.97	0.00	1.22	2.24	0.63
MeS-CN-IIN-A-21.out	49	1647.5	249.16	23.15	249.16	-0.17	1.78	2.45	0.51

file name	**mode no**	**frequency** [cm^{-1}]	**ROA1** **$ICP_u/SCP_u(180)$** [10^4 * K]	**ROA2** **$ICP_d/SCP_d(90)$** [10^4 * K]	**ROA3** **DCPI(180)** [10^4 * K]	***αG'*** [10^4 * A^5/AMU]	***β(G')²*** [10^4 * A^5/AMU]	***β(A)²*** [10^4 * A^5/AMU]	**RC180** degree of circularity
MeS-CN-IIN-A-23.out	49	1652.7	159.29	-1.20	159.29	-0.04	0.80	2.56	0.56
MeSO2-CN-IIN-A-22.out	55	1647.7	544.33	136.11	544.33	0.05	5.67	0.00	0.50
MeSO2-CN-IIN-A-62.out	55	1648.0	-63.50	-100.98	-63.50	-0.02	-2.43	5.32	0.50
NH2-CN-IIN-A-11.out	44	1669.3	129.78	9.55	129.78	0.01	0.87	1.43	0.65
NHNH2-CN-IIN-A-91.out	48	1656.7	-35.75	-86.47	-35.75	-0.03	-1.99	4.85	0.71
NHNH2-CN-IIN-A-92.out	48	1658.6	-17.90	6.96	-17.90	-0.01	0.05	-0.71	0.71
NMe2-CN-IIN-A-27.out	58	1666.8	249.11	21.20	249.11	0.03	1.74	2.57	0.58
NO-CN-IIN-A-13.out	43	1663.8	-105.73	-27.15	-105.73	0.11	-1.12	0.04	0.54
NO-CN-IIN-A-30.out	43	1661.6	108.59	-11.73	108.59	-0.01	0.32	2.43	0.70
OCF3-CN-IIN-A-25.out	52	1661.4	34.95	-1.42	34.95	0.01	0.15	0.63	0.70
OCF3-CN-IIN-A-74.out	52	1658.7	246.31	67.00	246.31	0.04	2.68	-0.34	0.37
OCF3-CN-IIN-A-75.out	52	1658.7	262.30	71.68	262.30	0.04	2.86	-0.38	0.37
OCF3-CN-IIN-A-76.out	52	1667.0	235.03	17.78	235.03	-0.04	1.59	2.56	0.49
OCF3-CN-IIN-A-77.out	52	1658.8	159.10	-25.16	159.10	-0.03	0.30	4.06	0.36
OCF3-CN-IIN-A-78.out	52	1658.8	153.28	-27.23	153.28	-0.03	0.23	4.10	0.36
OH-CN-IIN-A-31.out	42	1662.9	60.19	4.87	60.19	0.01	0.41	0.64	0.69
OMe-CN-IIN-A-24.out	49	1659.8	125.10	16.25	125.10	-0.01	0.99	0.94	0.70
OMe-CN-IIN-A-69.out	49	1666.0	140.31	6.58	140.31	-0.01	0.87	1.78	0.64
SH-CN-IIN-A-32.out	42	1651.3	236.33	18.01	236.33	-0.04	1.61	2.57	0.62
SiH3-CN-IIN-A-33.out	46	1648.2	210.49	13.42	210.49	0.00	1.38	2.45	0.62
SiMe3-CN-IIN-A-34.out	67	1647.6	231.90	10.31	231.90	0.00	1.42	2.98	0.69
SiMe3-CN-IIN-A-35.out	67	1649.1	310.10	41.95	310.10	0.01	2.49	2.22	0.68
tBu-CN-IIN-A-18.out	67	1661.3	188.33	12.56	188.33	0.00	1.24	2.16	0.69
tBu-CN-IIN-A-37.out	67	1664.5	209.13	16.97	209.13	0.02	1.44	2.21	0.65
Vin-CN-IIN-A-38.out	48	1660.3	1047.57	166.17	1047.57	0.81	8.92	5.98	0.21
Vin-CN-IIN-A-40.out	48	1661.4	-1147.45	-354.42	-1147.45	-1.75	-13.36	4.22	0.24

Correlations of spectral parameters of selected modes with substituent constants

ν(C*H) in IND

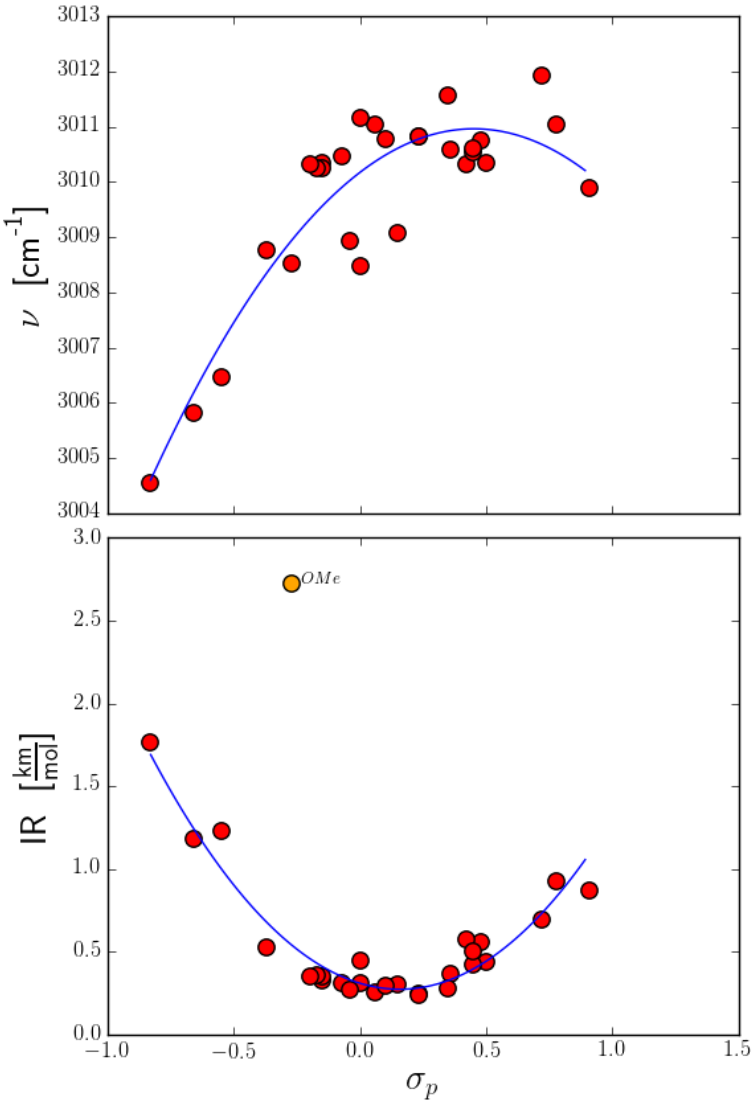

Figure S1. Correlations of frequencies and IR intensities of *ν*(C*H) in IND with σ_p.

Frequency = - 3.88 (± 0.68) σ_p^2 + 3.50 (± 0.36) σ_p + 3010.18 (± 0.19), *n* = 28, *r* = 0.90.

IR = 1.45 (± 0.09) σ_p^2 - 0.46 (± 0.05) σ_p + 0.31 (± 0.03) , *n* = 27, *r* = 0.96.

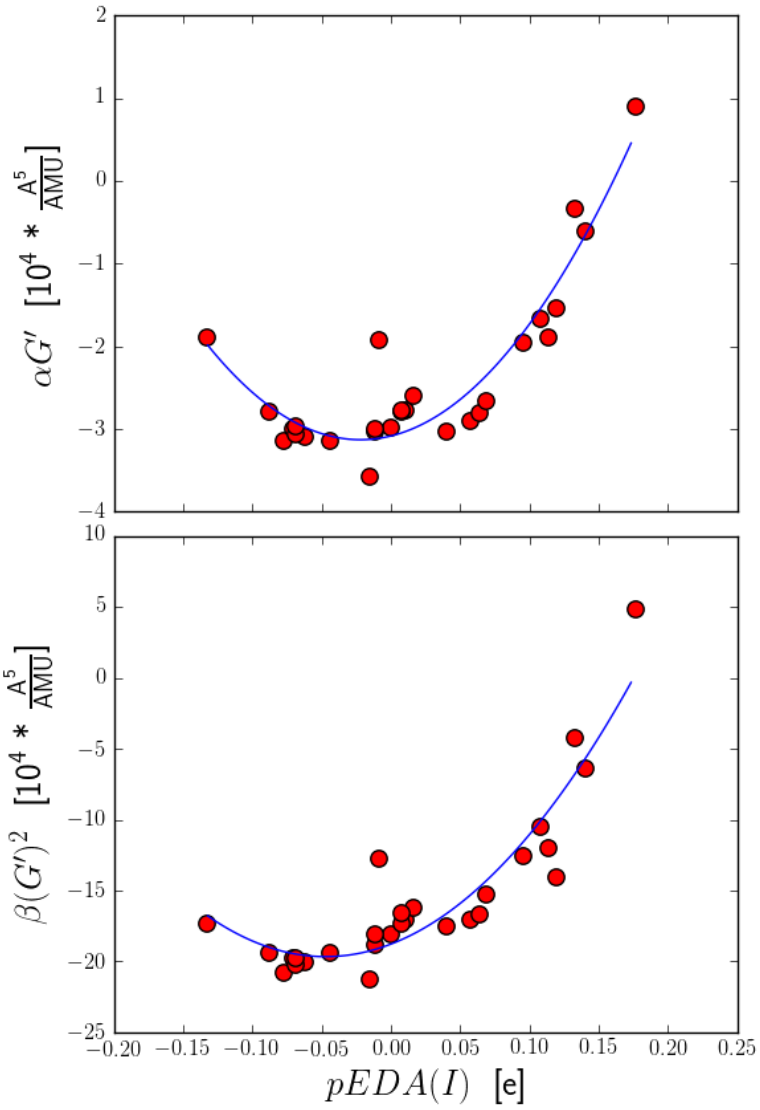

Figure S2. Correlations of $\alpha G'$ and $\beta(G')^2$ invariants of *v*(C*H) in IND with *pEDA(I)*.

$\alpha G'$ = 93.93 (± 10.65) *pEDA(I)*^{2} + 4.13 (± 1.03) *pEDA(I)* - 3.09 (± 0.09) , *n* = 28, *r* = 0.94.

$\beta(G')^2$ = 397.14 (± 67.23) *pEDA(I)*^{2} + 37.57 (± 6.47) *pEDA(I)* - 18.78 (± 0.59) , *n* = 28, *r* = 0.92.

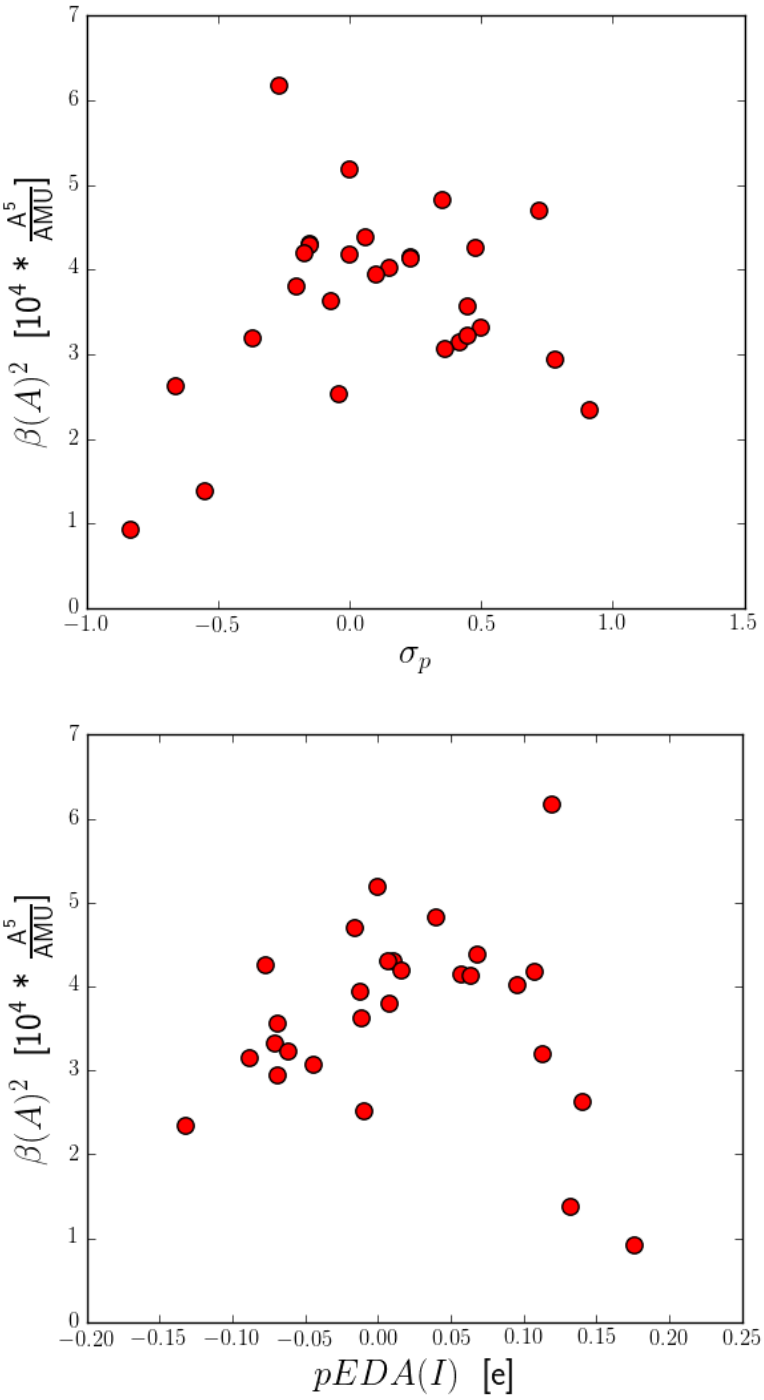

Figure S3. $\beta(A)^2$ invariant of *v*(C*H) in IND plotted against σ_p and *pEDA(I)*.

***v*(C*H) in IIN**

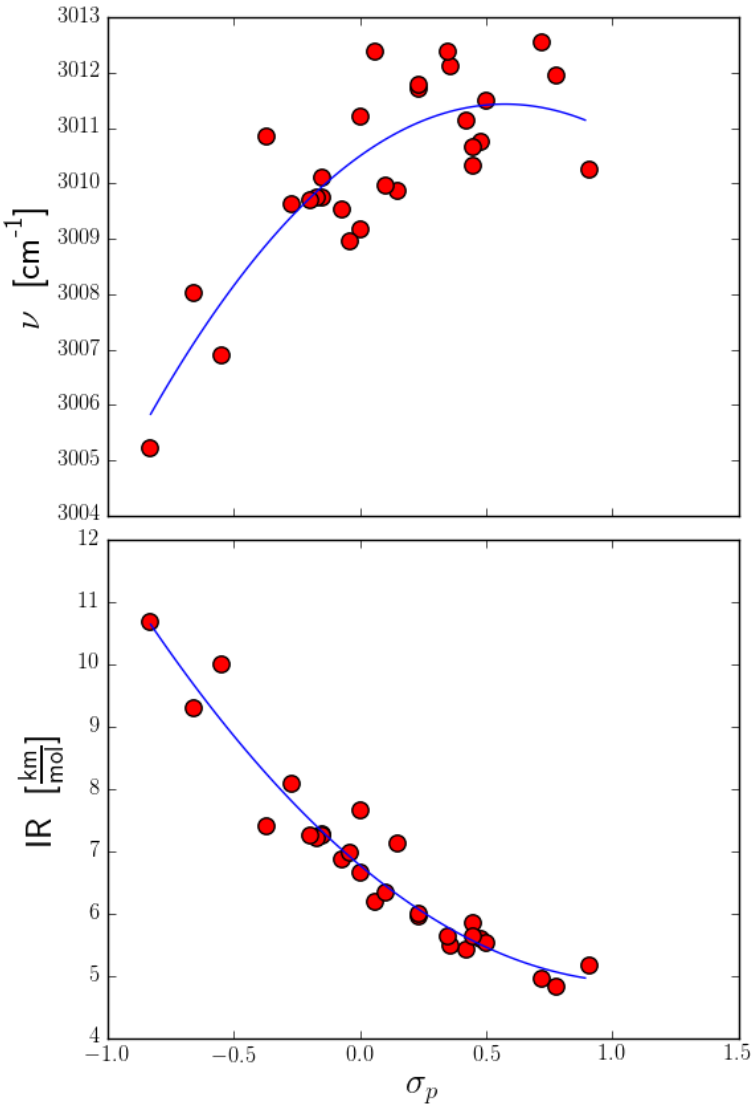

Figure S4. Correlations of frequencies and IR intensities of *v*(C*H) in IIN with σ_p.

Frequency = - 2.84 (± 0.82) σ_p^2 + 3.26 (± 0.44) σ_p + 3010.50 (± 0.23) , n = 28, r = 0.83.

IR = 1.53 (± 0.34) σ_p^2 - 3.39 (± 0.18) σ_p + 6.78 (± 0.10) , n = 28, r = 0.97.

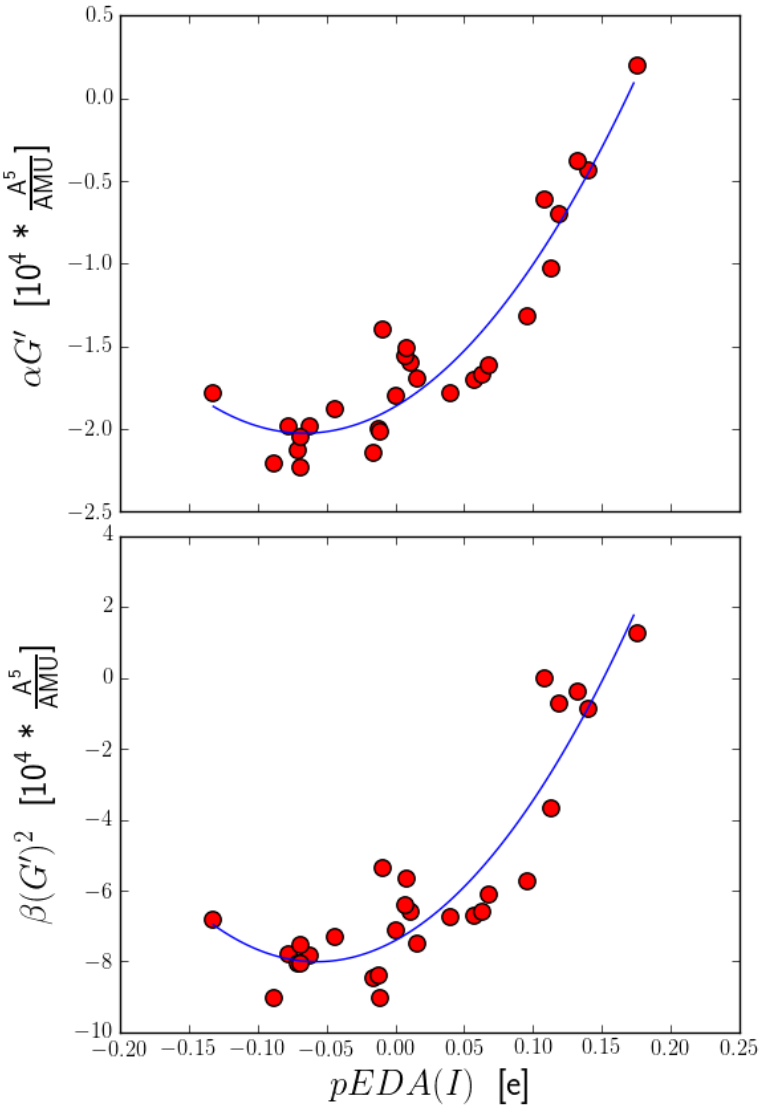

Figure S5. Correlations of $\alpha G'$ and $\beta(G')^2$ invariants of *ν*(C*H) in IIN with *pEDA(I)*.

$\alpha G'$ = 36.90 (± 6.16) *pEDA(I)*^{2} + 4.88 (± 0.59) *pEDA(I)* - 1.86 (± 0.05) , *n* = 28, *r* = 0.95.

$\beta(G')^2$ = 184.03 (± 34.98) *pEDA(I)*^{2} + 21.01 (± 3.37) *pEDA(I)* - 7.41 (± 0.31) , *n* = 28, *r* = 0.92.

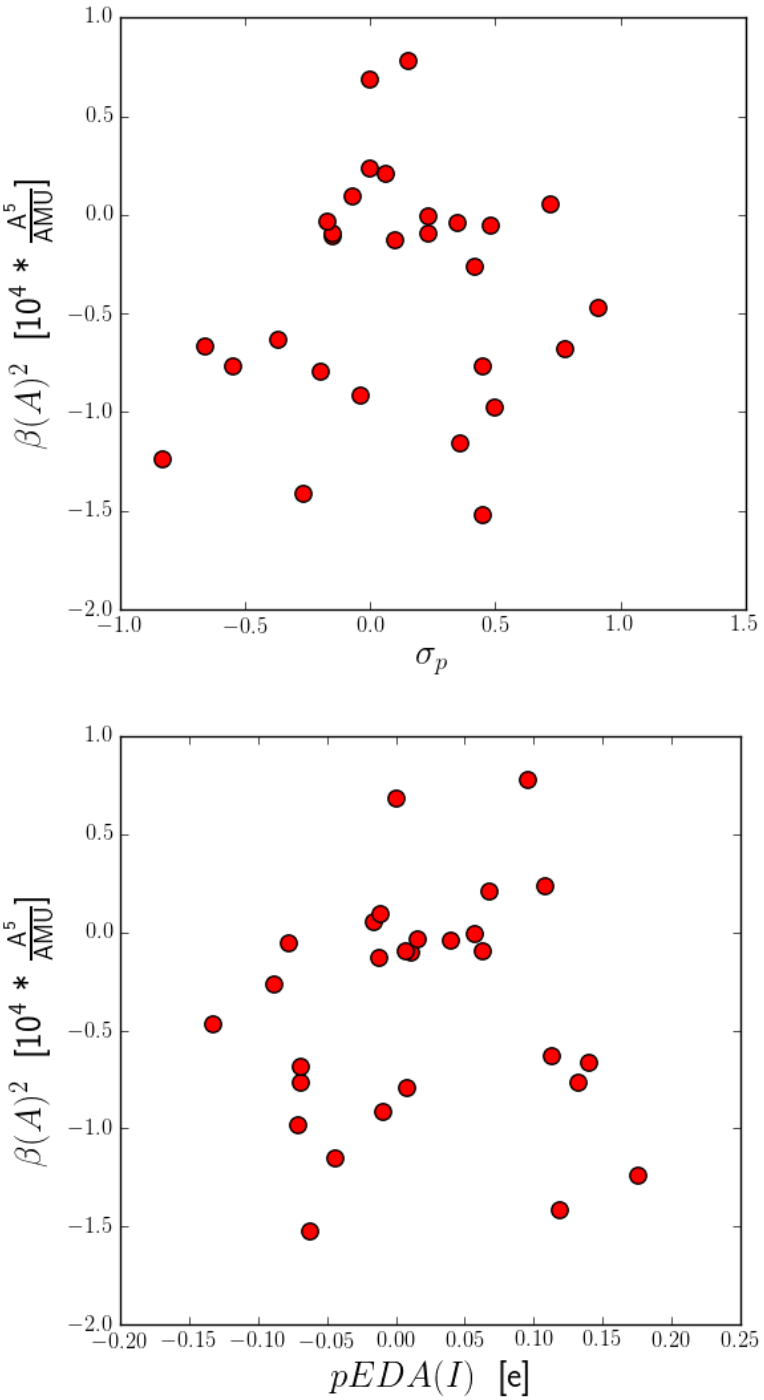

Figure S6. $\beta(A)^2$ invariant of *ν*(C*H) in IIN plotted against σ_p and *pEDA(I)*.

***v*(CN) in IND**

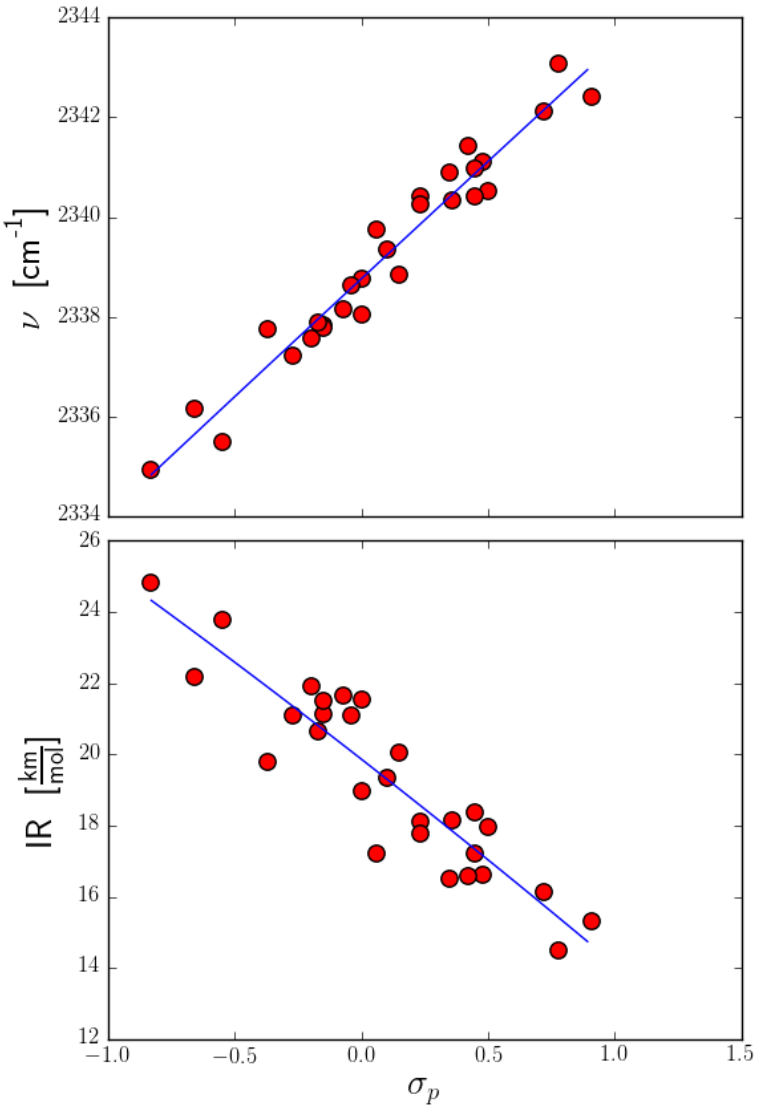

Figure S7. Correlations of frequencies and IR intensities of *v*(CN) in IND with σ_p.

Frequency = 4.70 (± 0.09) σ_p + 2338.77 (± 0.04), n = 28, r = 0.98.

IR = - 5.57 (± 0.21) σ_p - 19.83 (± 0.09), n = 28, r = 0.92.

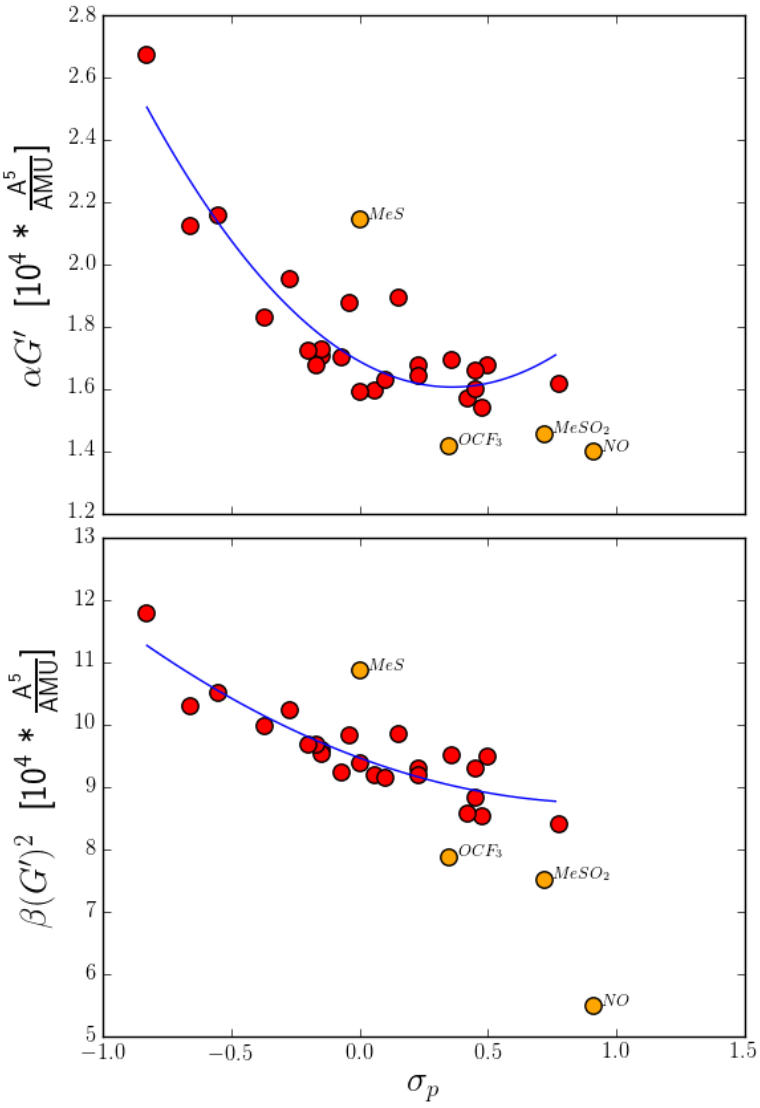

Figure S8. Correlations of $\alpha G'$ and $\beta(G')^2$ invariants of *ν*(CN) in IND with σ_p.

$\alpha G'$ = 0.63 (± 0.12) σ_p^2 - 0.46 (± 0.06) σ_p + 1.69 (± 0.03) , n = 24, r = 0.91.

$\beta(G')^2$ = 0.79 (± 0.38) σ_p^2 - 1.52 (± 0.18) σ_p + 9.47 (± 0.09) , n = 24, r = 0.89.

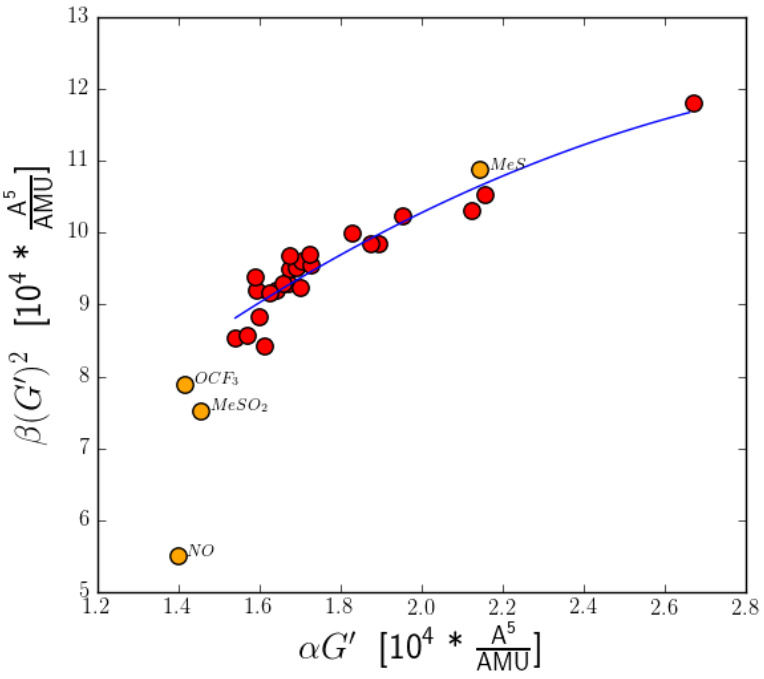

Figure S9. Mutual proportionality of $\alpha G'$ and $\beta(G')^2$ invariants of *ν*(CN) in IND.

$\beta(G')^2$ = - 0.96 (± 0.60) $(\alpha G')^2$ + 6.57 (± 2.46) $\alpha G'$ + 0.96 (± 2.45) , *n* = 24, *r* = 0.94

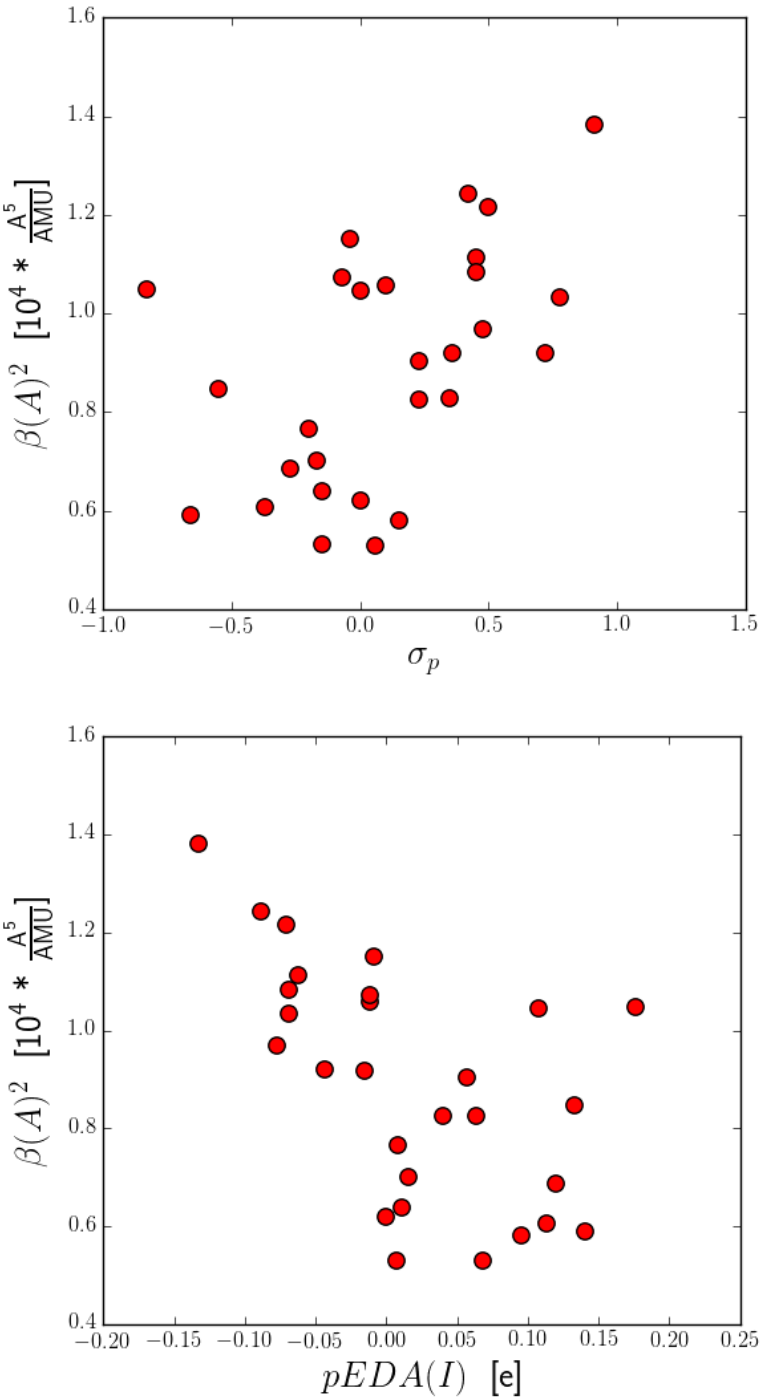

Figure S10. $\beta(A)^2$ invariant of *v*(CN) in IND plotted against σ_p and *pEDA(I)*.

***v*(CN) in IIN**

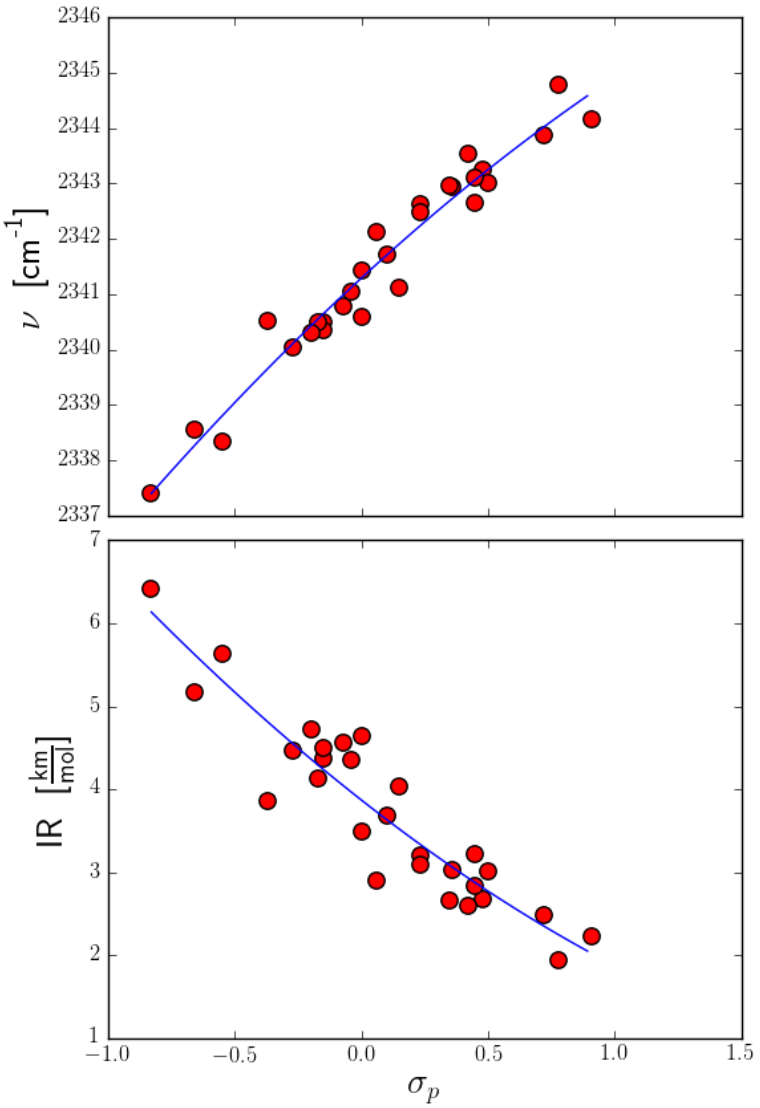

Figure S11. Correlations of frequencies and IR intensities of *v*(CN) in IIN with σ_p.

Frequency = - 0.58 (± 0.35) σ_p^2 + 4.21 (± 0.19) σ_p + 2341.29 (± 0.10) , n = 28, r = 0.98.

IR = 0.40 (± 0.36) σ_p^2 - 2.40 (± 0.19) σ_p + 3.87 (± 0.10) , n = 28, r = 0.93.

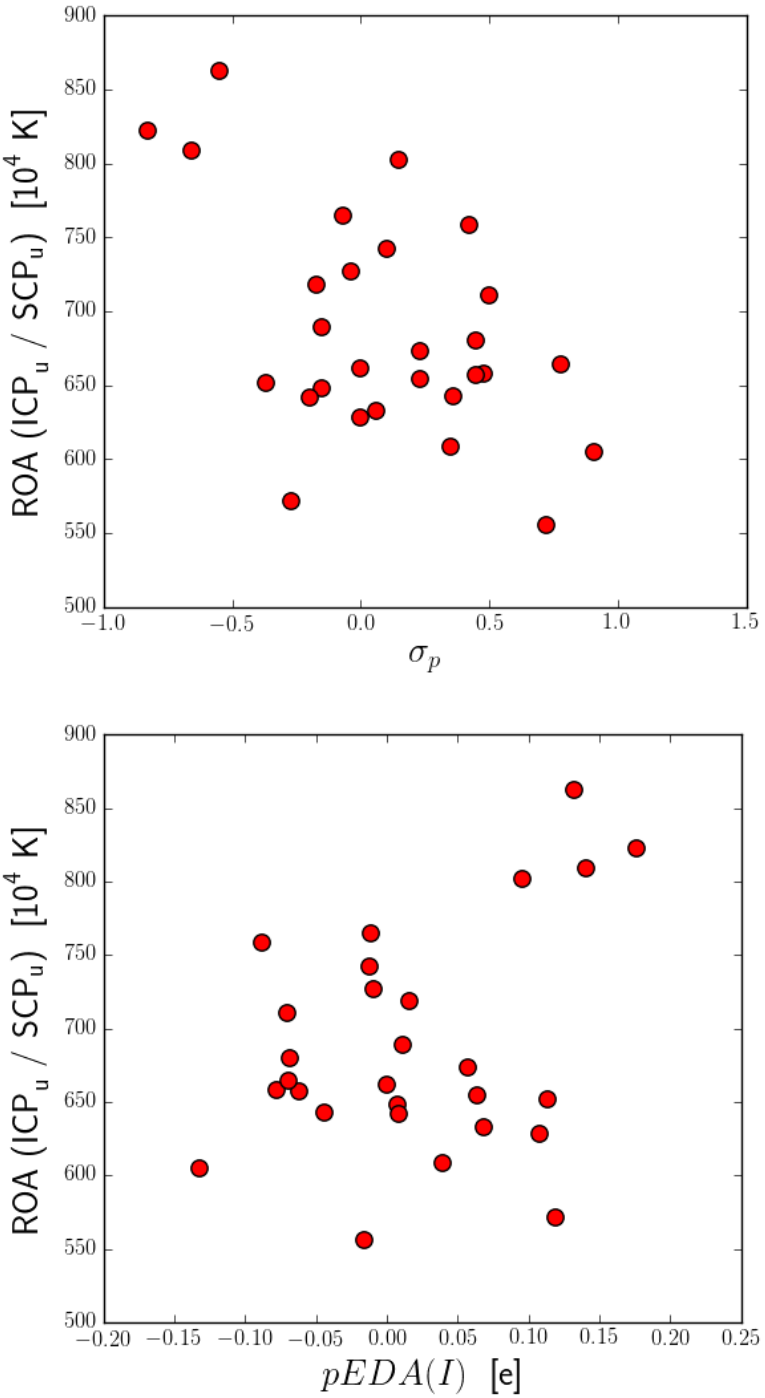

Figure S12. ROA intensities of *v*(CN) in IIN plotted against σ_p and *pEDA(I)*.

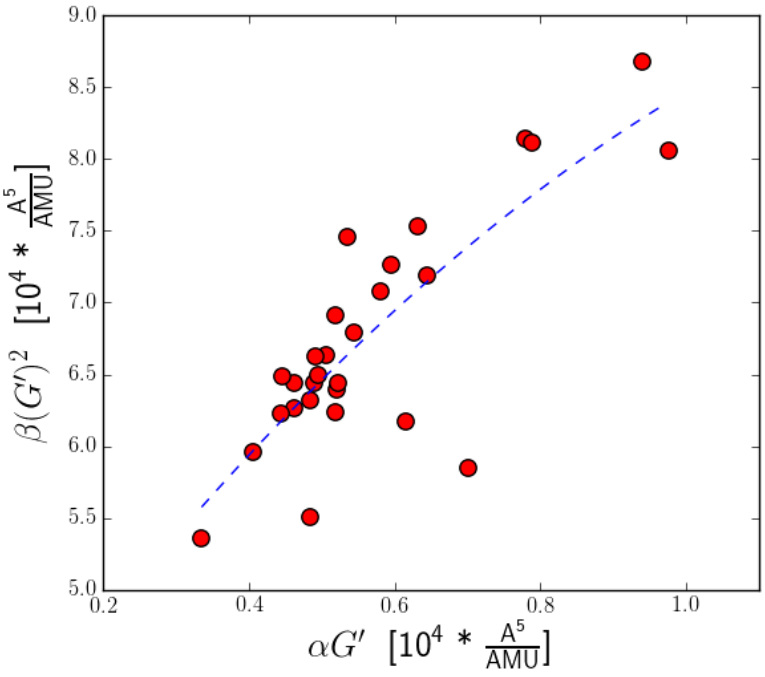

Figure S13. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of *v*(CN) in IIN.

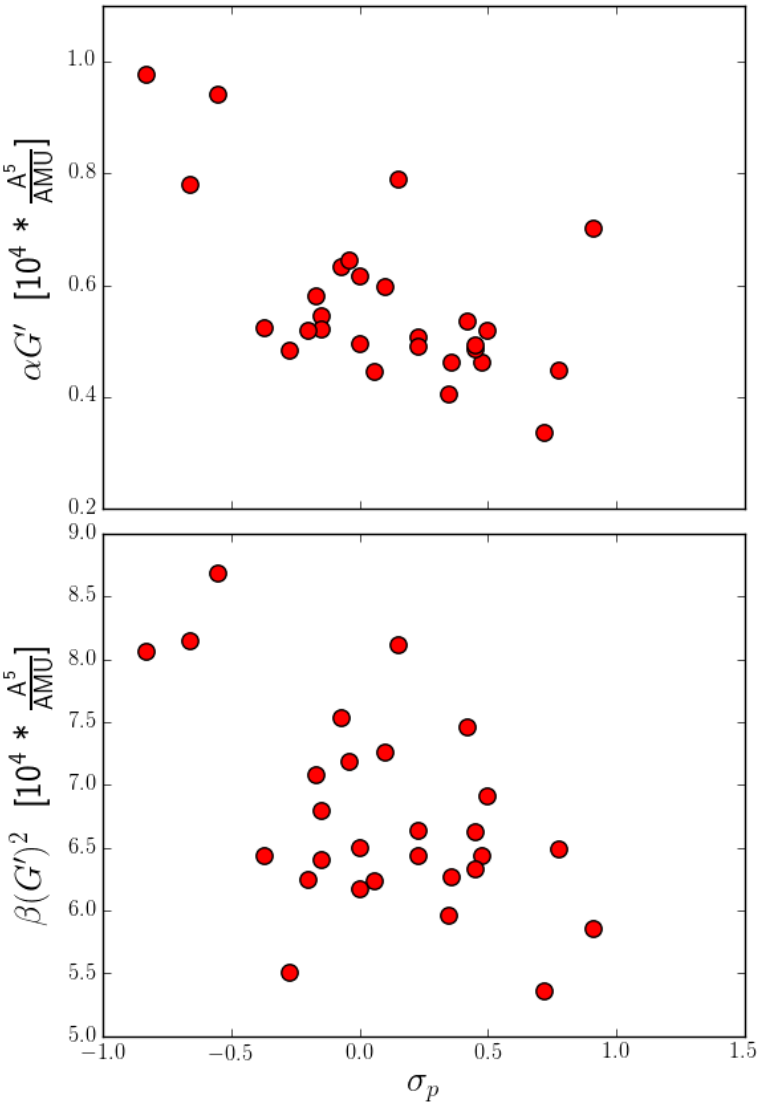

Figure S14. $\alpha G'$ and $\beta(G')^2$ invariants of *ν*(CN) in IIN plotted against σ_p.

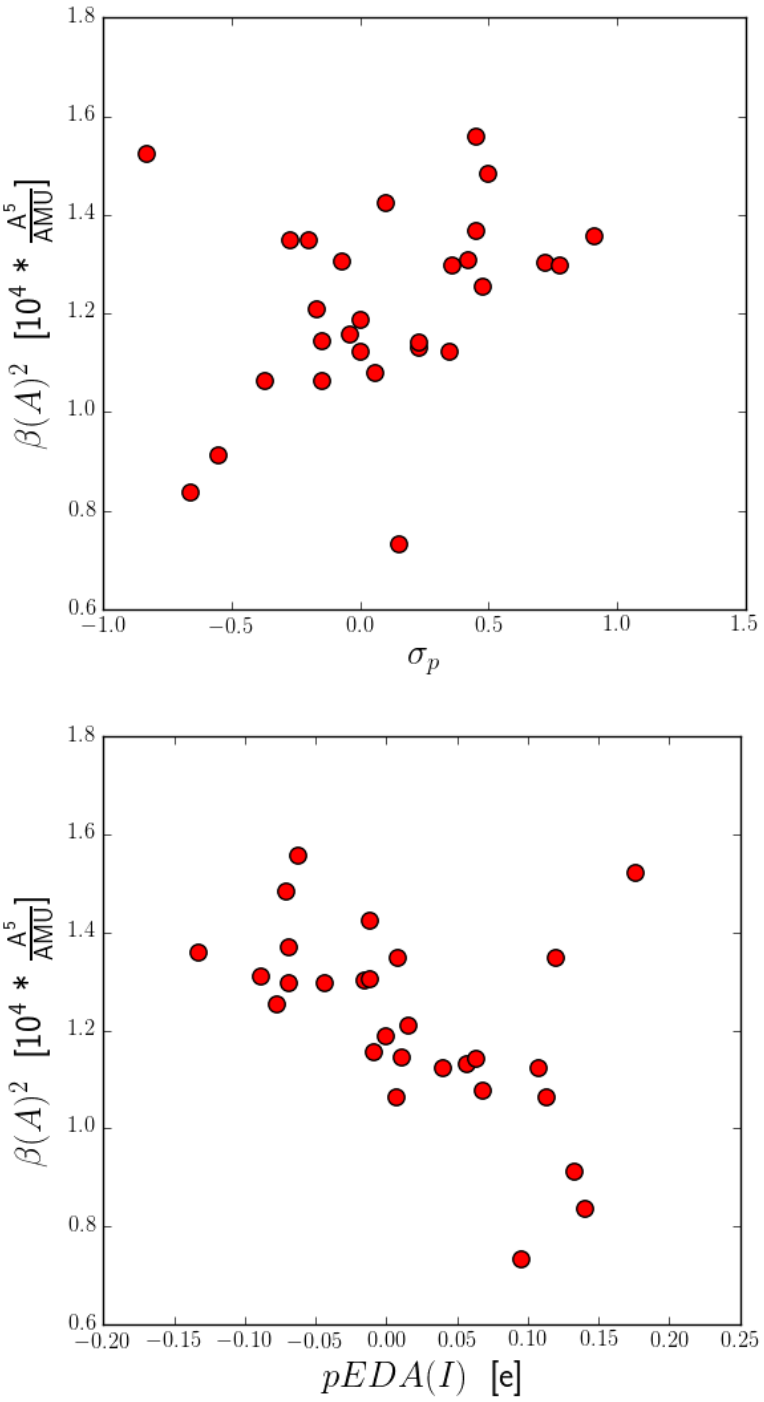

Figure S15. $\beta(A)^2$ invariant of *ν*(CN) in IIN plotted against σ_p and *pEDA(I)*.

ν_s(HC=CH) in IND

symmetric vibration of HC=CH in the five-membered ring of IND

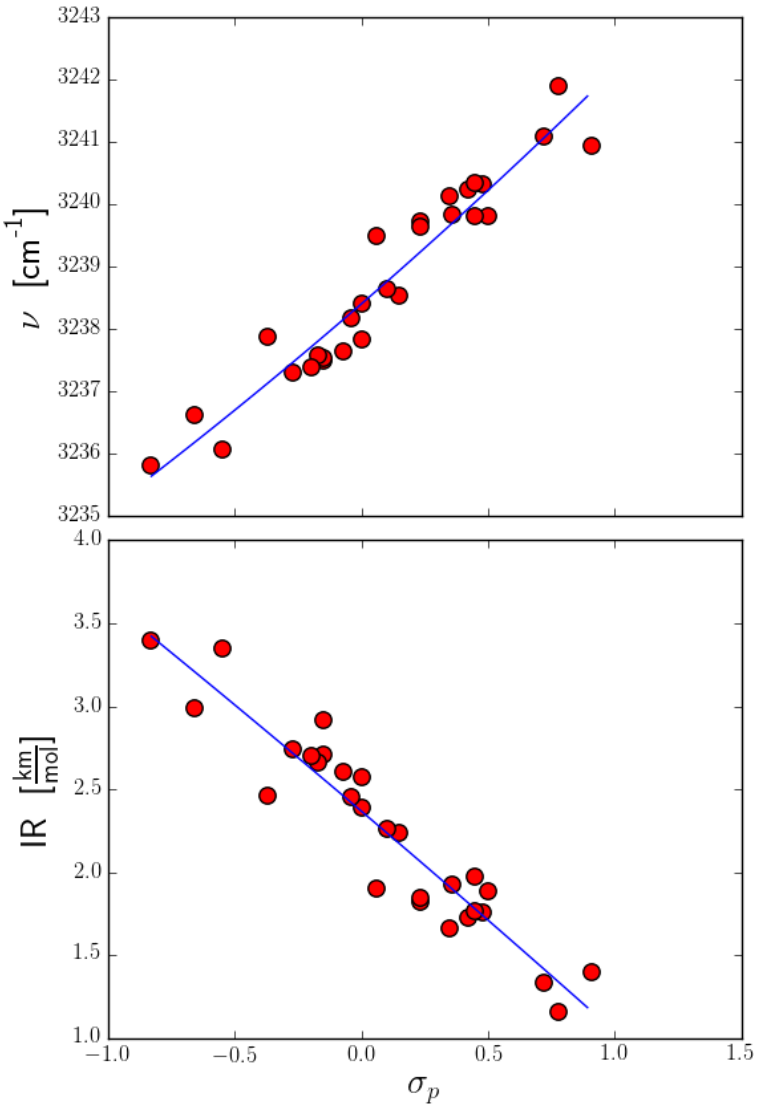

Figure S16. Correlations of frequencies and IR intensities of ν_s(HC=CH) in IND with σ_p.

Frequency = 3.56 (± 0.20) σ_p + 3238.44 (± 0.09), n = 28, r = 0.96.

IR = - 1.30 (± 0.09) σ_p - 2.36 (± 0.04), n = 28, r = 0.94.

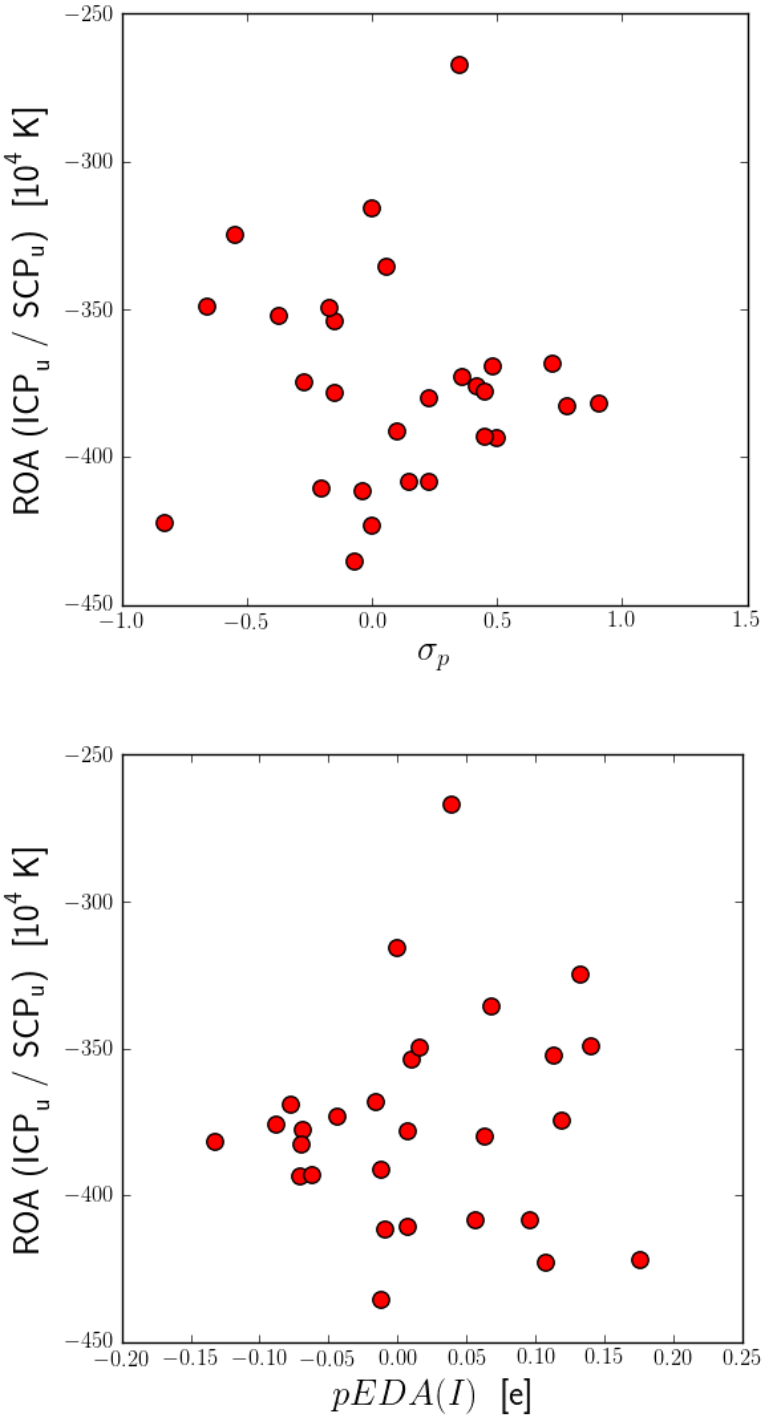

Figure S17. ROA intensities of ν_s(HC=CH) in IND plotted against σ_p and *pEDA(I)*.

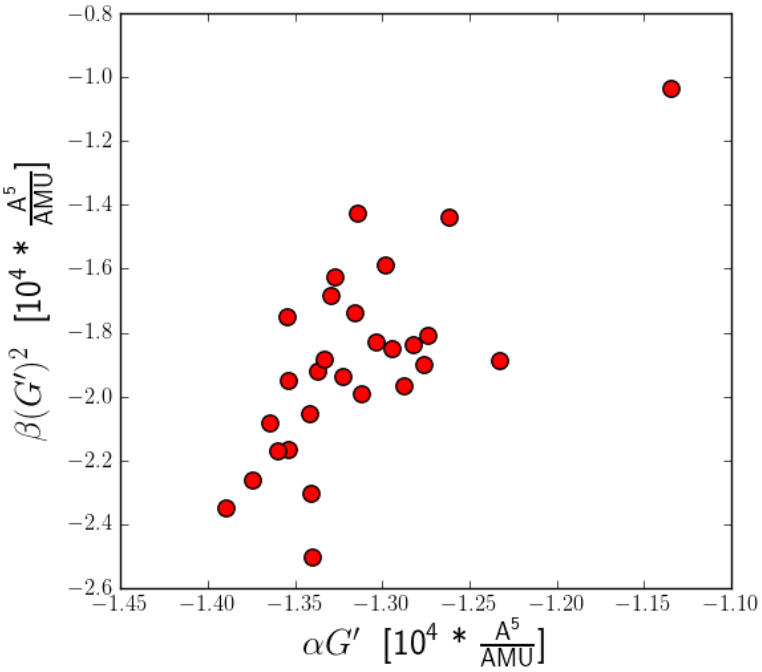

Figure S18. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of ν_s(HC=CH) in IND.

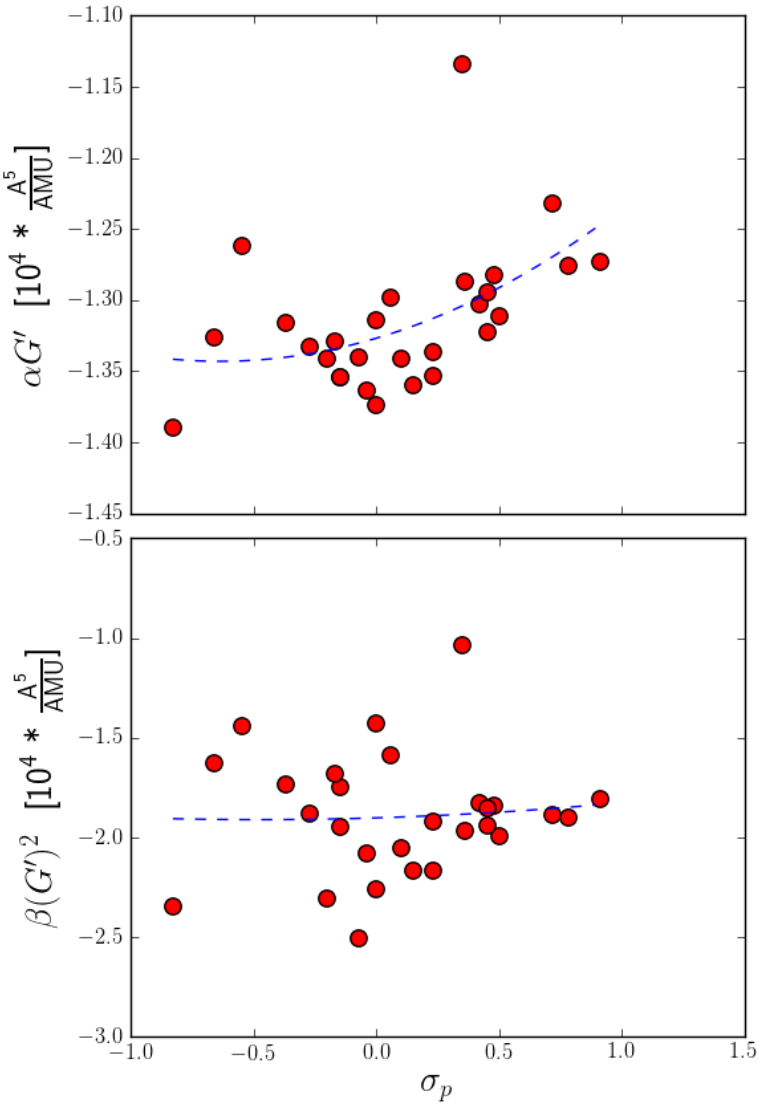

Figure S19. $\alpha G'$ and $\beta(G')^2$ invariants of ν_s(HC=CH) in IND plotted against σ_p.

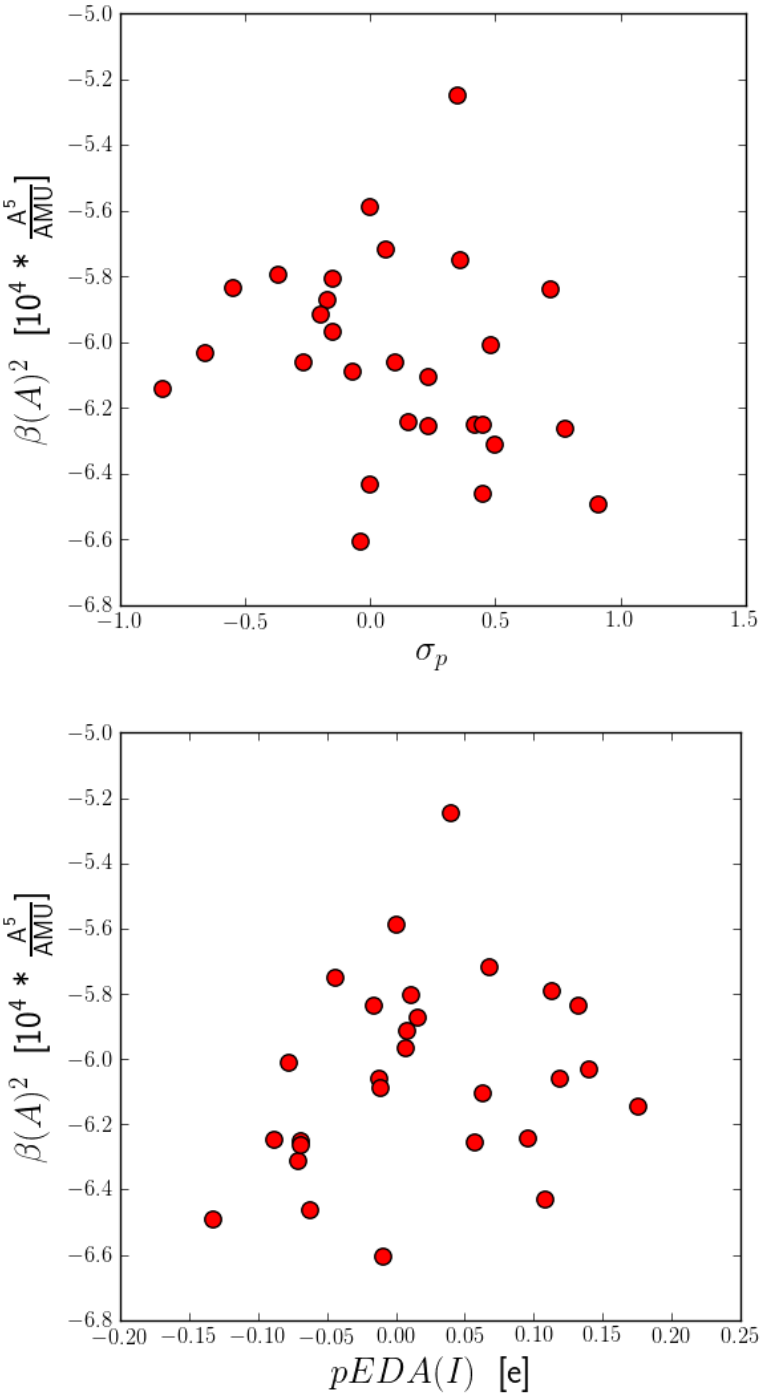

Figure S20. $\beta(A)^2$ invariant of ν_s(HC=CH) in IND plotted against σ_p and *pEDA(I)*.

v(NH) in IIN

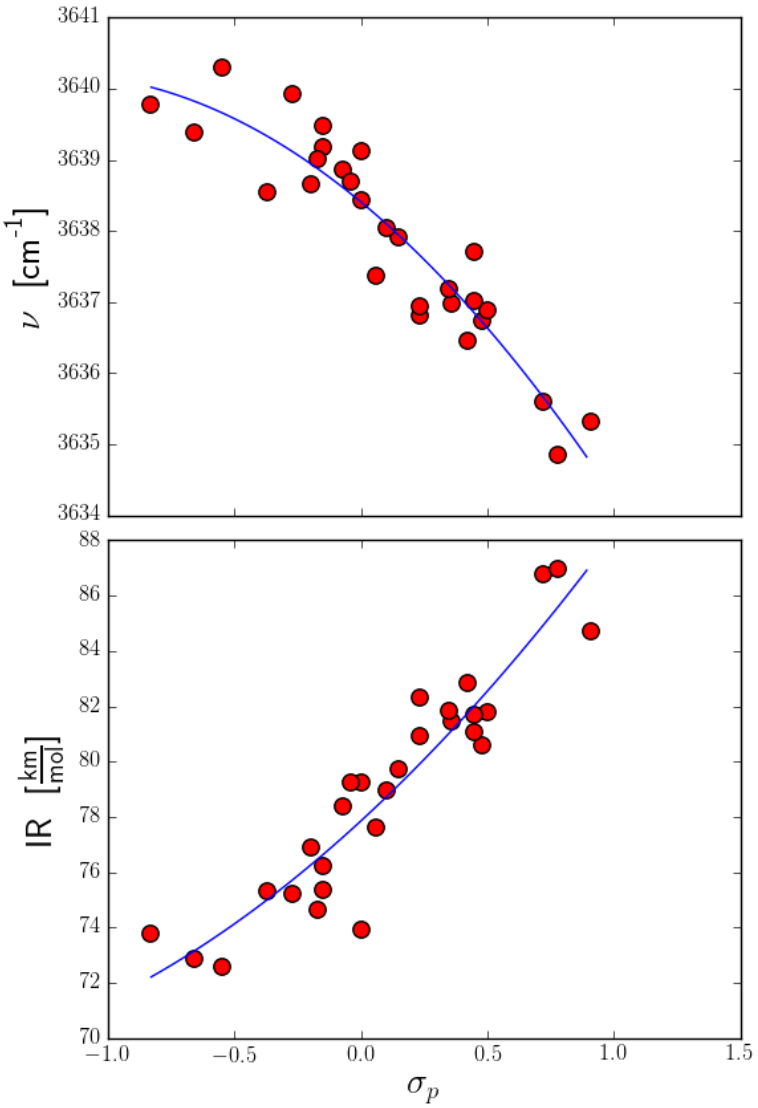

Figure S21. Correlations of frequencies and IR intensities of *v*(NH) in IIN with σ_p.

Frequency = 0.23 (± 0.39) σ_p^2 + 3.53 (± 0.21) σ_p + 3238.40 (± 0.11) , n = 28, r = 0.96.

IR = - 0.03 (± 0.17) σ_p^2 - 1.30 (± 0.09) σ_p + 2.37 (± 0.05) , n = 28, r = 0.94.

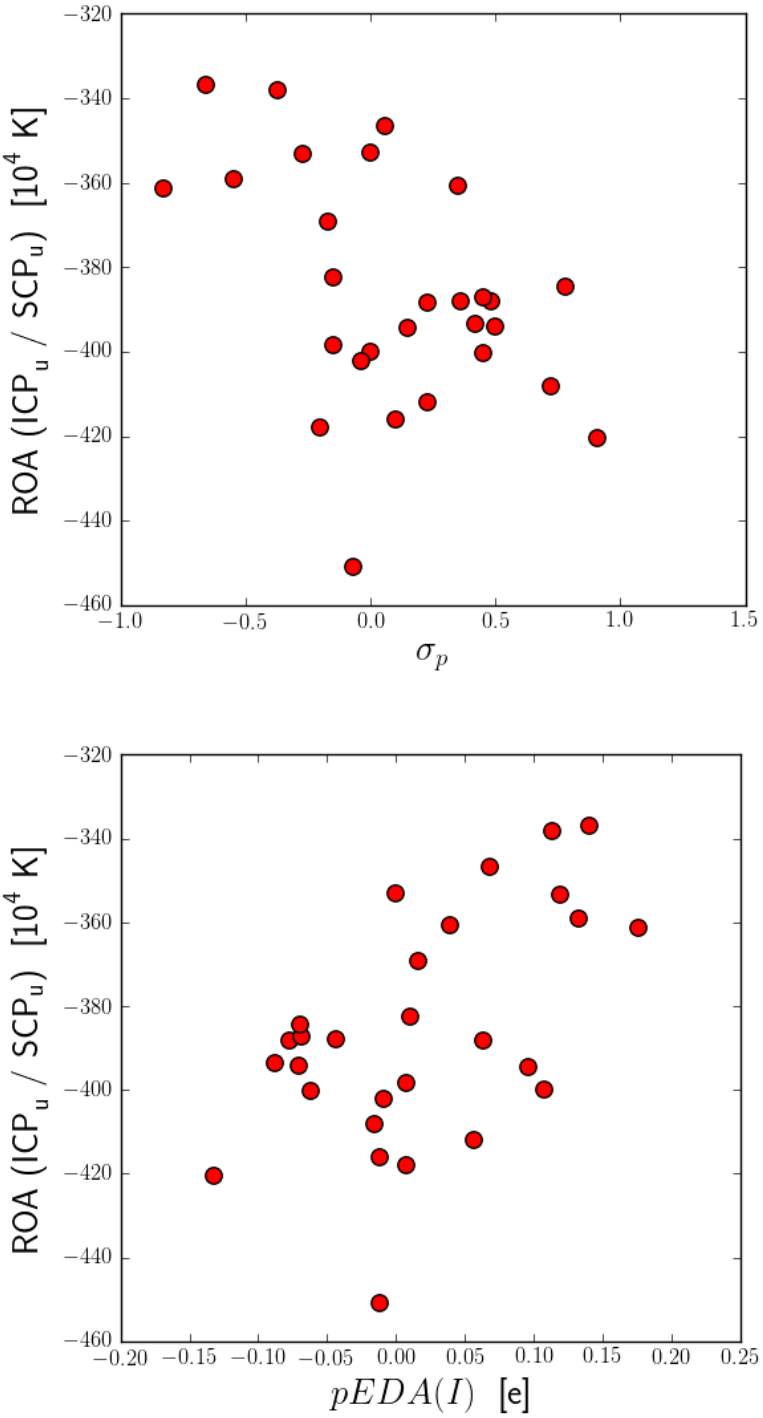

Figure S22. ROA intensities of *ν*(NH) in IIN plotted against σ_p and *pEDA(I)*.

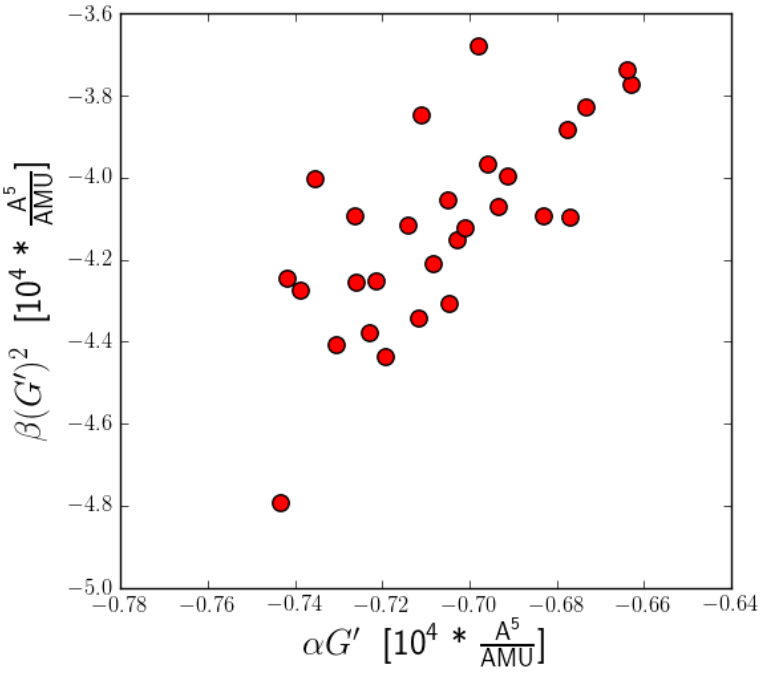

Figure S23. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of *v*(NH) in IIN.

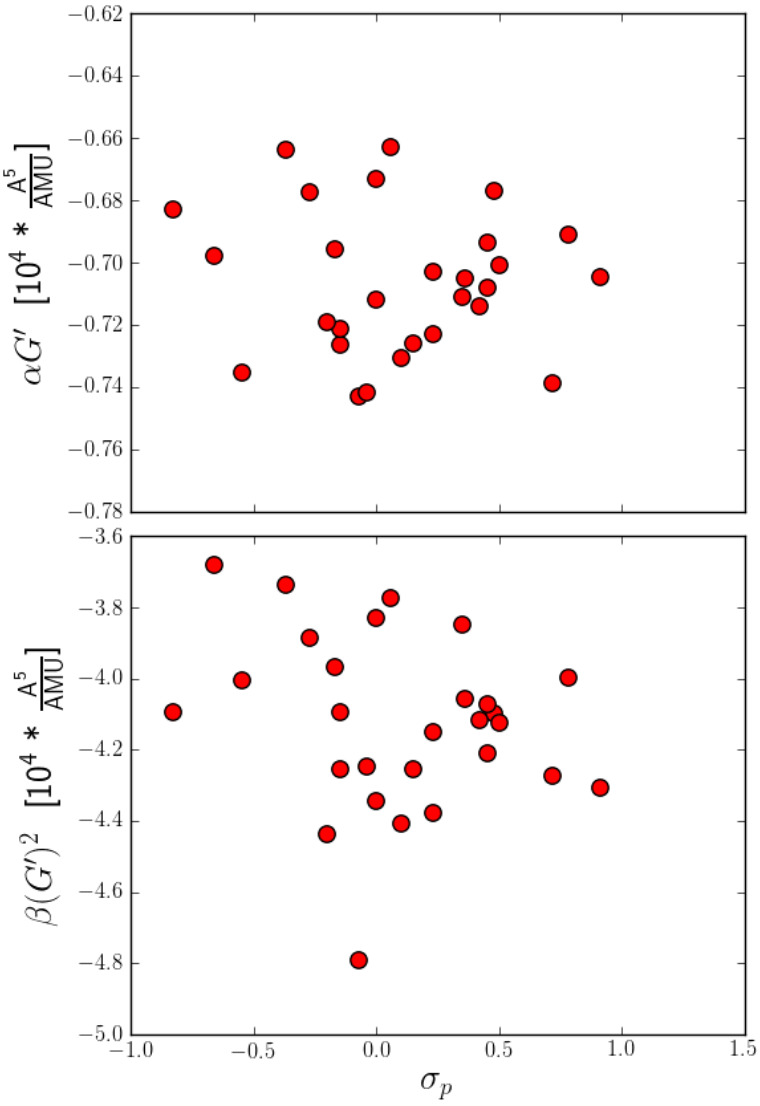

Figure S24. $\alpha G'$ and $\beta(G')^2$ invariants of *ν*(NH) in IIN plotted against *pEDA(I)*.

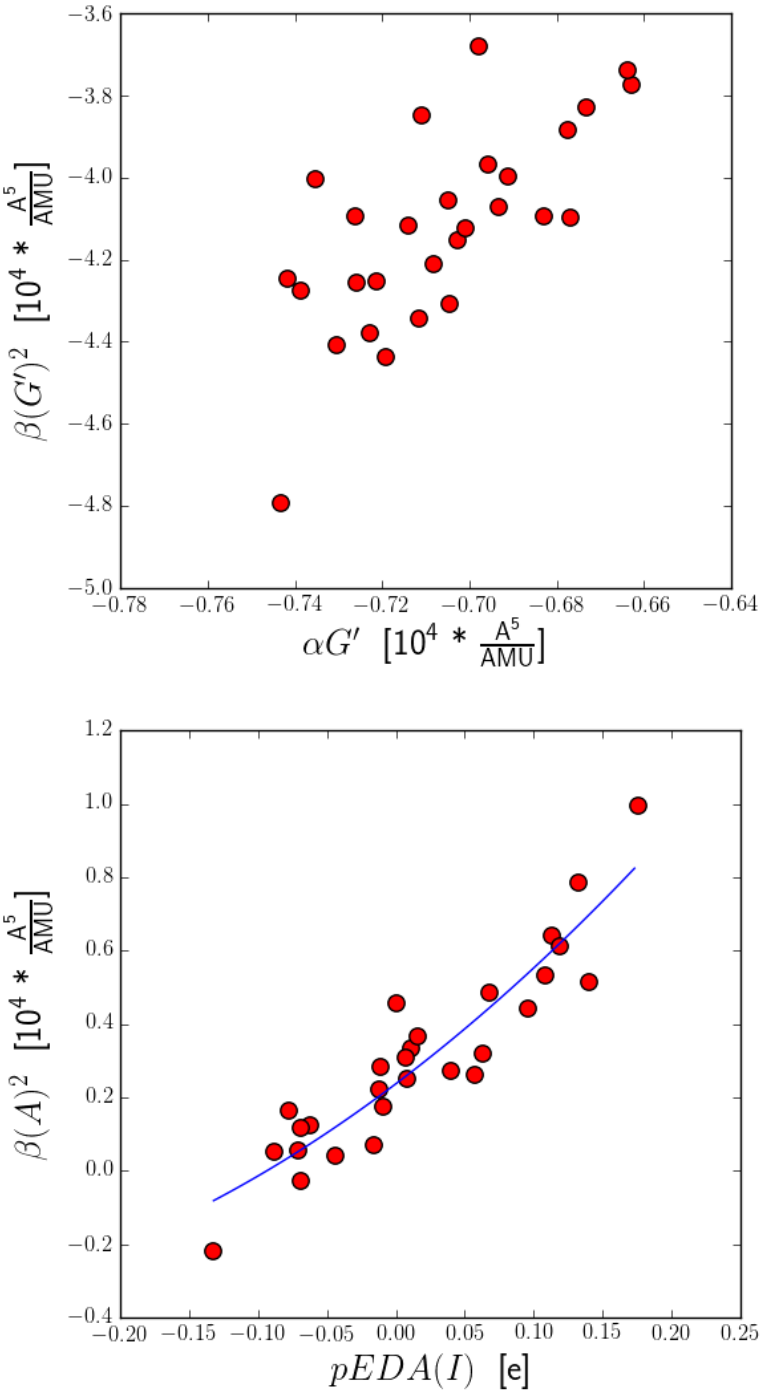

Figure S25. $\beta(A)^2$ invariant of *v*(NH) in IIN plotted against σ_p and *pEDA(I)*.

$\beta(A)^2$ is correlated with *pEDA(I)*:

$\beta(A)^2$ = 3.21 (± 3.02) *pEDA(I)*^{2} + 2.83 (± 0.29) *pEDA(I)* + 0.24 (± 0.03) , *n* = 28, *r* = 0.92.

$\nu(C{=}C)_1$ in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) parallel to C-R

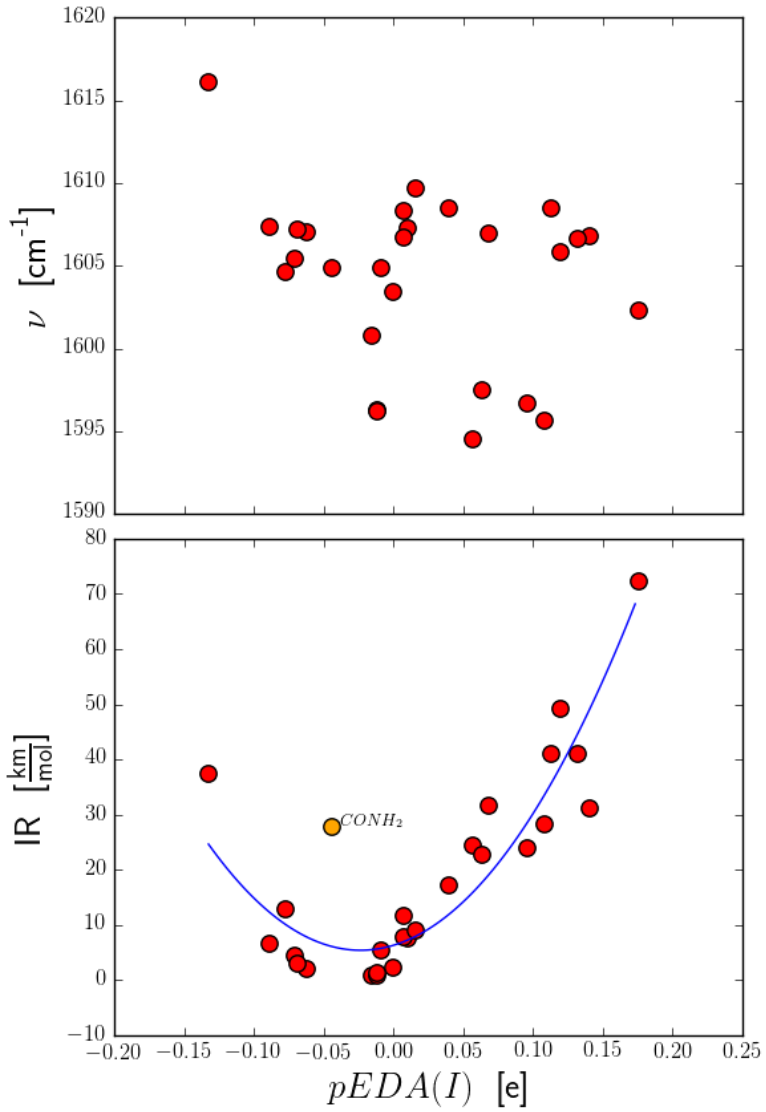

Figure S26. Frequencies and IR intensities of $\nu(C{=}C)_1$ in IND plotted against *pEDA(I)*.

IR = 1619.55 (± 211.07) $pEDA(I)^2$ + 75.90 (± 20.91) *pEDA(I)* + 6.28 (± 1.89) , *n* = 26, *r* = 0.93.

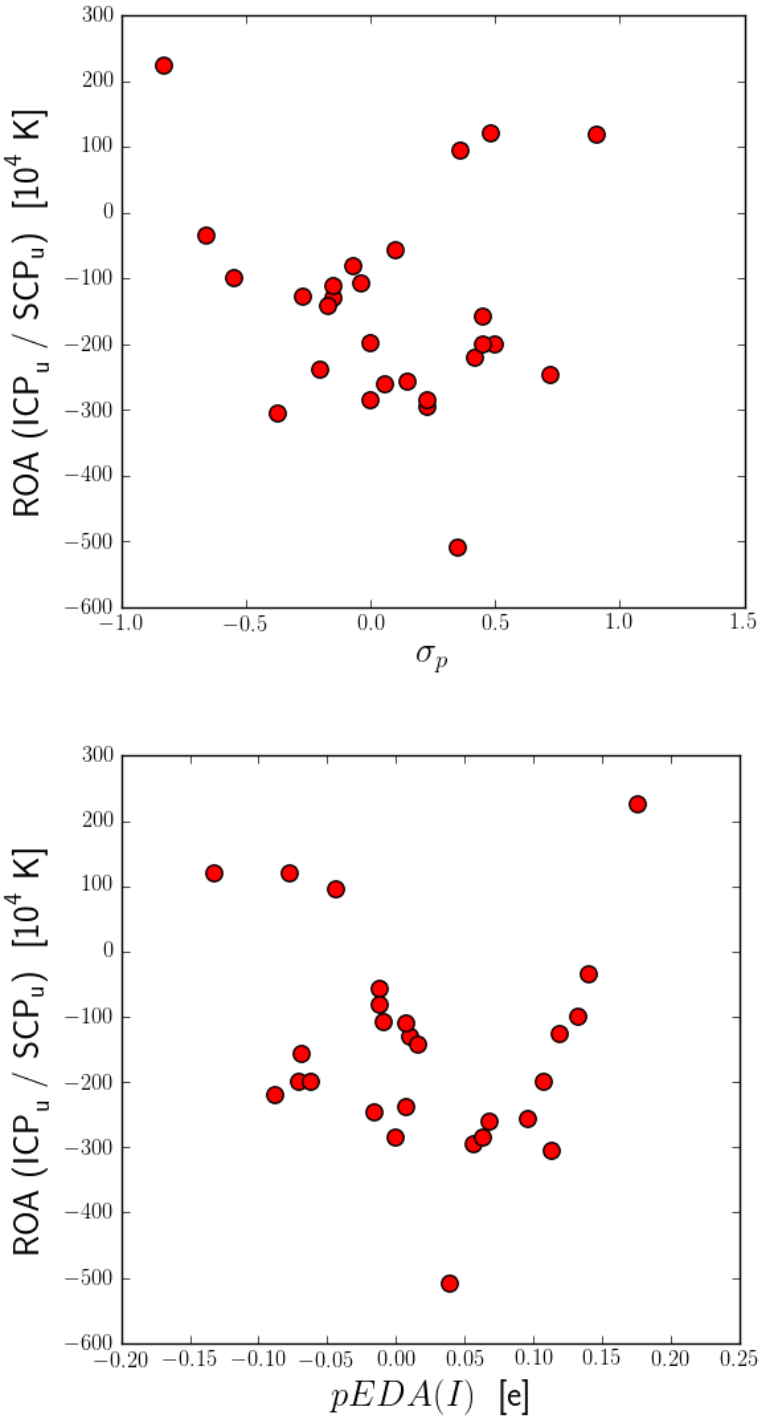

Figure S27. ROA intensities of *ν*(C=C)$_1$ in IND plotted against σ_p and *pEDA(I)*.

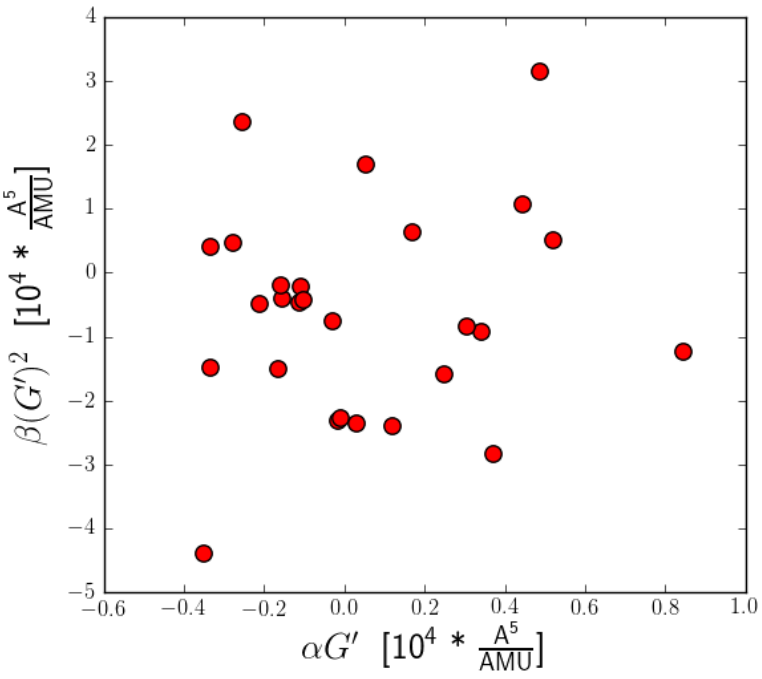

Figure S28. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_1$ in IND.

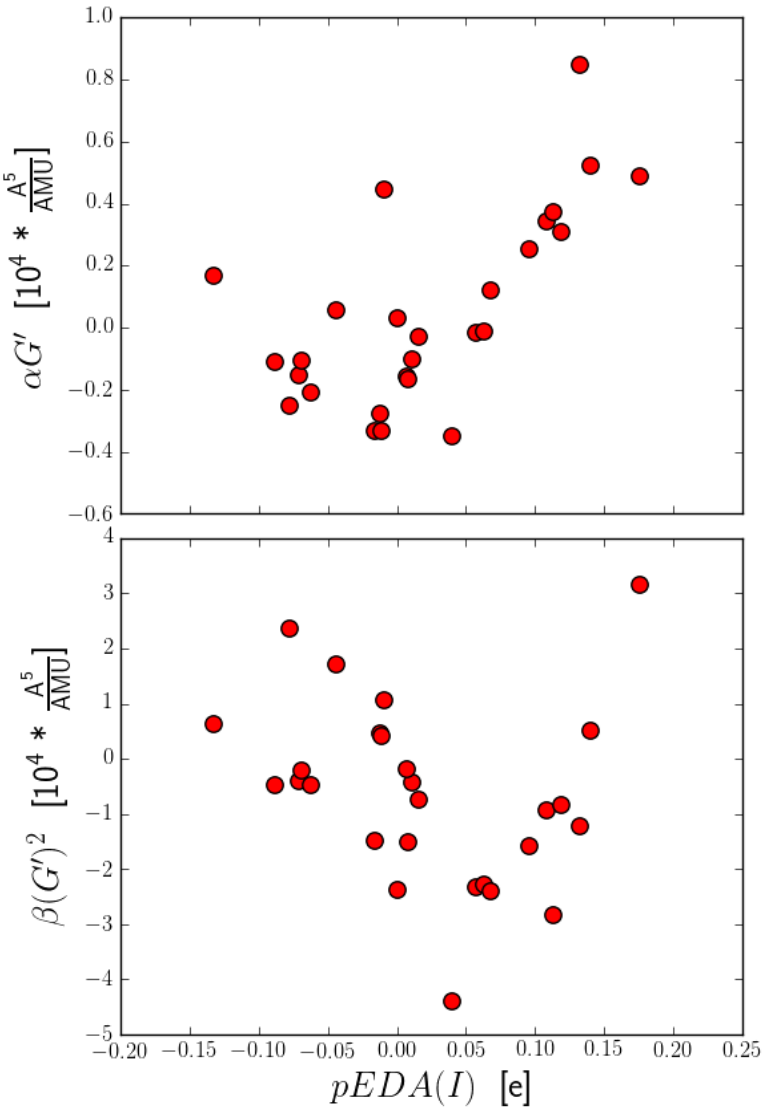

Figure S29. $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_1$ in IND plotted against *pEDA(I)*.

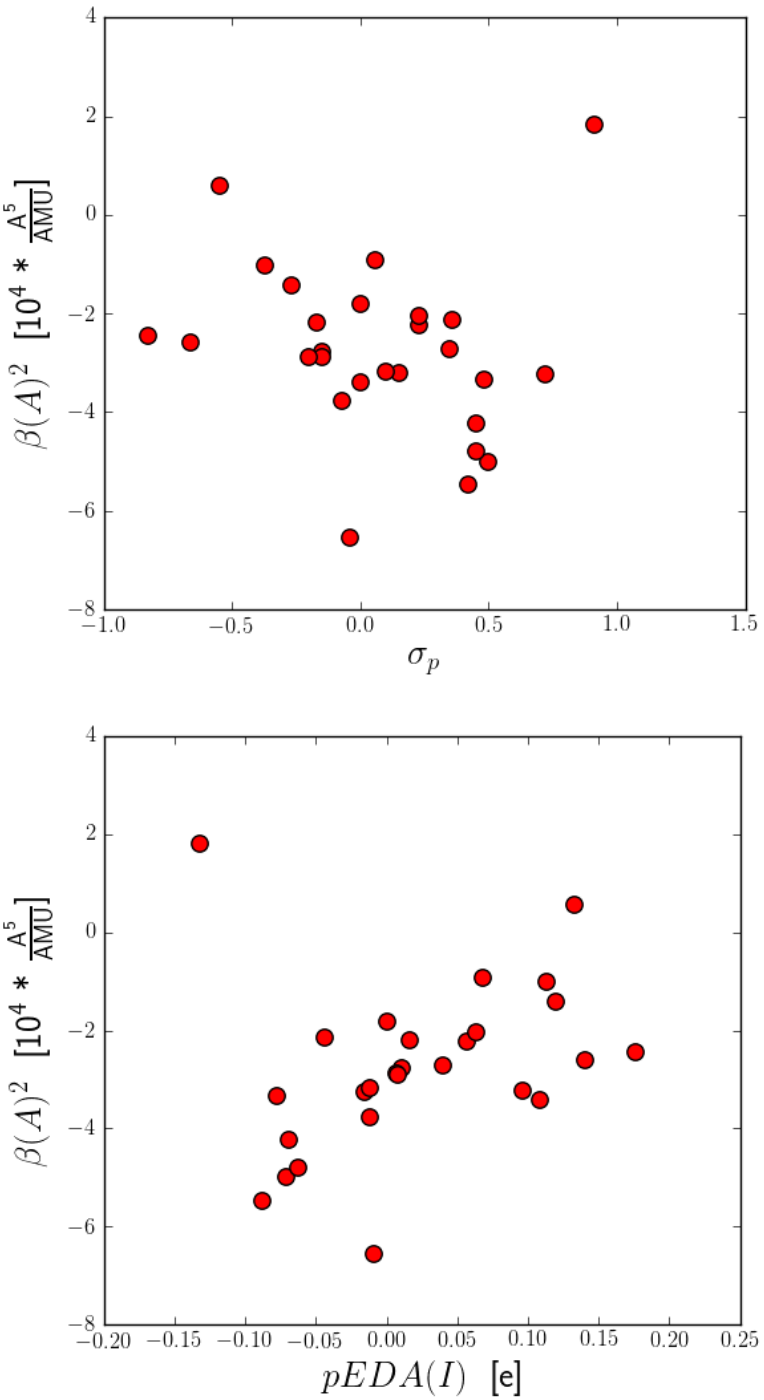

Figure S30. $\beta(A)^2$ invariant of *v*(C=C)$_1$ in IND plotted against σ_p and *pEDA(I)*.

ν(C=C)$_2$ in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) at 120° to C-R

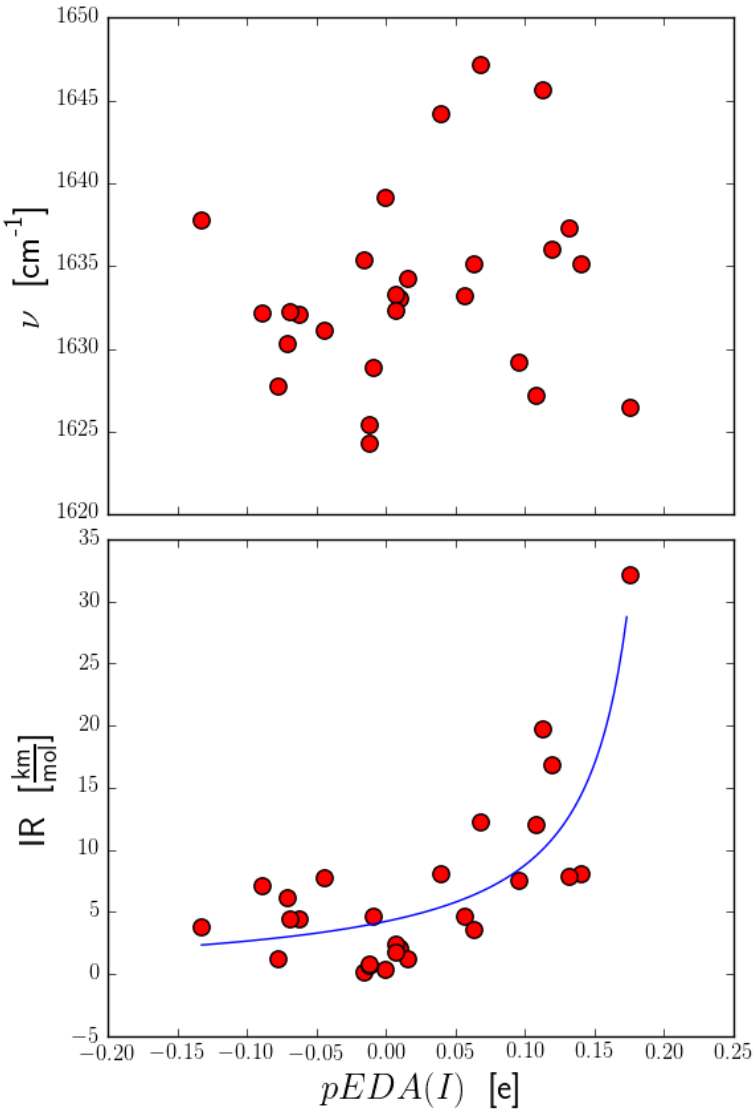

Figure S31. Frequencies and IR intensities of ν(C=C)$_2$ in IND plotted against *pEDA(I)*.

IR = (1 + *a* * *pEDA(I)*) / (*b* + *c* * *pEDA(I)*), *a* = 0.73 (± 2.69), *b* = 0.24 (± 0.05), *c* = - 1.14 (± 0.23), *n* = 27, *r* = 0.84.

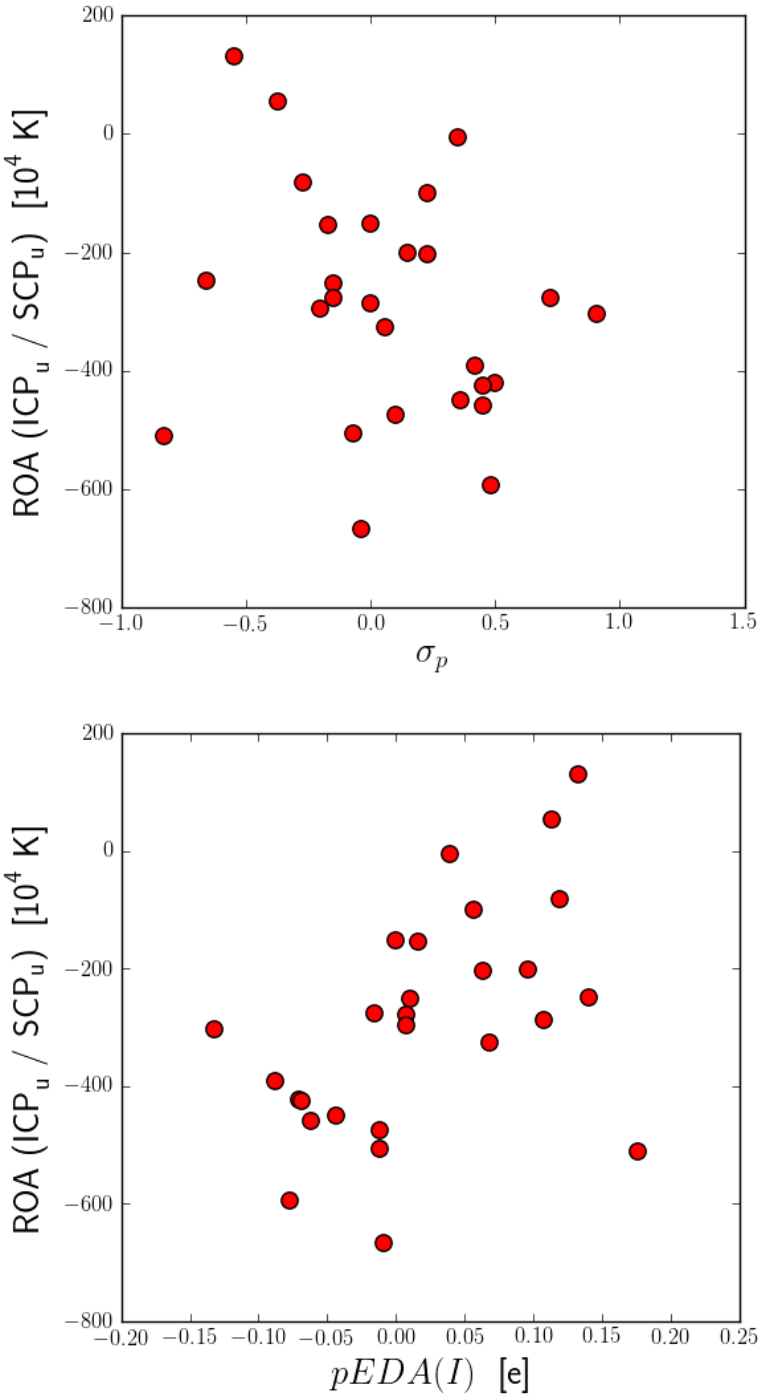

Figure S32. ROA intensities of *ν*(C=C)$_2$ in IND plotted against σ_p and *pEDA(I)*.

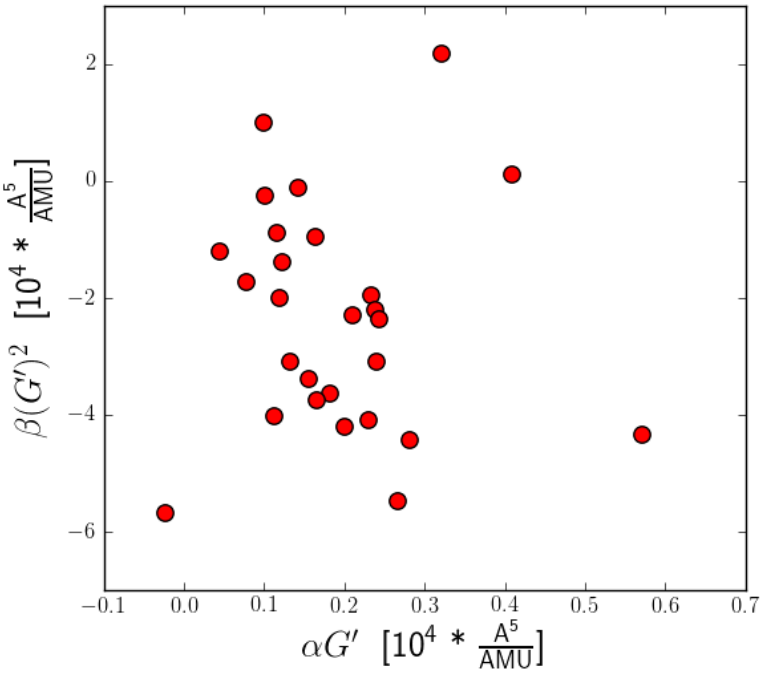

Figure S33. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of *v*(C=C)$_2$ in IND.

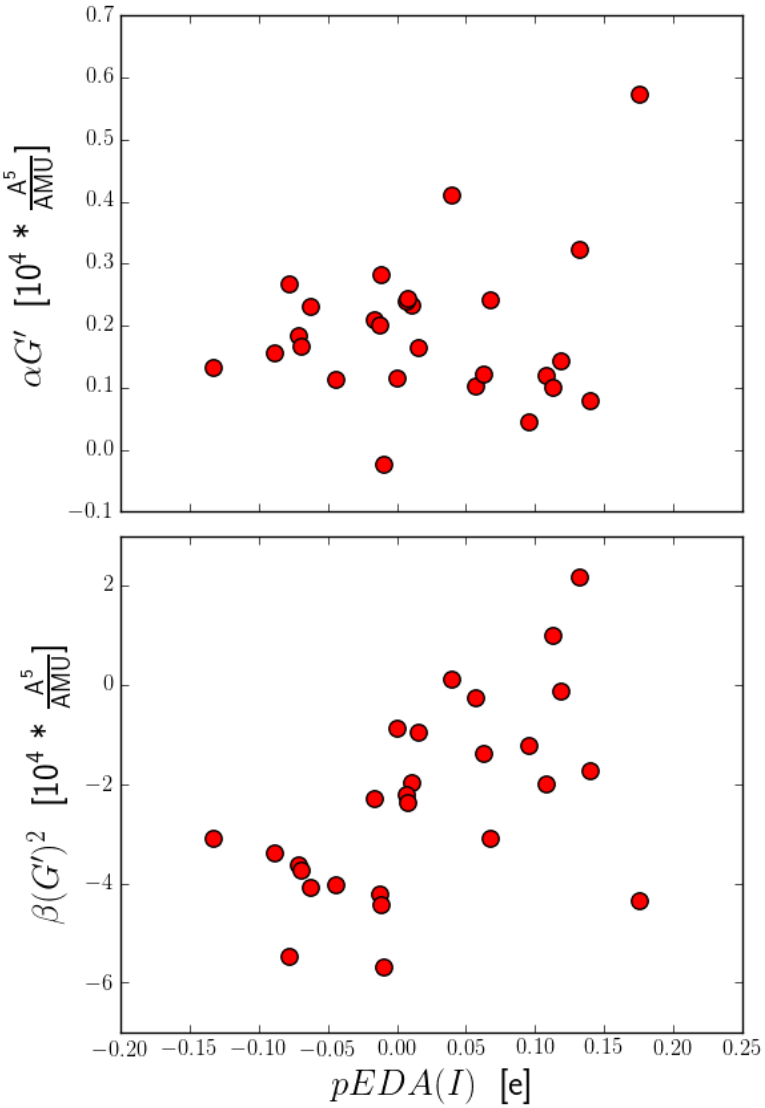

Figure S34. $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_2$ in IND plotted against *pEDA(I)*.

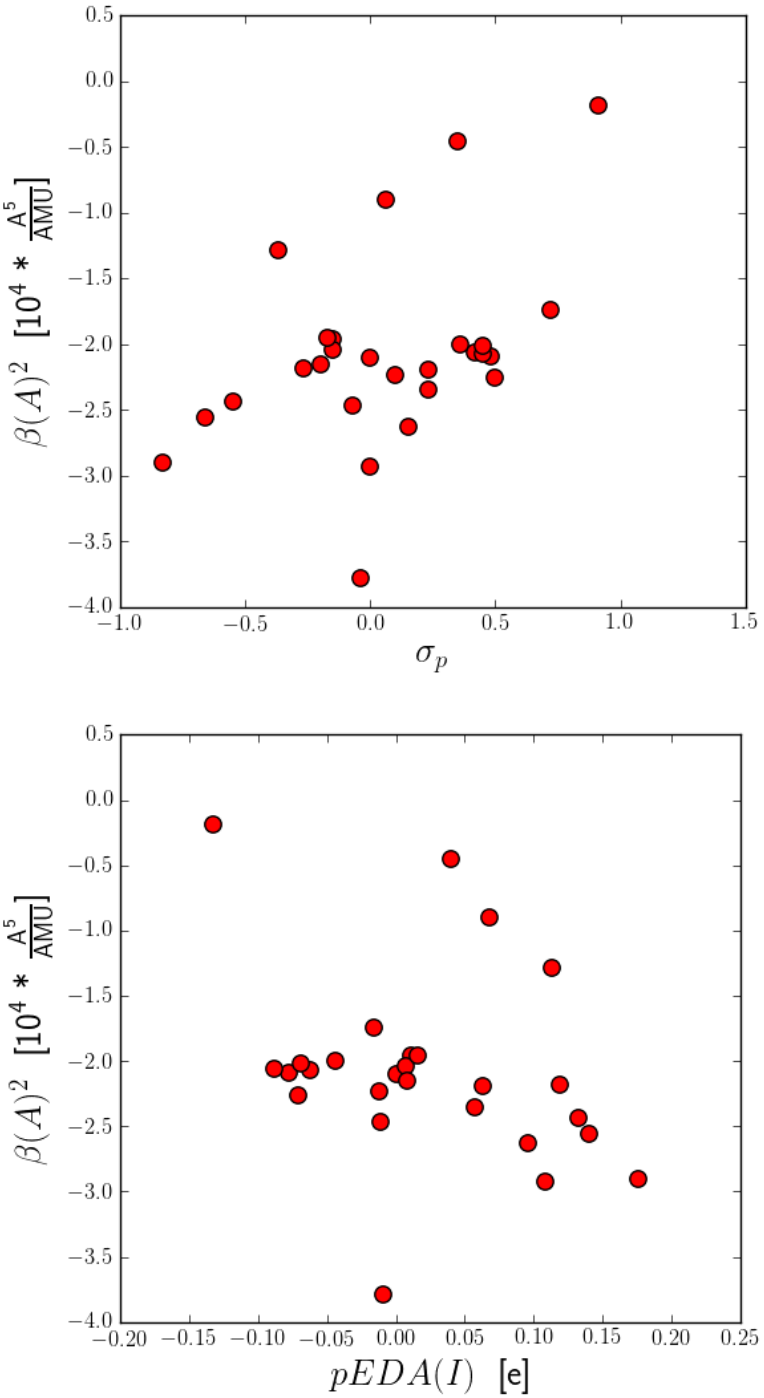

Figure S35. $\beta(A)^2$ invariant of ν(C=C)$_2$ in IND plotted against σ_p and *pEDA(I)*.

$\nu(C{=}C)_3$ in IND

in-phase vibration of C=C (5-membered ring) and two C=C (6-membered ring) at -120° to C-R

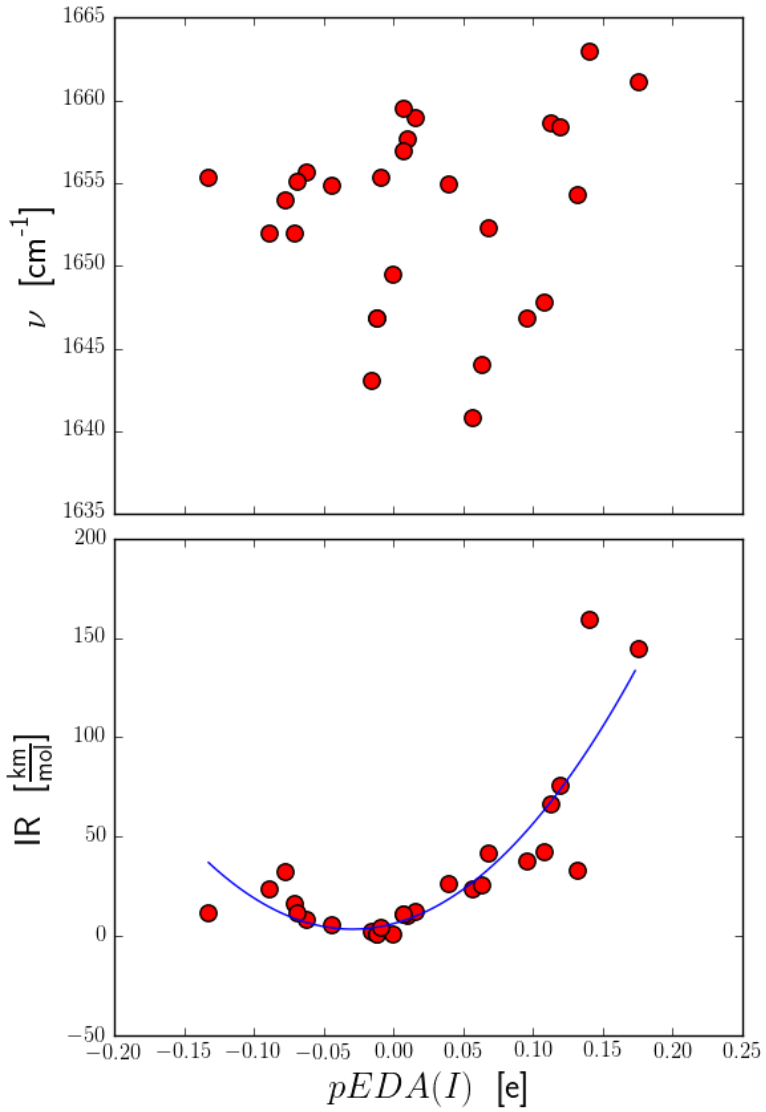

Figure S36. Frequencies and IR intensities of $\nu(C{=}C)_3$ in IND plotted against *pEDA(I)*.

IR = 3163.16 (± 574.45) $pEDA(I)^2$ + 186.03 (± 56.55) *pEDA* + 6.13 (± 5.04), n = 27, r = 0.88.

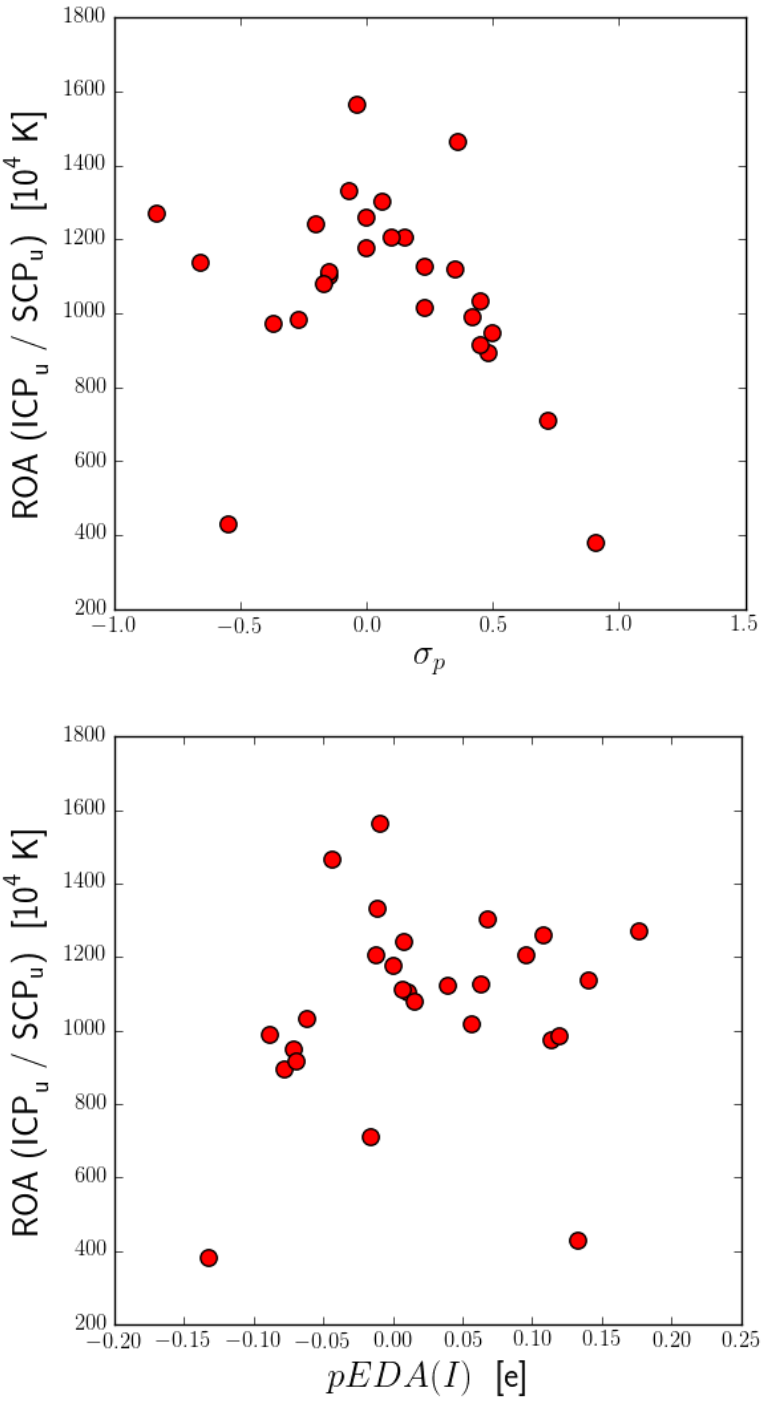

Figure S37. ROA intensities of *ν*(C=C)$_3$ in IND plotted against σ_p and *pEDA(I)*.

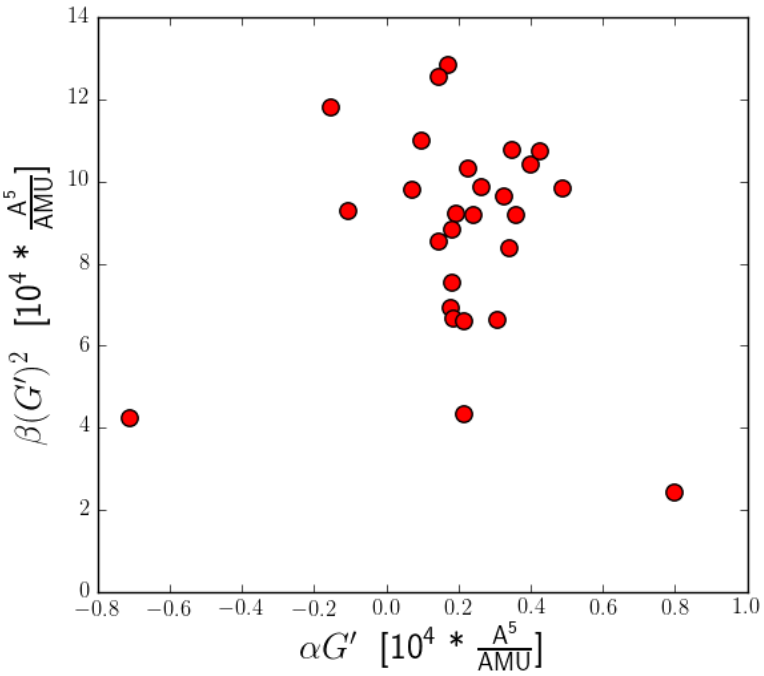

Figure S38. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of *v*(C=C)$_3$ in IND.

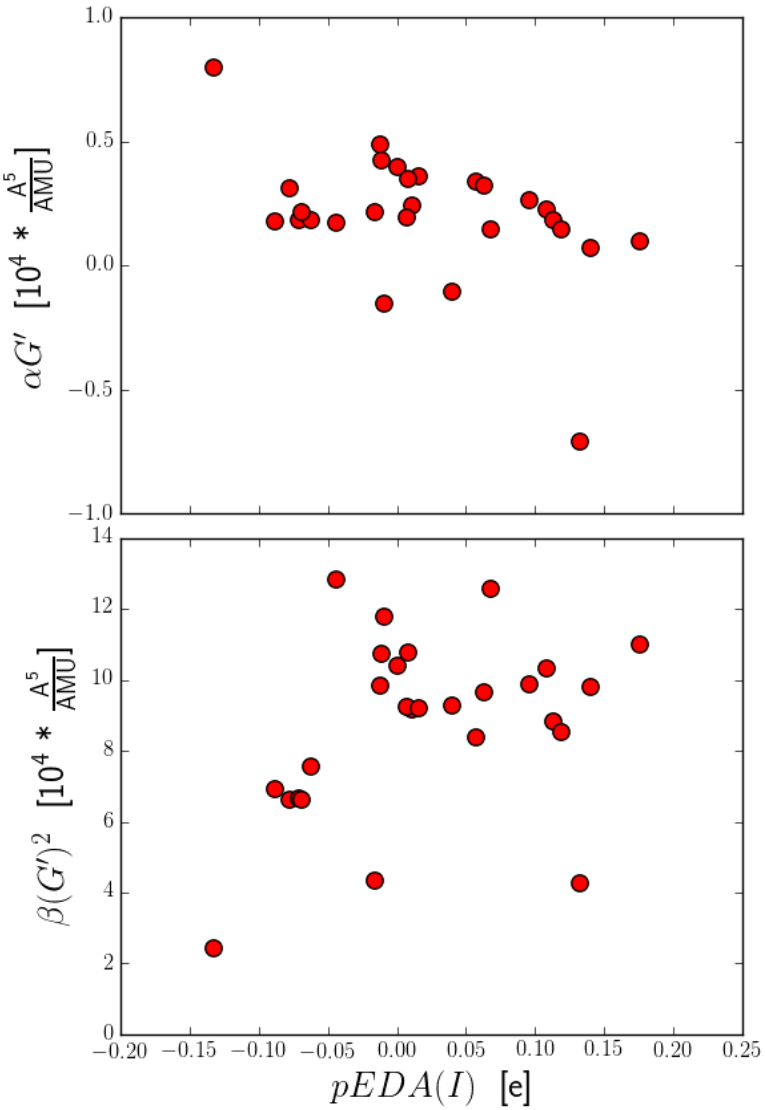

Figure S39. $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_3$ in IND plotted against *pEDA(I)*.

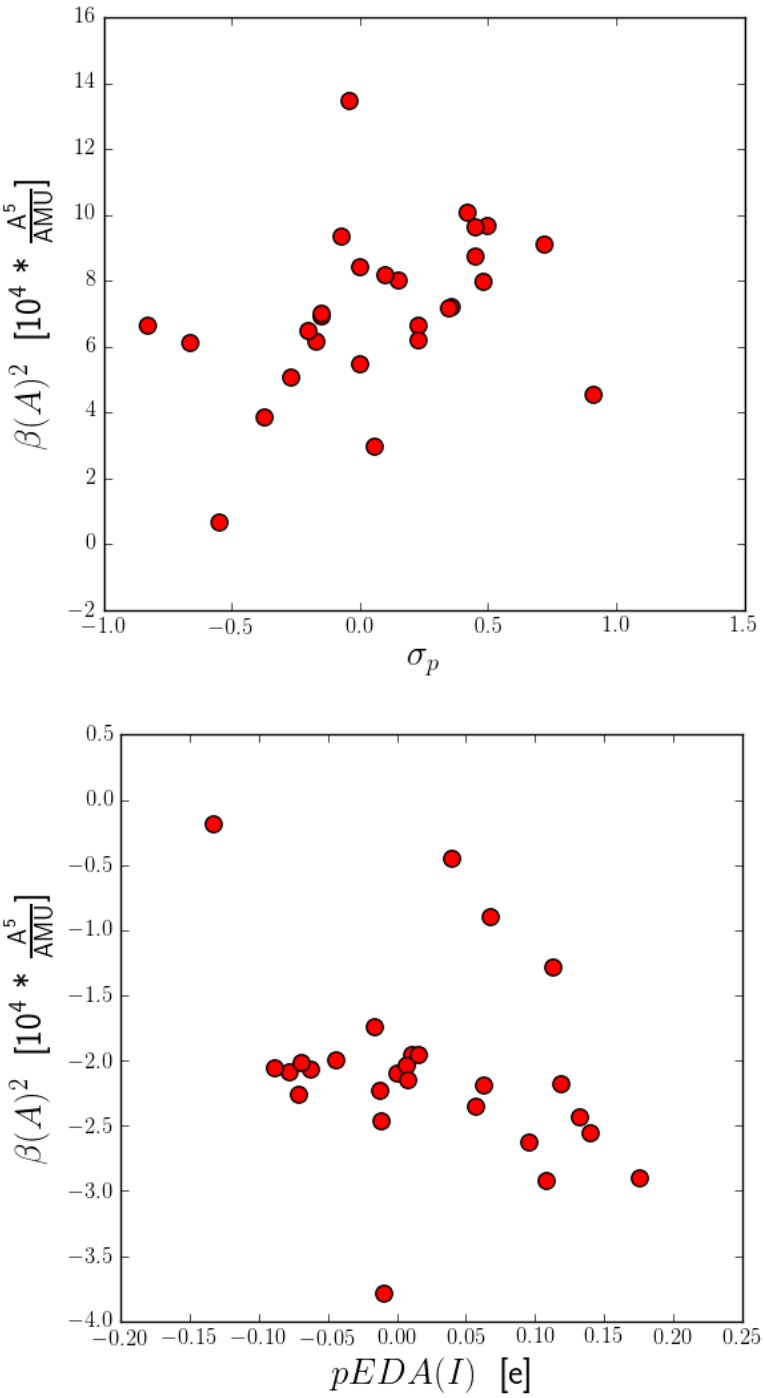

Figure S40. $\beta(A)^2$ invariant of *ν*(C=C)$_3$ in IND plotted against σ_p and *pEDA(I)*.

***v*(C=C)$_4$ in IIN**

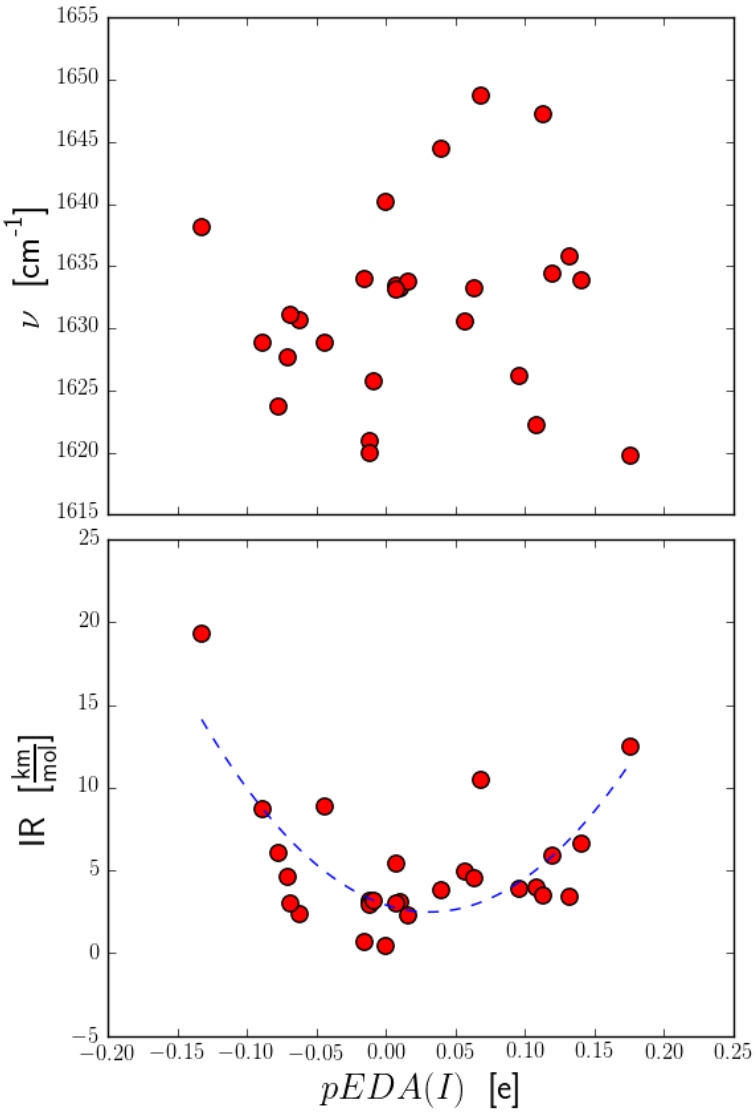

Figure S41. Frequencies and IR intensities of *v*(C=C)$_4$ in IIN plotted against *pEDA(I)*.

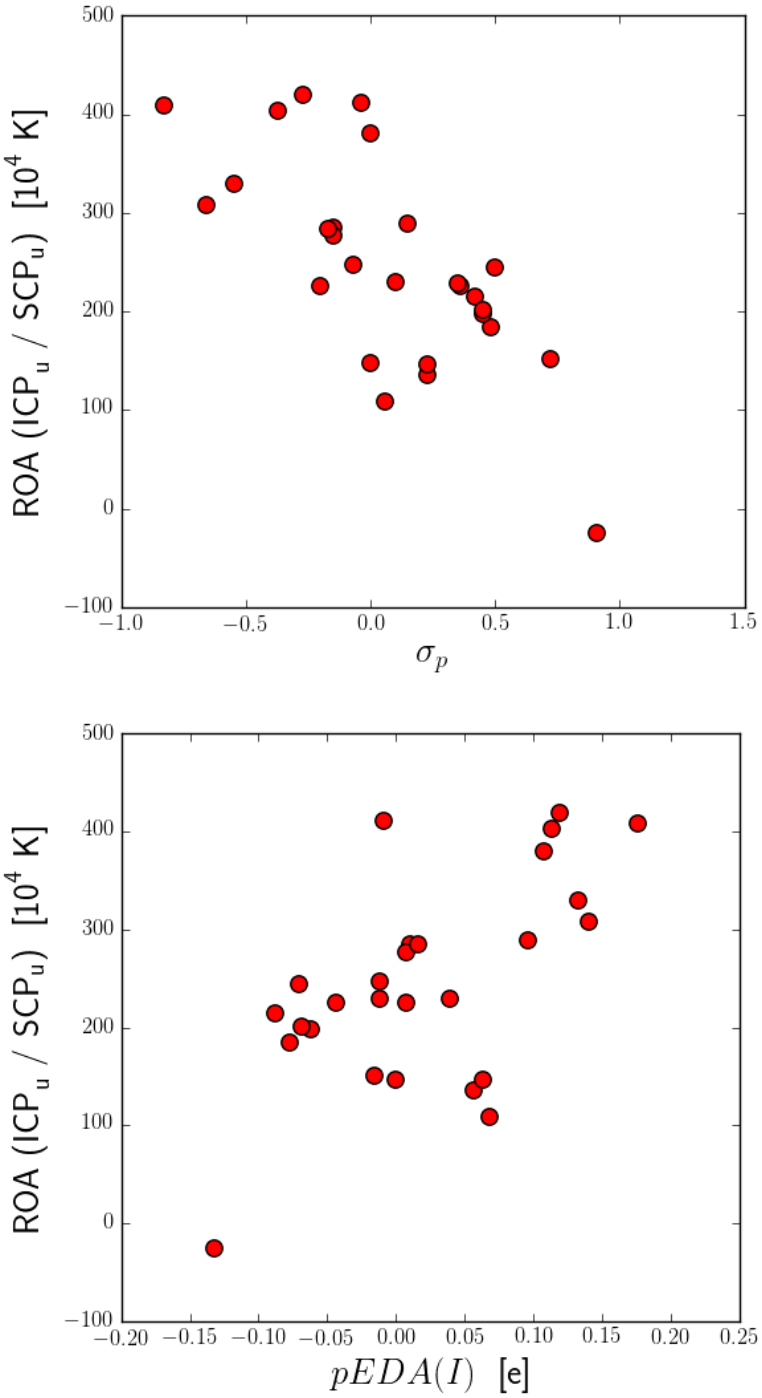

Figure S42. ROA intensities of *ν*(C=C)$_4$ in IIN plotted against σ_p and *pEDA(I)*.

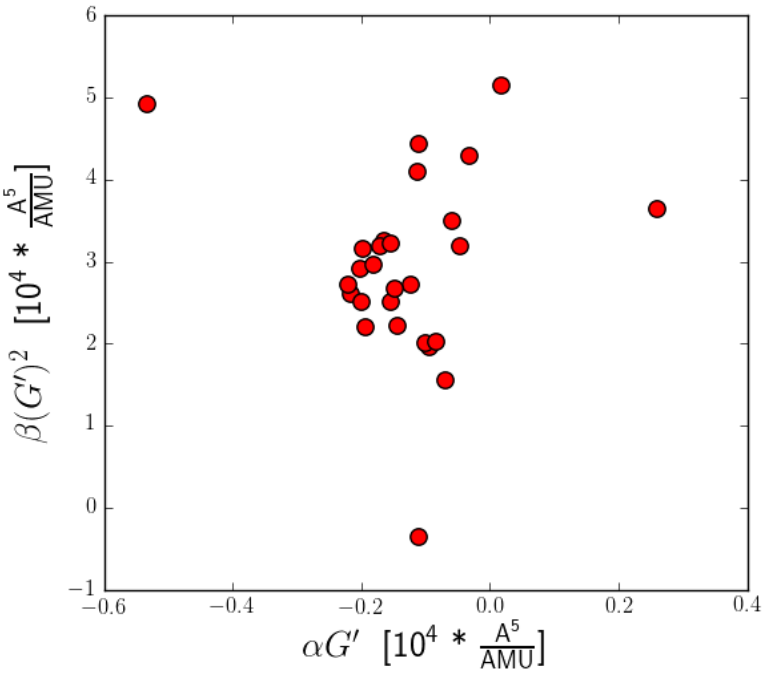

Figure S43. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of *v*(C=C)$_4$ in IIN.

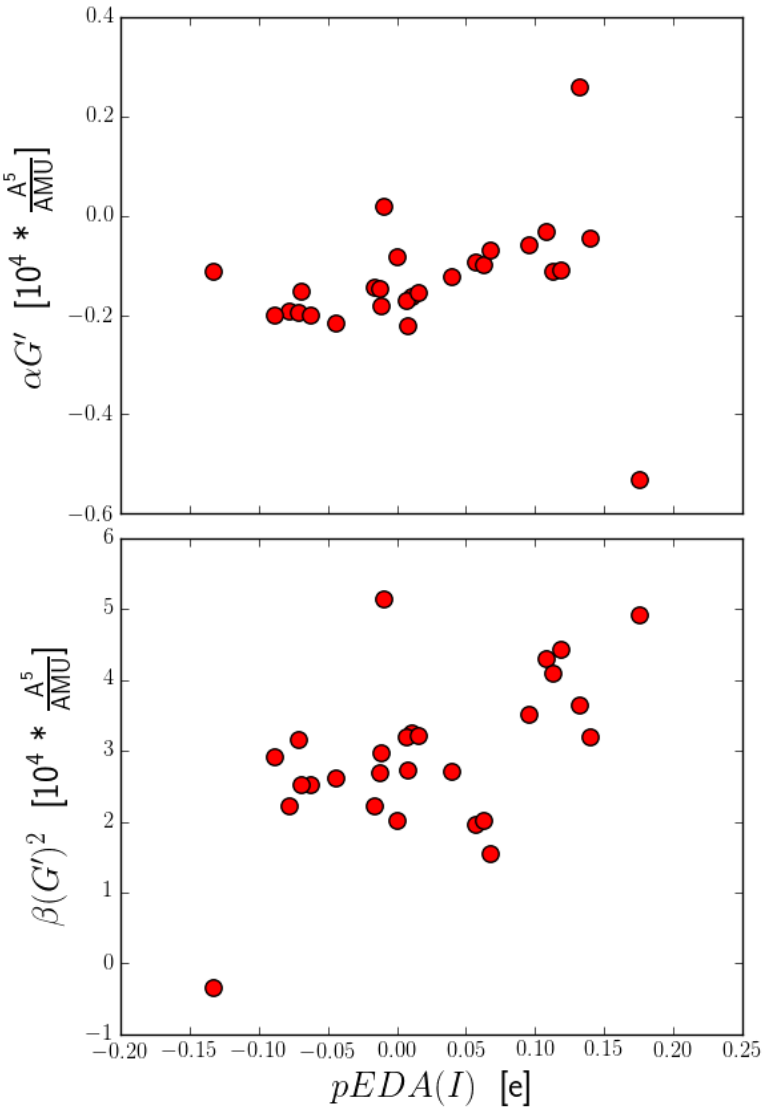

Figure S44. $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_4$ in IIN plotted against *pEDA(I)*.

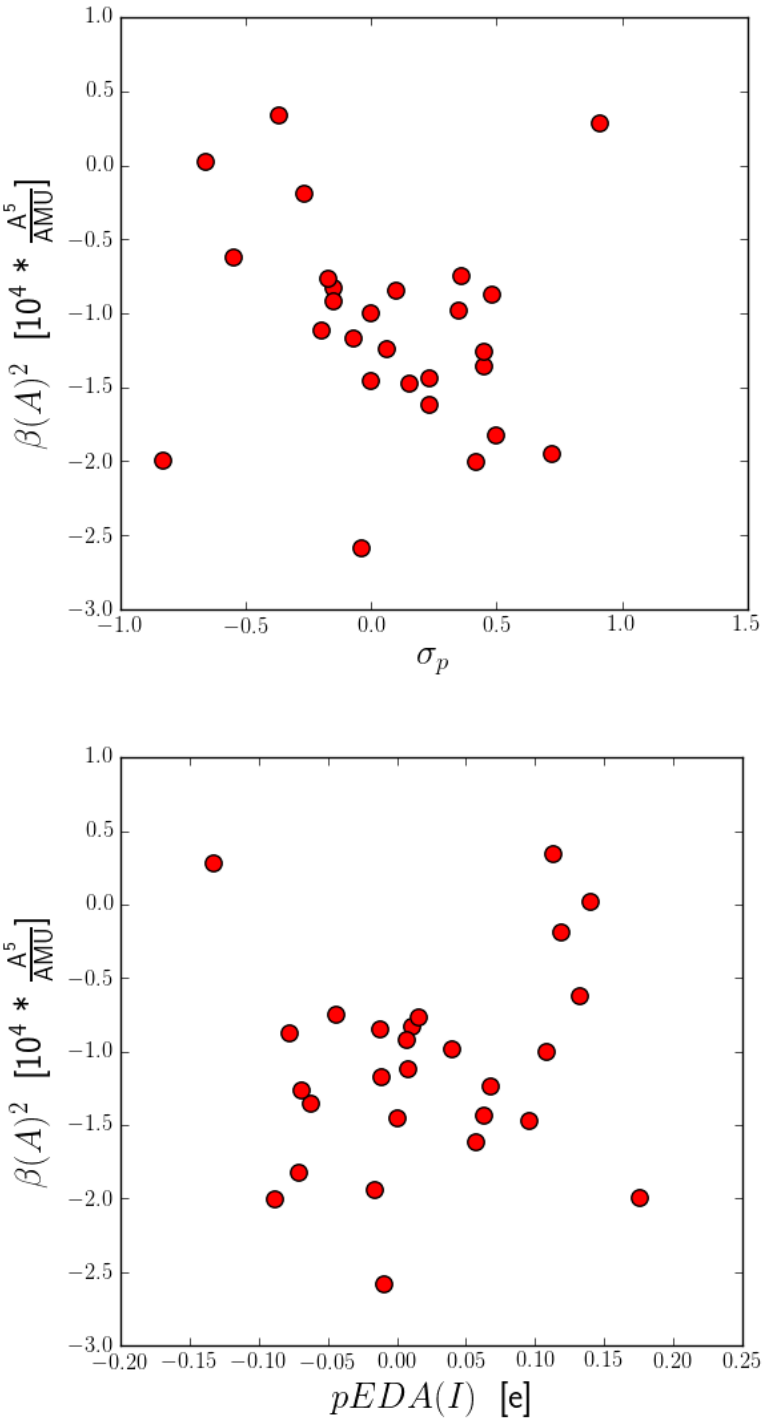

Figure S45. $\beta(A)^2$ invariant of *ν*(C=C)$_4$ in IIN plotted against σ_p and *pEDA(I)*.

$\nu(C{=}C)_5$ in IIN

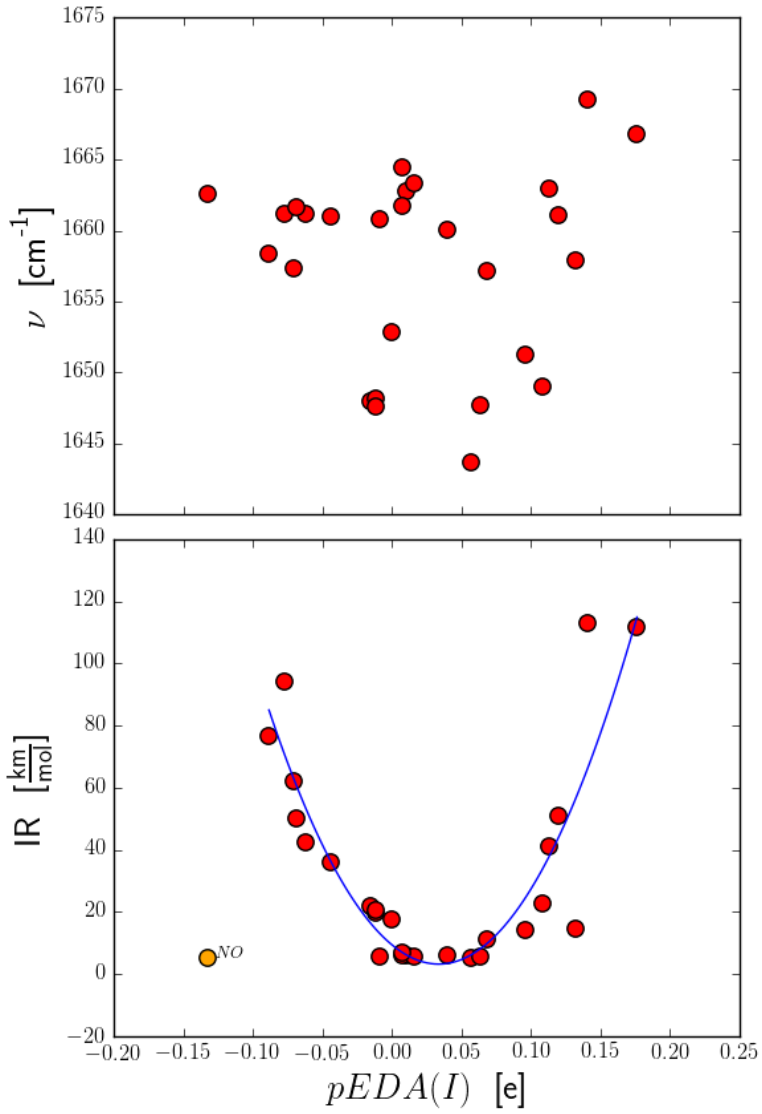

Figure S46. Frequencies and IR intensities of $\nu(C{=}C)_5$ in IIN plotted against *pEDA(I)*.

IR = 5486.46 (± 561.02) $pEDA(I)^2$ - 371.26 (± 57.44) *pEDA(I)* + 9.46 (± 3.97), *n* = 26, *r* = 0.90.

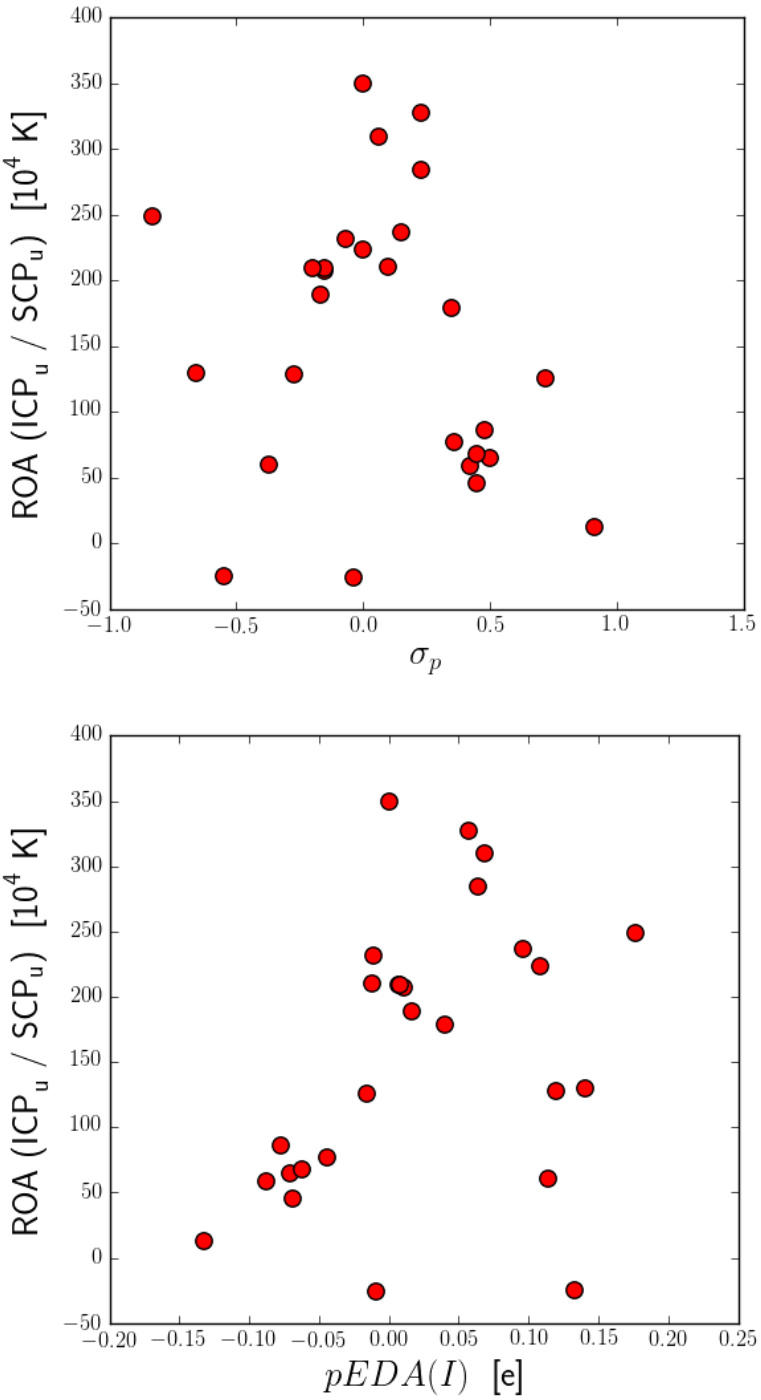

Figure S47. ROA intensities of *ν*(C=C)$_5$ in IIN plotted against σ_p and *pEDA(I)*.

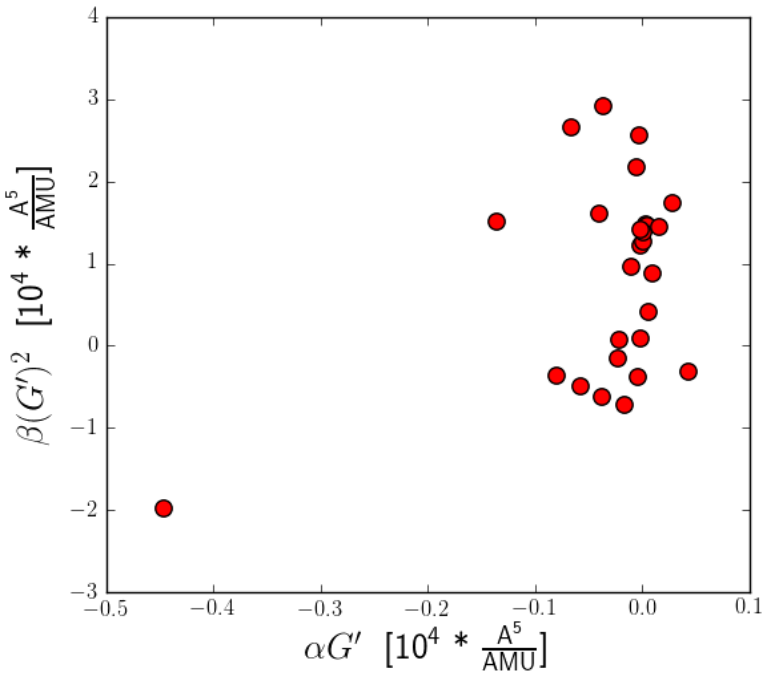

Figure S48. Relationship between $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_5$ in IIN.

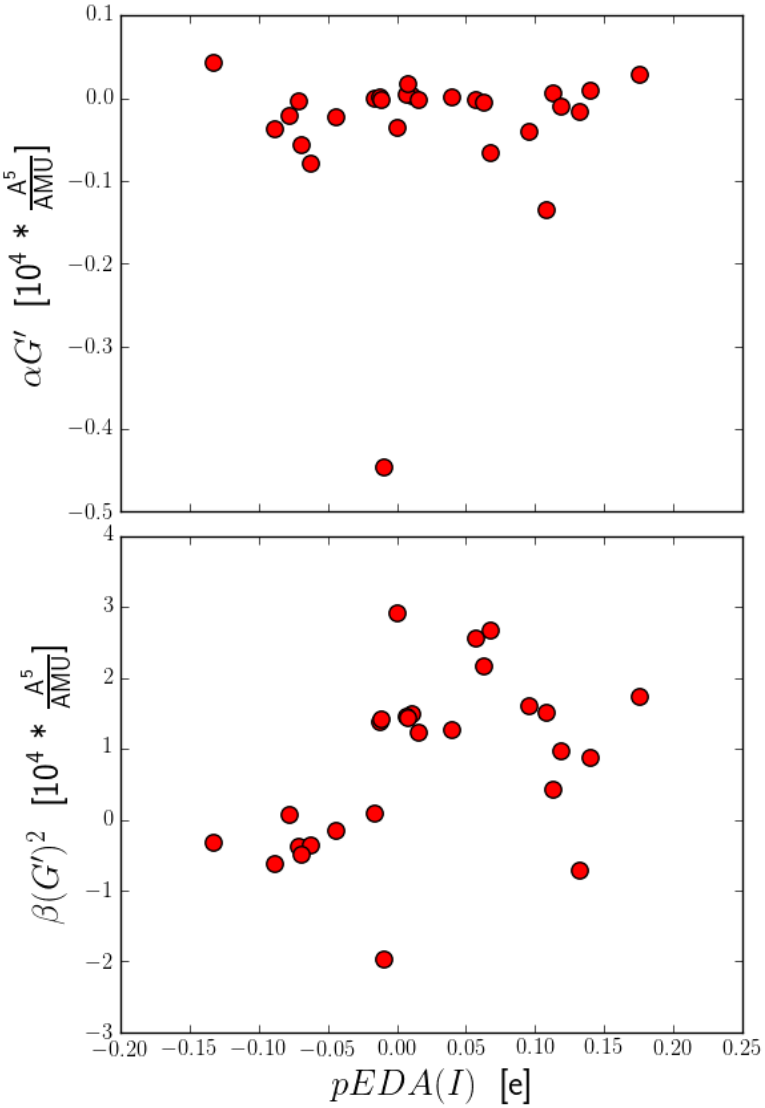

Figure S49. $\alpha G'$ and $\beta(G')^2$ invariants of ν(C=C)$_5$ in IIN plotted against *pEDA(I)*.

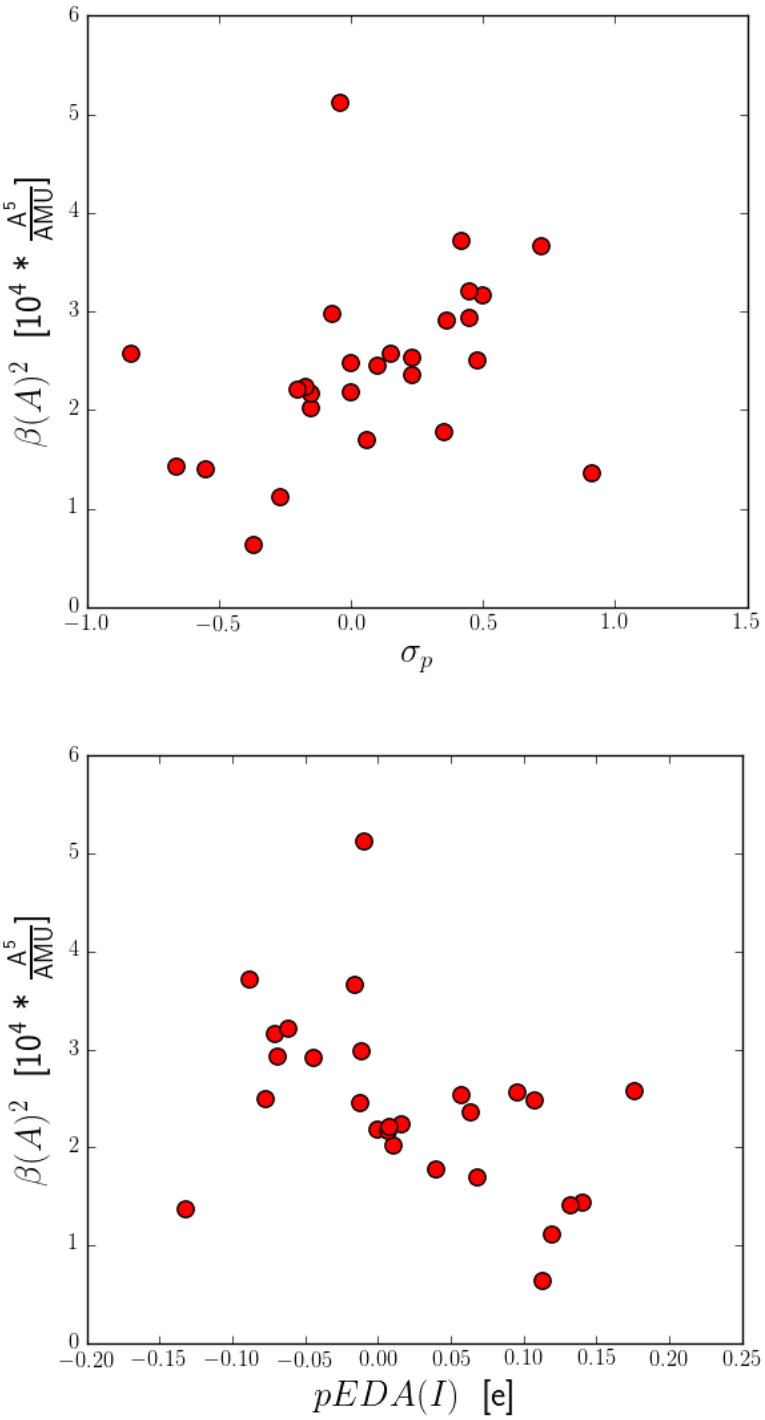

Figure S50. $\beta(A)^2$ invariant of ν(C=C)$_5$ in IIN plotted against σ_p and *pEDA(I)*.

Gaussian 09 input headings

Geometry optimization and harmonic frequencies

```
# opt=tight b3lyp/aug-cc-pvdz freq
```

ROA spectra

```
# freq=roa b3lyp/aug-cc-pvdz integral=ultrafine

[coordinates]

532.0 nm
```

Full Gaussian 09 citation

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Method dependence test

In order to test the dependence of the results on the theoretical level, we recalculated six INDs and IINs (substituents: BF_2, Cl, H, Me, NH_2, OH) with 55 other combinations of functionals and basis sets, namely:

a) functionals: BLYP, B3LYP, CAM-B3LYP, M06-2X
b) dispersion correction GD3 or no correction
c) basis sets: 6-31G*, 6-311++G**, 6-311++G(2d,2p), cc-pvDZ, aug-cc-pvDZ, cc-pvTZ, aug-cc-pvTZ.

The molecules were first optimized to minima and then ROA spectra were calculated. In total, this step included **1568** calculations: **7** molecules (6 substituents, OH – 2 conformers) * **2** model systems * **56** methods * (1 optimization + 1 ROA calculation)

All the chemistries are enumerated below:

1. BLYP/6-31G*
2. BLYP/6-311++G**
3. BLYP/6-311++G(2d,2p)
4. BLYP/cc-pvDZ
5. BLYP/aug-cc-pvDZ
6. BLYP/cc-pvTZ
7. BLYP/aug-cc-pvTZ
8. BLYP/6-31G* GD3
9. BLYP/6-311++G** GD3
10. BLYP/6-311++G(2d,2p) GD3
11. BLYP/cc-pvDZ GD3
12. BLYP/aug-cc-pvDZ GD3
13. BLYP/cc-pvTZ GD3
14. BLYP/aug-cc-pvTZ GD3
15. B3LYP/6-31G*
16. B3LYP/6-311++G**
17. B3LYP/6-311++G(2d,2p)
18. B3LYP/cc-pvDZ
19. B3LYP/aug-cc-pvDZ
20. B3LYP/cc-pvTZ
21. B3LYP/aug-cc-pvTZ
22. B3LYP/6-31G* GD3
23. B3LYP/6-311++G** GD3
24. B3LYP/6-311++G(2d,2p) GD3
25. B3LYP/cc-pvDZ GD3
26. B3LYP/aug-cc-pvDZ GD3
27. B3LYP/cc-pvTZ GD3
28. B3LYP/aug-cc-pvTZ GD3
29. CAM-B3LYP/6-31G*
30. CAM-B3LYP/6-311++G**
31. CAM-B3LYP/6-311++G(2d,2p)
32. CAM-B3LYP/cc-pvDZ
33. CAM-B3LYP/aug-cc-pvDZ
34. CAM-B3LYP/cc-pvTZ
35. CAM-B3LYP/aug-cc-pvTZ
36. CAM-B3LYP/6-31G* GD3
37. CAM-B3LYP/6-311++G** GD3
38. CAM-B3LYP/6-311++G(2d,2p) GD3
39. CAM-B3LYP/cc-pvDZ GD3
40. CAM-B3LYP/aug-cc-pvDZ GD3
41. CAM-B3LYP/cc-pvTZ GD3
42. CAM-B3LYP/aug-cc-pvTZ GD3
43. M06-2X/6-31G*
44. M06-2X/6-311++G**
45. M06-2X/6-311++G(2d,2p)
46. M06-2X/cc-pvDZ
47. M06-2X/aug-cc-pvDZ
48. M06-2X/cc-pvTZ
49. M06-2X/aug-cc-pvTZ
50. M06-2X/6-31G* GD3
51. M06-2X/6-311++G** GD3
52. M06-2X/6-311++G(2d,2p) GD3
53. M06-2X/cc-pvDZ GD3
54. M06-2X/aug-cc-pvDZ GD3
55. M06-2X/cc-pvTZ GD3
56. M06-2X/aug-cc-pvTZ GD3

Table S13 Method dependence of spectral parameters of ν(C*H) mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.98	0.99	1.00	1.00	0.62
BLYP/6-311++G**	1.00	1.00	1.00	1.00	0.91
BLYP/6-311++G(2d,2p)	1.00	1.00	1.00	1.00	0.94
BLYP/cc-pvDZ	0.99	1.00	1.00	1.00	0.51
BLYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	0.95
BLYP/cc-pvTZ	1.00	1.00	1.00	1.00	0.82
BLYP/aug-cc-pvTZ	1.00	1.00	1.00	1.00	0.98
BLYP/6-31G* GD3	0.99	0.99	0.99	1.00	0.64
BLYP/6-311++G** GD3	1.00	1.00	1.00	1.00	0.90
BLYP/6-311++G(2d,2p) GD3	1.00	1.00	1.00	1.00	0.93
BLYP/cc-pvDZ GD3	0.99	1.00	1.00	1.00	0.52
BLYP/aug-cc-pvDZ GD3	0.99	1.00	1.00	1.00	0.94
BLYP/cc-pvTZ GD3	1.00	1.00	1.00	1.00	0.79
BLYP/aug-cc-pvTZ GD3	1.00	1.00	1.00	1.00	0.98
B3LYP/6-31G*	0.99	0.99	0.99	1.00	0.74
B3LYP/6-311++G**	1.00	1.00	1.00	1.00	0.99
B3LYP/6-311++G(2d,2p)	0.99	1.00	1.00	1.00	1.00
B3LYP/cc-pvDZ	1.00	1.00	1.00	1.00	0.93
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	1.00	1.00	1.00	1.00	0.99
B3LYP/aug-cc-pvTZ	1.00	1.00	1.00	1.00	1.00
B3LYP/6-31G* GD3	0.99	0.99	0.99	0.99	0.72
B3LYP/6-311++G** GD3	0.99	1.00	1.00	1.00	0.99
B3LYP/6-311++G(2d,2p) GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvDZ GD3	0.99	1.00	1.00	1.00	0.93
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	1.00	1.00	1.00	1.00	0.99
B3LYP/aug-cc-pvTZ GD3	1.00	1.00	1.00	1.00	1.00
CAM-B3LYP/6-31G*	0.99	0.99	0.99	0.99	0.97
CAM-B3LYP/6-311++G**	1.00	0.99	1.00	0.99	1.00
CAM-B3LYP/6-311++G(2d,2p)	1.00	1.00	1.00	1.00	0.99
CAM-B3LYP/cc-pvDZ	0.99	0.99	0.99	0.99	0.99
CAM-B3LYP/aug-cc-pvDZ	0.99	0.99	1.00	0.99	0.99
CAM-B3LYP/cc-pvTZ	1.00	0.99	0.99	0.99	0.99
CAM-B3LYP/aug-cc-pvTZ	1.00	0.99	1.00	1.00	0.98
CAM-B3LYP/6-31G* GD3	0.99	0.99	0.98	0.99	0.97
CAM-B3LYP/6-311++G** GD3	0.99	0.99	1.00	0.99	1.00
CAM-B3LYP/6-311++G(2d,2p) GD3	0.99	1.00	1.00	1.00	0.99
CAM-B3LYP/cc-pvDZ GD3	0.99	0.99	0.99	0.99	0.99

CAM-B3LYP/aug-cc-pvDZ GD3	0.99	0.97	0.99	0.98	0.98
CAM-B3LYP/cc-pvTZ GD3	1.00	0.99	0.99	0.99	0.99
CAM-B3LYP/aug-cc-pvTZ GD3	1.00	0.99	1.00	0.99	0.98
M06-2X/6-31G*	0.96	0.98	0.99	0.98	0.97
M06-2X/6-311++G**	0.79	0.99	1.00	0.99	1.00
M06-2X/6-311++G(2d,2p)	0.74	0.99	1.00	0.99	0.99
M06-2X/cc-pvDZ	0.90	0.98	0.99	0.98	0.99
M06-2X/aug-cc-pvDZ	0.80	0.99	1.00	0.99	0.99
M06-2X/cc-pvTZ	0.79	0.99	0.99	0.99	0.98
M06-2X/aug-cc-pvTZ	0.79	0.99	1.00	0.99	0.98
M06-2X/6-31G* GD3	0.96	0.98	0.98	0.98	0.97
M06-2X/6-311++G** GD3	0.80	0.99	1.00	0.99	1.00
M06-2X/6-311++G(2d,2p) GD3	0.74	0.99	1.00	0.99	0.99
M06-2X/cc-pvDZ GD3	0.89	0.98	0.99	0.98	0.99
M06-2X/aug-cc-pvDZ GD3	0.78	0.99	1.00	0.99	0.99
M06-2X/cc-pvTZ GD3	0.80	0.99	0.99	0.99	0.98
M06-2X/aug-cc-pvTZ GD3	0.81	0.99	1.00	0.99	0.98

Table S14 Method dependence of spectral parameters of ν(CN) mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	**frequency**	**ROA1**	***αG'***	***β(G')²***	***β(A)²***
BLYP/6-31G*	0.99	1.00	1.00	1.00	0.91
BLYP/6-311++G**	0.99	0.98	0.99	0.98	0.95
BLYP/6-311++G(2d,2p)	1.00	0.97	0.99	0.98	0.97
BLYP/cc-pvDZ	0.99	0.98	0.99	0.98	0.82
BLYP/aug-cc-pvDZ	0.99	1.00	1.00	1.00	0.94
BLYP/cc-pvTZ	0.99	0.99	1.00	0.99	0.88
BLYP/aug-cc-pvTZ	0.99	0.98	0.99	0.98	0.96
BLYP/6-31G* GD3	1.00	0.99	1.00	0.99	0.91
BLYP/6-311++G** GD3	1.00	0.98	0.99	0.98	0.95
BLYP/6-311++G(2d,2p) GD3	1.00	0.97	0.99	0.98	0.97
BLYP/cc-pvDZ GD3	0.99	0.99	0.99	0.99	0.82
BLYP/aug-cc-pvDZ GD3	0.99	1.00	1.00	1.00	0.93
BLYP/cc-pvTZ GD3	1.00	0.99	1.00	0.99	0.88
BLYP/aug-cc-pvTZ GD3	1.00	0.97	0.99	0.97	0.95
B3LYP/6-31G*	1.00	0.99	1.00	1.00	0.90
B3LYP/6-311++G**	1.00	0.97	1.00	0.98	0.92
B3LYP/6-311++G(2d,2p)	1.00	0.97	0.99	0.98	0.91
B3LYP/cc-pvDZ	1.00	0.98	1.00	0.98	0.81
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	1.00	1.00	1.00	1.00	0.80
B3LYP/aug-cc-pvTZ	1.00	0.95	0.99	0.96	0.99

B3LYP/6-31G* GD3	1.00	0.99	1.00	0.99	0.90
B3LYP/6-311++G** GD3	1.00	0.94	0.99	0.95	0.92
B3LYP/6-311++G(2d,2p) GD3	1.00	0.93	0.99	0.95	0.91
B3LYP/cc-pvDZ GD3	1.00	0.98	1.00	0.98	0.81
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	1.00	0.98	0.99	0.98	0.81
B3LYP/aug-cc-pvTZ GD3	1.00	0.95	0.99	0.95	1.00
CAM-B3LYP/6-31G*	1.00	0.97	0.97	0.98	0.85
CAM-B3LYP/6-311++G**	1.00	0.88	0.99	0.93	0.80
CAM-B3LYP/6-311++G(2d,2p)	1.00	0.79	0.95	0.84	0.84
CAM-B3LYP/cc-pvDZ	0.99	0.95	0.98	0.96	0.66
CAM-B3LYP/aug-cc-pvDZ	1.00	0.97	0.99	0.97	0.98
CAM-B3LYP/cc-pvTZ	1.00	0.92	0.97	0.93	0.64
CAM-B3LYP/aug-cc-pvTZ	1.00	0.85	0.96	0.87	0.97
CAM-B3LYP/6-31G* GD3	0.99	0.96	0.97	0.97	0.85
CAM-B3LYP/6-311++G** GD3	1.00	0.79	0.97	0.85	0.80
CAM-B3LYP/6-311++G(2d,2p) GD3	1.00	0.79	0.96	0.84	0.84
CAM-B3LYP/cc-pvDZ GD3	1.00	0.95	0.98	0.96	0.65
CAM-B3LYP/aug-cc-pvDZ GD3	1.00	0.96	0.99	0.97	0.98
CAM-B3LYP/cc-pvTZ GD3	1.00	0.92	0.97	0.93	0.63
CAM-B3LYP/aug-cc-pvTZ GD3	1.00	0.92	0.98	0.93	0.98
M06-2X/6-31G*	0.99	0.94	0.97	0.95	0.83
M06-2X/6-311++G**	0.99	0.79	0.97	0.85	0.63
M06-2X/6-311++G(2d,2p)	0.99	0.92	0.97	0.95	0.79
M06-2X/cc-pvDZ	0.99	0.96	0.97	0.97	0.61
M06-2X/aug-cc-pvDZ	1.00	0.97	0.99	0.97	0.97
M06-2X/cc-pvTZ	1.00	0.95	0.97	0.96	0.62
M06-2X/aug-cc-pvTZ	1.00	0.99	0.97	0.99	0.99
M06-2X/6-31G* GD3	0.99	0.98	0.97	0.99	0.82
M06-2X/6-311++G** GD3	1.00	0.76	0.92	0.82	0.63
M06-2X/6-311++G(2d,2p) GD3	0.99	0.92	0.97	0.95	0.79
M06-2X/cc-pvDZ GD3	0.99	0.96	0.97	0.97	0.61
M06-2X/aug-cc-pvDZ GD3	1.00	0.97	0.99	0.97	0.97
M06-2X/cc-pvTZ GD3	1.00	0.95	0.97	0.96	0.62
M06-2X/aug-cc-pvTZ GD3	1.00	0.99	0.97	0.99	0.99

Table S15 Method dependence of spectral parameters of ν_s(HC=CH) mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.99	0.83	0.92	0.71	0.96
BLYP/6-311++G**	0.99	0.83	0.85	0.89	0.75
BLYP/6-311++G(2d,2p)	0.98	0.87	0.89	0.92	0.76
BLYP/cc-pvDZ	0.99	0.96	0.85	0.93	0.94
BLYP/aug-cc-pvDZ	1.00	0.81	0.98	0.83	0.85
BLYP/cc-pvTZ	0.97	0.80	0.90	0.84	0.75
BLYP/aug-cc-pvTZ	0.96	0.79	0.95	0.82	0.82
BLYP/6-31G* GD3	0.98	0.83	0.91	0.75	0.96
BLYP/6-311++G** GD3	1.00	0.83	0.85	0.91	0.72
BLYP/6-311++G(2d,2p) GD3	1.00	0.88	0.89	0.94	0.77
BLYP/cc-pvDZ GD3	0.99	0.96	0.86	0.94	0.94
BLYP/aug-cc-pvDZ GD3	0.99	0.82	0.97	0.87	0.78
BLYP/cc-pvTZ GD3	0.98	0.81	0.89	0.85	0.74
BLYP/aug-cc-pvTZ GD3	0.98	0.80	0.95	0.84	0.78
B3LYP/6-31G*	0.99	0.94	0.90	0.82	0.96
B3LYP/6-311++G**	0.97	0.97	0.85	0.93	0.98
B3LYP/6-311++G(2d,2p)	0.97	0.98	0.82	0.97	0.97
B3LYP/cc-pvDZ	1.00	0.95	0.79	0.90	0.99
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	1.00	0.94	0.89	0.89	0.95
B3LYP/aug-cc-pvTZ	1.00	0.93	0.91	0.90	0.97
B3LYP/6-31G* GD3	0.99	0.94	0.90	0.83	0.96
B3LYP/6-311++G** GD3	1.00	0.97	0.80	0.95	0.97
B3LYP/6-311++G(2d,2p) GD3	1.00	0.96	0.82	0.93	0.96
B3LYP/cc-pvDZ GD3	1.00	0.94	0.80	0.91	0.99
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	0.99	0.89	0.85	0.82	0.93
B3LYP/aug-cc-pvTZ GD3	1.00	0.93	0.92	0.91	0.96
CAM-B3LYP/6-31G*	0.99	0.91	0.83	0.80	0.91
CAM-B3LYP/6-311++G**	1.00	0.93	0.72	0.88	0.94
CAM-B3LYP/6-311++G(2d,2p)	1.00	0.91	0.64	0.83	0.96
CAM-B3LYP/cc-pvDZ	1.00	0.80	0.61	0.72	0.93
CAM-B3LYP/aug-cc-pvDZ	1.00	0.94	0.92	0.93	0.96
CAM-B3LYP/cc-pvTZ	0.99	0.83	0.80	0.74	0.96
CAM-B3LYP/aug-cc-pvTZ	1.00	0.90	0.78	0.82	0.97
CAM-B3LYP/6-31G* GD3	0.99	0.90	0.84	0.79	0.90
CAM-B3LYP/6-311++G** GD3	1.00	0.91	0.69	0.86	0.92
CAM-B3LYP/6-311++G(2d,2p) GD3	1.00	0.91	0.67	0.83	0.95
CAM-B3LYP/cc-pvDZ GD3	1.00	0.81	0.64	0.72	0.93

CAM-B3LYP/aug-cc-pvDZ GD3	1.00	0.94	0.95	0.92	0.96
CAM-B3LYP/cc-pvTZ GD3	0.99	0.83	0.81	0.74	0.97
CAM-B3LYP/aug-cc-pvTZ GD3	1.00	0.92	0.86	0.86	0.97
M06-2X/6-31G*	0.87	0.93	0.71	0.89	0.93
M06-2X/6-311++G**	0.76	0.29	0.96	0.36	0.95
M06-2X/6-311++G(2d,2p)	0.74	0.63	0.92	0.34	0.96
M06-2X/cc-pvDZ	0.82	0.83	0.59	0.75	0.94
M06-2X/aug-cc-pvDZ	0.77	0.95	0.89	0.91	0.99
M06-2X/cc-pvTZ	0.79	0.68	0.82	0.51	0.97
M06-2X/aug-cc-pvTZ	0.83	0.92	0.83	0.86	0.96
M06-2X/6-31G* GD3	0.83	0.89	0.83	0.78	0.94
M06-2X/6-311++G** GD3	0.74	0.33	0.85	0.45	0.94
M06-2X/6-311++G(2d,2p) GD3	0.73	0.63	0.92	0.33	0.96
M06-2X/cc-pvDZ GD3	0.83	0.83	0.59	0.75	0.94
M06-2X/aug-cc-pvDZ GD3	0.77	0.95	0.89	0.91	0.99
M06-2X/cc-pvTZ GD3	0.79	0.68	0.81	0.51	0.97
M06-2X/aug-cc-pvTZ GD3	0.83	0.92	0.83	0.87	0.97

Table S16 Method dependence of spectral parameters of $\nu(C=C)_1$ mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.93	0.77	0.94	0.83	0.71
BLYP/6-311++G**	0.97	0.99	0.98	0.99	0.89
BLYP/6-311++G(2d,2p)	0.96	1.00	0.97	1.00	0.83
BLYP/cc-pvDZ	0.97	0.75	0.98	0.89	0.69
BLYP/aug-cc-pvDZ	0.99	1.00	1.00	1.00	1.00
BLYP/cc-pvTZ	0.95	0.91	0.97	0.93	0.79
BLYP/aug-cc-pvTZ	0.96	1.00	0.96	0.99	0.83
BLYP/6-31G* GD3	0.96	0.77	0.95	0.83	0.73
BLYP/6-311++G** GD3	0.98	0.99	0.98	0.99	0.90
BLYP/6-311++G(2d,2p) GD3	0.98	1.00	0.97	0.99	0.86
BLYP/cc-pvDZ GD3	0.99	0.68	0.99	0.85	0.73
BLYP/aug-cc-pvDZ GD3	0.98	0.99	1.00	0.99	1.00
BLYP/cc-pvTZ GD3	0.97	0.91	0.98	0.92	0.80
BLYP/aug-cc-pvTZ GD3	0.98	1.00	0.96	1.00	0.85
B3LYP/6-31G*	0.92	0.84	0.92	0.89	0.76
B3LYP/6-311++G**	0.98	0.99	0.97	0.99	0.90
B3LYP/6-311++G(2d,2p)	0.97	1.00	0.97	0.99	0.87
B3LYP/cc-pvDZ	0.95	0.86	0.98	0.87	0.65
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.95	0.96	0.98	0.98	0.84
B3LYP/aug-cc-pvTZ	0.95	0.99	0.94	1.00	0.78

B3LYP/6-31G* GD3	0.94	0.83	0.92	0.88	0.78
B3LYP/6-311++G** GD3	0.98	0.99	0.95	0.99	0.82
B3LYP/6-311++G(2d,2p) GD3	0.97	1.00	0.96	0.99	0.80
B3LYP/cc-pvDZ GD3	0.98	0.88	0.98	0.95	0.72
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	0.96	0.96	0.95	0.97	0.77
B3LYP/aug-cc-pvTZ GD3	0.97	1.00	0.95	1.00	0.80
CAM-B3LYP/6-31G*	0.89	0.88	0.90	0.93	0.72
CAM-B3LYP/6-311++G**	0.97	0.97	0.97	0.99	0.88
CAM-B3LYP/6-311++G(2d,2p)	0.93	0.99	0.94	1.00	0.74
CAM-B3LYP/cc-pvDZ	0.60	0.36	0.95	0.35	0.46
CAM-B3LYP/aug-cc-pvDZ	0.89	0.64	0.95	0.59	0.42
CAM-B3LYP/cc-pvTZ	0.91	0.75	0.91	0.83	0.70
CAM-B3LYP/aug-cc-pvTZ	0.93	0.96	0.92	0.99	0.76
CAM-B3LYP/6-31G* GD3	0.91	0.88	0.90	0.94	0.75
CAM-B3LYP/6-311++G** GD3	0.96	0.97	0.93	0.99	0.78
CAM-B3LYP/6-311++G(2d,2p) GD3	0.95	0.99	0.94	0.99	0.75
CAM-B3LYP/cc-pvDZ GD3	0.66	0.39	0.95	0.36	0.46
CAM-B3LYP/aug-cc-pvDZ GD3	0.95	0.66	0.97	0.64	0.57
CAM-B3LYP/cc-pvTZ GD3	0.94	0.86	0.93	0.92	0.73
CAM-B3LYP/aug-cc-pvTZ GD3	0.97	0.99	0.97	1.00	0.86
M06-2X/6-31G*	0.93	0.83	0.97	0.83	0.71
M06-2X/6-311++G**	0.97	0.93	0.99	0.94	0.99
M06-2X/6-311++G(2d,2p)	0.97	0.98	1.00	0.98	0.98
M06-2X/cc-pvDZ	0.48	0.40	0.92	0.39	0.55
M06-2X/aug-cc-pvDZ	0.64	0.68	0.89	0.60	0.34
M06-2X/cc-pvTZ	0.91	0.42	0.93	0.53	0.64
M06-2X/aug-cc-pvTZ	0.96	0.89	0.99	0.89	0.92
M06-2X/6-31G* GD3	0.89	0.84	0.91	0.91	0.71
M06-2X/6-311++G** GD3	0.94	0.88	0.92	0.94	0.78
M06-2X/6-311++G(2d,2p) GD3	0.97	0.98	1.00	0.99	0.98
M06-2X/cc-pvDZ GD3	0.48	0.40	0.92	0.39	0.55
M06-2X/aug-cc-pvDZ GD3	0.64	0.67	0.89	0.60	0.34
M06-2X/cc-pvTZ GD3	0.91	0.43	0.93	0.54	0.64
M06-2X/aug-cc-pvTZ GD3	0.96	0.89	0.99	0.89	0.92

Table S17 Method dependence of spectral parameters of $\nu(C{=}C)_2$ mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.97	0.80	0.09	0.80	0.70
BLYP/6-311++G**	0.99	0.99	0.73	0.98	0.82
BLYP/6-311++G(2d,2p)	0.99	0.99	0.82	0.99	0.89
BLYP/cc-pvDZ	0.99	0.98	0.41	0.98	0.90
BLYP/aug-cc-pvDZ	1.00	0.98	0.91	0.98	0.95
BLYP/cc-pvTZ	0.98	0.96	0.32	0.95	0.90
BLYP/aug-cc-pvTZ	0.99	0.98	0.70	0.98	0.89
BLYP/6-31G* GD3	0.97	0.97	0.15	0.95	0.84
BLYP/6-311++G** GD3	0.99	0.98	0.74	0.98	0.71
BLYP/6-311++G(2d,2p) GD3	0.99	0.99	0.81	0.98	0.81
BLYP/cc-pvDZ GD3	0.98	0.98	0.38	0.97	0.92
BLYP/aug-cc-pvDZ GD3	1.00	0.98	0.88	0.97	0.86
BLYP/cc-pvTZ GD3	0.98	0.99	0.39	0.98	0.85
BLYP/aug-cc-pvTZ GD3	0.99	0.99	0.75	0.99	0.83
B3LYP/6-31G*	0.97	0.87	0.04	0.86	0.66
B3LYP/6-311++G**	1.00	1.00	0.83	1.00	0.89
B3LYP/6-311++G(2d,2p)	1.00	1.00	0.91	0.99	0.92
B3LYP/cc-pvDZ	0.95	0.62	0.26	0.61	0.95
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.99	0.96	0.41	0.95	0.94
B3LYP/aug-cc-pvTZ	0.99	0.98	0.79	0.98	0.90
B3LYP/6-31G* GD3	0.97	0.92	0.12	0.91	0.76
B3LYP/6-311++G** GD3	1.00	1.00	0.79	1.00	0.84
B3LYP/6-311++G(2d,2p) GD3	0.99	1.00	0.88	1.00	0.88
B3LYP/cc-pvDZ GD3	0.99	0.90	0.52	0.81	0.95
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	0.99	1.00	0.98
B3LYP/cc-pvTZ GD3	0.99	0.98	0.40	0.97	0.89
B3LYP/aug-cc-pvTZ GD3	0.99	0.99	0.82	0.99	0.90
CAM-B3LYP/6-31G*	0.97	0.87	0.21	0.91	0.93
CAM-B3LYP/6-311++G**	0.94	0.78	0.96	0.79	0.78
CAM-B3LYP/6-311++G(2d,2p)	0.99	0.81	0.92	0.83	0.76
CAM-B3LYP/cc-pvDZ	0.66	0.45	0.61	0.46	0.96
CAM-B3LYP/aug-cc-pvDZ	0.72	0.66	0.77	0.63	0.98
CAM-B3LYP/cc-pvTZ	0.83	0.71	0.54	0.72	0.83
CAM-B3LYP/aug-cc-pvTZ	0.88	0.80	0.89	0.82	0.74
CAM-B3LYP/6-31G* GD3	0.96	0.86	0.22	0.88	0.90
CAM-B3LYP/6-311++G** GD3	0.98	0.78	0.89	0.79	0.73
CAM-B3LYP/6-311++G(2d,2p) GD3	1.00	0.95	0.92	0.93	0.92
CAM-B3LYP/cc-pvDZ GD3	0.65	0.43	0.63	0.44	0.96

CAM-B3LYP/aug-cc-pvDZ GD3	0.74	0.66	0.89	0.64	0.98
CAM-B3LYP/cc-pvTZ GD3	0.88	0.74	0.60	0.75	0.82
CAM-B3LYP/aug-cc-pvTZ GD3	0.93	0.81	0.91	0.83	0.83
M06-2X/6-31G*	0.98	0.91	0.73	0.89	0.96
M06-2X/6-311++G**	0.90	0.71	0.93	0.73	0.90
M06-2X/6-311++G(2d,2p)	0.96	0.76	0.91	0.79	0.87
M06-2X/cc-pvDZ	0.67	0.46	0.43	0.48	0.97
M06-2X/aug-cc-pvDZ	0.71	0.66	0.51	0.62	0.97
M06-2X/cc-pvTZ	0.76	0.60	0.71	0.61	0.89
M06-2X/aug-cc-pvTZ	0.79	0.72	0.94	0.73	0.98
M06-2X/6-31G* GD3	0.98	0.95	0.53	0.95	0.95
M06-2X/6-311++G** GD3	0.91	0.72	0.91	0.74	0.77
M06-2X/6-311++G(2d,2p) GD3	0.96	0.76	0.91	0.79	0.87
M06-2X/cc-pvDZ GD3	0.67	0.46	0.43	0.48	0.97
M06-2X/aug-cc-pvDZ GD3	0.71	0.66	0.51	0.62	0.97
M06-2X/cc-pvTZ GD3	0.76	0.60	0.71	0.61	0.89
M06-2X/aug-cc-pvTZ GD3	0.79	0.72	0.94	0.73	0.98

Table S18 Method dependence of spectral parameters of $\nu(C{=}C)_3$ mode in IND

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	**frequency**	**ROA1**	***αG'***	***β(G')²***	***β(A)²***
BLYP/6-31G*	0.88	0.39	0.90	0.45	0.76
BLYP/6-311++G**	0.90	0.39	0.97	0.46	0.72
BLYP/6-311++G(2d,2p)	0.89	0.47	0.98	0.53	0.70
BLYP/cc-pvDZ	0.97	0.59	0.85	0.59	0.95
BLYP/aug-cc-pvDZ	0.98	0.55	0.99	0.62	0.66
BLYP/cc-pvTZ	0.91	0.42	0.94	0.47	0.69
BLYP/aug-cc-pvTZ	0.90	0.42	0.96	0.49	0.68
BLYP/6-31G* GD3	0.88	0.46	0.90	0.51	0.70
BLYP/6-311++G** GD3	0.90	0.32	0.95	0.41	0.72
BLYP/6-311++G(2d,2p) GD3	0.89	0.39	0.97	0.47	0.70
BLYP/cc-pvDZ GD3	0.98	0.52	0.82	0.51	0.95
BLYP/aug-cc-pvDZ GD3	0.97	0.45	0.98	0.54	0.63
BLYP/cc-pvTZ GD3	0.91	0.38	0.93	0.44	0.70
BLYP/aug-cc-pvTZ GD3	0.90	0.35	0.97	0.44	0.69
B3LYP/6-31G*	0.93	0.33	0.93	0.35	0.71
B3LYP/6-311++G**	0.98	0.38	0.98	0.49	0.76
B3LYP/6-311++G(2d,2p)	0.97	0.33	0.99	0.47	0.63
B3LYP/cc-pvDZ	0.98	0.92	0.86	0.87	0.96
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.99	0.54	0.96	0.54	0.79

B3LYP/aug-cc-pvTZ	0.98	0.48	0.99	0.60	0.70
B3LYP/6-31G* GD3	0.93	0.35	0.93	0.37	0.68
B3LYP/6-311++G** GD3	0.98	0.29	0.97	0.40	0.69
B3LYP/6-311++G(2d,2p) GD3	0.96	0.29	0.99	0.42	0.62
B3LYP/cc-pvDZ GD3	0.98	0.88	0.85	0.83	0.95
B3LYP/aug-cc-pvDZ GD3	1.00	0.99	1.00	0.99	1.00
B3LYP/cc-pvTZ GD3	0.98	0.40	0.94	0.42	0.68
B3LYP/aug-cc-pvTZ GD3	0.98	0.33	0.98	0.46	0.65
CAM-B3LYP/6-31G*	0.98	0.65	0.92	0.50	0.54
CAM-B3LYP/6-311++G**	0.99	0.93	0.98	0.97	0.67
CAM-B3LYP/6-311++G(2d,2p)	0.99	0.91	0.98	0.92	0.62
CAM-B3LYP/cc-pvDZ	0.97	0.99	0.79	0.91	0.89
CAM-B3LYP/aug-cc-pvDZ	0.99	0.92	0.99	0.96	0.88
CAM-B3LYP/cc-pvTZ	0.99	0.79	0.91	0.84	0.54
CAM-B3LYP/aug-cc-pvTZ	0.99	0.83	0.98	0.86	0.62
CAM-B3LYP/6-31G* GD3	0.98	0.66	0.92	0.50	0.54
CAM-B3LYP/6-311++G** GD3	0.99	0.94	0.97	0.97	0.59
CAM-B3LYP/6-311++G(2d,2p) GD3	0.99	0.93	0.98	0.95	0.63
CAM-B3LYP/cc-pvDZ GD3	0.98	0.99	0.80	0.91	0.89
CAM-B3LYP/aug-cc-pvDZ GD3	0.99	0.94	0.99	0.97	0.88
CAM-B3LYP/cc-pvTZ GD3	0.99	0.82	0.89	0.87	0.54
CAM-B3LYP/aug-cc-pvTZ GD3	0.99	0.87	0.97	0.91	0.71
M06-2X/6-31G*	0.97	0.68	0.99	0.50	0.82
M06-2X/6-311++G**	0.98	0.98	0.99	0.95	0.87
M06-2X/6-311++G(2d,2p)	0.98	0.98	0.99	0.97	0.92
M06-2X/cc-pvDZ	0.96	0.95	0.97	0.83	0.89
M06-2X/aug-cc-pvDZ	0.99	0.98	0.98	0.99	0.90
M06-2X/cc-pvTZ	0.97	0.88	0.95	0.85	0.57
M06-2X/aug-cc-pvTZ	0.98	0.94	0.97	0.94	0.91
M06-2X/6-31G* GD3	0.96	0.64	0.97	0.49	0.54
M06-2X/6-311++G** GD3	0.97	0.97	0.98	0.94	0.62
M06-2X/6-311++G(2d,2p) GD3	0.98	0.98	0.99	0.97	0.92
M06-2X/cc-pvDZ GD3	0.96	0.95	0.97	0.83	0.89
M06-2X/aug-cc-pvDZ GD3	0.99	0.98	0.98	0.99	0.90
M06-2X/cc-pvTZ GD3	0.97	0.88	0.96	0.85	0.57
M06-2X/aug-cc-pvTZ GD3	0.98	0.94	0.97	0.94	0.91

Table S19 Method dependence of spectral parameters of v(C*H) mode in IIN

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	1.00	0.99	0.99	0.99	0.35
BLYP/6-311++G**	0.99	0.99	0.99	0.99	0.54
BLYP/6-311++G(2d,2p)	0.97	0.99	1.00	1.00	0.89
BLYP/cc-pvDZ	1.00	0.99	0.99	0.99	0.28
BLYP/aug-cc-pvDZ	1.00	0.99	0.99	0.99	0.60
BLYP/cc-pvTZ	1.00	1.00	1.00	1.00	0.32
BLYP/aug-cc-pvTZ	1.00	0.99	1.00	0.99	0.89
BLYP/6-31G* GD3	1.00	0.99	0.99	0.99	0.33
BLYP/6-311++G** GD3	0.97	0.99	0.99	0.99	0.57
BLYP/6-311++G(2d,2p) GD3	0.95	1.00	1.00	1.00	0.90
BLYP/cc-pvDZ GD3	0.99	0.99	0.99	0.99	0.25
BLYP/aug-cc-pvDZ GD3	0.99	0.99	0.99	0.99	0.62
BLYP/cc-pvTZ GD3	0.99	1.00	1.00	1.00	0.36
BLYP/aug-cc-pvTZ GD3	0.99	0.99	0.99	1.00	0.90
B3LYP/6-31G*	0.99	0.99	0.98	0.99	0.47
B3LYP/6-311++G**	0.98	1.00	1.00	1.00	0.98
B3LYP/6-311++G(2d,2p)	0.98	1.00	1.00	1.00	0.99
B3LYP/cc-pvDZ	0.55	0.99	0.99	0.99	0.65
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.99	1.00	1.00	1.00	0.99
B3LYP/aug-cc-pvTZ	0.98	1.00	1.00	1.00	0.99
B3LYP/6-31G* GD3	0.99	0.98	0.98	0.98	0.49
B3LYP/6-311++G** GD3	0.98	1.00	1.00	1.00	0.98
B3LYP/6-311++G(2d,2p) GD3	0.97	1.00	1.00	1.00	0.99
B3LYP/cc-pvDZ GD3	1.00	0.99	0.99	0.99	0.73
B3LYP/aug-cc-pvDZ GD3	0.97	1.00	1.00	1.00	0.99
B3LYP/cc-pvTZ GD3	0.97	1.00	1.00	1.00	0.99
B3LYP/aug-cc-pvTZ GD3	0.97	1.00	1.00	1.00	0.99
CAM-B3LYP/6-31G*	0.92	0.95	0.96	0.96	0.93
CAM-B3LYP/6-311++G**	0.95	0.98	1.00	0.98	0.98
CAM-B3LYP/6-311++G(2d,2p)	0.95	0.97	1.00	0.98	0.98
CAM-B3LYP/cc-pvDZ	0.95	0.94	0.96	0.95	0.98
CAM-B3LYP/aug-cc-pvDZ	0.94	0.97	1.00	0.98	0.98
CAM-B3LYP/cc-pvTZ	0.97	0.96	0.99	0.97	0.98
CAM-B3LYP/aug-cc-pvTZ	0.96	0.97	1.00	0.98	0.97
CAM-B3LYP/6-31G* GD3	0.93	0.95	0.97	0.95	0.92
CAM-B3LYP/6-311++G** GD3	0.93	0.97	1.00	0.97	0.97
CAM-B3LYP/6-311++G(2d,2p) GD3	0.95	0.95	1.00	0.97	0.97
CAM-B3LYP/cc-pvDZ GD3	0.95	0.94	0.96	0.95	0.99

CAM-B3LYP/aug-cc-pvDZ GD3	0.93	0.95	1.00	0.96	0.97
CAM-B3LYP/cc-pvTZ GD3	0.98	0.96	0.99	0.97	0.98
CAM-B3LYP/aug-cc-pvTZ GD3	0.97	0.96	1.00	0.98	0.97
M06-2X/6-31G*	0.77	0.94	0.96	0.94	0.97
M06-2X/6-311++G**	0.86	0.94	1.00	0.96	0.97
M06-2X/6-311++G(2d,2p)	0.80	0.94	0.99	0.96	0.97
M06-2X/cc-pvDZ	0.51	0.85	0.95	0.86	0.99
M06-2X/aug-cc-pvDZ	0.55	0.45	0.94	0.45	0.36
M06-2X/cc-pvTZ	0.83	0.91	0.98	0.93	0.96
M06-2X/aug-cc-pvTZ	0.67	0.93	0.99	0.96	0.96
M06-2X/6-31G* GD3	0.76	0.94	0.96	0.94	0.98
M06-2X/6-311++G** GD3	0.85	0.94	1.00	0.96	0.97
M06-2X/6-311++G(2d,2p) GD3	0.74	0.94	0.99	0.96	0.97
M06-2X/cc-pvDZ GD3	0.55	0.85	0.95	0.86	0.99
M06-2X/aug-cc-pvDZ GD3	0.57	0.45	0.99	0.46	0.37
M06-2X/cc-pvTZ GD3	0.79	0.91	0.98	0.93	0.96
M06-2X/aug-cc-pvTZ GD3	0.69	0.93	0.99	0.96	0.96

Table S20 Method dependence of spectral parameters of v(CN) mode in IIN

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	**frequency**	**ROA1**	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.99	0.98	0.98	0.98	0.64
BLYP/6-311++G**	1.00	0.98	0.98	0.99	0.95
BLYP/6-311++G(2d,2p)	1.00	0.99	0.98	0.99	0.92
BLYP/cc-pvDZ	0.99	0.98	0.96	0.98	0.55
BLYP/aug-cc-pvDZ	0.99	0.98	0.98	0.99	0.88
BLYP/cc-pvTZ	0.99	0.98	0.98	0.99	0.72
BLYP/aug-cc-pvTZ	0.99	0.98	0.98	0.98	0.88
BLYP/6-31G* GD3	0.99	0.97	0.98	0.98	0.62
BLYP/6-311++G** GD3	0.98	0.99	0.98	0.99	0.96
BLYP/6-311++G(2d,2p) GD3	1.00	0.99	0.98	0.99	0.92
BLYP/cc-pvDZ GD3	0.99	0.97	0.97	0.98	0.51
BLYP/aug-cc-pvDZ GD3	1.00	0.98	0.98	0.99	0.89
BLYP/cc-pvTZ GD3	0.99	0.98	0.98	0.99	0.72
BLYP/aug-cc-pvTZ GD3	0.99	0.98	0.98	0.99	0.88
B3LYP/6-31G*	0.99	0.99	1.00	0.99	0.89
B3LYP/6-311++G**	1.00	1.00	1.00	1.00	0.95
B3LYP/6-311++G(2d,2p)	0.99	1.00	1.00	1.00	0.97
B3LYP/cc-pvDZ	0.99	0.99	1.00	0.99	0.74
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.98	1.00	1.00	1.00	0.86
B3LYP/aug-cc-pvTZ	1.00	1.00	1.00	1.00	0.99

B3LYP/6-31G* GD3	0.99	0.98	1.00	0.98	0.87
B3LYP/6-311++G** GD3	1.00	1.00	1.00	1.00	0.95
B3LYP/6-311++G(2d,2p) GD3	1.00	1.00	1.00	1.00	0.98
B3LYP/cc-pvDZ GD3	0.99	0.99	1.00	0.99	0.68
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	0.97	1.00	1.00	1.00	0.84
B3LYP/aug-cc-pvTZ GD3	0.98	1.00	1.00	1.00	0.99
CAM-B3LYP/6-31G*	0.99	0.91	0.93	0.92	0.55
CAM-B3LYP/6-311++G**	0.99	0.92	0.98	0.95	0.79
CAM-B3LYP/6-311++G(2d,2p)	0.99	0.93	0.98	0.96	0.87
CAM-B3LYP/cc-pvDZ	1.00	0.94	0.93	0.95	0.11
CAM-B3LYP/aug-cc-pvDZ	1.00	0.96	0.98	0.97	0.91
CAM-B3LYP/cc-pvTZ	0.99	0.96	0.97	0.97	0.29
CAM-B3LYP/aug-cc-pvTZ	1.00	0.97	0.98	0.98	0.89
CAM-B3LYP/6-31G* GD3	0.99	0.90	0.94	0.91	0.52
CAM-B3LYP/6-311++G** GD3	1.00	0.90	0.98	0.94	0.82
CAM-B3LYP/6-311++G(2d,2p) GD3	1.00	0.92	0.98	0.95	0.87
CAM-B3LYP/cc-pvDZ GD3	0.99	0.94	0.93	0.94	0.07
CAM-B3LYP/aug-cc-pvDZ GD3	1.00	0.95	0.98	0.97	0.91
CAM-B3LYP/cc-pvTZ GD3	0.99	0.96	0.97	0.97	0.26
CAM-B3LYP/aug-cc-pvTZ GD3	1.00	0.96	0.98	0.97	0.89
M06-2X/6-31G*	0.98	0.85	0.88	0.87	0.56
M06-2X/6-311++G**	0.99	0.80	0.95	0.88	0.74
M06-2X/6-311++G(2d,2p)	1.00	0.94	0.91	0.97	0.82
M06-2X/cc-pvDZ	0.99	0.90	0.90	0.91	0.22
M06-2X/aug-cc-pvDZ	1.00	0.95	0.90	0.96	0.87
M06-2X/cc-pvTZ	1.00	0.91	0.94	0.93	0.35
M06-2X/aug-cc-pvTZ	1.00	0.95	0.93	0.96	0.85
M06-2X/6-31G* GD3	0.99	0.84	0.88	0.87	0.56
M06-2X/6-311++G** GD3	0.99	0.80	0.95	0.88	0.74
M06-2X/6-311++G(2d,2p) GD3	1.00	0.94	0.90	0.97	0.82
M06-2X/cc-pvDZ GD3	0.99	0.90	0.90	0.91	0.22
M06-2X/aug-cc-pvDZ GD3	1.00	0.95	0.90	0.96	0.85
M06-2X/cc-pvTZ GD3	1.00	0.90	0.94	0.93	0.36
M06-2X/aug-cc-pvTZ GD3	1.00	0.95	0.93	0.96	0.85

Table S21 Method dependence of spectral parameters of v(NH) mode in IIN

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	**frequency**	**ROA1**	***αG'***	***β(G')²***	***β(A)²***
BLYP/6-31G*	0.77	0.91	0.64	0.90	0.88
BLYP/6-311++G**	0.97	0.96	0.81	0.96	0.90

BLYP/6-311++G(2d,2p)	0.68	0.93	0.73	0.93	0.84
BLYP/cc-pvDZ	0.68	0.93	0.79	0.91	0.95
BLYP/aug-cc-pvDZ	0.99	0.97	0.90	0.96	0.96
BLYP/cc-pvTZ	0.98	0.94	0.83	0.93	0.94
BLYP/aug-cc-pvTZ	0.94	0.97	0.84	0.96	0.95
BLYP/6-31G* GD3	0.87	0.90	0.63	0.89	0.85
BLYP/6-311++G** GD3	0.70	0.95	0.79	0.95	0.88
BLYP/6-311++G(2d,2p) GD3	0.08	0.93	0.72	0.92	0.80
BLYP/cc-pvDZ GD3	0.10	0.92	0.76	0.91	0.92
BLYP/aug-cc-pvDZ GD3	1.00	0.96	0.87	0.96	0.94
BLYP/cc-pvTZ GD3	0.82	0.94	0.80	0.93	0.92
BLYP/aug-cc-pvTZ GD3	0.93	0.96	0.81	0.96	0.93
B3LYP/6-31G*	0.93	0.97	0.78	0.97	0.98
B3LYP/6-311++G**	0.97	0.96	0.92	0.92	0.98
B3LYP/6-311++G(2d,2p)	0.90	0.98	0.91	0.96	0.97
B3LYP/cc-pvDZ	0.97	0.99	0.82	0.99	0.95
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	1.00	0.98	0.94	0.98	0.98
B3LYP/aug-cc-pvTZ	0.96	1.00	0.96	0.99	0.98
B3LYP/6-31G* GD3	0.81	0.96	0.80	0.97	0.89
B3LYP/6-311++G** GD3	0.99	0.97	0.86	0.94	0.96
B3LYP/6-311++G(2d,2p) GD3	0.98	0.99	0.72	0.98	0.92
B3LYP/cc-pvDZ GD3	0.99	0.97	0.86	0.96	0.99
B3LYP/aug-cc-pvDZ GD3	1.00	0.99	0.84	0.94	0.95
B3LYP/cc-pvTZ GD3	1.00	0.98	0.81	0.97	0.94
B3LYP/aug-cc-pvTZ GD3	1.00	0.99	0.83	0.97	0.95
CAM-B3LYP/6-31G*	0.96	0.98	0.91	0.98	0.98
CAM-B3LYP/6-311++G**	0.99	0.93	0.94	0.85	0.98
CAM-B3LYP/6-311++G(2d,2p)	1.00	0.99	0.93	0.98	0.96
CAM-B3LYP/cc-pvDZ	1.00	0.97	0.77	0.95	0.99
CAM-B3LYP/aug-cc-pvDZ	1.00	0.99	0.98	0.99	0.97
CAM-B3LYP/cc-pvTZ	0.98	0.98	0.91	0.97	0.98
CAM-B3LYP/aug-cc-pvTZ	1.00	0.99	0.95	0.99	0.96
CAM-B3LYP/6-31G* GD3	0.96	0.99	0.69	0.98	0.91
CAM-B3LYP/6-311++G** GD3	0.99	0.91	0.87	0.83	0.98
CAM-B3LYP/6-311++G(2d,2p) GD3	0.99	0.99	0.92	0.99	0.97
CAM-B3LYP/cc-pvDZ GD3	1.00	0.97	0.80	0.95	0.99
CAM-B3LYP/aug-cc-pvDZ GD3	1.00	0.99	0.98	0.99	0.97
CAM-B3LYP/cc-pvTZ GD3	0.99	0.98	0.89	0.97	0.98
CAM-B3LYP/aug-cc-pvTZ GD3	0.99	0.99	0.95	0.99	0.96
M06-2X/6-31G*	0.95	0.97	0.98	0.95	0.93
M06-2X/6-311++G**	1.00	0.80	0.90	0.67	0.98
M06-2X/6-311++G(2d,2p)	1.00	0.85	0.93	0.74	0.95
M06-2X/cc-pvDZ	0.77	0.98	0.94	0.97	0.97
M06-2X/aug-cc-pvDZ	0.86	0.99	0.84	1.00	0.95

M06-2X/cc-pvTZ	0.97	0.98	0.96	0.98	0.96
M06-2X/aug-cc-pvTZ	0.96	0.98	0.91	0.96	0.96
M06-2X/6-31G* GD3	0.94	0.97	0.96	0.96	0.91
M06-2X/6-311++G** GD3	0.99	0.81	0.90	0.68	0.98
M06-2X/6-311++G(2d,2p) GD3	1.00	0.85	0.93	0.74	0.95
M06-2X/cc-pvDZ GD3	0.77	0.98	0.94	0.97	0.97
M06-2X/aug-cc-pvDZ GD3	0.86	0.99	0.83	1.00	0.95
M06-2X/cc-pvTZ GD3	0.95	0.99	0.96	0.98	0.96
M06-2X/aug-cc-pvTZ GD3	0.95	0.98	0.91	0.96	0.96

Table S22 Method dependence of spectral parameters of $\nu(C=C)_4$ mode in IIN

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 but > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.96	0.95	0.94	0.91	0.91
BLYP/6-311++G**	0.99	0.96	0.98	0.95	0.99
BLYP/6-311++G(2d,2p)	0.99	0.94	1.00	0.92	0.99
BLYP/cc-pvDZ	0.97	0.97	0.94	0.97	0.99
BLYP/aug-cc-pvDZ	1.00	0.97	0.99	0.96	0.98
BLYP/cc-pvTZ	0.98	0.99	0.95	0.98	0.99
BLYP/aug-cc-pvTZ	0.98	0.97	0.99	0.95	0.98
BLYP/6-31G* GD3	0.95	0.92	0.94	0.86	0.92
BLYP/6-311++G** GD3	0.98	0.95	0.98	0.92	0.99
BLYP/6-311++G(2d,2p) GD3	0.99	0.91	0.99	0.85	0.99
BLYP/cc-pvDZ GD3	0.96	0.95	0.95	0.93	0.99
BLYP/aug-cc-pvDZ GD3	1.00	0.96	0.99	0.95	0.99
BLYP/cc-pvTZ GD3	0.97	0.98	0.95	0.97	0.99
BLYP/aug-cc-pvTZ GD3	0.98	0.96	0.98	0.94	0.99
B3LYP/6-31G*	0.98	0.89	0.92	0.88	0.86
B3LYP/6-311++G**	0.99	0.99	0.98	0.99	0.99
B3LYP/6-311++G(2d,2p)	1.00	1.00	0.99	0.99	1.00
B3LYP/cc-pvDZ	0.98	0.40	0.86	0.32	0.97
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.99	0.99	0.94	0.99	0.99
B3LYP/aug-cc-pvTZ	1.00	1.00	0.99	1.00	1.00
B3LYP/6-31G* GD3	0.97	0.89	0.81	0.86	0.87
B3LYP/6-311++G** GD3	0.99	0.98	0.98	0.97	0.99
B3LYP/6-311++G(2d,2p) GD3	0.99	0.99	0.99	0.98	0.99
B3LYP/cc-pvDZ GD3	0.98	0.82	0.95	0.73	0.99
B3LYP/aug-cc-pvDZ GD3	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ GD3	0.99	0.98	0.94	0.97	0.99
B3LYP/aug-cc-pvTZ GD3	0.99	1.00	0.98	0.99	0.99
CAM-B3LYP/6-31G*	0.98	0.79	0.91	0.76	0.85

CAM-B3LYP/6-311++G**	0.98	0.46	0.87	0.31	0.98
CAM-B3LYP/6-311++G(2d,2p)	1.00	0.95	0.99	0.88	0.98
CAM-B3LYP/cc-pvDZ	0.51	0.49	0.84	0.43	0.92
CAM-B3LYP/aug-cc-pvDZ	0.65	0.46	0.82	0.31	0.99
CAM-B3LYP/cc-pvTZ	0.95	0.44	0.86	0.33	0.99
CAM-B3LYP/aug-cc-pvTZ	0.98	0.46	0.84	0.30	0.98
CAM-B3LYP/6-31G* GD3	0.98	0.77	0.91	0.73	0.85
CAM-B3LYP/6-311++G** GD3	0.99	0.42	0.89	0.22	0.90
CAM-B3LYP/6-311++G(2d,2p) GD3	1.00	0.95	0.98	0.91	0.98
CAM-B3LYP/cc-pvDZ GD3	0.52	0.46	0.83	0.39	0.92
CAM-B3LYP/aug-cc-pvDZ GD3	0.67	0.42	0.82	0.28	0.98
CAM-B3LYP/cc-pvTZ GD3	0.97	0.40	0.86	0.28	0.98
CAM-B3LYP/aug-cc-pvTZ GD3	0.99	0.40	0.85	0.22	0.94
M06-2X/6-31G*	0.98	0.63	0.87	0.50	0.97
M06-2X/6-311++G**	0.93	0.39	0.93	0.23	0.97
M06-2X/6-311++G(2d,2p)	0.99	0.35	0.87	0.18	0.97
M06-2X/cc-pvDZ	0.45	0.34	0.80	0.27	0.84
M06-2X/aug-cc-pvDZ	0.54	0.38	0.83	0.22	0.96
M06-2X/cc-pvTZ	0.81	0.34	0.84	0.22	0.98
M06-2X/aug-cc-pvTZ	0.86	0.35	0.82	0.19	0.97
M06-2X/6-31G* GD3	0.98	0.62	0.88	0.49	0.97
M06-2X/6-311++G** GD3	0.93	0.39	0.93	0.23	0.97
M06-2X/6-311++G(2d,2p) GD3	0.99	0.34	0.87	0.17	0.97
M06-2X/cc-pvDZ GD3	0.45	0.34	0.80	0.27	0.84
M06-2X/aug-cc-pvDZ GD3	0.54	0.38	0.83	0.22	0.96
M06-2X/cc-pvTZ GD3	0.81	0.34	0.84	0.22	0.98
M06-2X/aug-cc-pvTZ GD3	0.86	0.35	0.82	0.19	0.97

Table S23 Method dependence of spectral parameters of $\nu(C{=}C)_5$ mode in IIN

The table presents correlation coefficients of a given property calculated at a theoretical level with the results at the B3LYP/aug-cc-pvDZ level used in the main body of the paper. Yellow are values < 0.90 ut > 0.80, orange > 0.70 and red below 0.70.

method	frequency	ROA1	$\alpha G'$	$\beta(G')^2$	$\beta(A)^2$
BLYP/6-31G*	0.83	0.99	0.73	0.95	0.86
BLYP/6-311++G**	0.86	0.93	0.90	0.96	0.86
BLYP/6-311++G(2d,2p)	0.83	0.95	0.93	0.98	0.85
BLYP/cc-pvDZ	0.96	0.98	0.73	0.98	0.96
BLYP/aug-cc-pvDZ	0.98	0.99	0.95	0.98	0.99
BLYP/cc-pvTZ	0.89	0.95	0.98	0.97	0.87
BLYP/aug-cc-pvTZ	0.86	0.92	0.87	0.95	0.85

BLYP/6-31G* GD3	0.83	0.94	0.78	0.86	0.86
BLYP/6-311++G** GD3	0.85	0.94	0.87	0.97	0.86
BLYP/6-311++G(2d,2p) GD3	0.82	0.96	0.90	0.96	0.85
BLYP/cc-pvDZ GD3	0.97	0.97	0.81	0.96	0.93
BLYP/aug-cc-pvDZ GD3	0.97	0.98	0.96	0.98	0.99
BLYP/cc-pvTZ GD3	0.88	0.96	0.97	0.98	0.87
BLYP/aug-cc-pvTZ GD3	0.85	0.93	0.86	0.96	0.85
B3LYP/6-31G*	0.92	0.90	0.63	0.91	0.94
B3LYP/6-311++G**	0.97	0.95	0.94	0.95	0.98
B3LYP/6-311++G(2d,2p)	0.96	0.87	0.97	0.86	0.97
B3LYP/cc-pvDZ	0.97	0.99	0.77	0.99	0.98
B3LYP/aug-cc-pvDZ	1.00	1.00	1.00	1.00	1.00
B3LYP/cc-pvTZ	0.98	0.97	0.96	0.97	0.99
B3LYP/aug-cc-pvTZ	0.98	0.94	0.92	0.93	1.00
B3LYP/6-31G* GD3	0.91	0.90	0.61	0.84	0.72
B3LYP/6-311++G** GD3	0.97	0.93	0.95	0.94	0.98
B3LYP/6-311++G(2d,2p) GD3	0.94	0.89	0.98	0.89	0.96
B3LYP/cc-pvDZ GD3	0.98	0.98	0.71	0.98	0.99
B3LYP/aug-cc-pvDZ GD3	1.00	0.99	1.00	0.99	1.00
B3LYP/cc-pvTZ GD3	0.98	0.95	0.96	0.94	1.00
B3LYP/aug-cc-pvTZ GD3	0.98	0.91	0.92	0.89	1.00
CAM-B3LYP/6-31G*	0.99	0.92	0.27	0.93	0.95
CAM-B3LYP/6-311++G**	1.00	0.97	0.95	0.94	0.95
CAM-B3LYP/6-311++G(2d,2p)	1.00	0.98	0.84	0.95	0.98
CAM-B3LYP/cc-pvDZ	0.98	0.98	0.67	0.96	0.94
CAM-B3LYP/aug-cc-pvDZ	0.99	0.99	0.92	0.97	0.98
CAM-B3LYP/cc-pvTZ	0.99	0.98	0.74	0.95	0.95
CAM-B3LYP/aug-cc-pvTZ	0.99	0.98	0.96	0.96	0.97
CAM-B3LYP/6-31G* GD3	0.99	0.93	0.28	0.95	0.95
CAM-B3LYP/6-311++G** GD3	1.00	0.97	0.95	0.94	0.96
CAM-B3LYP/6-311++G(2d,2p) GD3	0.99	0.97	0.85	0.95	0.98
CAM-B3LYP/cc-pvDZ GD3	0.98	0.98	0.68	0.96	0.95
CAM-B3LYP/aug-cc-pvDZ GD3	0.98	0.99	0.93	0.97	0.98
CAM-B3LYP/cc-pvTZ GD3	0.99	0.97	0.77	0.95	0.96
CAM-B3LYP/aug-cc-pvTZ GD3	1.00	0.97	0.95	0.96	0.98
M06-2X/6-31G*	0.96	0.88	0.09	0.85	0.96
M06-2X/6-311++G**	0.97	0.96	0.09	0.96	0.99
M06-2X/6-311++G(2d,2p)	0.97	0.95	0.14	0.95	1.00
M06-2X/cc-pvDZ	0.94	0.98	0.06	0.98	0.98
M06-2X/aug-cc-pvDZ	0.99	0.97	0.74	0.97	0.99
M06-2X/cc-pvTZ	0.97	0.97	0.05	0.97	0.99
M06-2X/aug-cc-pvTZ	0.97	0.96	0.65	0.95	0.99
M06-2X/6-31G* GD3	0.96	0.89	0.09	0.86	0.97
M06-2X/6-311++G** GD3	0.97	0.96	0.09	0.96	0.99
M06-2X/6-311++G(2d,2p) GD3	0.97	0.95	0.09	0.95	1.00

M06-2X/cc-pvDZ GD3	0.94	0.98	0.06	0.98	0.98
M06-2X/aug-cc-pvDZ GD3	0.99	0.97	0.74	0.97	0.99
M06-2X/cc-pvTZ GD3	0.97	0.96	0.04	0.96	0.99
M06-2X/aug-cc-pvTZ GD3	0.97	0.95	0.64	0.95	0.99

Table S24 ROA intensity correlations with *pEDA(I)* descriptor in IND

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***ν*(C*H)**	***ν*(CN)**	***ν*$_s$(HC=CH)**	***ν*(C=C)$_1$**	***ν*(C=C)$_2$**	***ν*(C=C)$_3$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, IS THERE A CORRELATION?	**YES**	**YES, BUT BETTER IS WITH S-P**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.98	0.88	0.36	0.87	0.77	0.83
BLYP/6-311++G**	0.95	0.88	0.34	0.84	0.68	0.91
BLYP/6-311++G(2d,2p)	0.96	0.85	0.29	0.80	0.68	0.94
BLYP/cc-pvDZ	0.98	0.96	0.06	0.91	0.57	0.93
BLYP/aug-cc-pvDZ	0.95	0.92	0.33	0.86	0.61	0.93
BLYP/cc-pvTZ	0.97	0.90	0.34	0.79	0.75	0.92
BLYP/aug-cc-pvTZ	0.96	0.85	0.41	0.78	0.75	0.94
BLYP/6-31G* GD3	0.98	0.86	0.35	0.88	0.75	0.93
BLYP/6-311++G** GD3	0.95	0.87	0.32	0.85	0.67	0.91
BLYP/6-311++G(2d,2p) GD3	0.96	0.85	0.26	0.82	0.66	0.92
BLYP/cc-pvDZ GD3	0.98	0.95	0.08	0.94	0.54	0.94
BLYP/aug-cc-pvDZ GD3	0.95	0.92	0.32	0.89	0.59	0.92
BLYP/cc-pvTZ GD3	0.97	0.89	0.32	0.80	0.59	0.90
BLYP/aug-cc-pvTZ GD3	0.96	0.84	0.39	0.79	0.65	0.92
B3LYP/6-31G*	0.98	0.84	0.11	0.82	0.90	0.87
B3LYP/6-311++G**	0.95	0.83	0.18	0.83	0.87	0.89
B3LYP/6-311++G(2d,2p)	0.96	0.81	0.17	0.82	0.87	0.88
B3LYP/cc-pvDZ	0.97	0.94	0.51	0.82	0.91	0.84
B3LYP/aug-cc-pvDZ	0.96	0.90	0.25	0.88	0.87	0.66
B3LYP/cc-pvTZ	0.97	0.87	0.18	0.78	0.86	0.90
B3LYP/aug-cc-pvTZ	0.96	0.77	0.19	0.77	0.88	0.90
B3LYP/6-31G* GD3	0.98	0.82	0.11	0.81	0.89	0.89
B3LYP/6-311++G** GD3	0.96	0.76	0.19	0.80	0.83	0.89
B3LYP/6-311++G(2d,2p) GD3	0.96	0.75	0.13	0.78	0.83	0.88
B3LYP/cc-pvDZ GD3	0.97	0.94	0.52	0.89	0.93	0.86
B3LYP/aug-cc-pvDZ GD3	0.96	0.89	0.23	0.87	0.80	0.73
B3LYP/cc-pvTZ GD3	0.97	0.82	0.16	0.72	0.81	0.86
B3LYP/aug-cc-pvTZ GD3	0.96	0.76	0.18	0.77	0.85	0.89
CAM-B3LYP/6-31G*	0.97	0.77	0.37	0.61	0.90	0.91
CAM-B3LYP/6-311++G**	0.94	0.65	0.49	0.79	0.90	0.55
CAM-B3LYP/6-311++G(2d,2p)	0.96	0.56	0.38	0.71	0.90	0.66

CAM-B3LYP/cc-pvDZ	0.96	0.92	0.73	0.78	0.86	0.46
CAM-B3LYP/aug-cc-pvDZ	0.95	0.82	0.52	0.91	0.87	0.59
CAM-B3LYP/cc-pvTZ	0.97	0.70	0.35	0.69	0.88	0.78
CAM-B3LYP/aug-cc-pvTZ	0.95	0.59	0.37	0.73	0.90	0.72
CAM-B3LYP/6-31G* GD3	0.97	0.75	0.37	0.61	0.88	0.90
CAM-B3LYP/6-311++G** GD3	0.95	0.55	0.44	0.73	0.90	0.51
CAM-B3LYP/6-311++G(2d,2p) GD3	0.95	0.56	0.38	0.71	0.92	0.60
CAM-B3LYP/cc-pvDZ GD3	0.96	0.91	0.73	0.77	0.86	0.54
CAM-B3LYP/aug-cc-pvDZ GD3	0.89	0.80	0.52	0.92	0.87	0.55
CAM-B3LYP/cc-pvTZ GD3	0.96	0.71	0.35	0.64	0.88	0.65
CAM-B3LYP/aug-cc-pvTZ GD3	0.94	0.69	0.42	0.77	0.90	0.65
M06-2X/6-31G*	0.96	0.91	0.52	0.64	0.87	0.97
M06-2X/6-311++G**	0.95	0.54	0.75	0.88	0.92	0.46
M06-2X/6-311++G(2d,2p)	0.95	0.75	0.68	0.86	0.93	0.40
M06-2X/cc-pvDZ	0.96	0.91	0.68	0.78	0.87	0.83
M06-2X/aug-cc-pvDZ	0.94	0.79	0.46	0.91	0.89	0.50
M06-2X/cc-pvTZ	0.96	0.74	0.48	0.81	0.88	0.44
M06-2X/aug-cc-pvTZ	0.94	0.85	0.54	0.90	0.91	0.26
M06-2X/6-31G* GD3	0.97	0.79	0.33	0.67	0.96	0.92
M06-2X/6-311++G** GD3	0.95	0.39	0.70	0.80	0.92	0.33
M06-2X/6-311++G(2d,2p) GD3	0.95	0.75	0.68	0.86	0.93	0.39
M06-2X/cc-pvDZ GD3	0.96	0.91	0.68	0.78	0.87	0.82
M06-2X/aug-cc-pvDZ GD3	0.94	0.79	0.46	0.91	0.89	0.50
M06-2X/cc-pvTZ GD3	0.96	0.74	0.48	0.81	0.88	0.45
M06-2X/aug-cc-pvTZ GD3	0.94	0.85	0.54	0.90	0.91	0.26

Table S25 ROA intensity correlations with σ_p descriptor in IND

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***ν*(C*H)**	***ν*(CN)**	***ν*$_s$(HC=CH)**	***ν*(C=C)$_1$**	***ν*(C=C)$_2$**	***ν*(C=C)$_3$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, IS THERE A CORRELATION?	**YES, BUT BETTER IS WITH pEDA**	**YES**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.95	0.98	0.60	0.97	0.61	0.79
BLYP/6-311++G**	0.97	0.95	0.59	0.86	0.82	0.99
BLYP/6-311++G(2d,2p)	0.96	0.94	0.50	0.82	0.76	1.00
BLYP/cc-pvDZ	0.96	0.96	0.50	0.97	0.77	0.94
BLYP/aug-cc-pvDZ	0.97	0.97	0.65	0.86	0.81	0.98
BLYP/cc-pvTZ	0.96	0.97	0.49	0.89	0.70	0.97

BLYP/aug-cc-pvTZ	0.97	0.95	0.58	0.81	0.69	0.99
BLYP/6-31G* GD3	0.95	0.98	0.57	0.97	0.79	0.98
BLYP/6-311++G** GD3	0.97	0.95	0.56	0.87	0.83	0.99
BLYP/6-311++G(2d,2p) GD3	0.96	0.95	0.46	0.85	0.80	1.00
BLYP/cc-pvDZ GD3	0.96	0.96	0.47	1.00	0.77	0.96
BLYP/aug-cc-pvDZ GD3	0.97	0.97	0.63	0.89	0.80	0.99
BLYP/cc-pvTZ GD3	0.96	0.97	0.45	0.90	0.78	0.99
BLYP/aug-cc-pvTZ GD3	0.97	0.95	0.55	0.80	0.78	1.00
B3LYP/6-31G*	0.95	0.99	0.26	0.92	0.87	0.91
B3LYP/6-311++G**	0.97	0.95	0.38	0.86	0.92	0.99
B3LYP/6-311++G(2d,2p)	0.97	0.97	0.39	0.84	0.89	0.98
B3LYP/cc-pvDZ	0.96	0.97	0.54	0.71	0.95	0.71
B3LYP/aug-cc-pvDZ	0.97	0.99	0.35	0.86	0.93	0.49
B3LYP/cc-pvTZ	0.96	0.99	0.22	0.83	0.87	0.98
B3LYP/aug-cc-pvTZ	0.97	0.93	0.17	0.77	0.85	0.97
B3LYP/6-31G* GD3	0.95	0.99	0.25	0.92	0.91	0.97
B3LYP/6-311++G** GD3	0.97	0.92	0.31	0.83	0.92	0.99
B3LYP/6-311++G(2d,2p) GD3	0.96	0.93	0.34	0.82	0.90	0.99
B3LYP/cc-pvDZ GD3	0.96	0.97	0.54	0.86	0.96	0.76
B3LYP/aug-cc-pvDZ GD3	0.97	0.99	0.33	0.88	0.93	0.48
B3LYP/cc-pvTZ GD3	0.96	0.97	0.13	0.80	0.90	0.98
B3LYP/aug-cc-pvTZ GD3	0.97	0.93	0.17	0.78	0.89	0.98
CAM-B3LYP/6-31G*	0.96	0.99	0.31	0.66	0.92	0.90
CAM-B3LYP/6-311++G**	0.98	0.95	0.48	0.75	0.91	0.72
CAM-B3LYP/6-311++G(2d,2p)	0.97	0.86	0.40	0.72	0.89	0.83
CAM-B3LYP/cc-pvDZ	0.96	0.97	0.72	0.83	0.91	0.39
CAM-B3LYP/aug-cc-pvDZ	0.98	1.00	0.45	0.81	0.92	0.77
CAM-B3LYP/cc-pvTZ	0.96	0.96	0.34	0.48	0.89	0.90
CAM-B3LYP/aug-cc-pvTZ	0.97	0.88	0.30	0.65	0.87	0.90
CAM-B3LYP/6-31G* GD3	0.96	0.98	0.31	0.70	0.94	0.94
CAM-B3LYP/6-311++G** GD3	0.97	0.86	0.42	0.72	0.92	0.62
CAM-B3LYP/6-311++G(2d,2p) GD3	0.97	0.86	0.40	0.74	0.91	0.75
CAM-B3LYP/cc-pvDZ GD3	0.96	0.96	0.72	0.85	0.92	0.44
CAM-B3LYP/aug-cc-pvDZ GD3	0.98	1.00	0.45	0.82	0.93	0.70
CAM-B3LYP/cc-pvTZ GD3	0.97	0.97	0.35	0.49	0.91	0.83
CAM-B3LYP/aug-cc-pvTZ GD3	0.98	0.95	0.36	0.75	0.89	0.85
M06-2X/6-31G*	0.96	0.96	0.51	0.58	0.70	0.87
M06-2X/6-311++G**	0.97	0.83	0.76	0.83	0.94	0.43
M06-2X/6-311++G(2d,2p)	0.97	0.96	0.51	0.84	0.91	0.46
M06-2X/cc-pvDZ	0.96	0.97	0.68	0.82	0.92	0.65
M06-2X/aug-cc-pvDZ	0.98	1.00	0.33	0.84	0.92	0.58
M06-2X/cc-pvTZ	0.97	0.98	0.43	0.68	0.92	0.52
M06-2X/aug-cc-pvTZ	0.98	1.00	0.25	0.76	0.88	0.59
M06-2X/6-31G* GD3	0.96	0.99	0.26	0.62	0.85	0.89
M06-2X/6-311++G** GD3	0.97	0.81	0.78	0.71	0.94	0.29

M06-2X/6-311++G(2d,2p) GD3	0.97	0.96	0.50	0.84	0.91	0.46
M06-2X/cc-pvDZ GD3	0.96	0.97	0.68	0.82	0.92	0.64
M06-2X/aug-cc-pvDZ GD3	0.98	1.00	0.33	0.84	0.92	0.57
M06-2X/cc-pvTZ GD3	0.97	0.98	0.43	0.68	0.92	0.52
M06-2X/aug-cc-pvTZ GD3	0.98	1.00	0.26	0.76	0.88	0.59

Table S26 Proportionality of $\alpha G'$ and $\beta(G')^2$ invariants in IND

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***ν*(C*H)**	***ν*(CN)**	***ν*$_s$(HC=CH)**	***ν*(C=C)$_1$**	***ν*(C=C)$_2$**	***ν*(C=C)$_3$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, ARE THE INVARIANTS PROPORTIONAL?	**YES**	**YES**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.99	0.82	0.46	0.09	0.54	0.61
BLYP/6-311++G**	0.99	0.79	0.16	0.09	0.75	0.77
BLYP/6-311++G(2d,2p)	0.99	0.75	0.46	0.08	0.74	0.86
BLYP/cc-pvDZ	0.99	0.84	0.38	0.15	0.52	0.56
BLYP/aug-cc-pvDZ	0.99	0.79	0.44	0.04	0.87	0.75
BLYP/cc-pvTZ	0.99	0.79	0.81	0.09	0.66	0.78
BLYP/aug-cc-pvTZ	0.99	0.80	0.59	0.04	0.68	0.73
BLYP/6-31G* GD3	0.99	0.77	0.53	0.09	0.66	0.90
BLYP/6-311++G** GD3	0.99	0.75	0.26	0.09	0.83	0.72
BLYP/6-311++G(2d,2p) GD3	0.99	0.72	0.49	0.08	0.84	0.82
BLYP/cc-pvDZ GD3	0.99	0.80	0.48	0.21	0.61	0.52
BLYP/aug-cc-pvDZ GD3	0.99	0.74	0.56	0.03	0.91	0.70
BLYP/cc-pvTZ GD3	0.99	0.75	0.84	0.09	0.70	0.80
BLYP/aug-cc-pvTZ GD3	0.99	0.76	0.67	0.08	0.76	0.76
B3LYP/6-31G*	0.99	0.91	0.63	0.13	0.52	0.92
B3LYP/6-311++G**	0.98	0.82	0.33	0.16	0.89	0.83
B3LYP/6-311++G(2d,2p)	0.98	0.80	0.25	0.12	0.91	0.87
B3LYP/cc-pvDZ	0.99	0.92	0.65	0.65	0.76	0.32
B3LYP/aug-cc-pvDZ	0.98	0.84	0.74	0.22	0.90	0.15
B3LYP/cc-pvTZ	0.98	0.86	0.90	0.16	0.69	0.86
B3LYP/aug-cc-pvTZ	0.98	0.84	0.81	0.12	0.79	0.76
B3LYP/6-31G* GD3	0.99	0.89	0.69	0.12	0.61	0.96
B3LYP/6-311++G** GD3	0.98	0.79	0.41	0.14	0.86	0.85
B3LYP/6-311++G(2d,2p) GD3	0.98	0.75	0.41	0.10	0.88	0.88
B3LYP/cc-pvDZ GD3	0.99	0.91	0.69	0.49	0.72	0.34
B3LYP/aug-cc-pvDZ GD3	0.98	0.82	0.81	0.17	0.88	0.02
B3LYP/cc-pvTZ GD3	0.98	0.83	0.94	0.13	0.68	0.83

B3LYP/aug-cc-pvTZ GD3	0.98	0.81	0.86	0.12	0.83	0.81
CAM-B3LYP/6-31G*	0.99	0.92	0.78	0.41	0.36	0.94
CAM-B3LYP/6-311++G**	0.96	0.74	0.33	0.46	0.86	0.16
CAM-B3LYP/6-311++G(2d,2p)	0.97	0.72	0.47	0.24	0.91	0.21
CAM-B3LYP/cc-pvDZ	0.99	0.93	0.74	0.70	0.57	0.36
CAM-B3LYP/aug-cc-pvDZ	0.97	0.82	0.70	0.83	0.15	0.51
CAM-B3LYP/cc-pvTZ	0.98	0.82	0.90	0.60	0.39	0.36
CAM-B3LYP/aug-cc-pvTZ	0.97	0.78	0.78	0.36	0.87	0.39
CAM-B3LYP/6-31G* GD3	0.99	0.91	0.79	0.37	0.54	0.96
CAM-B3LYP/6-311++G** GD3	0.96	0.71	0.46	0.36	0.84	0.03
CAM-B3LYP/6-311++G(2d,2p) GD3	0.96	0.70	0.48	0.20	0.93	0.10
CAM-B3LYP/cc-pvDZ GD3	0.98	0.93	0.76	0.66	0.47	0.38
CAM-B3LYP/aug-cc-pvDZ GD3	0.90	0.81	0.77	0.89	0.14	0.41
CAM-B3LYP/cc-pvTZ GD3	0.97	0.80	0.91	0.55	0.51	0.63
CAM-B3LYP/aug-cc-pvTZ GD3	0.97	0.79	0.77	0.31	0.97	0.37
M06-2X/6-31G*	0.99	0.93	0.61	0.70	0.80	0.93
M06-2X/6-311++G**	0.96	0.67	0.05	0.58	0.94	0.13
M06-2X/6-311++G(2d,2p)	0.97	0.78	0.31	0.39	0.97	0.04
M06-2X/cc-pvDZ	0.98	0.92	0.67	0.56	0.78	0.72
M06-2X/aug-cc-pvDZ	0.96	0.75	0.70	0.62	0.52	0.15
M06-2X/cc-pvTZ	0.97	0.83	0.94	0.71	0.39	0.77
M06-2X/aug-cc-pvTZ	0.97	0.85	0.70	0.73	0.90	0.25
M06-2X/6-31G* GD3	0.98	0.92	0.77	0.56	0.43	0.94
M06-2X/6-311++G** GD3	0.96	0.70	0.11	0.54	0.85	0.26
M06-2X/6-311++G(2d,2p) GD3	0.97	0.78	0.30	0.39	0.97	0.04
M06-2X/cc-pvDZ GD3	0.98	0.92	0.67	0.56	0.77	0.72
M06-2X/aug-cc-pvDZ GD3	0.96	0.75	0.70	0.62	0.52	0.14
M06-2X/cc-pvTZ GD3	0.97	0.83	0.94	0.72	0.39	0.77
M06-2X/aug-cc-pvTZ GD3	0.97	0.85	0.69	0.73	0.91	0.25

Table S27 ROA intensity correlations with *pEDA(I)* descriptor in IIN

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***ν*(C*H)**	***ν*(CN)**	***ν*(NH)**	***ν*(C=C)$_4$**	***ν*(C=C)$_5$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, IS THERE A CORRELATION?	**YES**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.98	0.22	0.85	0.55	0.76
BLYP/6-311++G**	0.84	0.21	0.75	0.41	0.66
BLYP/6-311++G(2d,2p)	0.98	0.19	0.85	0.79	0.87
BLYP/cc-pvDZ	0.79	0.23	0.79	0.52	0.59

BLYP/aug-cc-pvDZ	0.83	0.21	0.71	0.34	0.52
BLYP/cc-pvTZ	0.81	0.21	0.76	0.36	0.59
BLYP/aug-cc-pvTZ	0.98	0.21	0.78	0.78	0.89
BLYP/6-31G* GD3	0.98	0.23	0.85	0.60	0.71
BLYP/6-311++G** GD3	0.97	0.20	0.81	0.81	0.88
BLYP/6-311++G(2d,2p) GD3	0.83	0.19	0.80	0.50	0.72
BLYP/cc-pvDZ GD3	0.98	0.23	0.87	0.79	0.85
BLYP/aug-cc-pvDZ GD3	0.98	0.20	0.78	0.80	0.82
BLYP/cc-pvTZ GD3	0.81	0.21	0.77	0.42	0.60
BLYP/aug-cc-pvTZ GD3	0.83	0.21	0.74	0.41	0.67
B3LYP/6-31G*	0.76	0.18	0.69	0.63	0.63
B3LYP/6-311++G**	0.98	0.12	0.59	0.73	0.84
B3LYP/6-311++G(2d,2p)	0.97	0.13	0.67	0.71	0.92
B3LYP/cc-pvDZ	0.95	0.14	0.68	0.63	0.74
B3LYP/aug-cc-pvDZ	0.82	0.14	0.57	0.29	0.40
B3LYP/cc-pvTZ	0.97	0.12	0.67	0.60	0.82
B3LYP/aug-cc-pvTZ	0.82	0.14	0.58	0.29	0.59
B3LYP/6-31G* GD3	0.95	0.16	0.73	0.83	0.93
B3LYP/6-311++G** GD3	0.98	0.12	0.60	0.74	0.87
B3LYP/6-311++G(2d,2p) GD3	0.83	0.15	0.65	0.40	0.70
B3LYP/cc-pvDZ GD3	0.95	0.14	0.73	0.59	0.79
B3LYP/aug-cc-pvDZ GD3	0.98	0.12	0.59	0.69	0.73
B3LYP/cc-pvTZ GD3	0.97	0.13	0.69	0.61	0.87
B3LYP/aug-cc-pvTZ GD3	0.97	0.13	0.63	0.69	0.91
CAM-B3LYP/6-31G*	0.70	0.14	0.61	0.75	0.48
CAM-B3LYP/6-311++G**	0.79	0.13	0.51	0.80	0.33
CAM-B3LYP/6-311++G(2d,2p)	0.89	0.15	0.59	0.59	0.63
CAM-B3LYP/cc-pvDZ	0.69	0.10	0.61	0.81	0.29
CAM-B3LYP/aug-cc-pvDZ	0.89	0.11	0.56	0.62	0.65
CAM-B3LYP/cc-pvTZ	0.87	0.09	0.62	0.63	0.63
CAM-B3LYP/aug-cc-pvTZ	0.75	0.09	0.53	0.79	0.31
CAM-B3LYP/6-31G* GD3	0.70	0.16	0.60	0.77	0.48
CAM-B3LYP/6-311++G** GD3	0.78	0.13	0.51	0.81	0.31
CAM-B3LYP/6-311++G(2d,2p) GD3	0.88	0.18	0.57	0.65	0.64
CAM-B3LYP/cc-pvDZ GD3	0.69	0.11	0.61	0.83	0.29
CAM-B3LYP/aug-cc-pvDZ GD3	0.88	0.12	0.56	0.65	0.67
CAM-B3LYP/cc-pvTZ GD3	0.87	0.10	0.62	0.66	0.64
CAM-B3LYP/aug-cc-pvTZ GD3	0.88	0.11	0.55	0.65	0.67
M06-2X/6-31G*	0.68	0.15	0.62	0.81	0.51
M06-2X/6-311++G**	0.77	0.13	0.51	0.83	0.40
M06-2X/6-311++G(2d,2p)	0.85	0.17	0.62	0.71	0.76
M06-2X/cc-pvDZ	0.63	0.12	0.61	0.86	0.35
M06-2X/aug-cc-pvDZ	0.51	0.14	0.54	0.81	0.39
M06-2X/cc-pvTZ	0.83	0.12	0.61	0.72	0.77
M06-2X/aug-cc-pvTZ	0.70	0.11	0.53	0.82	0.40

M06-2X/6-31G* GD3	0.68	0.16	0.61	0.82	0.51
M06-2X/6-311++G** GD3	0.88	0.22	0.56	0.69	0.75
M06-2X/6-311++G(2d,2p) GD3	0.85	0.18	0.61	0.71	0.77
M06-2X/cc-pvDZ GD3	0.78	0.16	0.65	0.79	0.77
M06-2X/aug-cc-pvDZ GD3	0.52	0.14	0.54	0.81	0.39
M06-2X/cc-pvTZ GD3	0.83	0.12	0.61	0.72	0.77
M06-2X/aug-cc-pvTZ GD3	0.70	0.11	0.53	0.82	0.40

Table S28 ROA intensity correlations with σ_p descriptor in IIN

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***v*(C*H)**	***v*(CN)**	***v*(NH)**	***v*(C=C)$_4$**	***v*(C=C)$_5$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, IS THERE A CORRELATION?	**YES**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.98	0.22	0.85	0.55	0.76
BLYP/6-311++G**	0.84	0.21	0.75	0.41	0.66
BLYP/6-311++G(2d,2p)	0.98	0.19	0.85	0.79	0.87
BLYP/cc-pvDZ	0.79	0.23	0.79	0.52	0.59
BLYP/aug-cc-pvDZ	0.83	0.21	0.71	0.34	0.52
BLYP/cc-pvTZ	0.81	0.21	0.76	0.36	0.59
BLYP/aug-cc-pvTZ	0.98	0.21	0.78	0.78	0.89
BLYP/6-31G* GD3	0.98	0.23	0.85	0.60	0.71
BLYP/6-311++G** GD3	0.97	0.20	0.81	0.81	0.88
BLYP/6-311++G(2d,2p) GD3	0.83	0.19	0.80	0.50	0.72
BLYP/cc-pvDZ GD3	0.98	0.23	0.87	0.79	0.85
BLYP/aug-cc-pvDZ GD3	0.98	0.20	0.78	0.80	0.82
BLYP/cc-pvTZ GD3	0.81	0.21	0.77	0.42	0.60
BLYP/aug-cc-pvTZ GD3	0.83	0.21	0.74	0.41	0.67
B3LYP/6-31G*	0.76	0.18	0.69	0.63	0.63
B3LYP/6-311++G**	0.98	0.12	0.59	0.73	0.84
B3LYP/6-311++G(2d,2p)	0.97	0.13	0.67	0.71	0.92
B3LYP/cc-pvDZ	0.95	0.14	0.68	0.63	0.74
B3LYP/aug-cc-pvDZ	0.82	0.14	0.57	0.29	0.40
B3LYP/cc-pvTZ	0.97	0.12	0.67	0.60	0.82
B3LYP/aug-cc-pvTZ	0.82	0.14	0.58	0.29	0.59
B3LYP/6-31G* GD3	0.95	0.16	0.73	0.83	0.93
B3LYP/6-311++G** GD3	0.98	0.12	0.60	0.74	0.87
B3LYP/6-311++G(2d,2p) GD3	0.83	0.15	0.65	0.40	0.70
B3LYP/cc-pvDZ GD3	0.95	0.14	0.73	0.59	0.79
B3LYP/aug-cc-pvDZ GD3	0.98	0.12	0.59	0.69	0.73

B3LYP/cc-pvTZ GD3	0.97	0.13	0.69	0.61	0.87
B3LYP/aug-cc-pvTZ GD3	0.97	0.13	0.63	0.69	0.91
CAM-B3LYP/6-31G*	0.70	0.14	0.61	0.75	0.48
CAM-B3LYP/6-311++G**	0.79	0.13	0.51	0.80	0.33
CAM-B3LYP/6-311++G(2d,2p)	0.89	0.15	0.59	0.59	0.63
CAM-B3LYP/cc-pvDZ	0.69	0.10	0.61	0.81	0.29
CAM-B3LYP/aug-cc-pvDZ	0.89	0.11	0.56	0.62	0.65
CAM-B3LYP/cc-pvTZ	0.87	0.09	0.62	0.63	0.63
CAM-B3LYP/aug-cc-pvTZ	0.75	0.09	0.53	0.79	0.31
CAM-B3LYP/6-31G* GD3	0.70	0.16	0.60	0.77	0.48
CAM-B3LYP/6-311++G** GD3	0.78	0.13	0.51	0.81	0.31
CAM-B3LYP/6-311++G(2d,2p) GD3	0.88	0.18	0.57	0.65	0.64
CAM-B3LYP/cc-pvDZ GD3	0.69	0.11	0.61	0.83	0.29
CAM-B3LYP/aug-cc-pvDZ GD3	0.88	0.12	0.56	0.65	0.67
CAM-B3LYP/cc-pvTZ GD3	0.87	0.10	0.62	0.66	0.64
CAM-B3LYP/aug-cc-pvTZ GD3	0.88	0.11	0.55	0.65	0.67
M06-2X/6-31G*	0.68	0.15	0.62	0.81	0.51
M06-2X/6-311++G**	0.77	0.13	0.51	0.83	0.40
M06-2X/6-311++G(2d,2p)	0.85	0.17	0.62	0.71	0.76
M06-2X/cc-pvDZ	0.63	0.12	0.61	0.86	0.35
M06-2X/aug-cc-pvDZ	0.51	0.14	0.54	0.81	0.39
M06-2X/cc-pvTZ	0.83	0.12	0.61	0.72	0.77
M06-2X/aug-cc-pvTZ	0.70	0.11	0.53	0.82	0.40
M06-2X/6-31G* GD3	0.68	0.16	0.61	0.82	0.51
M06-2X/6-311++G** GD3	0.88	0.22	0.56	0.69	0.75
M06-2X/6-311++G(2d,2p) GD3	0.85	0.18	0.61	0.71	0.77
M06-2X/cc-pvDZ GD3	0.78	0.16	0.65	0.79	0.77
M06-2X/aug-cc-pvDZ GD3	0.52	0.14	0.54	0.81	0.39
M06-2X/cc-pvTZ GD3	0.83	0.12	0.61	0.72	0.77
M06-2X/aug-cc-pvTZ GD3	0.70	0.11	0.53	0.82	0.40

Table S29 Proportionality of $\alpha G'$ and $\beta(G')^2$ invariants in IIN

The figures in the table are correlation coefficients. These are coloured with a red-yellow-green gradient, the more green the field, the better the correlation.

Method	***ν*(C*H)**	***ν*(CN)**	***ν*(NH)**	***ν*(C=C)$_4$**	***ν*(C=C)$_5$**
IN DATASET USED IN THE MAIN BODY OF THE PAPER, ARE THE INVARIANTS PROPORTIONAL?	**YES**	**NO**	**NO**	**NO**	**NO**
BLYP/6-31G*	0.99	0.87	0.26	0.30	0.64
BLYP/6-311++G**	1.00	0.92	0.71	0.49	0.61
BLYP/6-311++G(2d,2p)	1.00	0.91	0.38	0.20	0.67

BLYP/cc-pvDZ	0.99	0.93	0.63	0.57	0.52
BLYP/aug-cc-pvDZ	1.00	0.93	0.81	0.39	0.37
BLYP/cc-pvTZ	0.99	0.93	0.73	0.51	0.15
BLYP/aug-cc-pvTZ	0.99	0.92	0.77	0.31	0.77
BLYP/6-31G* GD3	0.99	0.86	0.20	0.32	0.71
BLYP/6-311++G** GD3	1.00	0.90	0.65	0.41	0.78
BLYP/6-311++G(2d,2p) GD3	1.00	0.93	0.33	0.49	0.01
BLYP/cc-pvDZ GD3	0.99	0.88	0.52	0.59	0.30
BLYP/aug-cc-pvDZ GD3	1.00	0.91	0.77	0.40	0.59
BLYP/cc-pvTZ GD3	0.99	0.93	0.68	0.55	0.09
BLYP/aug-cc-pvTZ GD3	0.99	0.93	0.72	0.48	0.60
B3LYP/6-31G*	0.99	0.93	0.82	0.18	0.11
B3LYP/6-311++G**	0.99	0.92	0.94	0.35	0.64
B3LYP/6-311++G(2d,2p)	0.99	0.92	0.89	0.29	0.66
B3LYP/cc-pvDZ	0.99	0.92	0.94	0.66	0.28
B3LYP/aug-cc-pvDZ	0.99	0.93	0.95	0.26	0.06
B3LYP/cc-pvTZ	0.99	0.93	0.94	0.31	0.28
B3LYP/aug-cc-pvTZ	0.99	0.93	0.94	0.30	0.49
B3LYP/6-31G* GD3	0.99	0.91	0.77	0.72	0.32
B3LYP/6-311++G** GD3	0.99	0.91	0.93	0.38	0.66
B3LYP/6-311++G(2d,2p) GD3	0.99	0.93	0.79	0.36	0.22
B3LYP/cc-pvDZ GD3	0.99	0.92	0.88	0.05	0.36
B3LYP/aug-cc-pvDZ GD3	0.99	0.91	0.98	0.27	0.33
B3LYP/cc-pvTZ GD3	0.98	0.93	0.90	0.33	0.36
B3LYP/aug-cc-pvTZ GD3	0.99	0.92	0.92	0.25	0.74
CAM-B3LYP/6-31G*	0.99	0.97	0.94	0.06	0.54
CAM-B3LYP/6-311++G**	0.98	0.95	0.97	0.65	0.64
CAM-B3LYP/6-311++G(2d,2p)	0.98	0.93	0.94	0.07	0.08
CAM-B3LYP/cc-pvDZ	0.99	0.99	0.97	0.46	0.69
CAM-B3LYP/aug-cc-pvDZ	0.97	0.94	0.97	0.79	0.03
CAM-B3LYP/cc-pvTZ	0.98	0.96	0.95	0.69	0.19
CAM-B3LYP/aug-cc-pvTZ	0.98	0.96	0.97	0.72	0.48
CAM-B3LYP/6-31G* GD3	0.99	0.97	0.95	0.05	0.65
CAM-B3LYP/6-311++G** GD3	0.97	0.94	0.96	0.65	0.65
CAM-B3LYP/6-311++G(2d,2p) GD3	0.96	0.93	0.95	0.19	0.18
CAM-B3LYP/cc-pvDZ GD3	0.99	0.99	0.96	0.49	0.72
CAM-B3LYP/aug-cc-pvDZ GD3	0.96	0.94	0.97	0.79	0.11
CAM-B3LYP/cc-pvTZ GD3	0.97	0.96	0.95	0.70	0.08
CAM-B3LYP/aug-cc-pvTZ GD3	0.97	0.94	0.96	0.79	0.36
M06-2X/6-31G*	0.99	0.98	0.93	0.10	0.71
M06-2X/6-311++G**	0.97	0.96	0.96	0.62	0.85
M06-2X/6-311++G(2d,2p)	0.97	0.95	0.93	0.72	0.26
M06-2X/cc-pvDZ	0.95	0.99	0.94	0.55	0.88
M06-2X/aug-cc-pvDZ	0.69	0.93	0.93	0.74	0.74
M06-2X/cc-pvTZ	0.95	0.94	0.95	0.73	0.66

M06-2X/aug-cc-pvTZ	0.96	0.96	0.96	0.76	0.80
M06-2X/6-31G* GD3	0.99	0.98	0.92	0.10	0.71
M06-2X/6-311++G** GD3	0.96	0.90	0.95	0.67	0.21
M06-2X/6-311++G(2d,2p) GD3	0.97	0.95	0.93	0.71	0.28
M06-2X/cc-pvDZ GD3	0.94	0.96	0.94	0.63	0.84
M06-2X/aug-cc-pvDZ GD3	0.52	0.93	0.93	0.75	0.74
M06-2X/cc-pvTZ GD3	0.95	0.94	0.95	0.73	0.66
M06-2X/aug-cc-pvTZ GD3	0.96	0.96	0.96	0.76	0.80

Correlations of ROA robustness parameters with substituents volume

We have calculated *cos φ* and *cos ψ* parameters according to equations found in:

Tommasini, M.; Longhi, G.; Mazzeo, G.; Abbate, S.; Nieto-Ortega, B.; Ramírez, F. J.; Casado, J.; López Navarrete, J. T. Mode Robustness in Raman Optical Activity. *J. Chem. Theory Comput.* **2014**, *10* (12), 5520–5527.

Tensor elements required for the calculation were obtained by transforming tensor derivatives in Cartesian coordinates (as found in Gaussian output files) into normal mode representation. Then it was attempted to correlate the parameters with electronic substituent constants, however without success. On the other hand, we found some relationships of *cos φ* to substituents volume. These are presented in Figures S51-S53.

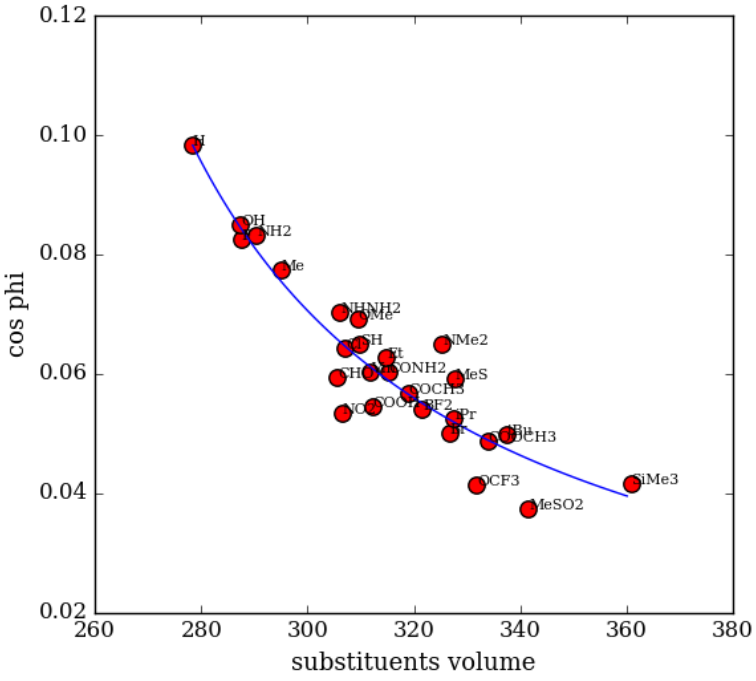

Figure S51. Correlation of *cos φ* with substituents volume, IND, ν(CN) mode.

n = 26, r = 0.93, SiH_3 and NO excluded

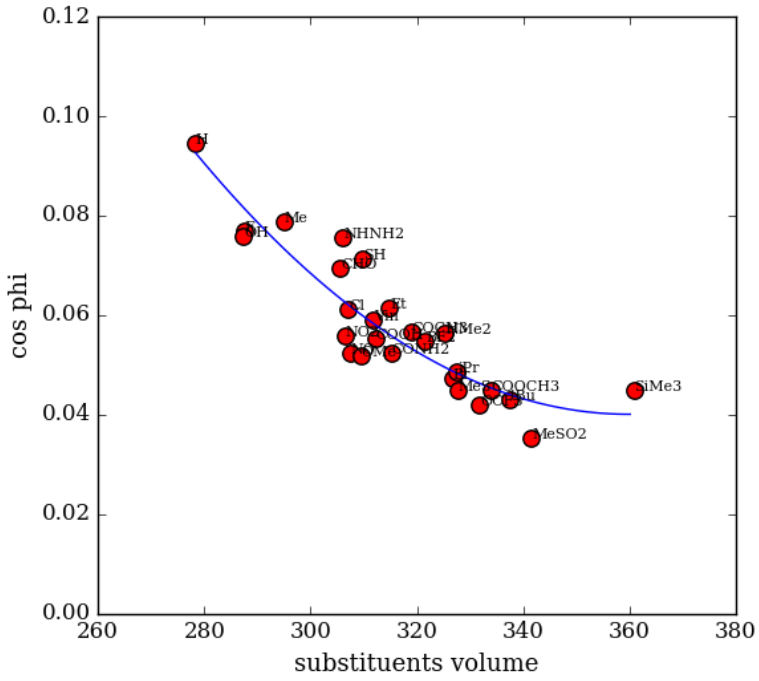

Figure S52. Correlation of *cos φ* with substituents volume, IIN, ν(CN) mode.

n = 26, *r* = 0.91, SiH_3 and NH_2 excluded

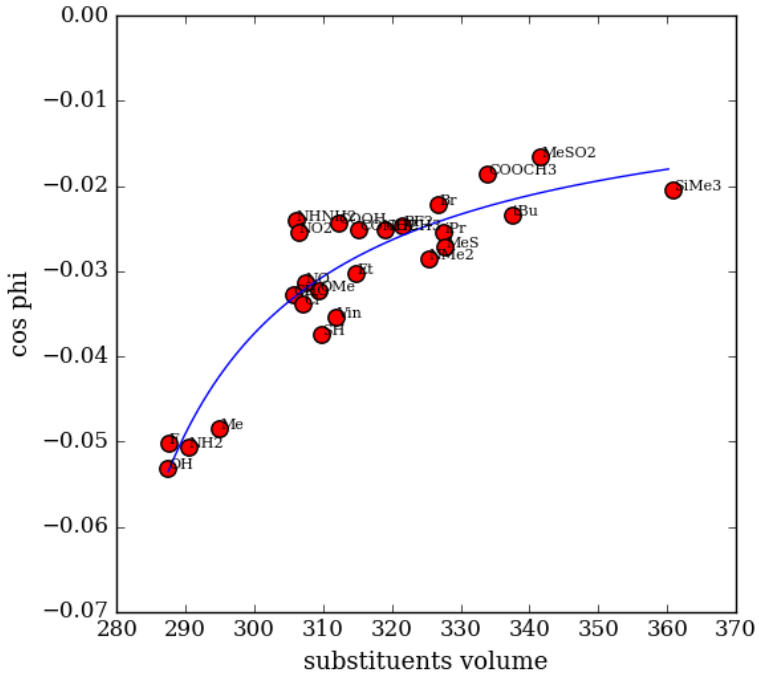

Figure S53. Correlation of *cos φ* with substituents volume, IND, ν_s(CH=CH) mode.

n = 25, *r* = 0.92, H, SiH_3 and OCF_3 excluded

Coordinates and energies of CN-IND

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

BF2-CN-IND-A-5.out
Total energy (hartree): -664.144789
Corrected energy (hartree): -664.044660

C	1.5122	2.0348	0.0087
C	2.7274	1.4979	-0.2153
C	2.6007	0.0070	-0.5156
C	1.1040	-0.2378	-0.3588
C	0.3726	-1.4133	-0.4752
C	-1.0172	-1.3458	-0.3107
C	-1.6686	-0.1250	-0.0355
C	-0.9060	1.0560	0.0844
C	0.4782	0.9941	-0.0739
H	1.3133	3.0835	0.2219
H	3.6850	2.0124	-0.2109
H	0.8608	-2.3662	-0.6793
H	-1.6092	-2.2569	-0.3959
H	-1.3991	2.0036	0.3016
H	2.8993	-0.1873	-1.5611
C	3.4383	-0.8433	0.3403
N	4.1076	-1.5176	1.0069
B	-3.2026	-0.0799	0.1376
F	-3.8507	1.0654	0.4005
F	-3.9649	-1.1781	0.0325

Br-CN-IND-A-8.out
Total energy (hartree): -3013.600737
Corrected energy (hartree): -3013.509236

C	-1.8615	2.0344	-0.0760
C	-3.0773	1.5040	0.1616
C	-2.9515	0.0249	0.5154
C	-1.4542	-0.2226	0.3753
C	-0.7142	-1.3861	0.5359
C	0.6790	-1.3289	0.3767
C	1.2891	-0.1100	0.0636
C	0.5587	1.0697	-0.1070

C	-0.8285	0.9973	0.0492
H	-1.6626	3.0750	-0.3259
H	-4.0349	2.0179	0.1337
H	-1.1929	-2.3366	0.7720
H	1.2827	-2.2266	0.4937
H	1.0575	2.0046	-0.3551
H	-3.2607	-0.1304	1.5643
C	-3.7856	-0.8526	-0.3167
N	-4.4520	-1.5496	-0.9626
Br	3.1957	-0.0554	-0.1432

CHO-CN-IND-A-16.out
Total energy (hartree): -553.386724
Corrected energy (hartree): -553.275490

C	0.9748	2.0379	0.0224
C	2.2254	1.5954	-0.2126
C	2.2115	0.1013	-0.5227
C	0.7392	-0.2585	-0.3571
C	0.1018	-1.4862	-0.4734
C	-1.2882	-1.5258	-0.2958
C	-2.0137	-0.3575	-0.0109
C	-1.3598	0.8830	0.1105
C	0.0212	0.9229	-0.0596
H	0.6984	3.0670	0.2438
H	3.1411	2.1814	-0.2112
H	0.6601	-2.3977	-0.6864
H	-1.8186	-2.4758	-0.3776
H	-1.9446	1.7739	0.3370
H	2.5167	-0.0621	-1.5717
C	3.1175	-0.6892	0.3207
N	3.8401	-1.3173	0.9767
C	-3.4850	-0.4486	0.1647
H	-3.9072	-1.4756	0.0570
O	-4.2118	0.4953	0.4069

CHO-CN-IND-A-17.out
Total energy (hartree): -553.386220
Corrected energy (hartree): -553.275032

C	-1.2714	2.0282	-0.0918
C	-2.4425	1.4233	0.1880
C	-2.2103	-0.0434	0.5389
C	-0.7057	-0.1975	0.3481
C	0.1043	-1.3210	0.4897
C	1.4798	-1.1788	0.2862

C	2.0278	0.0723	-0.0533
C	1.2036	1.2004	-0.2005
C	-0.1707	1.0594	-0.0008
H	-1.1479	3.0785	-0.3494
H	-3.4313	1.8747	0.1928
H	-0.3190	-2.2927	0.7444
H	2.1516	-2.0305	0.3847
H	1.6394	2.1644	-0.4685
H	-2.4680	-0.2154	1.5991
C	-3.0137	-0.9772	-0.2608
N	-3.6558	-1.7169	-0.8832
C	3.4908	0.2154	-0.2639
H	3.8250	1.2447	-0.5365
O	4.2985	-0.6865	-0.1579

Cl-CN-IND-A-19.out
Total energy (hartree): -899.664910
Corrected energy (hartree): -899.571723

C	-1.1775	2.0348	-0.0770
C	-2.3925	1.5142	0.1858
C	-2.2718	0.0333	0.5333
C	-0.7800	-0.2264	0.3607
C	-0.0467	-1.3967	0.5028
C	1.3425	-1.3512	0.3134
C	1.9560	-0.1370	-0.0108
C	1.2327	1.0494	-0.1628
C	-0.1509	0.9888	0.0235
H	-0.9753	3.0743	-0.3288
H	-3.3459	2.0365	0.1798
H	-0.5286	-2.3434	0.7475
H	1.9453	-2.2515	0.4143
H	1.7387	1.9780	-0.4202
H	-2.5607	-0.1221	1.5880
C	-3.1307	-0.8347	-0.2833
N	-3.8163	-1.5245	-0.9168
Cl	3.7032	-0.1027	-0.2398

COCH3-CN-IND-A-77.out
Total energy (hartree): -592.711713
Corrected energy (hartree): -592.574952

C	1.4429	2.0399	-0.0183
C	2.6723	1.5323	-0.2344
C	2.5840	0.0347	-0.5149
C	1.0939	-0.2456	-0.3577

C	0.3873	-1.4387	-0.4614
C	-1.0014	-1.4046	-0.3009
C	-1.6765	-0.1970	-0.0406
C	-0.9503	1.0031	0.0680
C	0.4367	0.9713	-0.0889
H	1.2179	3.0861	0.1814
H	3.6161	2.0717	-0.2353
H	0.8966	-2.3831	-0.6540
H	-1.5922	-2.3160	-0.3731
H	-1.4541	1.9461	0.2728
H	2.8912	-0.1658	-1.5568
C	3.4417	-0.7803	0.3554
N	4.1279	-1.4254	1.0336
C	-3.1723	-0.2382	0.1160
O	-3.7786	-1.2922	0.0027
C	-3.9155	1.0502	0.4167
H	-3.7546	1.7901	-0.3808
H	-4.9836	0.8283	0.4978
H	-3.5607	1.4957	1.3574

COCH3-CN-IND-A-78.out
Total energy (hartree): -592.712179
Corrected energy (hartree): -592.575392

C	1.5484	2.0255	0.0243
C	2.7490	1.4596	-0.2077
C	2.5847	-0.0254	-0.5205
C	1.0831	-0.2332	-0.3601
C	0.3188	-1.3850	-0.4803
C	-1.0695	-1.2831	-0.3079
C	-1.6794	-0.0481	-0.0233
C	-0.8915	1.1120	0.1007
C	0.4876	1.0120	-0.0632
H	1.3765	3.0770	0.2466
H	3.7192	1.9500	-0.2023
H	0.7775	-2.3505	-0.6932
H	-1.6742	-2.1834	-0.3971
H	-1.3812	2.0580	0.3258
H	2.8764	-0.2172	-1.5685
C	3.4034	-0.9042	0.3249
N	4.0567	-1.6032	0.9820
C	-3.1669	0.0812	0.1601
O	-3.6667	1.1715	0.3923
C	-4.0354	-1.1581	0.0529
H	-3.7391	-1.9092	0.7993

H	-5.0780	-0.8706	0.2174
H	-3.9352	-1.6218	-0.9392

CONH2-CN-IND-A-24.out
Total energy (hartree): -608.779655
Corrected energy (hartree): -608.652785

C	1.4728	2.0267	-0.1392
C	2.6922	1.4838	-0.3243
C	2.5759	-0.0260	-0.5145
C	1.0801	-0.2677	-0.3452
C	0.3477	-1.4472	-0.3982
C	-1.0427	-1.3760	-0.2511
C	-1.6875	-0.1455	-0.0407
C	-0.9392	1.0435	0.0095
C	0.4469	0.9750	-0.1442
H	1.2680	3.0872	-0.0035
H	3.6459	2.0045	-0.3562
H	0.8355	-2.4107	-0.5465
H	-1.6538	-2.2753	-0.3011
H	-1.4277	2.0102	0.1302
H	2.8833	-0.2955	-1.5404
C	3.4150	-0.8010	0.4090
N	4.0861	-1.4146	1.1303
C	-3.1866	-0.1694	0.0981
O	-3.8633	-1.0887	-0.3472
N	-3.7603	0.9092	0.7271
H	-4.7534	0.8449	0.9038
H	-3.2196	1.5065	1.3342

CONH2-CN-IND-A-25.out
Total energy (hartree): -608.779990
Corrected energy (hartree): -608.653423

C	1.5013	2.0278	-0.0894
C	2.7113	1.4722	-0.2968
C	2.5729	-0.0303	-0.5275
C	1.0762	-0.2559	-0.3465
C	0.3316	-1.4262	-0.3901
C	-1.0577	-1.3391	-0.2186
C	-1.6871	-0.1001	-0.0063
C	-0.9209	1.0759	0.0563
C	0.4598	0.9915	-0.1153
H	1.3108	3.0864	0.0770
H	3.6723	1.9797	-0.3229
H	0.8070	-2.3962	-0.5354

H	-1.6381	-2.2610	-0.2167
H	-1.4249	2.0217	0.2470
H	2.8626	-0.2723	-1.5656
C	3.4132	-0.8474	0.3576
N	4.0841	-1.4990	1.0450
C	-3.1734	0.0427	0.1948
O	-3.6605	1.0493	0.6975
N	-3.9555	-1.0155	-0.1922
H	-4.9553	-0.8843	-0.1301
H	-3.6127	-1.7329	-0.8118

COOCH3-CN-IND-A-71.out
Total energy (hartree): -667.956046
Corrected energy (hartree): -667.815360

C	1.7451	2.0585	-0.0486
C	3.0014	1.6050	-0.2265
C	2.9893	0.1008	-0.4848
C	1.5101	-0.2463	-0.3580
C	0.8635	-1.4721	-0.4575
C	-0.5300	-1.5008	-0.3288
C	-1.2583	-0.3197	-0.1055
C	-0.5986	0.9173	-0.0008
C	0.7906	0.9439	-0.1252
H	1.4667	3.0958	0.1282
H	3.9192	2.1874	-0.2139
H	1.4196	-2.3949	-0.6221
H	-1.0748	-2.4404	-0.3982
H	-1.1668	1.8277	0.1760
H	3.3303	-0.1009	-1.5158
C	3.8625	-0.6606	0.4180
N	4.5614	-1.2635	1.1216
C	-2.7430	-0.4347	0.0173
O	-3.3608	-1.4769	-0.0733
O	-3.3398	0.7591	0.2424
C	-4.7743	0.7175	0.3715
H	-5.2286	0.3302	-0.5483
H	-5.0626	0.0768	1.2134
H	-5.0793	1.7523	0.5491

COOCH3-CN-IND-A-73.out
Total energy (hartree): -667.937312
Corrected energy (hartree): -667.797814

C	-1.5873	1.9665	-0.5531
C	-2.8256	1.6258	-0.1453

C	-2.8031	0.2584	0.5313
C	-1.3462	-0.1634	0.3785
C	-0.7069	-1.3400	0.7472
C	0.6660	-1.4598	0.4960
C	1.3877	-0.4037	-0.0851
C	0.7343	0.7817	-0.4610
C	-0.6400	0.8878	-0.2405
H	-1.3183	2.9000	-1.0442
H	-3.7354	2.2124	-0.2452
H	-1.2551	-2.1649	1.2022
H	1.1889	-2.3835	0.7384
H	1.2805	1.5889	-0.9470
H	-3.0455	0.3735	1.6029
C	-3.7680	-0.6959	-0.0301
N	-4.5392	-1.4488	-0.4607
C	2.8415	-0.6342	-0.3903
O	3.2320	-1.6509	-0.9154
O	3.7455	0.3396	-0.0963
C	3.4730	1.3748	0.8655
H	3.1303	2.2872	0.3613
H	2.7298	1.0562	1.6049
H	4.4271	1.5734	1.3648

COOCH3-CN-IND-A-75.out
Total energy (hartree): -667.956200
Corrected energy (hartree): -667.815601

C	2.0473	1.9962	0.0432
C	3.2221	1.3761	-0.1825
C	2.9901	-0.0970	-0.5079
C	1.4786	-0.2347	-0.3632
C	0.6616	-1.3491	-0.5017
C	-0.7213	-1.1870	-0.3435
C	-1.2673	0.0755	-0.0537
C	-0.4343	1.1983	0.0900
C	0.9414	1.0344	-0.0620
H	1.9232	3.0529	0.2722
H	4.2142	1.8200	-0.1644
H	1.0776	-2.3329	-0.7188
H	-1.3822	-2.0445	-0.4438
H	-0.8795	2.1649	0.3191
H	3.2823	-0.2952	-1.5544
C	3.7589	-1.0187	0.3387
N	4.3739	-1.7506	0.9969
C	-2.7375	0.2809	0.1170

O	-3.2533	1.3537	0.3622
O	-3.4460	-0.8615	-0.0314
C	-4.8724	-0.7288	0.1236
H	-5.1135	-0.3593	1.1275
H	-5.2736	-0.0327	-0.6227
H	-5.2748	-1.7340	-0.0270

COOCH3-CN-IND-A-76.out
Total energy (hartree): -667.938077
Corrected energy (hartree): -667.798547

C	1.9065	1.9407	0.5939
C	3.0857	1.3759	0.2681
C	2.8583	0.0586	-0.4682
C	1.3394	-0.0712	-0.4522
C	0.5188	-1.0730	-0.9515
C	-0.8693	-0.9289	-0.8153
C	-1.4187	0.2140	-0.2111
C	-0.5825	1.2353	0.2700
C	0.7989	1.0764	0.1640
H	1.7806	2.8959	1.1002
H	4.0796	1.7708	0.4626
H	0.9332	-1.9585	-1.4332
H	-1.5242	-1.7033	-1.2110
H	-1.0222	2.1313	0.7054
H	3.2139	0.1503	-1.5098
C	3.5598	-1.0836	0.1325
N	4.1186	-1.9882	0.5980
C	-2.9029	0.4472	-0.1596
O	-3.3906	1.5081	-0.4771
O	-3.7275	-0.5627	0.2235
C	-3.2653	-1.6909	0.9894
H	-2.3542	-1.4566	1.5507
H	-4.0762	-1.9286	1.6860
H	-3.0879	-2.5507	0.3315

COOH-CN-IND-A-26.out
Total energy (hartree): -628.654413
Corrected energy (hartree): -628.538830

C	1.4552	2.0363	0.0050
C	2.6767	1.5140	-0.2202
C	2.5677	0.0212	-0.5178
C	1.0745	-0.2413	-0.3586
C	0.3548	-1.4246	-0.4726
C	-1.0340	-1.3762	-0.3073

C	-1.6833	-0.1599	-0.0338
C	-0.9505	1.0339	0.0864
C	0.4342	0.9826	-0.0747
H	1.2439	3.0828	0.2169
H	3.6277	2.0405	-0.2179
H	0.8515	-2.3730	-0.6763
H	-1.6351	-2.2800	-0.3866
H	-1.4596	1.9706	0.3025
H	2.8677	-0.1709	-1.5633
C	3.4174	-0.8166	0.3385
N	4.0970	-1.4804	1.0052
C	-3.1648	-0.1862	0.1250
O	-3.8578	-1.1781	0.0300
O	-3.6936	1.0386	0.3936
H	-4.6518	0.9096	0.4776

COOH-CN-IND-A-29.out
Total energy (hartree): -628.654584
Corrected energy (hartree): -628.538987

C	1.5055	2.0341	0.0218
C	2.7133	1.4838	-0.2101
C	2.5681	-0.0035	-0.5199
C	1.0695	-0.2315	-0.3583
C	0.3219	-1.3956	-0.4778
C	-1.0668	-1.3170	-0.3076
C	-1.6846	-0.0866	-0.0246
C	-0.9221	1.0877	0.1007
C	0.4591	1.0061	-0.0635
H	1.3197	3.0836	0.2424
H	3.6769	1.9871	-0.2061
H	0.7954	-2.3542	-0.6893
H	-1.6751	-2.2144	-0.3932
H	-1.4237	2.0276	0.3248
H	2.8606	-0.1935	-1.5679
C	3.3996	-0.8695	0.3262
N	4.0639	-1.5570	0.9844
C	-3.1596	0.0247	0.1567
O	-3.7521	1.0565	0.3985
O	-3.8072	-1.1635	0.0236
H	-4.7499	-0.9781	0.1604

COOH-CN-IND-A-30.out
Total energy (hartree): -628.644035
Corrected energy (hartree): -628.529582

C	1.4867	2.0333	-0.0753
C	2.6971	1.4802	-0.2862
C	2.5618	-0.0208	-0.5266
C	1.0659	-0.2501	-0.3471
C	0.3250	-1.4220	-0.3994
C	-1.0644	-1.3387	-0.2285
C	-1.6962	-0.1025	-0.0066
C	-0.9328	1.0758	0.0649
C	0.4475	0.9951	-0.1075
H	1.2942	3.0904	0.0976
H	3.6572	1.9894	-0.3094
H	0.8019	-2.3898	-0.5524
H	-1.6359	-2.2680	-0.2360
H	-1.4377	2.0203	0.2592
H	2.8510	-0.2553	-1.5666
C	3.4021	-0.8432	0.3534
N	4.0716	-1.4992	1.0378
C	-3.1796	0.0366	0.1946
O	-3.6905	1.0237	0.6674
O	-3.9674	-1.0069	-0.1851
H	-3.4481	-1.6898	-0.6300

Et-CN-IND-A-109.out
Total energy (hartree): -518.683180
Corrected energy (hartree): -518.527153

C	-1.1918	2.0297	-0.1153
C	-2.3908	1.5456	0.2655
C	-2.2760	0.0632	0.6122
C	-0.8128	-0.2357	0.3045
C	-0.0970	-1.4224	0.3824
C	1.2672	-1.4016	0.0565
C	1.9165	-0.2192	-0.3395
C	1.1741	0.9713	-0.4195
C	-0.1858	0.9589	-0.1011
H	-0.9888	3.0623	-0.3945
H	-3.3267	2.0931	0.3443
H	-0.5779	-2.3564	0.6744
H	1.8380	-2.3302	0.1042
H	1.6586	1.8961	-0.7376
H	-2.4724	-0.0810	1.6893
C	-3.2287	-0.7844	-0.1173
N	-3.9886	-1.4569	-0.6812
C	3.3995	-0.2227	-0.6453
H	3.6838	-1.2009	-1.0594

H	3.6125	0.5245	-1.4239
C	4.2653	0.0742	0.5919
H	5.3329	0.0647	0.3318
H	4.0243	1.0602	1.0128
H	4.0978	-0.6756	1.3775

Et-CN-IND-A-110.out
Total energy (hartree): -518.682039
Corrected energy (hartree): -518.525732

C	1.4532	2.0077	0.1020
C	2.6066	1.3685	-0.1768
C	2.3301	-0.0886	-0.5401
C	0.8196	-0.1928	-0.3587
C	-0.0383	-1.2707	-0.5066
C	-1.4143	-1.0702	-0.2999
C	-1.9341	0.1865	0.0479
C	-1.0455	1.2690	0.1969
C	0.3208	1.0771	-0.0012
H	1.3643	3.0598	0.3678
H	3.6092	1.7888	-0.1723
H	0.3358	-2.2610	-0.7679
H	-2.0840	-1.9207	-0.4123
H	-1.4301	2.2530	0.4717
H	2.5972	-0.2629	-1.5974
C	3.0992	-1.0486	0.2632
N	3.7146	-1.8109	0.8861
C	-3.4185	0.4254	0.2733
H	-3.5460	0.8559	1.2790
H	-3.7483	1.2118	-0.4241
C	-4.3375	-0.7890	0.1288
H	-5.3788	-0.4973	0.3189
H	-4.2919	-1.2155	-0.8831
H	-4.0781	-1.5815	0.8445

Et-CN-IND-A-111.out
Total energy (hartree): -518.683178
Corrected energy (hartree): -518.527264

C	1.2389	2.0247	0.1473
C	2.4636	1.4863	-0.0169
C	2.3454	0.0260	-0.4457
C	0.8374	-0.2006	-0.4355
C	0.0918	-1.3378	-0.7141
C	-1.3072	-1.2480	-0.6625
C	-1.9614	-0.0462	-0.3400

C	-1.1902	1.0951	-0.0610
C	0.2034	1.0132	-0.1046
H	1.0365	3.0572	0.4274
H	3.4228	1.9817	0.1106
H	0.5727	-2.2841	-0.9633
H	-1.9037	-2.1349	-0.8815
H	-1.6806	2.0381	0.1863
H	2.7368	-0.0905	-1.4718
C	3.0979	-0.8997	0.4115
N	3.7017	-1.6338	1.0780
C	-3.4724	0.0077	-0.2571
H	-3.8186	1.0057	-0.5641
H	-3.9018	-0.7095	-0.9717
C	-4.0059	-0.3016	1.1529
H	-5.1036	-0.2536	1.1730
H	-3.7012	-1.3063	1.4769
H	-3.6185	0.4184	1.8868

F-CN-IND-A-33.out
Total energy (hartree): -539.295927
Corrected energy (hartree): -539.200550

C	-0.7479	2.0356	-0.0774
C	-1.9612	1.5288	0.2185
C	-1.8485	0.0453	0.5571
C	-0.3653	-0.2318	0.3416
C	0.3559	-1.4130	0.4603
C	1.7396	-1.3855	0.2315
C	2.3446	-0.1760	-0.1053
C	1.6472	1.0225	-0.2360
C	0.2685	0.9776	-0.0098
H	-0.5409	3.0736	-0.3316
H	-2.9080	2.0626	0.2414
H	-0.1332	-2.3528	0.7163
H	2.3472	-2.2857	0.3085
H	2.1710	1.9378	-0.5062
H	-2.1118	-0.1106	1.6183
C	-2.7407	-0.8077	-0.2398
N	-3.4522	-1.4859	-0.8571
F	3.6875	-0.1664	-0.3213

H-CN-IND-A-35.out
Total energy (hartree): -440.045876
Corrected energy (hartree): -439.940965

C	-0.2787	2.0299	-0.0852

C	-1.4971	1.5666	0.2573
C	-1.4237	0.0770	0.5813
C	0.0394	-0.2522	0.3024
C	0.7181	-1.4610	0.3849
C	2.0919	-1.4738	0.0970
C	2.7588	-0.2950	-0.2618
C	2.0715	0.9221	-0.3480
C	0.7021	0.9363	-0.0668
H	-0.0453	3.0621	-0.3410
H	-2.4224	2.1336	0.3228
H	0.2019	-2.3825	0.6554
H	2.6448	-2.4117	0.1510
H	2.5945	1.8355	-0.6319
H	-1.6455	-0.0799	1.6518
C	-2.3781	-0.7385	-0.1815
N	-3.1399	-1.3853	-0.7721
H	3.8264	-0.3284	-0.4811

iPr-CN-IND-A-112.out
Total energy (hartree): -557.999806
Corrected energy (hartree): -557.817476

C	1.7190	2.0076	0.2606
C	2.8916	1.4240	-0.0580
C	2.6555	-0.0039	-0.5437
C	1.1470	-0.1608	-0.3877
C	0.3186	-1.2477	-0.6367
C	-1.0597	-1.0998	-0.4293
C	-1.6172	0.1123	0.0187
C	-0.7633	1.1988	0.2666
C	0.6134	1.0592	0.0677
H	1.5991	3.0312	0.6117
H	3.8828	1.8676	-0.0078
H	0.7229	-2.2018	-0.9760
H	-1.7106	-1.9532	-0.6199
H	-1.1764	2.1457	0.6178
H	2.9348	-0.0827	-1.6093
C	3.4422	-1.0084	0.1846
N	4.0718	-1.8045	0.7481
C	-3.1179	0.2480	0.2390
H	-3.2950	1.2770	0.5882
C	-3.6251	-0.7039	1.3375
H	-4.6943	-0.5354	1.5281
H	-3.4988	-1.7553	1.0429
H	-3.0801	-0.5500	2.2782

C	-3.9105	0.0643	-1.0679
H	-3.7983	-0.9556	-1.4622
H	-4.9816	0.2406	-0.8956
H	-3.5680	0.7644	-1.8416

iPr-CN-IND-A-114.out
Total energy (hartree): -557.999849
Corrected energy (hartree): -557.817387

C	1.4026	2.0217	0.1559
C	2.6592	1.6035	-0.0947
C	2.6541	0.1359	-0.5152
C	1.1793	-0.2350	-0.4014
C	0.5297	-1.4403	-0.6216
C	-0.8650	-1.4844	-0.4670
C	-1.6099	-0.3514	-0.1003
C	-0.9324	0.8613	0.1224
C	0.4544	0.9137	-0.0249
H	1.1215	3.0314	0.4508
H	3.5722	2.1906	-0.0349
H	1.0802	-2.3398	-0.8987
H	-1.3860	-2.4281	-0.6344
H	-1.4825	1.7569	0.4127
H	2.9850	0.0506	-1.5653
C	3.5488	-0.7070	0.2894
N	4.2645	-1.3746	0.9136
C	-3.1213	-0.4448	0.0601
H	-3.4024	-1.4808	-0.1832
C	-3.8636	0.4766	-0.9247
H	-4.9501	0.3360	-0.8377
H	-3.6463	1.5350	-0.7219
H	-3.5728	0.2652	-1.9624
C	-3.5600	-0.1780	1.5114
H	-3.3312	0.8540	1.8135
H	-4.6438	-0.3256	1.6189
H	-3.0506	-0.8545	2.2104

Me-CN-IND-A-41.out
Total energy (hartree): -479.366380
Corrected energy (hartree): -479.237175

C	0.7854	2.0300	0.0778
C	2.0026	1.5273	-0.2096
C	1.8950	0.0431	-0.5505
C	0.4098	-0.2356	-0.3471
C	-0.3150	-1.4112	-0.4724

C	-1.7012	-1.3689	-0.2514
C	-2.3605	-0.1768	0.0889
C	-1.6091	1.0057	0.2152
C	-0.2306	0.9712	0.0015
H	0.5761	3.0679	0.3317
H	2.9487	2.0627	-0.2245
H	0.1711	-2.3534	-0.7270
H	-2.2808	-2.2881	-0.3444
H	-2.1039	1.9411	0.4824
H	2.1673	-0.1137	-1.6093
C	2.7816	-0.8087	0.2537
N	3.4899	-1.4847	0.8774
C	-3.8532	-0.1567	0.3247
H	-4.0874	0.1459	1.3560
H	-4.3514	0.5595	-0.3450
H	-4.2981	-1.1449	0.1544

MeS-CN-IND-A-45.out
Total energy (hartree): -877.570634
Corrected energy (hartree): -877.442501

C	-1.7694	2.0018	-0.0738
C	-2.9261	1.3601	0.1839
C	-2.6571	-0.1018	0.5320
C	-1.1458	-0.2065	0.3659
C	-0.2904	-1.2878	0.5076
C	1.0884	-1.0958	0.3206
C	1.5996	0.1720	-0.0040
C	0.7259	1.2677	-0.1520
C	-0.6402	1.0672	0.0305
H	-1.6750	3.0569	-0.3250
H	-3.9279	1.7824	0.1737
H	-0.6681	-2.2812	0.7511
H	1.7530	-1.9491	0.4295
H	1.1173	2.2521	-0.4099
H	-2.9384	-0.2878	1.5837
C	-3.4191	-1.0503	-0.2921
N	-4.0277	-1.8051	-0.9305
S	3.3346	0.5137	-0.2555
C	4.1351	-1.1100	-0.0258
H	3.9847	-1.4911	0.9916
H	3.7834	-1.8371	-0.7678
H	5.2047	-0.9289	-0.1834

MeS-CN-IND-A-46.out

Total energy (hartree): -877.570554
Corrected energy (hartree): -877.442357

C	1.3586	2.0334	-0.0457
C	2.6259	1.6188	-0.2419
C	2.6548	0.1161	-0.5080
C	1.1882	-0.2718	-0.3671
C	0.5620	-1.5095	-0.4652
C	-0.8270	-1.5749	-0.3179
C	-1.5884	-0.4131	-0.0768
C	-0.9530	0.8352	0.0254
C	0.4370	0.8908	-0.1175
H	1.0531	3.0616	0.1409
H	3.5259	2.2286	-0.2365
H	1.1319	-2.4218	-0.6429
H	-1.3296	-2.5397	-0.3877
H	-1.5173	1.7453	0.2145
H	2.9984	-0.0684	-1.5414
C	3.5599	-0.6189	0.3861
N	4.2835	-1.2031	1.0809
S	-3.3511	-0.6518	0.0830
C	-3.9849	1.0268	0.4139
H	-3.5728	1.4332	1.3457
H	-3.7857	1.7039	-0.4258
H	-5.0690	0.9093	0.5259

MeSO2-CN-IND-A-83.out
Total energy (hartree): -1027.970794
Corrected energy (hartree): -1027.836697

C	-2.0938	2.0379	-0.0961
C	-3.3039	1.5115	0.1759
C	-3.1714	0.0372	0.5450
C	-1.6786	-0.2168	0.3698
C	-0.9492	-1.3905	0.5111
C	0.4389	-1.3428	0.3139
C	1.0443	-0.1255	-0.0121
C	0.3230	1.0615	-0.1744
C	-1.0592	1.0014	0.0188
H	-1.8987	3.0742	-0.3648
H	-4.2616	2.0256	0.1640
H	-1.4362	-2.3358	0.7501
H	1.0450	-2.2444	0.3836
H	0.8311	1.9785	-0.4684
H	-3.4477	-0.1033	1.6053
C	-4.0292	-0.8533	-0.2474

N	-4.7154	-1.5601	-0.8608
S	2.8446	-0.0861	-0.2531
O	3.2894	-1.4591	-0.6335
O	3.1630	1.0931	-1.1121
C	3.5019	0.2581	1.4069
H	4.5904	0.2905	1.2871
H	3.1134	1.2255	1.7403
H	3.2034	-0.5564	2.0744

MeSO2-CN-IND-A-84.out
Total energy (hartree): -1027.971341
Corrected energy (hartree): -1027.837239

C	2.1087	2.0314	0.1082
C	3.3238	1.4893	-0.1039
C	3.1900	0.0194	-0.4898
C	1.6859	-0.2125	-0.4007
C	0.9457	-1.3665	-0.6243
C	-0.4507	-1.2974	-0.5111
C	-1.0527	-0.0803	-0.1778
C	-0.3230	1.0915	0.0455
C	1.0670	1.0103	-0.0656
H	1.9143	3.0697	0.3699
H	4.2867	1.9895	-0.0388
H	1.4281	-2.3090	-0.8829
H	-1.0708	-2.1711	-0.7041
H	-0.8367	2.0244	0.2721
H	3.5256	-0.1218	-1.5325
C	3.9827	-0.8873	0.3510
N	4.6139	-1.6059	1.0082
S	-2.8630	-0.0137	-0.0383
O	-3.2809	1.4068	-0.2329
O	-3.4306	-1.1053	-0.8835
C	-3.1873	-0.4436	1.6978
H	-4.2768	-0.4088	1.8068
H	-2.8048	-1.4523	1.8834
H	-2.7033	0.3025	2.3358

NH2-CN-IND-A-47.out
Total energy (hartree): -495.415180
Corrected energy (hartree): -495.295515

C	-0.7685	2.0278	-0.0719
C	-1.9846	1.5253	0.2207
C	-1.8769	0.0399	0.5568
C	-0.3942	-0.2377	0.3456

C	0.3400	-1.4110	0.4631
C	1.7206	-1.3747	0.2370
C	2.3735	-0.1720	-0.1042
C	1.6226	1.0141	-0.2253
C	0.2467	0.9676	-0.0036
H	-0.5602	3.0663	-0.3250
H	-2.9299	2.0620	0.2409
H	-0.1402	-2.3561	0.7185
H	2.3037	-2.2932	0.3171
H	2.1146	1.9488	-0.4983
H	-2.1518	-0.1181	1.6149
C	-2.7697	-0.8049	-0.2492
N	-3.4825	-1.4777	-0.8715
N	3.7421	-0.1713	-0.3853
H	4.2131	0.7191	-0.2963
H	4.2762	-0.9327	0.0117

NHNH2-CN-IND-A-115.out
Total energy (hartree): -550.739226
Corrected energy (hartree): -550.604154

C	-1.3809	2.0131	-0.0613
C	-2.5428	1.3985	0.2374
C	-2.2955	-0.0727	0.5626
C	-0.7949	-0.2113	0.3377
C	0.0474	-1.3097	0.4467
C	1.4198	-1.1508	0.2136
C	1.9482	0.1085	-0.1294
C	1.0919	1.2240	-0.2362
C	-0.2716	1.0508	-0.0088
H	-1.2720	3.0679	-0.3092
H	-3.5336	1.8452	0.2679
H	-0.3420	-2.2957	0.7026
H	2.0941	-1.9996	0.2891
H	1.4938	2.2029	-0.5040
H	-2.5455	-0.2622	1.6217
C	-3.1144	-0.9904	-0.2422
N	-3.7696	-1.7199	-0.8639
N	3.3080	0.2795	-0.4321
H	3.6215	1.2418	-0.3537
N	4.2131	-0.6913	0.0486
H	4.6326	-0.4116	0.9357
H	4.9479	-0.8270	-0.6391

NHNH2-CN-IND-A-116.out

Total energy (hartree): -550.739820
Corrected energy (hartree): -550.604703

C	1.0305	2.0250	-0.0348
C	2.2958	1.6009	-0.2248
C	2.3136	0.0999	-0.5043
C	0.8422	-0.2744	-0.3800
C	0.2006	-1.5023	-0.4896
C	-1.1899	-1.5529	-0.3487
C	-1.9428	-0.3837	-0.1077
C	-1.2913	0.8573	0.0117
C	0.0972	0.8930	-0.1243
H	0.7328	3.0543	0.1587
H	3.2012	2.2025	-0.2072
H	0.7601	-2.4211	-0.6674
H	-1.7034	-2.5125	-0.4303
H	-1.8719	1.7552	0.2067
H	2.6705	-0.0786	-1.5343
C	3.2027	-0.6491	0.3949
N	3.9126	-1.2465	1.0930
N	-3.3411	-0.4912	-0.0470
H	-3.6630	-1.4283	0.1738
N	-4.0459	0.5535	0.5908
H	-4.2256	0.3434	1.5732
H	-4.9315	0.6926	0.1136

NMe2-CN-IND-A-50.out
Total energy (hartree): -574.027127
Corrected energy (hartree): -573.855889

C	1.5494	2.0202	-0.0188
C	2.7668	1.4921	-0.2552
C	2.6493	-0.0049	-0.5334
C	1.1578	-0.2539	-0.3543
C	0.4030	-1.4148	-0.4511
C	-0.9825	-1.3523	-0.2681
C	-1.6415	-0.1277	0.0205
C	-0.8572	1.0519	0.1062
C	0.5223	0.9698	-0.0725
H	1.3477	3.0708	0.1850
H	3.7192	2.0164	-0.2696
H	0.8702	-2.3774	-0.6619
H	-1.5522	-2.2735	-0.3489
H	-1.3132	2.0161	0.3138
H	2.9542	-0.2103	-1.5751
C	3.5066	-0.8257	0.3340

N	4.1918	-1.4799	1.0053
N	-3.0122	-0.0881	0.2279
C	-3.8152	-1.2703	-0.0349
H	-4.8614	-1.0491	0.1967
H	-3.7560	-1.5989	-1.0883
H	-3.5039	-2.1102	0.6033
C	-3.6828	1.1957	0.3402
H	-3.5682	1.8150	-0.5679
H	-4.7508	1.0273	0.5076
H	-3.2990	1.7696	1.1964

NMe2-CN-IND-A-51.out
Total energy (hartree): -574.027179
Corrected energy (hartree): -573.855858

C	1.5564	2.0202	-0.0168
C	2.7771	1.4860	-0.2202
C	2.6591	-0.0085	-0.5113
C	1.1612	-0.2490	-0.3797
C	0.4044	-1.4076	-0.4879
C	-0.9851	-1.3380	-0.3416
C	-1.6478	-0.1069	-0.0926
C	-0.8581	1.0651	0.0353
C	0.5249	0.9769	-0.1098
H	1.3551	3.0707	0.1877
H	3.7326	2.0047	-0.2040
H	0.8737	-2.3747	-0.6715
H	-1.5549	-2.2594	-0.4189
H	-1.3131	2.0288	0.2477
H	2.9945	-0.2099	-1.5443
C	3.4836	-0.8399	0.3774
N	4.1424	-1.5030	1.0662
N	-3.0306	-0.0500	0.0121
C	-3.6617	1.1742	0.4753
H	-4.7473	1.0369	0.4777
H	-3.3459	1.4568	1.4962
H	-3.4357	2.0136	-0.1979
C	-3.7970	-1.2835	0.0757
H	-3.5382	-1.9021	0.9542
H	-4.8621	-1.0382	0.1297
H	-3.6420	-1.8899	-0.8280

NO-CN-IND-A-52.out
Total energy (hartree): -569.357742
Corrected energy (hartree): -569.259127

C	-1.2529	2.0328	-0.0980
C	-2.4207	1.4239	0.1861
C	-2.1823	-0.0406	0.5410
C	-0.6784	-0.1910	0.3452
C	0.1322	-1.3169	0.4869
C	1.5058	-1.1783	0.2804
C	2.0357	0.0787	-0.0611
C	1.2240	1.2124	-0.2112
C	-0.1490	1.0675	-0.0077
H	-1.1323	3.0825	-0.3586
H	-3.4113	1.8715	0.1928
H	-0.2933	-2.2871	0.7441
H	2.1832	-2.0253	0.3763
H	1.6832	2.1631	-0.4817
H	-2.4333	-0.2091	1.6036
C	-2.9850	-0.9824	-0.2499
N	-3.6255	-1.7294	-0.8652
N	3.4442	0.3115	-0.2881
O	4.1620	-0.6633	-0.1592

NO-CN-IND-A-53.out
Total energy (hartree): -569.358216
Corrected energy (hartree): -569.259507

C	0.9448	2.0390	0.0249
C	2.1947	1.5982	-0.2156
C	2.1827	0.1045	-0.5269
C	0.7122	-0.2593	-0.3559
C	0.0815	-1.4908	-0.4720
C	-1.3073	-1.5375	-0.2908
C	-2.0213	-0.3654	-0.0038
C	-1.3867	0.8834	0.1207
C	-0.0080	0.9232	-0.0543
H	0.6677	3.0675	0.2484
H	3.1095	2.1856	-0.2172
H	0.6443	-2.3987	-0.6877
H	-1.8589	-2.4743	-0.3666
H	-1.9787	1.7681	0.3501
H	2.4830	-0.0580	-1.5775
C	3.0937	-0.6849	0.3121
N	3.8207	-1.3108	0.9652
N	-3.4448	-0.5517	0.1541
O	-4.0769	0.4606	0.3982

NO2-CN-IND-A-86.out

Total energy (hartree): -644.582826
Corrected energy (hartree): -644.479658

C	1.4455	2.0388	0.0199
C	2.6585	1.5012	-0.2144
C	2.5304	0.0125	-0.5230
C	1.0356	-0.2333	-0.3582
C	0.3037	-1.4085	-0.4754
C	-1.0852	-1.3524	-0.3035
C	-1.6888	-0.1235	-0.0228
C	-0.9703	1.0690	0.1054
C	0.4123	0.9979	-0.0628
H	1.2471	3.0858	0.2402
H	3.6161	2.0155	-0.2127
H	0.7888	-2.3609	-0.6868
H	-1.7025	-2.2432	-0.3828
H	-1.4894	1.9971	0.3297
H	2.8214	-0.1736	-1.5722
C	3.3732	-0.8443	0.3211
N	4.0455	-1.5245	0.9783
N	-3.1573	-0.0815	0.1503
O	-3.7780	-1.1349	0.0371
O	-3.6707	1.0071	0.3963

NO2-CN-IND-A-87.out
Total energy (hartree): -644.582826
Corrected energy (hartree): -644.479659

C	1.4455	2.0388	0.0199
C	2.6585	1.5012	-0.2144
C	2.5304	0.0125	-0.5230
C	1.0356	-0.2333	-0.3582
C	0.3037	-1.4085	-0.4754
C	-1.0852	-1.3524	-0.3035
C	-1.6888	-0.1235	-0.0228
C	-0.9703	1.0690	0.1054
C	0.4123	0.9979	-0.0628
H	1.2471	3.0858	0.2402
H	3.6161	2.0155	-0.2127
H	0.7888	-2.3609	-0.6868
H	-1.7025	-2.2432	-0.3828
H	-1.4894	1.9971	0.3297
H	2.8214	-0.1736	-1.5722
C	3.3732	-0.8443	0.3211
N	4.0455	-1.5245	0.9783
N	-3.1573	-0.0815	0.1503

O	-3.7780	-1.1349	0.0371
O	-3.6707	1.0071	0.3963

OCF3-CN-IND-A-97.out
Total energy (hartree): -852.361967
Corrected energy (hartree): -852.256190

C	1.8426	2.0013	-0.0482
C	3.1364	1.6606	-0.2104
C	3.2605	0.1648	-0.4843
C	1.8158	-0.3093	-0.3858
C	1.2702	-1.5809	-0.5071
C	-0.1171	-1.7286	-0.4000
C	-0.9248	-0.6086	-0.1774
C	-0.3960	0.6783	-0.0485
C	0.9926	0.8077	-0.1521
H	1.4714	3.0081	0.1347
H	3.9989	2.3214	-0.1766
H	1.8974	-2.4567	-0.6724
H	-0.5870	-2.7068	-0.4845
H	-1.0239	1.5464	0.1276
H	3.6389	0.0087	-1.5100
C	4.1819	-0.5259	0.4279
N	4.9181	-1.0753	1.1373
O	-2.2913	-0.9159	-0.1018
C	-3.2237	0.0284	0.1498
F	-3.2657	0.9984	-0.7971
F	-3.0438	0.6485	1.3411
F	-4.4152	-0.5795	0.1727

OCF3-CN-IND-A-98.out
Total energy (hartree): -852.361797
Corrected energy (hartree): -852.256087

C	-2.5187	2.0022	-0.1491
C	-3.6338	1.2949	0.1199
C	-3.2752	-0.1335	0.5205
C	-1.7585	-0.1457	0.3720
C	-0.8401	-1.1667	0.5599
C	0.5278	-0.9032	0.3816
C	0.9324	0.3846	0.0187
C	0.0195	1.4249	-0.1794
C	-1.3347	1.1456	-0.0022
H	-2.4890	3.0518	-0.4357
H	-4.6606	1.6506	0.0861
H	-1.1582	-2.1722	0.8347

H	1.2483	-1.7020	0.5266
H	0.3796	2.4113	-0.4663
H	-3.5532	-0.3003	1.5762
C	-3.9646	-1.1574	-0.2761
N	-4.5158	-1.9710	-0.8937
O	2.2660	0.7715	-0.1791
C	3.2873	-0.1100	-0.1001
F	3.1809	-1.1263	-0.9885
F	3.4113	-0.6695	1.1286
F	4.4155	0.5593	-0.3653

OCF3-CN-IND-A-99.out
Total energy (hartree): -852.362205
Corrected energy (hartree): -852.256986

C	2.1579	2.0293	0.1314
C	3.3790	1.4617	0.0801
C	3.2701	0.0065	-0.3651
C	1.7637	-0.1877	-0.4977
C	1.0308	-1.3136	-0.8488
C	-0.3655	-1.2078	-0.9281
C	-0.9781	0.0154	-0.6533
C	-0.2591	1.1592	-0.3053
C	1.1305	1.0411	-0.2217
H	1.9514	3.0645	0.3966
H	4.3328	1.9350	0.2994
H	1.5173	-2.2669	-1.0539
H	-0.9789	-2.0635	-1.2030
H	-0.7760	2.0965	-0.1103
H	3.7517	-0.1140	-1.3517
C	3.9182	-0.9408	0.5516
N	4.4400	-1.6926	1.2654
O	-2.3757	0.1173	-0.8235
C	-3.1584	-0.0719	0.2649
F	-2.9191	0.8298	1.2484
F	-3.0036	-1.2982	0.8175
F	-4.4336	0.0585	-0.1209

OH-CN-IND-A-54.out
Total energy (hartree): -515.282992
Corrected energy (hartree): -515.175261

C	-0.7652	2.0310	-0.0776
C	-1.9780	1.5219	0.2167
C	-1.8627	0.0384	0.5573
C	-0.3784	-0.2331	0.3454

C	0.3540	-1.4057	0.4641
C	1.7370	-1.3656	0.2350
C	2.3656	-0.1582	-0.1067
C	1.6308	1.0291	-0.2321
C	0.2554	0.9765	-0.0072
H	-0.5613	3.0695	-0.3327
H	-2.9261	2.0535	0.2370
H	-0.1251	-2.3509	0.7203
H	2.3284	-2.2792	0.3195
H	2.1417	1.9520	-0.5028
H	-2.1329	-0.1175	1.6168
C	-2.7505	-0.8158	-0.2438
N	-3.4582	-1.4965	-0.8631
O	3.7147	-0.0770	-0.3363
H	4.1170	-0.9480	-0.2320

OH-CN-IND-A-55.out
Total energy (hartree): -515.282679
Corrected energy (hartree): -515.174964

C	-0.7497	2.0308	-0.0716
C	-1.9666	1.5310	0.2218
C	-1.8619	0.0457	0.5568
C	-0.3798	-0.2368	0.3445
C	0.3456	-1.4167	0.4624
C	1.7264	-1.3908	0.2362
C	2.3651	-0.1881	-0.1028
C	1.6401	1.0057	-0.2274
C	0.2614	0.9672	-0.0041
H	-0.5381	3.0687	-0.3238
H	-2.9105	2.0701	0.2438
H	-0.1427	-2.3577	0.7170
H	2.3256	-2.2966	0.3154
H	2.1432	1.9368	-0.4952
H	-2.1332	-0.1123	1.6157
C	-2.7569	-0.7974	-0.2481
N	-3.4714	-1.4672	-0.8713
O	3.7199	-0.2463	-0.3051
H	4.0541	0.6280	-0.5400

OMe-CN-IND-A-88.out
Total energy (hartree): -554.583688
Corrected energy (hartree): -554.449898

C	0.9975	2.0239	-0.0060
C	2.2627	1.6168	-0.2308

C	2.2900	0.1190	-0.5226
C	0.8266	-0.2744	-0.3647
C	0.1995	-1.5125	-0.4747
C	-1.1846	-1.5843	-0.3062
C	-1.9375	-0.4265	-0.0309
C	-1.3110	0.8246	0.0844
C	0.0779	0.8804	-0.0823
H	0.6927	3.0480	0.2036
H	3.1611	2.2290	-0.2297
H	0.7686	-2.4197	-0.6787
H	-1.7093	-2.5357	-0.3805
H	-1.8742	1.7290	0.3006
H	2.6196	-0.0470	-1.5636
C	3.2108	-0.6273	0.3459
N	3.9469	-1.2205	1.0199
O	-3.2816	-0.6262	0.1106
C	-4.1042	0.4983	0.4029
H	-3.8199	0.9625	1.3599
H	-4.0552	1.2489	-0.4012
H	-5.1242	0.1092	0.4757

OMe-CN-IND-A-90.out
Total energy (hartree): -554.583814
Corrected energy (hartree): -554.450025

C	-1.3927	2.0133	-0.1019
C	-2.5512	1.3860	0.1822
C	-2.2908	-0.0741	0.5449
C	-0.7830	-0.1949	0.3581
C	0.0651	-1.2801	0.5031
C	1.4445	-1.1075	0.2942
C	1.9531	0.1544	-0.0563
C	1.0930	1.2575	-0.2081
C	-0.2702	1.0703	-0.0029
H	-1.2929	3.0641	-0.3684
H	-3.5489	1.8179	0.1815
H	-0.3180	-2.2663	0.7666
H	2.1046	-1.9637	0.4052
H	1.5119	2.2240	-0.4849
H	-2.5612	-0.2446	1.6020
C	-3.0743	-1.0235	-0.2581
N	-3.6997	-1.7790	-0.8792
O	3.2766	0.4135	-0.2759
C	4.2071	-0.6571	-0.1502
H	4.2070	-1.0685	0.8708

H	3.9922	-1.4596	-0.8723
H	5.1880	-0.2240	-0.3682

SH-CN-IND-A-58.out
Total energy (hartree): -838.255901
Corrected energy (hartree): -838.154955

C	-1.1891	2.0311	-0.0722
C	-2.4055	1.5121	0.1874
C	-2.2876	0.0300	0.5328
C	-0.7959	-0.2298	0.3629
C	-0.0578	-1.3970	0.5025
C	1.3307	-1.3470	0.3145
C	1.9672	-0.1371	-0.0095
C	1.2187	1.0433	-0.1562
C	-0.1632	0.9841	0.0287
H	-0.9862	3.0711	-0.3222
H	-3.3583	2.0356	0.1801
H	-0.5366	-2.3461	0.7449
H	1.9160	-2.2598	0.4205
H	1.7087	1.9825	-0.4134
H	-2.5821	-0.1271	1.5857
C	-3.1456	-0.8343	-0.2892
N	-3.8303	-1.5220	-0.9261
S	3.7375	-0.0190	-0.2535
H	4.0192	-1.3309	-0.0668

SH-CN-IND-A-59.out
Total energy (hartree): -838.255821
Corrected energy (hartree): -838.154997

C	-1.1893	2.0317	-0.0697
C	-2.4055	1.5126	0.1905
C	-2.2872	0.0301	0.5330
C	-0.7955	-0.2295	0.3624
C	-0.0571	-1.3971	0.5021
C	1.3302	-1.3459	0.3132
C	1.9671	-0.1348	-0.0102
C	1.2195	1.0450	-0.1555
C	-0.1633	0.9844	0.0289
H	-0.9867	3.0721	-0.3183
H	-3.3582	2.0364	0.1847
H	-0.5358	-2.3462	0.7442
H	1.9201	-2.2567	0.4157
H	1.7050	1.9870	-0.4093
H	-2.5817	-0.1294	1.5856

C	-3.1457	-0.8317	-0.2911
N	-3.8316	-1.5163	-0.9302
S	3.7446	-0.1792	-0.2236
H	3.9070	1.1293	-0.5357

SiH3-CN-IND-A-60.out
Total energy (hartree): -730.753260
Corrected energy (hartree): -730.638443

C	1.2314	2.0328	0.0788
C	2.4479	1.5122	-0.1769
C	2.3272	0.0313	-0.5264
C	0.8333	-0.2270	-0.3625
C	0.1011	-1.3955	-0.5109
C	-1.2903	-1.3376	-0.3275
C	-1.9479	-0.1346	-0.0025
C	-1.1815	1.0399	0.1474
C	0.2025	0.9892	-0.0286
H	1.0300	3.0727	0.3301
H	3.4020	2.0331	-0.1646
H	0.5855	-2.3417	-0.7538
H	-1.8693	-2.2551	-0.4403
H	-1.6605	1.9873	0.4024
H	2.6199	-0.1253	-1.5798
C	3.1800	-0.8392	0.2937
N	3.8620	-1.5295	0.9306
Si	-3.8258	-0.1012	0.2350
H	-4.1741	0.3358	1.6216
H	-4.3705	-1.4706	-0.0045
H	-4.4580	0.8578	-0.7224

SiH3-CN-IND-A-62.out
Total energy (hartree): -730.753260
Corrected energy (hartree): -730.638444

C	1.2314	2.0328	0.0788
C	2.4479	1.5122	-0.1769
C	2.3272	0.0313	-0.5264
C	0.8333	-0.2270	-0.3625
C	0.1011	-1.3955	-0.5109
C	-1.2903	-1.3376	-0.3275
C	-1.9479	-0.1346	-0.0025
C	-1.1815	1.0399	0.1474
C	0.2025	0.9892	-0.0286
H	1.0300	3.0727	0.3301
H	3.4020	2.0331	-0.1646

H	0.5855	-2.3417	-0.7538
H	-1.8693	-2.2551	-0.4403
H	-1.6605	1.9873	0.4024
H	2.6199	-0.1253	-1.5798
C	3.1800	-0.8392	0.2937
N	3.8620	-1.5295	0.9306
Si	-3.8258	-0.1012	0.2350
H	-4.1741	0.3359	1.6216
H	-4.3705	-1.4706	-0.0045
H	-4.4580	0.8578	-0.7224

SiMe3-CN-IND-A-65.out
Total energy (hartree): -848.745922
Corrected energy (hartree): -848.551657

C	2.1942	2.0234	0.0685
C	3.4158	1.5005	-0.1569
C	3.2996	0.0207	-0.5134
C	1.8008	-0.2329	-0.3900
C	1.0660	-1.3967	-0.5615
C	-0.3298	-1.3315	-0.4144
C	-0.9976	-0.1302	-0.1027
C	-0.2234	1.0367	0.0705
C	1.1649	0.9834	-0.0687
H	1.9898	3.0634	0.3176
H	4.3708	2.0185	-0.1182
H	1.5520	-2.3446	-0.7951
H	-0.9040	-2.2487	-0.5467
H	-0.7010	1.9873	0.3172
H	3.6210	-0.1350	-1.5584
C	4.1276	-0.8533	0.3283
N	4.7906	-1.5462	0.9823
Si	-2.8916	-0.0551	0.0972
C	-3.6428	-1.7613	-0.2305
H	-3.2696	-2.5177	0.4748
H	-4.7358	-1.7185	-0.1173
H	-3.4319	-2.1155	-1.2498
C	-3.5925	1.2022	-1.1371
H	-4.6833	1.2946	-1.0288
H	-3.1599	2.2019	-0.9853
H	-3.3822	0.9045	-2.1743
C	-3.3053	0.4988	1.8623
H	-2.8808	1.4884	2.0860
H	-4.3935	0.5654	2.0099
H	-2.9082	-0.2072	2.6055

tBu-CN-IND-A-66.out
Total energy (hartree): -597.314011
Corrected energy (hartree): -597.104273

C	1.8294	2.0203	0.0707
C	3.0520	1.5057	-0.1686
C	2.9423	0.0252	-0.5261
C	1.4468	-0.2367	-0.3883
C	0.7087	-1.3971	-0.5520
C	-0.6861	-1.3382	-0.3889
C	-1.3528	-0.1431	-0.0680
C	-0.5788	1.0233	0.0974
C	0.8057	0.9737	-0.0578
H	1.6214	3.0587	0.3238
H	4.0037	2.0301	-0.1386
H	1.1887	-2.3461	-0.7926
H	-1.2497	-2.2588	-0.5171
H	-1.0540	1.9700	0.3518
H	3.2575	-0.1271	-1.5735
C	3.7836	-0.8430	0.3086
N	4.4569	-1.5317	0.9568
C	-2.8802	-0.0692	0.1134
C	-3.2014	0.4022	1.5508
H	-2.7862	1.3970	1.7556
H	-4.2893	0.4557	1.6992
H	-2.7886	-0.2949	2.2924
C	-3.5633	-1.4304	-0.1100
H	-4.6475	-1.3228	0.0272
H	-3.3942	-1.8109	-1.1264
H	-3.2133	-2.1868	0.6053
C	-3.4685	0.9381	-0.9019
H	-3.2519	0.6268	-1.9329
H	-4.5597	1.0006	-0.7855
H	-3.0589	1.9464	-0.7609

tBu-CN-IND-A-67.out
Total energy (hartree): -597.314011
Corrected energy (hartree): -597.104270

C	1.8294	2.0203	0.0707
C	3.0520	1.5057	-0.1686
C	2.9423	0.0252	-0.5261
C	1.4468	-0.2367	-0.3883
C	0.7087	-1.3971	-0.5520
C	-0.6861	-1.3382	-0.3889

C	-1.3528	-0.1431	-0.0680
C	-0.5788	1.0233	0.0975
C	0.8057	0.9737	-0.0578
H	1.6214	3.0587	0.3238
H	4.0037	2.0301	-0.1386
H	1.1887	-2.3461	-0.7926
H	-1.2497	-2.2588	-0.5171
H	-1.0540	1.9700	0.3518
H	3.2575	-0.1271	-1.5735
C	3.7836	-0.8430	0.3086
N	4.4569	-1.5317	0.9568
C	-2.8802	-0.0692	0.1134
C	-3.4685	0.9381	-0.9019
H	-3.2519	0.6268	-1.9329
H	-4.5597	1.0006	-0.7855
H	-3.0589	1.9464	-0.7609
C	-3.2014	0.4022	1.5508
H	-4.2893	0.4557	1.6992
H	-2.7886	-0.2949	2.2924
H	-2.7862	1.3970	1.7556
C	-3.5633	-1.4304	-0.1100
H	-3.2133	-2.1868	0.6053
H	-4.6475	-1.3228	0.0272
H	-3.3942	-1.8109	-1.1264

tBu-CN-IND-A-68.out
Total energy (hartree): -597.314011
Corrected energy (hartree): -597.104281

C	1.8294	2.0203	0.0707
C	3.0520	1.5057	-0.1686
C	2.9423	0.0252	-0.5261
C	1.4468	-0.2367	-0.3883
C	0.7087	-1.3971	-0.5520
C	-0.6861	-1.3382	-0.3889
C	-1.3528	-0.1431	-0.0680
C	-0.5788	1.0233	0.0974
C	0.8057	0.9737	-0.0578
H	1.6214	3.0587	0.3238
H	4.0037	2.0301	-0.1386
H	1.1887	-2.3461	-0.7926
H	-1.2497	-2.2588	-0.5172
H	-1.0540	1.9700	0.3518
H	3.2575	-0.1271	-1.5735
C	3.7836	-0.8430	0.3086

N	4.4569	-1.5317	0.9567
C	-2.8802	-0.0692	0.1134
C	-3.5633	-1.4304	-0.1100
H	-3.2133	-2.1868	0.6053
H	-4.6475	-1.3228	0.0272
H	-3.3942	-1.8109	-1.1264
C	-3.4685	0.9381	-0.9019
H	-4.5597	1.0006	-0.7855
H	-3.0589	1.9464	-0.7609
H	-3.2520	0.6268	-1.9329
C	-3.2014	0.4022	1.5508
H	-2.7861	1.3970	1.7556
H	-4.2893	0.4558	1.6991
H	-2.7886	-0.2949	2.2924

Vin-CN-IND-A-69.out
Total energy (hartree): -517.453920
Corrected energy (hartree): -517.319332

C	0.9815	2.0301	0.0085
C	2.2385	1.6015	-0.2193
C	2.2422	0.1047	-0.5196
C	0.7726	-0.2674	-0.3595
C	0.1333	-1.4931	-0.4712
C	-1.2573	-1.5361	-0.2984
C	-2.0118	-0.3790	-0.0195
C	-1.3417	0.8576	0.0947
C	0.0401	0.9044	-0.0712
H	0.6952	3.0583	0.2232
H	3.1473	2.1982	-0.2169
H	0.6895	-2.4076	-0.6780
H	-1.7735	-2.4932	-0.3799
H	-1.8958	1.7692	0.3149
H	2.5614	-0.0625	-1.5636
C	3.1528	-0.6649	0.3389
N	3.8807	-1.2758	1.0056
C	-3.4712	-0.5126	0.1451
H	-3.8505	-1.5326	0.0393
C	-4.3550	0.4638	0.4036
H	-4.0664	1.5082	0.5241
H	-5.4162	0.2397	0.5044

Vin-CN-IND-A-70.out
Total energy (hartree): -517.453776
Corrected energy (hartree): -517.319198

C	-1.3063	2.0185	-0.0901
C	-2.4774	1.4105	0.1848
C	-2.2415	-0.0561	0.5363
C	-0.7357	-0.2019	0.3524
C	0.0909	-1.3113	0.4943
C	1.4659	-1.1545	0.2929
C	2.0265	0.0954	-0.0473
C	1.1715	1.2060	-0.1905
C	-0.2022	1.0534	0.0053
H	-1.1861	3.0695	-0.3474
H	-3.4676	1.8591	0.1851
H	-0.3165	-2.2901	0.7481
H	2.1127	-2.0237	0.4011
H	1.5888	2.1781	-0.4569
H	-2.5099	-0.2301	1.5936
C	-3.0381	-0.9898	-0.2711
N	-3.6747	-1.7314	-0.8975
C	3.4732	0.2859	-0.2629
H	3.7637	1.3077	-0.5229
C	4.4417	-0.6390	-0.1763
H	4.2458	-1.6812	0.0762
H	5.4816	-0.3722	-0.3606

Coordinates and energies of CN-IIN

Files are named according to the convention:

[**5-substituent**]-[**model system** (three elements)]-[**conformer number**].out

Conformer numeration is not continous since many of the starting conformers converged to one or a few optimized geometries. The redundant ones were excluded.

BF2-CN-IIN-A-1.out
Total energy (hartree): -755.457802
Corrected energy (hartree): -755.365569

C	1.5087	1.7311	-0.0560
N	2.6709	1.0136	-0.2976
C	2.4654	-0.4061	-0.5424
C	0.9534	-0.5392	-0.3826
C	0.1480	-1.6706	-0.4803
C	-1.2292	-1.5001	-0.3075
C	-1.7983	-0.2332	-0.0411
C	-0.9578	0.8919	0.0579
C	0.4122	0.7181	-0.1140
O	1.4372	2.9278	0.1476
H	3.5783	1.4576	-0.3171
H	2.7668	-0.6849	-1.5665
H	0.5679	-2.6572	-0.6750
H	-1.8840	-2.3687	-0.3780
H	-1.3611	1.8824	0.2662
B	-3.3283	-0.0860	0.1437
F	-3.8957	1.0988	0.3990
F	-4.1527	-1.1384	0.0543
C	3.2241	-1.2685	0.3877
N	3.8367	-1.9571	1.0920

Br-CN-IIN-A-2.out
Total energy (hartree): -3104.914173
Corrected energy (hartree): -3104.830547

C	1.8447	1.7361	-0.0230
N	3.0076	1.0245	-0.2738
C	2.8044	-0.3906	-0.5496
C	1.2924	-0.5262	-0.4011
C	0.4797	-1.6491	-0.5252
C	-0.9004	-1.4862	-0.3565

C	-1.4318	-0.2196	-0.0694
C	-0.6217	0.9093	0.0623
C	0.7491	0.7231	-0.1084
O	1.7700	2.9282	0.2058
H	3.9147	1.4694	-0.2782
H	3.1159	-0.6455	-1.5767
H	0.8902	-2.6358	-0.7387
H	-1.5658	-2.3428	-0.4455
H	-1.0291	1.8923	0.2888
Br	-3.3256	-0.0427	0.1492
C	3.5603	-1.2696	0.3675
N	4.1709	-1.9722	1.0599

CHO-CN-IIN-A-3.out
Total energy (hartree): -644.699612
Corrected energy (hartree): -644.596347

C	1.2977	1.7053	-0.0104
N	2.3921	0.9058	-0.3019
C	2.0676	-0.4865	-0.5755
C	0.5544	-0.5040	-0.3781
C	-0.3427	-1.5677	-0.4829
C	-1.6951	-1.2999	-0.2691
C	-2.1384	0.0025	0.0446
C	-1.2244	1.0595	0.1518
C	0.1237	0.7834	-0.0630
O	1.3240	2.8982	0.2251
H	3.3313	1.2767	-0.3355
H	2.3204	-0.7611	-1.6138
H	-0.0056	-2.5777	-0.7151
H	-2.4379	-2.0939	-0.3383
H	-1.5501	2.0711	0.3971
C	-3.5861	0.2638	0.2665
H	-3.8393	1.3206	0.5145
O	-4.4546	-0.5817	0.1912
C	2.7785	-1.4296	0.3130
N	3.3527	-2.1811	0.9846

CHO-CN-IIN-A-6.out
Total energy (hartree): -644.698573
Corrected energy (hartree): -644.595408

C	0.9886	1.7612	-0.0506
N	2.2074	1.1492	-0.3037
C	2.1276	-0.2822	-0.5523
C	0.6356	-0.5510	-0.3783

C	-0.0630	-1.7505	-0.4700
C	-1.4486	-1.7044	-0.2819
C	-2.1121	-0.4933	-0.0103
C	-1.3916	0.7095	0.0846
C	-0.0159	0.6543	-0.1010
O	0.8137	2.9459	0.1563
H	3.0711	1.6729	-0.3321
H	2.4427	-0.5294	-1.5804
H	0.4421	-2.6950	-0.6703
H	-2.0315	-2.6248	-0.3445
H	-1.9028	1.6470	0.2988
C	-3.5882	-0.5049	0.1782
H	-4.0648	-1.5097	0.0907
O	-4.2577	0.4805	0.4097
C	2.9694	-1.0771	0.3664
N	3.6474	-1.7123	1.0610

Cl-CN-IIN-A-8.out

Total energy (hartree): -990.978354

Corrected energy (hartree): -990.893061

C	1.1965	1.7381	-0.0219
N	2.3575	1.0331	-0.2984
C	2.1565	-0.3834	-0.5684
C	0.6491	-0.5276	-0.3855
C	-0.1597	-1.6556	-0.4901
C	-1.5359	-1.5007	-0.2900
C	-2.0675	-0.2370	0.0084
C	-1.2621	0.8972	0.1204
C	0.1051	0.7188	-0.0815
O	1.1199	2.9299	0.2077
H	3.2617	1.4833	-0.3238
H	2.4464	-0.6374	-1.6020
H	0.2518	-2.6399	-0.7122
H	-2.2025	-2.3581	-0.3619
H	-1.6747	1.8761	0.3557
Cl	-3.8024	-0.0860	0.2500
C	2.9380	-1.2571	0.3323
N	3.5680	-1.9555	1.0113

COCH3-CN-IIN-A-56.out

Total energy (hartree): -684.024533

Corrected energy (hartree): -683.895924

C	1.5479	1.7151	-0.0450

N	2.6879	0.9633	-0.2927
C	2.4400	-0.4473	-0.5489
C	0.9257	-0.5360	-0.3848
C	0.0851	-1.6389	-0.4848
C	-1.2871	-1.4291	-0.3038
C	-1.8095	-0.1489	-0.0306
C	-0.9412	0.9517	0.0707
C	0.4200	0.7354	-0.1065
O	1.5161	2.9118	0.1654
H	3.6075	1.3810	-0.3143
H	2.7309	-0.7262	-1.5760
H	0.4713	-2.6377	-0.6867
H	-1.9569	-2.2839	-0.3766
H	-1.3375	1.9425	0.2854
C	-3.2863	0.0860	0.1628
O	-3.7016	1.2119	0.3810
C	-4.2375	-1.0919	0.0822
H	-3.9862	-1.8503	0.8378
H	-5.2564	-0.7315	0.2515
H	-4.1795	-1.5755	-0.9038
C	3.1754	-1.3403	0.3714
N	3.7687	-2.0550	1.0663

COCH3-CN-IIN-A-57.out
Total energy (hartree): -684.026131
Corrected energy (hartree): -683.897178

C	1.4394	1.7414	-0.0713
N	2.6223	1.0589	-0.3099
C	2.4592	-0.3696	-0.5399
C	0.9521	-0.5454	-0.3798
C	0.1733	-1.6978	-0.4696
C	-1.2057	-1.5641	-0.2998
C	-1.8023	-0.3110	-0.0435
C	-1.0002	0.8366	0.0493
C	0.3750	0.6958	-0.1212
O	1.3300	2.9373	0.1249
H	3.5165	1.5290	-0.3285
H	2.7712	-0.6491	-1.5605
H	0.6170	-2.6754	-0.6573
H	-1.8581	-2.4337	-0.3609
H	-1.4158	1.8224	0.2491
C	-3.2994	-0.2571	0.1242
O	-3.9634	-1.2764	0.0271
C	-3.9551	1.0780	0.4121

H	-3.7502	1.7956	-0.3957
H	-5.0348	0.9278	0.5027
H	-3.5643	1.5125	1.3436
C	3.2438	-1.1968	0.4005
N	3.8786	-1.8556	1.1135

COCH3-CN-IIN-A-59.out
Total energy (hartree): -684.026130
Corrected energy (hartree): -683.897177

C	1.4390	1.7419	-0.0709
N	2.6223	1.0594	-0.3075
C	2.4592	-0.3687	-0.5394
C	0.9522	-0.5450	-0.3793
C	0.1737	-1.6976	-0.4690
C	-1.2054	-1.5642	-0.2995
C	-1.8023	-0.3111	-0.0434
C	-1.0005	0.8366	0.0495
C	0.3749	0.6961	-0.1208
O	1.3291	2.9381	0.1240
H	3.5159	1.5303	-0.3299
H	2.7710	-0.6469	-1.5605
H	0.6177	-2.6750	-0.6566
H	-1.8575	-2.4339	-0.3607
H	-1.4163	1.8223	0.2492
C	-3.2994	-0.2576	0.1240
O	-3.9632	-1.2770	0.0266
C	-3.9554	1.0773	0.4118
H	-5.0351	0.9269	0.5025
H	-3.5648	1.5120	1.3434
H	-3.7507	1.7949	-0.3959
C	3.2443	-1.1971	0.3996
N	3.8794	-1.8570	1.1115

CONH2-CN-IIN-A-10.out
Total energy (hartree): -700.094241
Corrected energy (hartree): -699.976239

C	1.4640	1.7359	-0.0142
N	2.6337	1.0427	-0.2830
C	2.4455	-0.3754	-0.5572
C	0.9363	-0.5310	-0.3954
C	0.1352	-1.6641	-0.5111
C	-1.2411	-1.5102	-0.3259
C	-1.8130	-0.2552	-0.0365
C	-0.9888	0.8724	0.0875

C	0.3821	0.7113	-0.0947
O	1.3748	2.9266	0.2225
H	3.5363	1.4967	-0.2850
H	2.7487	-0.6265	-1.5878
H	0.5574	-2.6452	-0.7278
H	-1.9099	-2.3663	-0.3952
H	-1.3696	1.8607	0.3426
C	-3.3114	-0.2190	0.1463
O	-3.9649	-1.2507	0.2521
N	-3.8997	1.0136	0.2010
H	-4.9059	1.0417	0.2805
H	-3.4129	1.8662	-0.0239
C	3.2218	-1.2444	0.3518
N	3.8508	-1.9358	1.0387

CONH2-CN-IIN-A-11.out
Total energy (hartree): -700.092655
Corrected energy (hartree): -699.973881

C	1.5024	1.7280	0.0411
N	2.6587	1.0115	-0.2345
C	2.4404	-0.3900	-0.5581
C	0.9269	-0.5147	-0.4120
C	0.1069	-1.6254	-0.5786
C	-1.2699	-1.4518	-0.3951
C	-1.8152	-0.1968	-0.0615
C	-0.9740	0.9158	0.0885
C	0.3946	0.7313	-0.0790
O	1.4459	2.9115	0.3123
H	3.5704	1.4468	-0.2247
H	2.7459	-0.6152	-1.5941
H	0.5110	-2.6028	-0.8415
H	-1.9277	-2.3068	-0.5487
H	-1.3917	1.8922	0.3271
C	-3.2962	0.0251	0.1142
O	-3.8000	1.1290	-0.0452
N	-4.0475	-1.0787	0.4328
H	-5.0229	-0.9108	0.6385
H	-3.6253	-1.9036	0.8315
C	3.1848	-1.3105	0.3272
N	3.7843	-2.0456	0.9952

CONH2-CN-IIN-A-9.out
Total energy (hartree): -700.094395
Corrected energy (hartree): -699.975946

C	1.4699	1.7259	-0.1254
N	2.6375	1.0127	-0.3471
C	2.4449	-0.4193	-0.5299
C	0.9341	-0.5583	-0.3664
C	0.1278	-1.6919	-0.4314
C	-1.2496	-1.5215	-0.2701
C	-1.8139	-0.2516	-0.0369
C	-0.9870	0.8790	0.0230
C	0.3842	0.7021	-0.1433
O	1.3855	2.9288	0.0395
H	3.5422	1.4619	-0.3713
H	2.7530	-0.7387	-1.5398
H	0.5464	-2.6843	-0.5977
H	-1.9242	-2.3741	-0.3264
H	-1.3759	1.8864	0.1656
C	-3.3143	-0.1886	0.1118
O	-4.0314	-1.1101	-0.2603
N	-3.8304	0.9531	0.6616
H	-4.8279	0.9744	0.8194
H	-3.2589	1.6237	1.1512
C	3.2113	-1.2297	0.4398
N	3.8312	-1.8764	1.1766

COOCH3-CN-IIN-A-42.out
Total energy (hartree): -759.269062
Corrected energy (hartree): -759.136425

C	2.0084	1.6815	-0.0325
N	3.1178	0.8829	-0.2714
C	2.8120	-0.5147	-0.5363
C	1.2931	-0.5385	-0.3906
C	0.4066	-1.6047	-0.5074
C	-0.9568	-1.3404	-0.3422
C	-1.4186	-0.0382	-0.0667
C	-0.5125	1.0261	0.0521
C	0.8413	0.7516	-0.1115
O	2.0251	2.8777	0.1840
H	4.0548	1.2604	-0.2793
H	3.1027	-0.8024	-1.5610
H	0.7527	-2.6178	-0.7110
H	-1.6769	-2.1512	-0.4252
H	-0.8664	2.0324	0.2682
C	-2.8737	0.2630	0.1121
O	-3.3144	1.3698	0.3440
O	-3.6504	-0.8356	-0.0131

C	-5.0662	-0.6131	0.1512
H	-5.2737	-0.2146	1.1513
H	-5.4289	0.0954	-0.6028
H	-5.5303	-1.5939	0.0192
C	3.4977	-1.4414	0.3889
N	4.0531	-2.1815	1.0884

COOCH3-CN-IIN-A-47.out
Total energy (hartree): -759.251713
Corrected energy (hartree): -759.119863

C	1.6240	1.6951	-0.3889
N	2.8372	1.0261	-0.4362
C	2.7274	-0.4259	-0.4334
C	1.2173	-0.6281	-0.3512
C	0.4751	-1.8057	-0.3161
C	-0.9175	-1.6964	-0.2771
C	-1.5548	-0.4400	-0.2438
C	-0.7940	0.7364	-0.2764
C	0.5921	0.6169	-0.3371
O	1.4704	2.9019	-0.3931
H	3.7186	1.5193	-0.4651
H	3.1231	-0.8595	-1.3673
H	0.9520	-2.7855	-0.3228
H	-1.5349	-2.5934	-0.2836
H	-1.2517	1.7239	-0.2831
C	-3.0596	-0.4247	-0.2966
O	-3.6675	-1.1442	-1.0555
O	-3.7502	0.4291	0.4976
C	-3.1756	1.0381	1.6706
H	-2.3664	0.4293	2.0887
H	-2.8080	2.0448	1.4373
H	-3.9934	1.1089	2.3948
C	3.4569	-1.0549	0.6876
N	4.0474	-1.5615	1.5480

COOCH3-CN-IIN-A-49.out
Total energy (hartree): -759.269830
Corrected energy (hartree): -759.137098

C	1.7148	1.7755	-0.0883
N	2.9398	1.1559	-0.2859
C	2.8622	-0.2812	-0.5037
C	1.3636	-0.5392	-0.3783
C	0.6560	-1.7350	-0.4708
C	-0.7334	-1.6794	-0.3350

C	-1.3986	-0.4582	-0.1106
C	-0.6733	0.7385	-0.0145
C	0.7107	0.6717	-0.1506
O	1.5374	2.9660	0.0878
H	3.8061	1.6757	-0.2926
H	3.2146	-0.5535	-1.5130
H	1.1588	-2.6878	-0.6343
H	-1.3319	-2.5866	-0.3990
H	-1.1679	1.6906	0.1619
C	-2.8890	-0.4960	0.0212
O	-3.5536	-1.5094	-0.0612
O	-3.4174	0.7254	0.2421
C	-4.8526	0.7662	0.3803
H	-5.3320	0.3955	-0.5334
H	-5.1691	0.1512	1.2310
H	-5.0962	1.8183	0.5487
C	3.6676	-1.0548	0.4647
N	4.3200	-1.6712	1.1994

COOCH3-CN-IIN-A-54.out
Total energy (hartree): -759.251236
Corrected energy (hartree): -759.119587

C	-1.5661	1.7460	-0.2414
N	-2.7752	1.2069	0.1690
C	-2.6958	-0.1697	0.6366
C	-1.2161	-0.4858	0.4375
C	-0.5142	-1.6648	0.6750
C	0.8567	-1.6722	0.4033
C	1.5184	-0.5213	-0.0701
C	0.7964	0.6553	-0.3118
C	-0.5730	0.6457	-0.0596
O	-1.3867	2.8795	-0.6454
H	-3.6336	1.7393	0.1445
H	-2.9639	-0.2451	1.7042
H	-1.0095	-2.5640	1.0404
H	1.4352	-2.5843	0.5417
H	1.2646	1.5522	-0.7128
C	2.9781	-0.6567	-0.4143
O	3.3974	-1.6311	-0.9954
O	3.8401	0.3400	-0.0948
C	3.5451	1.3391	0.9002
H	3.1723	2.2539	0.4235
H	2.8198	0.9767	1.6371
H	4.4978	1.5507	1.3962

C	-3.5912	-1.0828	-0.1039
N	-4.3131	-1.8046	-0.6547

COOH-CN-IIN-A-15.out
Total energy (hartree): -719.967703
Corrected energy (hartree): -719.860068

C	1.4563	1.7359	-0.0587
N	2.6267	1.0329	-0.3028
C	2.4382	-0.3899	-0.5448
C	0.9287	-0.5411	-0.3814
C	0.1346	-1.6813	-0.4772
C	-1.2428	-1.5295	-0.3032
C	-1.8098	-0.2672	-0.0379
C	-0.9988	0.8728	0.0623
C	0.3726	0.7090	-0.1128
O	1.3702	2.9319	0.1442
H	3.5283	1.4883	-0.3250
H	2.7413	-0.6662	-1.5690
H	0.5633	-2.6639	-0.6724
H	-1.9071	-2.3895	-0.3683
H	-1.4184	1.8544	0.2704
C	-3.2913	-0.1970	0.1322
O	-4.0402	-1.1481	0.0518
O	-3.7337	1.0592	0.3904
H	-4.6980	1.0019	0.4847
C	3.2104	-1.2403	0.3852
N	3.8349	-1.9183	1.0894

COOH-CN-IIN-A-6.out
Total energy (hartree): -719.967101
Corrected energy (hartree): -719.859514

C	1.5078	1.7271	-0.0482
N	2.6578	0.9919	-0.2968
C	2.4297	-0.4230	-0.5484
C	0.9168	-0.5334	-0.3827
C	0.0929	-1.6505	-0.4814
C	-1.2816	-1.4645	-0.3024
C	-1.8129	-0.1882	-0.0303
C	-0.9699	0.9286	0.0718
C	0.3951	0.7309	-0.1063
O	1.4570	2.9235	0.1606
H	3.5716	1.4223	-0.3194
H	2.7228	-0.7008	-1.5752
H	0.4949	-2.6431	-0.6822

H	-1.9544	-2.3162	-0.3717
H	-1.3788	1.9143	0.2858
C	-3.2781	0.0246	0.1612
O	-3.7938	1.0967	0.3933
O	-4.0003	-1.1209	0.0482
H	-4.9291	-0.8769	0.1891
C	3.1791	-1.3023	0.3736
N	3.7845	-2.0046	1.0706

Et-CN-IIN-A-79.out

Total energy (hartree): -609.997370

Corrected energy (hartree): -609.848688

C	1.4620	1.6778	-0.0080
N	2.5320	0.8458	-0.3040
C	2.1655	-0.5365	-0.5783
C	0.6524	-0.5040	-0.3857
C	-0.2886	-1.5194	-0.4919
C	-1.6358	-1.1942	-0.2744
C	-2.0507	0.1125	0.0441
C	-1.0755	1.1198	0.1484
C	0.2593	0.7961	-0.0659
O	1.5339	2.8690	0.2338
H	3.4828	1.1863	-0.3242
H	2.4197	-0.8191	-1.6139
H	-0.0019	-2.5444	-0.7271
H	-2.3759	-1.9882	-0.3553
H	-1.3501	2.1459	0.3959
C	-3.5075	0.4744	0.2821
H	-3.5886	0.9124	1.2892
H	-3.7722	1.2883	-0.4108
C	-4.5273	-0.6568	0.1417
H	-5.5389	-0.2742	0.3293
H	-4.5187	-1.0894	-0.8687
H	-4.3411	-1.4660	0.8617
C	2.8469	-1.4977	0.3151
N	3.3980	-2.2651	0.9885

Et-CN-IIN-A-81.out

Total energy (hartree): -609.998556

Corrected energy (hartree): -609.850317

C	1.2565	1.7267	0.0060
N	2.4263	1.0011	-0.1669

C	2.2227	-0.4045	-0.4871
C	0.7012	-0.5146	-0.4643
C	-0.1208	-1.6150	-0.6847
C	-1.5052	-1.4172	-0.6230
C	-2.0741	-0.1572	-0.3479
C	-1.2219	0.9355	-0.1291
C	0.1558	0.7378	-0.1878
O	1.1882	2.9166	0.2550
H	3.3374	1.4293	-0.0843
H	2.6146	-0.6466	-1.4895
H	0.2882	-2.6033	-0.8947
H	-2.1668	-2.2673	-0.7967
H	-1.6186	1.9291	0.0818
C	-3.5763	0.0028	-0.2533
H	-3.8554	1.0100	-0.5945
H	-4.0623	-0.7099	-0.9352
C	-4.1086	-0.2154	1.1743
H	-5.1998	-0.0919	1.2039
H	-3.8685	-1.2254	1.5342
H	-3.6634	0.5051	1.8740
C	2.8873	-1.3130	0.4716
N	3.4293	-2.0379	1.1974

Et-CN-IIN-A-82.out

Total energy (hartree): -609.997762

Corrected energy (hartree): -609.848856

C	1.0128	1.7563	-0.0754
N	2.2627	1.2022	-0.3115
C	2.2503	-0.2354	-0.5403
C	0.7692	-0.5650	-0.3845
C	0.1058	-1.7867	-0.4720
C	-1.2806	-1.7865	-0.2993
C	-2.0143	-0.6069	-0.0429
C	-1.3215	0.6075	0.0436
C	0.0636	0.6062	-0.1274
O	0.7839	2.9362	0.1205
H	3.1023	1.7636	-0.3247
H	2.5979	-0.4808	-1.5582
H	0.6403	-2.7182	-0.6585
H	-1.8182	-2.7342	-0.3619
H	-1.8309	1.5484	0.2418
C	-3.5203	-0.7070	0.1304
H	-3.9400	-1.1628	-0.7803

H	-3.7236	-1.4281	0.9377
C	-4.2561	0.6009	0.4256
H	-5.3316	0.4101	0.5352
H	-3.9034	1.0631	1.3579
H	-4.1291	1.3310	-0.3858
C	3.1145	-0.9743	0.4049
N	3.8122	-1.5646	1.1196

Et-CN-IIN-A-83.out

Total energy (hartree): -609.998533

Corrected energy (hartree): -609.850410

C	-1.1984	1.7403	0.0049
N	-2.3478	1.0711	0.3999
C	-2.1617	-0.3507	0.6517
C	-0.6824	-0.5362	0.3279
C	0.1047	-1.6830	0.3565
C	1.4572	-1.5538	0.0200
C	2.0289	-0.3166	-0.3402
C	1.2108	0.8227	-0.3678
C	-0.1353	0.6937	-0.0333
O	-1.1171	2.9303	-0.2398
H	-3.2335	1.5458	0.5020
H	-2.3617	-0.5987	1.7079
H	-0.3103	-2.6568	0.6167
H	2.0891	-2.4433	0.0291
H	1.6075	1.7981	-0.6511
C	3.5048	-0.2174	-0.6606
H	3.8387	-1.1518	-1.1347
H	3.6624	0.5855	-1.3947
C	4.3663	0.0568	0.5850
H	5.4287	0.1253	0.3138
H	4.0738	1.0010	1.0644
H	4.2541	-0.7461	1.3267
C	-3.0504	-1.1996	-0.1704
N	-3.7635	-1.8767	-0.7861

F-CN-IIN-A-17.out

Total energy (hartree): -630.609609

Corrected energy (hartree): -630.522093

C	0.8009	1.7414	-0.0207
N	1.9591	1.0465	-0.3317
C	1.7623	-0.3723	-0.5930

C	0.2624	-0.5295	-0.3646
C	-0.5380	-1.6665	-0.4438
C	-1.9088	-1.5246	-0.2029
C	-2.4276	-0.2639	0.1076
C	-1.6449	0.8818	0.1970
C	-0.2828	0.7133	-0.0460
O	0.7205	2.9330	0.2098
H	2.8581	1.5045	-0.3842
H	2.0246	-0.6253	-1.6341
H	-0.1218	-2.6463	-0.6770
H	-2.5827	-2.3788	-0.2493
H	-2.0722	1.8518	0.4444
F	-3.7610	-0.1626	0.3338
C	2.5790	-1.2364	0.2857
N	3.2358	-1.9276	0.9465

H-CN-IIN-A-8.out

Total energy (hartree): -531.360644

Corrected energy (hartree): -531.263607

C	-0.3174	1.7507	0.0133
N	-1.5060	1.1312	0.3710
C	-1.3904	-0.2984	0.6187
C	0.0855	-0.5518	0.3234
C	0.8087	-1.7402	0.3645
C	2.1752	-1.6802	0.0624
C	2.7932	-0.4639	-0.2712
C	2.0565	0.7232	-0.3137
C	0.6964	0.6558	-0.0134
O	-0.1735	2.9379	-0.2140
H	-2.3691	1.6472	0.4673
H	-1.6203	-0.5422	1.6698
H	0.3353	-2.6902	0.6125
H	2.7686	-2.5945	0.0842
H	2.5156	1.6764	-0.5733
H	3.8585	-0.4502	-0.5019
C	-2.2995	-1.1034	-0.2246
N	-3.0297	-1.7456	-0.8572

iPr-CN-IIN-A-86.out

Total energy (hartree): -649.315207

Corrected energy (hartree): -649.140778

C	1.7077	1.7008	0.0530

N	2.8090	0.9177	-0.2615
C	2.4914	-0.4634	-0.5951
C	0.9758	-0.4871	-0.4226
C	0.0704	-1.5319	-0.5846
C	-1.2855	-1.2603	-0.3740
C	-1.7500	0.0210	-0.0081
C	-0.8154	1.0533	0.1507
C	0.5364	0.7828	-0.0574
O	1.7359	2.8829	0.3438
H	3.7483	1.2892	-0.2537
H	2.7677	-0.6962	-1.6374
H	0.3973	-2.5354	-0.8574
H	-2.0014	-2.0730	-0.4971
H	-1.1282	2.0583	0.4352
C	-3.2331	0.2791	0.2173
H	-3.3319	1.3452	0.4717
C	-3.7792	-0.5317	1.4068
H	-4.8303	-0.2734	1.5953
H	-3.7301	-1.6120	1.2093
H	-3.2071	-0.3292	2.3218
C	-4.0612	0.0308	-1.0564
H	-4.0320	-1.0274	-1.3528
H	-5.1127	0.3004	-0.8867
H	-3.6861	0.6286	-1.8976
C	3.1914	-1.4376	0.2692
N	3.7577	-2.2139	0.9195

iPr-CN-IIN-A-87.out

Total energy (hartree): -649.315264

Corrected energy (hartree): -649.140919

C	1.3858	1.7524	-0.0130
N	2.6120	1.1582	-0.2737
C	2.5430	-0.2674	-0.5616
C	1.0500	-0.5452	-0.4167
C	0.3408	-1.7327	-0.5525
C	-1.0487	-1.6857	-0.3774
C	-1.7327	-0.4927	-0.0730
C	-0.9899	0.6915	0.0619
C	0.3904	0.6447	-0.1101
O	1.2046	2.9315	0.2311
H	3.4732	1.6860	-0.2659
H	2.8803	-0.4836	-1.5895
H	0.8380	-2.6764	-0.7772

H	-1.6221	-2.6083	-0.4775
H	-1.4662	1.6419	0.3003
C	-3.2445	-0.4958	0.1051
H	-3.5783	-1.5370	-0.0210
C	-3.9438	0.3493	-0.9755
H	-5.0352	0.2818	-0.8680
H	-3.6631	1.4089	-0.8944
H	-3.6772	0.0057	-1.9840
C	-3.6546	-0.0456	1.5190
H	-3.3718	1.0006	1.7019
H	-4.7433	-0.1249	1.6444
H	-3.1749	-0.6650	2.2884
C	3.3785	-1.0775	0.3504
N	4.0534	-1.7231	1.0387

Me-CN-IIN-A-9.out

Total energy (hartree): -570.681731

Corrected energy (hartree): -570.560165

C	0.8345	1.7355	-0.0209
N	1.9977	1.0445	-0.325
C	1.8050	-0.3751	-0.5871
C	0.3034	-0.5327	-0.3703
C	-0.5016	-1.6655	-0.4570
C	-1.8716	-1.5113	-0.2237
C	-2.4458	-0.2613	0.0921
C	-1.6128	0.8620	0.1767
C	-0.2464	0.7070	-0.0548
O	0.7563	2.9279	0.2124
H	2.8972	1.5027	-0.3651
H	2.0764	-0.6322	-1.6250
H	-0.0872	-2.6467	-0.6894
H	-2.5187	-2.3878	-0.2852
H	-2.0129	1.8461	0.4207
C	-3.9325	-0.1527	0.3365
H	-4.5035	-0.4820	-0.5437
H	-4.2411	-0.7865	1.1806
H	-4.2242	0.8795	0.5637
C	2.6162	-1.2351	0.3010
N	3.2700	-1.9217	0.9697

MeS-CN-IIN-A-21.out

Total energy (hartree): -968.886116

Corrected energy (hartree): -968.765642

C	1.3439	1.7598	-0.0885
N	2.5859	1.1838	-0.3059
C	2.5527	-0.2550	-0.5289
C	1.0657	-0.5596	-0.3876
C	0.3802	-1.7704	-0.4744
C	-1.0062	-1.7538	-0.3181
C	-1.7104	-0.5510	-0.0771
C	-1.0084	0.6598	0.0123
C	0.3763	0.6242	-0.1443
O	1.1287	2.9439	0.0972
H	3.4344	1.7318	-0.3174
H	2.9087	-0.5090	-1.5418
H	0.8988	-2.7130	-0.6495
H	-1.5609	-2.6904	-0.3801
H	-1.4987	1.6120	0.1984
S	-3.4779	-0.6967	0.0970
C	-4.0137	1.0198	0.4104
H	-3.5734	1.4116	1.3350
H	-3.7783	1.6727	-0.4386
H	-5.1020	0.9650	0.5279
C	3.3955	-1.0022	0.4293
N	4.0760	-1.6001	1.1541

MeS-CN-IIN-A-23.out
Total energy (hartree): -968.885060
Corrected energy (hartree): -968.764763

C	1.7581	1.6735	-0.0187
N	2.8363	0.8444	-0.2891
C	2.4820	-0.5411	-0.5645
C	0.9668	-0.5160	-0.3955
C	0.0320	-1.5379	-0.5057
C	-1.3203	-1.2275	-0.3109
C	-1.7339	0.0855	-0.0085
C	-0.7754	1.1100	0.1046
C	0.5602	0.7837	-0.0902
O	1.8177	2.8664	0.2147
H	3.7850	1.1912	-0.3026
H	2.7557	-0.8249	-1.5948
H	0.3270	-2.5634	-0.7285
H	-2.0520	-2.0272	-0.3952
H	-1.0605	2.1347	0.3418
S	-3.4328	0.5603	0.2520
C	-4.3561	-1.0022	0.0600
H	-4.2479	-1.4114	-0.9518

H	-4.0549	-1.7405	0.8130
H	-5.4066	-0.7356	0.2243
C	3.1542	-1.4958	0.3431
N	3.6967	-2.2604	1.0266

MeSO2-CN-IIN-A-22.out
Total energy (hartree): -1119.282657
Corrected energy (hartree): -1119.156404

C	-2.0657	1.7384	0.0114
N	-3.2246	1.0316	0.2928
C	-3.0190	-0.3802	0.5810
C	-1.5105	-0.5239	0.4002
C	-0.7099	-1.6575	0.5124
C	0.6673	-1.5062	0.3121
C	1.1950	-0.2442	0.0066
C	0.3965	0.8932	-0.1257
C	-0.9706	0.7227	0.0833
O	-1.9906	2.9278	-0.2260
H	-4.1305	1.4786	0.3134
H	-3.3032	-0.6219	1.6192
H	-1.1312	-2.6383	0.7314
H	1.3364	-2.3637	0.3639
H	0.8149	1.8598	-0.4021
S	2.9907	-0.0965	-0.2580
O	3.5127	-1.4623	-0.5575
O	3.2173	1.0423	-1.1934
C	3.6339	0.3922	1.3699
H	4.7173	0.4849	1.2360
H	3.1885	1.3533	1.6456
H	3.3924	-0.3960	2.0900
C	-3.7978	-1.2712	-0.3041
N	-4.4277	-1.9824	-0.9694

MeSO2-CN-IIN-A-62.out
Total energy (hartree): -1119.283209
Corrected energy (hartree): -1119.157154

C	2.0815	1.7283	-0.0177
N	3.2429	1.0058	-0.2445
C	3.0330	-0.4060	-0.5292
C	1.5153	-0.5278	-0.4260
C	0.7048	-1.6478	-0.5908
C	-0.6786	-1.4766	-0.4630
C	-1.2029	-0.2083	-0.1790
C	-0.3970	0.9205	-0.0197

C	0.9775	0.7276	-0.1421
O	2.0122	2.9170	0.2248
H	4.1554	1.4385	-0.2115
H	3.3690	-0.6643	-1.5477
H	1.1211	-2.6302	-0.8120
H	-1.3599	-2.3142	-0.6042
H	-0.8196	1.9062	0.1689
S	-3.0096	-0.0285	-0.0384
O	-3.3561	1.3668	-0.4343
O	-3.6297	-1.2033	-0.7189
C	-3.3287	-0.1921	1.7428
H	-4.4142	-0.0915	1.8521
H	-2.9904	-1.1812	2.0673
H	-2.8048	0.6146	2.2653
C	3.7478	-1.2960	0.4095
N	4.3242	-2.0055	1.1236

NH2-CN-IIN-A-11.out
Total energy (hartree): -586.731337
Corrected energy (hartree): -586.619488

C	0.8148	1.7334	-0.0241
N	1.9785	1.0461	-0.3329
C	1.7907	-0.3754	-0.5904
C	0.2912	-0.5363	-0.3734
C	-0.5193	-1.6661	-0.4519
C	-1.8874	-1.5198	-0.2161
C	-2.4571	-0.2635	0.0994
C	-1.6238	0.8679	0.1792
C	-0.2645	0.7025	-0.0573
O	0.7331	2.9259	0.2105
H	2.8763	1.5074	-0.3707
H	2.0698	-0.6305	-1.6267
H	-0.1096	-2.6498	-0.6817
H	-2.5367	-2.3944	-0.2769
H	-2.0229	1.8535	0.4196
N	-3.8336	-0.1439	0.2689
H	-4.1564	0.6726	0.7699
H	-4.3346	-0.9854	0.5189
C	2.6063	-1.2284	0.3017
N	3.2614	-1.9116	0.9728

NHNH2-CN-IIN-A-91.out
Total energy (hartree): -642.055281
Corrected energy (hartree): -641.928171

C	1.0185	1.7561	-0.0466
N	2.2532	1.1865	-0.3217
C	2.2152	-0.2482	-0.5670
C	0.7355	-0.5573	-0.3774
C	0.0461	-1.7647	-0.4647
C	-1.3336	-1.7540	-0.2593
C	-2.0314	-0.5582	0.0368
C	-1.3263	0.6553	0.1202
C	0.0492	0.6205	-0.0864
O	0.8152	2.9377	0.1674
H	3.1001	1.7362	-0.3469
H	2.5396	-0.4837	-1.5950
H	0.5572	-2.7031	-0.6805
H	-1.8887	-2.6920	-0.3183
H	-1.8393	1.5864	0.3438
N	-3.4029	-0.6352	0.2929
H	-3.8551	-1.4619	-0.0834
N	-4.1505	0.5575	0.2466
H	-4.6151	0.6796	-0.6529
H	-4.8461	0.5466	0.9864
C	3.0945	-1.0080	0.3487
N	3.8030	-1.6170	1.0368

NHNH2-CN-IIN-A-92.out
Total energy (hartree): -642.055841
Corrected energy (hartree): -641.928631

C	1.3934	1.6885	-0.0278
N	2.4779	0.8849	-0.3440
C	2.1433	-0.5109	-0.5943
C	0.6362	-0.5164	-0.3680
C	-0.2893	-1.5529	-0.4480
C	-1.6368	-1.2720	-0.2060
C	-2.0634	0.0356	0.1186
C	-1.1187	1.0774	0.1932
C	0.2147	0.7740	-0.0480
O	1.4372	2.8845	0.2015
H	3.4189	1.2498	-0.3826
H	2.3884	-0.7973	-1.6311
H	0.0149	-2.5726	-0.6857
H	-2.3806	-2.0627	-0.2598
H	-1.4114	2.0987	0.4395
N	-3.3982	0.3132	0.4261
H	-3.6411	1.2969	0.3732
N	-4.3846	-0.5923	-0.0152

H	-4.8175	-0.2824	-0.8852
H	-5.1003	-0.6789	0.7003
C	2.8740	-1.4393	0.2961
N	3.4636	-2.1816	0.9652

NMe2-CN-IIN-A-27.out
Total energy (hartree): -665.343931
Corrected energy (hartree): -665.180901

C	1.5483	1.7144	-0.0716
N	2.7154	1.0038	-0.3074
C	2.5185	-0.4211	-0.5399
C	1.0076	-0.5526	-0.4006
C	0.1774	-1.6656	-0.4914
C	-1.1981	-1.4939	-0.3287
C	-1.7772	-0.2163	-0.0772
C	-0.9084	0.8994	0.0247
C	0.4554	0.6999	-0.1400
O	1.4760	2.9131	0.1350
H	3.6219	1.4491	-0.2989
H	2.8511	-0.7063	-1.5525
H	0.5767	-2.6636	-0.6736
H	-1.8329	-2.3730	-0.3944
H	-1.2706	1.9027	0.2300
N	-3.1437	-0.0702	0.0576
C	-4.0030	-1.2423	0.0862
H	-3.7687	-1.9151	0.9297
H	-5.0430	-0.9187	0.1866
H	-3.9219	-1.8197	-0.8471
C	-3.6942	1.2205	0.4403
H	-4.7847	1.1455	0.4797
H	-3.3343	1.5532	1.4293
H	-3.4374	1.9960	-0.2964
C	3.2713	-1.2627	0.4162
N	3.8785	-1.9383	1.1383

NO-CN-IIN-A-13.out
Total energy (hartree): -660.669598
Corrected energy (hartree): -660.578987

C	0.9633	1.7631	-0.0497
N	2.1807	1.1525	-0.3089
C	2.1018	-0.2794	-0.5572
C	0.6111	-0.5516	-0.3775
C	-0.0824	-1.7547	-0.4678
C	-1.4672	-1.7140	-0.2756

C	-2.1167	-0.4988	-0.0025
C	-1.4143	0.7124	0.0943
C	-0.0409	0.6551	-0.0969
O	0.7856	2.9467	0.1593
H	3.0443	1.6764	-0.3392
H	2.4121	-0.5259	-1.5869
H	0.4260	-2.6967	-0.6704
H	-2.0718	-2.6193	-0.3314
H	-1.9306	1.6461	0.3113
N	-3.5527	-0.6072	0.1702
O	-4.1233	0.4404	0.4011
C	2.9484	-1.0730	0.3580
N	3.6298	-1.7069	1.0504

NO-CN-IIN-A-30.out
Total energy (hartree): -660.669794
Corrected energy (hartree): -660.579187

C	1.2891	1.7063	-0.0075
N	2.3754	0.8980	-0.3067
C	2.0391	-0.4910	-0.5800
C	0.5269	-0.4975	-0.3770
C	-0.3749	-1.5602	-0.4807
C	-1.7245	-1.2912	-0.2628
C	-2.1441	0.0168	0.0525
C	-1.2388	1.0779	0.1617
C	0.1067	0.7931	-0.0585
O	1.3259	2.8970	0.2322
H	3.3183	1.2600	-0.3372
H	2.2843	-0.7669	-1.6199
H	-0.0392	-2.5702	-0.7156
H	-2.4756	-2.0772	-0.3286
H	-1.5852	2.0805	0.4105
N	-3.5309	0.3675	0.2893
O	-4.3195	-0.5526	0.1928
C	2.7443	-1.4425	0.3040
N	3.3132	-2.2015	0.9716

NO2-CN-IIN-A-23.out
Total energy (hartree): -735.894108
Corrected energy (hartree): -735.798941

C	1.4553	1.7344	-0.0504
N	2.6114	1.0122	-0.3022
C	2.3992	-0.4059	-0.5521
C	0.8884	-0.5344	-0.3822

C	0.0785	-1.6635	-0.4777
C	-1.2975	-1.4982	-0.2965
C	-1.8136	-0.2238	-0.0271
C	-1.0127	0.9133	0.0778
C	0.3539	0.7238	-0.1054
O	1.3854	2.9289	0.1587
H	3.5208	1.4523	-0.3267
H	2.6914	-0.6802	-1.5800
H	0.4914	-2.6514	-0.6782
H	-1.9803	-2.3417	-0.3589
H	-1.4374	1.8908	0.2923
N	-3.2772	-0.0813	0.1566
O	-3.7111	1.0409	0.3932
O	-3.9634	-1.0946	0.0595
C	3.1603	-1.2763	0.3682
N	3.7737	-1.9719	1.0647

OCF3-CN-IIN-A-25.out
Total energy (hartree): -943.675354
Corrected energy (hartree): -943.577377

C	1.8027	1.7472	-0.0930
N	3.0831	1.2504	-0.2782
C	3.1478	-0.1864	-0.5046
C	1.6794	-0.5858	-0.4069
C	1.0797	-1.8382	-0.5169
C	-0.3091	-1.9105	-0.4004
C	-1.0691	-0.7514	-0.1783
C	-0.4781	0.5071	-0.0625
C	0.9104	0.5514	-0.1805
O	1.5048	2.9117	0.0914
H	3.8962	1.8498	-0.2583
H	3.5457	-0.4141	-1.5080
H	1.6623	-2.7444	-0.6794
H	-0.8275	-2.8649	-0.4766
H	-1.0389	1.4208	0.1116
O	-2.4408	-1.0002	-0.0924
C	-3.3311	-0.0068	0.1551
F	-3.1119	0.6100	1.3380
F	-4.5458	-0.5632	0.1888
F	-3.3285	0.9492	-0.8021
C	4.0068	-0.8847	0.4750
N	4.7010	-1.4439	1.2174

OCF3-CN-IIN-A-74.out

Total energy (hartree): -943.675267
Corrected energy (hartree): -943.577435

C	-2.0831	1.7426	0.0033
N	-3.2182	1.0690	0.4267
C	-3.0263	-0.3552	0.6595
C	-1.5585	-0.5408	0.2865
C	-0.7817	-1.6959	0.2758
C	0.5604	-1.5788	-0.1009
C	1.0842	-0.3276	-0.4480
C	0.3120	0.8313	-0.4539
C	-1.0223	0.6932	-0.0774
O	-2.0021	2.9321	-0.2350
H	-4.1008	1.5424	0.5602
H	-3.1895	-0.6121	1.7198
H	-1.1954	-2.6695	0.5369
H	1.2083	-2.4525	-0.1361
H	0.7267	1.7943	-0.7443
O	2.4151	-0.2628	-0.9008
C	3.3830	-0.0291	0.0208
F	3.2181	1.1497	0.6639
F	4.5566	-0.0040	-0.6177
F	3.4359	-0.9896	0.9754
C	-3.9397	-1.1978	-0.1408
N	-4.6699	-1.8710	-0.7400

OCF3-CN-IIN-A-75.out
Total energy (hartree): -943.675267
Corrected energy (hartree): -943.577433

C	-2.0828	1.7437	0.0025
N	-3.2192	1.0695	0.4212
C	-3.0265	-0.3538	0.6585
C	-1.5587	-0.5397	0.2855
C	-0.7822	-1.6952	0.2747
C	0.5600	-1.5782	-0.1016
C	1.0841	-0.3271	-0.4485
C	0.3122	0.8320	-0.4545
C	-1.0223	0.6940	-0.0784
O	-2.0006	2.9338	-0.2326
H	-4.0994	1.5448	0.5636
H	-3.1890	-0.6076	1.7196
H	-1.1963	-2.6686	0.5356
H	1.2078	-2.4521	-0.1369
H	0.7271	1.7950	-0.7447
O	2.4152	-0.2622	-0.9009

C	3.3828	-0.0297	0.0212
F	3.2176	1.1480	0.6662
F	4.5566	-0.0035	-0.6170
F	3.4359	-0.9917	0.9744
C	-3.9398	-1.1993	-0.1390
N	-4.6693	-1.8753	-0.7360

OCF3-CN-IIN-A-76.out
Total energy (hartree): -943.675000
Corrected energy (hartree): -943.576959

C	-2.4672	1.6640	-0.0209
N	-3.4954	0.7774	0.2576
C	-3.0620	-0.5796	0.5607
C	-1.5490	-0.4670	0.4061
C	-0.5586	-1.4316	0.5477
C	0.7777	-1.0535	0.3651
C	1.0877	0.2759	0.0430
C	0.0981	1.2491	-0.1059
C	-1.2195	0.8477	0.0806
O	-2.5902	2.8457	-0.2803
H	-4.4639	1.0652	0.2507
H	-3.3268	-0.8612	1.5939
H	-0.7962	-2.4676	0.7875
H	1.5588	-1.7994	0.4745
H	0.3529	2.2764	-0.3593
O	2.3850	0.7582	-0.1535
C	3.4683	-0.0537	-0.1092
F	3.6378	-0.6400	1.1008
F	4.5422	0.6991	-0.3617
F	3.4195	-1.0471	-1.0274
C	-3.6653	-1.5888	-0.3354
N	-4.1534	-2.3957	-1.0109

OCF3-CN-IIN-A-77.out
Total energy (hartree): -943.675156
Corrected energy (hartree): -943.577484

C	2.1342	1.7276	-0.0022
N	3.3014	0.9823	-0.0630
C	3.1081	-0.4198	-0.4031
C	1.5898	-0.5084	-0.5248
C	0.7831	-1.6031	-0.8226
C	-0.5988	-1.3975	-0.8940
C	-1.1308	-0.1230	-0.6644
C	-0.3319	0.9793	-0.3704

C	1.0412	0.7531	-0.3008
O	2.0544	2.9168	0.2376
H	4.2078	1.3960	0.1049
H	3.5865	-0.6669	-1.3659
H	1.1999	-2.5956	-0.9912
H	-1.2741	-2.2180	-1.1292
H	-0.7564	1.9675	-0.2064
O	-2.5164	0.0581	-0.8307
C	-3.3019	-0.0444	0.2716
F	-3.2149	-1.2611	0.8599
F	-4.5675	0.1507	-0.1113
F	-2.9943	0.8703	1.2194
C	3.6647	-1.3407	0.6102
N	4.1237	-2.0766	1.3805

OCF3-CN-IIN-A-78.out
Total energy (hartree): -943.675156
Corrected energy (hartree): -943.577491

C	2.1351	1.7268	-0.0025
N	3.3022	0.9817	-0.0661
C	3.1082	-0.4210	-0.4039
C	1.5897	-0.5088	-0.5255
C	0.7824	-1.6031	-0.8234
C	-0.5993	-1.3969	-0.8945
C	-1.1308	-0.1222	-0.6644
C	-0.3313	0.9797	-0.3706
C	1.0417	0.7529	-0.3013
O	2.0557	2.9157	0.2392
H	4.2084	1.3938	0.1072
H	3.5866	-0.6697	-1.3662
H	1.1987	-2.5958	-0.9922
H	-1.2750	-2.2172	-1.1296
H	-0.7553	1.9681	-0.2063
O	-2.5163	0.0597	-0.8304
C	-3.3019	-0.0441	0.2718
F	-3.2144	-1.2611	0.8592
F	-4.5675	0.1507	-0.1112
F	-2.9949	0.8701	1.2203
C	3.6636	-1.3407	0.6112
N	4.1217	-2.0753	1.3832

OH-CN-IIN-A-31.out
Total energy (hartree): -606.598277
Corrected energy (hartree): -606.498323

C	0.7953	1.7381	-0.0247
N	1.9609	1.0555	-0.3344
C	1.7776	-0.3666	-0.5917
C	0.2791	-0.5353	-0.3678
C	-0.5221	-1.6731	-0.4466
C	-1.8909	-1.5371	-0.2084
C	-2.4471	-0.2821	0.1054
C	-1.6406	0.8588	0.1887
C	-0.2779	0.7010	-0.0512
O	0.7042	2.9304	0.2056
H	2.8560	1.5213	-0.3817
H	2.0495	-0.6199	-1.6303
H	-0.1042	-2.6526	-0.6787
H	-2.5542	-2.3996	-0.2572
H	-2.0486	1.8405	0.4333
O	-3.7968	-0.2504	0.3204
H	-4.0762	0.6484	0.5355
C	2.6010	-1.2175	0.2942
N	3.2637	-1.8978	0.9606

OMe-CN-IIN-A-24.out
Total energy (hartree): -645.899823
Corrected energy (hartree): -645.773827

C	0.9988	1.7546	-0.0683
N	2.2401	1.1886	-0.3130
C	2.2106	-0.2483	-0.5483
C	0.7278	-0.5617	-0.3859
C	0.0458	-1.7761	-0.4741
C	-1.3356	-1.7687	-0.2949
C	-2.0346	-0.5698	-0.0294
C	-1.3462	0.6477	0.0626
C	0.0368	0.6148	-0.1191
O	0.7799	2.9358	0.1330
H	3.0854	1.7414	-0.3317
H	2.5534	-0.4909	-1.5684
H	0.5666	-2.7138	-0.6676
H	-1.9094	-2.6928	-0.3523
H	-1.8381	1.5947	0.2681
O	-3.3804	-0.7060	0.1235
C	-4.1471	0.4637	0.4082
H	-3.8291	0.9242	1.3554
H	-4.0671	1.1983	-0.4071
H	-5.1830	0.1238	0.4950
C	3.0725	-0.9985	0.3907

N	3.7675	-1.5986	1.0999

OMe-CN-IIN-A-69.out
Total energy (hartree): -645.898456
Corrected energy (hartree): -645.772528

C	1.4126	1.6858	-0.0048
N	2.4880	0.8621	-0.3020
C	2.1332	-0.5226	-0.5809
C	0.6208	-0.5023	-0.3889
C	-0.3127	-1.5242	-0.4943
C	-1.6648	-1.2233	-0.2763
C	-2.0674	0.0887	0.0441
C	-1.1161	1.1174	0.1530
C	0.2153	0.7947	-0.0651
O	1.4748	2.8766	0.2394
H	3.4359	1.2105	-0.3216
H	2.3942	-0.7988	-1.6165
H	-0.0182	-2.5466	-0.7312
H	-2.3973	-2.0223	-0.3559
H	-1.4232	2.1312	0.4039
O	-3.3597	0.4565	0.2681
C	-4.3783	-0.5374	0.1849
H	-4.4251	-0.9764	-0.8233
H	-4.2211	-1.3319	0.9301
H	-5.3159	-0.0166	0.3995
C	2.8223	-1.4802	0.3111
N	3.3778	-2.2470	0.9818

SH-CN-IIN-A-32.out
Total energy (hartree): -929.570094
Corrected energy (hartree): -929.476939

C	1.2040	1.7347	-0.0247
N	2.3681	1.0332	-0.2990
C	2.1718	-0.3846	-0.5669
C	0.6649	-0.5316	-0.3874
C	-0.1472	-1.6567	-0.4905
C	-1.5228	-1.5000	-0.2922
C	-2.0792	-0.2399	0.0066
C	-1.2503	0.8876	0.1140
C	0.1155	0.7131	-0.0855
O	1.1259	2.9272	0.2039
H	3.2710	1.4859	-0.3209
H	2.4678	-0.6394	-1.5987
H	0.2624	-2.6425	-0.7108

H	-2.1708	-2.3726	-0.3693
H	-1.6482	1.8745	0.3481
S	-3.8326	-0.0023	0.2631
H	-4.2018	-1.2947	0.0921
C	2.9543	-1.2533	0.3383
N	3.5847	-1.9487	1.0202

SiH3-CN-IIN-A-33.out
Total energy (hartree): -822.067654
Corrected energy (hartree): -821.960748

C	1.2391	1.7354	-0.0217
N	2.4051	1.0351	-0.2948
C	2.2093	-0.3822	-0.5621
C	0.7007	-0.5301	-0.3878
C	-0.1036	-1.6607	-0.4980
C	-1.4805	-1.4998	-0.3045
C	-2.0613	-0.2455	-0.0052
C	-1.2204	0.8762	0.1040
C	0.1515	0.7144	-0.0880
O	1.1617	2.9277	0.2096
H	3.3088	1.4865	-0.3077
H	2.5045	-0.6394	-1.5936
H	0.3150	-2.6429	-0.7178
H	-2.1184	-2.3818	-0.3872
H	-1.6144	1.8658	0.3369
Si	-3.9345	-0.0819	0.2453
H	-4.3858	-0.9767	1.3532
H	-4.6568	-0.4787	-1.0012
H	-4.2517	1.3368	0.5799
C	2.9878	-1.2522	0.3446
N	3.6168	-1.9464	1.0290

SiMe3-CN-IIN-A-34.out
Total energy (hartree): -940.061218
Corrected energy (hartree): -939.874645

C	2.1777	1.7218	-0.0265
N	3.3424	1.0080	-0.2710
C	3.1356	-0.4059	-0.5485
C	1.6209	-0.5341	-0.4162
C	0.8030	-1.6515	-0.5532
C	-0.5762	-1.4692	-0.3941
C	-1.1545	-0.2111	-0.1034
C	-0.2952	0.8943	0.0305
C	1.0795	0.7162	-0.1259

O	2.1117	2.9148	0.2076
H	4.2517	1.4476	-0.2560
H	3.4572	-0.6640	-1.5717
H	1.2128	-2.6388	-0.7671
H	-1.2204	-2.3444	-0.4991
H	-0.6761	1.8900	0.2561
Si	-3.0469	-0.0487	0.1030
C	-3.4899	1.7506	0.4784
H	-3.1889	2.4278	-0.3335
H	-4.5781	1.8495	0.6020
H	-3.0207	2.1059	1.4069
C	-3.6025	-1.1667	1.5281
H	-4.6933	-1.1163	1.6617
H	-3.3406	-2.2189	1.3452
H	-3.1346	-0.8679	2.4768
C	-3.8854	-0.6017	-1.5039
H	-3.6378	-1.6436	-1.7537
H	-4.9799	-0.5353	-1.4162
H	-3.5789	0.0261	-2.3526
C	3.8777	-1.2878	0.3773
N	4.4787	-1.9913	1.0772

tBu-CN-IIN-A-37.out
Total energy (hartree): -688.629629
Corrected energy (hartree): -688.427685

C	1.8072	1.7205	-0.0301
N	2.9803	1.0259	-0.2872
C	2.7952	-0.3926	-0.5605
C	1.2845	-0.5448	-0.4161
C	0.4750	-1.6651	-0.5439
C	-0.9076	-1.5026	-0.3715
C	-1.4955	-0.2562	-0.0762
C	-0.6457	0.8581	0.0490
C	0.7248	0.6973	-0.1197
O	1.7239	2.9122	0.2060
H	3.8826	1.4800	-0.2770
H	3.1157	-0.6464	-1.5852
H	0.8883	-2.6499	-0.7619
H	-1.5349	-2.3850	-0.4705
H	-1.0321	1.8496	0.2788
C	-3.0118	-0.0796	0.1185
C	-3.5424	0.9452	-0.9108
H	-3.3622	0.5997	-1.9378
H	-4.6250	1.0830	-0.7816

H	-3.0643	1.9259	-0.7950
C	-3.2810	0.4403	1.5499
H	-4.3608	0.5700	1.7077
H	-2.9086	-0.2688	2.3015
H	-2.7976	1.4086	1.7306
C	-3.7836	-1.3979	-0.0701
H	-3.4761	-2.1611	0.6578
H	-4.8567	-1.2177	0.0757
H	-3.6529	-1.8096	-1.0803
C	3.5602	-1.2584	0.3621
N	4.1793	-1.9488	1.0593

Vin-CN-IIN-A-38.out
Total energy (hartree): -608.768597
Corrected energy (hartree): -608.642019

C	1.3224	1.6978	-0.0103
N	2.4192	0.8981	-0.2961
C	2.0956	-0.4943	-0.5713
C	0.5824	-0.5080	-0.3816
C	-0.3264	-1.5595	-0.4872
C	-1.6780	-1.2823	-0.2768
C	-2.1392	0.0184	0.0368
C	-1.1989	1.0590	0.1406
C	0.1485	0.7773	-0.0684
O	1.3533	2.8917	0.2246
H	3.3582	1.2696	-0.3241
H	2.3586	-0.7689	-1.6070
H	-0.0017	-2.5740	-0.7178
H	-2.3940	-2.0990	-0.3561
H	-1.5106	2.0750	0.3831
C	-3.5646	0.3239	0.2612
H	-3.7737	1.3710	0.4947
C	-4.5980	-0.5303	0.2091
H	-4.4823	-1.5906	-0.0159
H	-5.6135	-0.1833	0.3956
C	2.8030	-1.4360	0.3226
N	3.3741	-2.1882	0.9964

Vin-CN-IIN-A-40.out
Total energy (hartree): -608.768659
Corrected energy (hartree): -608.641978

C	0.9845	1.7552	-0.0601
N	2.2146	1.1648	-0.3084
C	2.1598	-0.2707	-0.5465

C	0.6716	-0.5601	-0.3808
C	-0.0246	-1.7600	-0.4696
C	-1.4111	-1.7226	-0.2872
C	-2.1094	-0.5235	-0.0198
C	-1.3767	0.6762	0.0691
C	-0.0002	0.6337	-0.1111
O	0.7911	2.9395	0.1439
H	3.0701	1.7018	-0.3267
H	2.4916	-0.5187	-1.5691
H	0.4818	-2.7052	-0.6648
H	-1.9770	-2.6528	-0.3510
H	-1.8584	1.6302	0.2766
C	-3.5725	-0.5826	0.1572
H	-4.0052	-1.5824	0.0655
C	-4.3982	0.4435	0.4125
H	-4.0517	1.4714	0.5193
H	-5.4690	0.2786	0.5244
C	3.0107	-1.0402	0.3862
N	3.6976	-1.6551	1.0905