Organic and Biomolecular Chemistry

Electronic Supplementary Information

New donor-acceptor chromophores by formal [2+2] cycloaddition of donor-substituted alkynes to dicyanovinyl derivatives

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ESI 1. General Experimental Details.

Reagents were purchased at reagent grade from Acros, Aldrich and Fluka, and anhydrous DMF (absolute, over molecular sieves 4Å, H_2O < 0.005%) was purchased from Fluka and used as received. Anhydrous CH_2Cl_2 was freshly distilled from CaH_2 under N_2 atmosphere. THF was freshly distilled from Na/benzophenone and toluene from Na under N_2 atmosphere. Column chromatography was carried out with SiO_2 60 (particle size 0.040–0.063 mm, 230–400 mesh; Fluka) and distilled technical solvents. Thin-layer chromatography (TLC) was conducted on aluminum sheets coated with SiO_2 60 F_{254} obtained from Macherey-Nagel; visualisation with a UV lamp (254 or 366 nm). Melting points (mp) were measured on a Büchi B-540 melting-point apparatus in open capillaries and are uncorrected. "Dec." refers to decomposition, and "subl." refers to sublimation. ^{1}H NMR and ^{13}C NMR spectra were measured on a Varian Gemini 300 at 20 °C. Chemical shifts are reported in ppm relative to the signal of tetramethylsilane. Residual solvent signals in the ^{1}H and ^{13}C NMR spectra were used as an internal reference. Coupling constants (*J*) are given in Hz. The apparent resonance multiplicity is described as s (singlet), br s (broad singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quartet) and m (multiplet). Infrared spectra (IR) were recorded on a Perkin-Elmer Spectrum BX instrument. UV-Vis spectra were recorded on a Varian Cary-5 spectrophotometer. The spectra were measured in CH_2Cl_2 in a quartz cuvette (1 cm). The absorption wavelengths are reported in nm with the extinction coefficient ε (M^{-1} cm^{-1}) in parenthesis; shoulders are indicated as sh. High-resolution HR-EI-MS spectra were measured on a Hitachi-Perkin-Elmer VG-Tribrid spectrometer. The most important signals are reported in *m*/*z* units with M^+ as the molecular ion. Compounds **1**,[1] **4**,[2] **5**,[3] **7**,[4] **12**,[5] **16**,[6] **17**,[7] **18**[8] and **22**[9] were prepared according to the literature procedures. Dicyanovinyl precursor molecules **2a**,[10] **2b**,[5] **2c**,[11] **2e**,[12] **2f**,[13] **2g**,[5] **2h**[13] and **6**[14] were prepared by the general method (A) (see below) using Al_2O_3-catalyzed condensation with $CH_2(CN)_2$; their NMR data and melting points are in accord with the literature values.

Geometries were optimized using the program Gaussian 03 at the B3LYP/6-31G(d) level of theory.[15] Stationary points were characterized by harmonic vibrational frequency analysis.[16] Time-dependant calculations were done on these optimised structures.

Electrochemical measurements were carried out in CH_2Cl_2 containing 0.1M nBu$_4$NPF$_6$ in a classical three-electrode cell by cyclic voltammetry (CV) and rotating-disk voltammetry (RDV). The working electrode was a glassy carbon disk (3 mm in diameter), the auxiliary electrode was a Pt wire, and the pseudo reference electrode was a Pt wire. The cell was connected to an Autolab PGSTAT20 potentiostat (Eco Chemie, Holland) driven by a GPSE

software running on a personal computer. All potentials are given vs. Fc^+/Fc used as internal reference and are uncorrected from Ohmic drop.

X-ray measurements were carried out on a Bruker Kappa CCD diffractometer equipped with graphite monochromator (MoK_α radiation, λ = 0.71073 Å) and an Oxford Cryostream low-temperature device. Unit cell dimensions were obtained by least-squares refinement of all measured reflections (HKL, Scalepack[17a]). All structures were solved by direct methods (SIR97[17b] and SHELX-97[17c]). Non-hydrogen atoms were refined anisotropically by full-matrix least-squares analysis.

ESI 2. X-ray analysis of **3e**, **3g** and **10**.

Single crystals of **3e** (red needles) were obtained by slow diffusion of pentane into a solution of compound **3e** in $CHCl_3$ at r.t. Crystal data of **3e** at 223(2) K $C_{20}H_{16}BrN_3$, M_r = 378.273: monoclinic, space group $P2_1/c$ (no. 14), D_c 1.389 g cm^{-3}, Z = 4, a = 9.4778 (3), b = 7.9420 (3), c = 24.0757(3) Å, α = 90.00, β = 93.4125 (14), γ = 90°, V = 1809.03 (11) $Å^3$. Crystal dimensions ca. 0.2 x 0.12 x 0.05 mm. The numbers of measured and unique reflections are 6188 and 3690, respectively. (R_{int} = 0.045). Final $R(F) = 0.050$, $wR(F^2) = 0.146$ for 217 parameters and 2650 reflections with $I > 2\sigma(I)$ and $2.4 < \theta < 27.5°$ (corresponding R-values based on all 3690 reflections are 0.074 and 0.168, respectively). CCDC 699250.

Single crystals of **3g** (orange-red plates) were obtained by slow diffusion of pentane into a solution of compound **3g** in $CHCl_3$ at r.t. Crystal data of **3g** at 203(2) K $C_{21}H_{19}N_3O$, M_r = 329.403: triclinic, space group $P\bar{1}$, (no. 2), D_c 1.242 g cm^{-3}, Z = 4, a = 7.8176 (2), b = 15.0473 (4), c = 16.0532 (5) Å, α = 104.702 (2), β =90.581 (2), γ = 104.638 (2)°, V = 1761.71 (9) $Å^3$. Crystal dimensions ca. 0.3 x 0.2 x 0.006 mm. The numbers of measured and unique reflections are 10655 and 6111, respectively. (R_{int} = 0.041). Final $R(F) = 0.044$, $wR(F^2) = 0.126$ for 604 parameters and 4731 reflections with $I > 2\sigma(I)$ and $2.4 < \theta < 25.0°$ (corresponding R-values based on all 6111 reflections are 0.062 and 0.143, respectively). CCDC 699251.

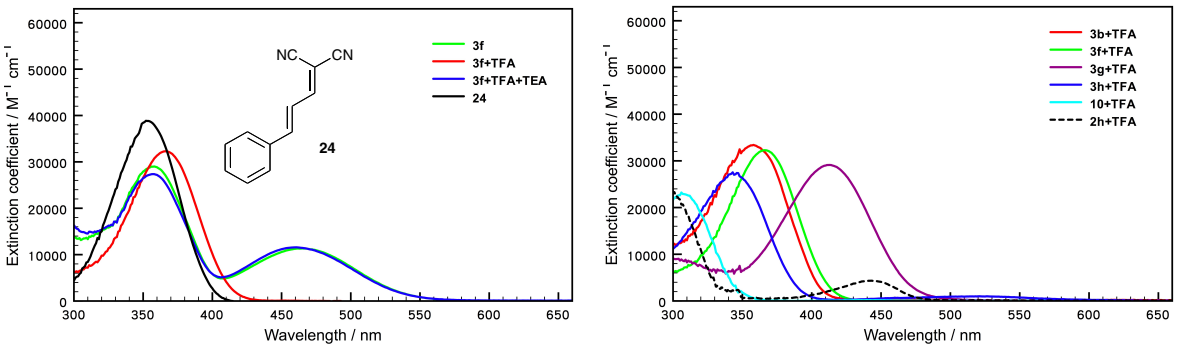
Single crystals of **10** (orange-plates) were obtained by slow diffusion of pentane into a solution of compound **10** in $CHCl_3$ at r.t. Crystal data of **10** at 173(2) K $C_{20}H_{23}N_3$, M_r = 305.425: monoclinic, space group $P2_1/c$ (no. 14), D_c 1.155 g cm^{-3}, Z = 4, a = 10.0678 (3), b =

15.9325 (5), c = 11.7652 (4) Å, α = 90.00, β = 111.406 (2), γ = 90.00°, V = 1757.01 (10) Å^3. Crystal dimensions ca. 0.2 x 0.12 x 0.05 mm. The numbers of measured and unique reflections are 5645 and 3185, respectively. (R_{int} = 0.042). Final $R(F)$ = 0.045, w$R(F^2)$ = 0.132 for 300 parameters and 2515 reflections with $I > 2\sigma(I)$ and 3.3 < θ < 25.4° (corresponding R-values based on all 3185 reflections are 0.059 and 0.146, respectively). CCDC 699249.

ESI 3. Experimental electronic absorption maxima (λ_{max}), molar extinction coefficients (ε) and calculated TD B3LYP/6-31G(d)//B3LYP/6-31G(d) transition energies and oscillator strengths (f) for selected molecules **3b**, **3c**, **3f**, **3g**, **3h**, **10** and **11** (H = HOMO, L = LUMO).

	Experimental value			Calculated value			
	λ_{max} (nm)	E	ε (M^{-1} cm^{-1})	λ (nm)	E	Assignment	f
3b	491	2.53	8.52x10^3	569	2.21	H→L	0.09
				388	3.20	H-1→L, H→L+1	0.43
	352	3.52	3.18x10^4	364	3.40	H-1→L, H→L+1	0.41
3c	483	2.57	9.83x10^3	527	2.35	H→L	0.12
	360	3.44	3.06x10^4	367	3.37	H-1→L, H→L+1	0.96
3f	465	2.67	1.13x10^4	476	2.60	H→L	0.16
	358	3.46	2.90x10^4	352	3.52	H-1→L, H→1	0.83
3g	460 (sh)	2.70	1.22x10^4	463	2.67	H→L	0.18
	394	3.15	3.57x10^4	377	3.29	H-1→L, H→1	0.94
3h	477	2.60	4.11x10^4	455	2.73	H-1→L	0.26
				416	2.98	H→L	0.89
10	440	2.82	1.62x10^4	428	2.90	H→L	0.24
	302	4.11	2.01x10^4	297	4.17	H-1→L	0.47
11	436	2.84	2.58x10^4	405	3.06	H→L	0.33
	323	3.84	1.38x10^4	316	3.93	H-1→L	0.41

ESI 4. Quenching by acidification and reconstitution by neutralisation of the CT absorption transitions of **2h**, **3b**, **3f**, **3g**, **3h** and **10** with comparison to **24**.[18]



ESI 5. B3LYP/6-31G(d) optimised geometries of **2h**, **3**, **8**–**11** and stationary points along the reaction coordinate of the reaction of 1,1-dicyanoethene (DCE), 1,1,2-tricyanoethene (TCE), 1,1,4,4-tetracyanoethene (TCNE) and **2f** with **1** (Å). Imaginary frequencies (ν_i[cm^{-1}]) are reported as appropriate.

[4-(Dimethylamino)benzylidene]malononitrile (2h)

6	0.583757	-0.513820	-0.000434
6	-0.332589	-1.592033	-0.000837
6	0.031775	0.790381	-0.000161
6	-1.700136	-1.401483	-0.000935
1	0.052491	-2.609127	-0.001052
6	-1.333232	0.996382	-0.000327
1	0.681120	1.657296	0.000372
6	-2.248196	-0.091850	-0.000805
1	-2.348991	-2.268397	-0.001358
1	-1.699949	2.015356	0.000167
7	-3.603185	0.115994	-0.001275
6	-4.139572	1.470550	-0.000339
1	-3.821650	2.032463	-0.888282
1	-5.229056	1.423035	-0.003308
1	-3.826068	2.030193	0.890719
6	-4.517832	-1.017019	0.002478
1	-4.380738	-1.645034	0.892812
1	-5.544163	-0.648453	0.004029
1	-4.384493	-1.647816	-0.886453
6	1.986128	-0.832925	-0.000299
6	3.107965	-0.038508	0.000067
6	3.101958	1.390678	0.000123
6	4.400120	-0.656207	0.000339
7	3.107552	2.555550	0.000680
7	5.446803	-1.166534	0.000536
1	2.202431	-1.899468	-0.000456

[(2*E*)-1-[4-(Dimethylamino)phenyl]-3-(4-nitrophenyl)-2-propen-1-ylidene]malononitrile (3b)

6	2.058212	0.542443	0.040028
6	1.950948	-0.544275	0.931109
6	3.141716	0.528992	-0.859493
6	2.874431	-1.576719	0.938903
1	1.147072	-0.558661	1.660813
6	4.060050	-0.506924	-0.879027
1	3.253912	1.335137	-1.577031
6	3.959586	-1.593565	0.026244
1	2.759520	-2.369195	1.668137
1	4.863292	-0.471597	-1.604387
7	4.873222	-2.621356	0.016842
6	6.032268	-2.559434	-0.861796
1	6.658193	-1.680203	-0.655151
1	6.640823	-3.452436	-0.713517
1	5.734711	-2.527046	-1.917984
6	4.772022	-3.695449	0.992557
1	3.809914	-4.217728	0.913544
1	5.562584	-4.423605	0.806626
1	4.879615	-3.330153	2.024110
6	1.090501	1.651242	0.073309
6	1.509083	2.975213	0.038782
6	2.881402	3.371538	0.092585
6	0.571840	4.054994	-0.018481
7	3.985051	3.740304	0.144840
7	-0.199498	4.927195	-0.057842
6	-0.340135	1.385140	0.147728
1	-0.965094	2.236264	0.402848
6	-0.921143	0.195866	-0.138541
1	-0.285203	-0.628883	-0.450107
6	-2.350758	-0.105727	-0.098350
6	-2.775113	-1.383182	-0.517679
6	-3.329254	0.812256	0.339807
6	-4.117573	-1.740236	-0.508673
1	-2.035089	-2.102432	-0.857812
6	-4.673704	0.470070	0.354521
1	-3.039213	1.802374	0.675327
6	-5.051964	-0.804697	-0.070623
1	-4.450253	-2.719129	-0.830695
1	-5.432071	1.167134	0.688953
7	-6.475328	-1.172113	-0.052738
8	-7.278104	-0.327030	0.342190
8	-6.777064	-2.303386	-0.433296

[(2*E*)-1-[4-(Dimethylamino)phenyl]-3-(4-formylphenyl)-2-propen-1-ylidene]malononitrile (3c)

6	1.716009	0.557793	0.043825
6	1.682617	-0.535702	0.931594
6	2.794927	0.618462	-0.858426
6	2.672883	-1.505025	0.933952
1	0.882185	-0.604857	1.661969
6	3.779704	-0.354773	-0.883827
1	2.852109	1.433173	-1.572850
6	3.753533	-1.447904	0.018266
1	2.613529	-2.305492	1.661082
1	4.577454	-0.263370	-1.610368
7	4.733716	-2.413985	0.002524
6	5.88727	-2.265790	-0.872302
1	6.452745	-1.347900	-0.658128
1	6.554635	-3.117002	-0.730890
1	5.589575	-2.244963	-1.928654
6	4.716583	-3.485006	0.986470
1	3.789385	-4.068928	0.924286
1	5.549837	-4.161966	0.792921
1	4.81409	-3.107071	2.014780
6	0.677458	1.602044	0.081157
6	1.014804	2.949533	0.063942
6	2.360144	3.427520	0.133070
6	0.014597	3.971326	0.009533
7	3.439282	3.861380	0.197636
7	-0.806129	4.797342	-0.028229
6	-0.732214	1.244340	0.140009
1	-1.413841	2.052375	0.389858
6	-1.232252	0.019894	-0.155331
1	-0.539377	-0.760131	-0.461507
6	-2.638294	-0.374994	-0.133059
6	-2.972892	-1.674232	-0.563537
6	-3.68053	0.477367	0.298511
6	-4.293821	-2.107217	-0.569864
1	-2.182095	-2.341166	-0.897387
6	-4.996118	0.045556	0.293034
1	-3.454149	1.481669	0.642139
6	-5.316398	-1.252245	-0.141939
1	-4.537665	-3.112483	-0.906813
1	-5.801346	0.694508	0.623169
6	-6.722149	-1.715544	-0.145656

[(2*E*)-1-[4-(Dimethylamino)phenyl]-3-(4-ethynylphenyl)-2-propen-1-ylidene]malononitrile (3d)

6	1.653393	0.545190	0.041418
6	1.605766	-0.540670	0.937186
6	2.722166	0.574767	-0.873793
6	2.573058	-1.533361	0.934018
1	0.812716	-0.585987	1.677398
6	3.684076	-0.421459	-0.904140
1	2.789887	1.384079	-1.593484
6	3.642816	-1.507995	0.004758
1	2.503622	-2.327375	1.667350
1	4.475620	-0.352957	-1.639978

7	4.599617	-2.498569	-0.017231
6	5.750994	-2.377320	-0.898654
1	6.340224	-1.473423	-0.688042
1	6.398156	-3.244940	-0.762369
1	5.447128	-2.348548	-1.953013
6	4.572773	-3.557580	0.978925
1	3.630742	-4.119074	0.937832
1	5.385705	-4.257264	0.779315
1	4.696032	-3.171825	2.001782
6	0.638503	1.613720	0.083596
6	1.011505	2.952679	0.063378
6	2.369000	3.395167	0.125431
6	0.037810	3.999702	0.014969
7	3.459503	3.801023	0.183717
7	-0.762096	4.846314	-0.017867
6	-0.776300	1.289345	0.152060
1	-1.438202	2.115099	0.397180
6	-1.307197	0.073273	-0.129345
1	-0.633077	-0.725061	-0.430699
6	-2.718638	-0.291820	-0.097161
6	-3.086772	-1.591157	-0.500140
6	-3.744162	0.584891	0.316191
6	-4.412207	-2.002965	-0.498264
1	-2.312775	-2.283498	-0.822139
6	-5.069778	0.181268	0.321194
1	-3.502538	1.592612	0.639067
6	-5.428773	-1.120883	-0.086561
1	-4.675467	-3.007373	-0.814050
1	-5.847036	0.867665	0.641485
6	-6.794263	-1.533843	-0.079708

{(2*E*)-3-(4-Bromophenyl)-1-[4-(dimethylamino)phenyl]-2-propen-1-ylidene}malononitrile (3e)

6	2.527135	0.518475	0.038267
6	2.385122	-0.562706	0.930561
6	3.598931	0.461105	-0.872910
6	3.266299	-1.632703	0.928360
1	1.588481	-0.544389	1.668085
6	4.474788	-0.611909	-0.901935
1	3.737239	1.263684	-1.589970
6	4.339206	-1.694030	0.003665
1	3.126211	-2.419836	1.659129
1	5.272570	-0.607211	-1.634269
7	5.209896	-2.761061	-0.016878
6	6.370898	-2.736045	-0.894135
1	7.039892	-1.892126	-0.672623
1	6.935292	-3.660924	-0.766053
1	6.073948	-2.668633	-1.948605
6	5.093965	-3.812495	0.981028
1	4.111553	-4.299601	0.934688
1	5.851591	-4.573625	0.788814
1	5.240271	-3.434813	2.003792
6	1.605249	1.667332	0.082263
6	2.084765	2.971737	0.058802
6	3.473848	3.303933	0.113446
6	1.197402	4.093257	0.014554
7	4.593473	3.621266	0.166322
7	0.467686	5.001080	-0.014878
6	0.167397	1.460398	0.158168
1	-0.421825	2.336874	0.412577
6	-0.464399	0.295472	-0.126691
1	0.137601	-0.554941	-0.437797
6	-1.904049	0.051802	-0.086246
6	-2.385472	-1.205685	-0.498503
6	-2.844563	1.009856	0.344568
6	-3.745873	-1.505523	-0.491527
1	-1.679308	-1.961063	-0.834162
6	-4.205892	0.726823	0.358075
1	-2.515528	1.989548	0.676384
6	-4.641211	-0.530414	-0.061914
1	-4.099503	-2.478230	-0.814492
1	-4.918374	1.472926	0.691358
35	-6.563965	-0.931678	-0.044177

{(2*E*)-1-[4-(Dimethylamino)phenyl]-3-phenyl-2-propen-1-ylidene}malononitrile (3f)

6	-0.197298	1.469321	0.086577
6	-0.061712	2.852518	0.072921
6	-1.201988	3.715200	0.024415
7	-2.135657	4.411507	-0.008950
6	0.988297	0.593471	0.044825
6	1.127652	-0.488017	0.936046
6	2.251640	-1.299418	0.930487
6	3.300942	-1.088161	0.001888
6	3.156653	-0.004837	-0.899917
6	2.037638	0.811146	-0.867085
7	4.411594	-1.903962	-0.027846
6	4.578919	-2.938982	0.979590
6	5.533117	-1.570846	-0.892952
6	1.198462	3.523303	0.141649
7	2.202224	4.111303	0.205403
1	0.353531	-0.673592	1.674493
1	1.967256	1.624284	-1.582211
1	2.317703	-2.095355	1.662222
1	3.925993	0.205142	-1.632614
1	5.974121	-0.593899	-0.646721
1	6.306784	-2.332340	-0.783575
1	5.230545	-1.552265	-1.947457
1	3.741534	-3.647554	0.962481
1	5.491151	-3.499161	0.768634
1	4.656927	-2.526303	1.996669
6	-1.534240	0.902984	0.146624
6	-1.843416	-0.385544	-0.140363
6	-3.171159	-0.993551	-0.119151
6	-3.295074	-2.343911	-0.500281
6	-4.338738	-0.300787	0.262076
6	-5.574755	-0.937037	0.257028
6	-5.678810	-2.278744	-0.125693
6	-4.533487	-2.980682	-0.504469
1	-2.330980	1.599709	0.391048
1	-1.037712	-1.053200	-0.436647
1	-6.463119	-0.386004	0.552900
1	-6.647259	-2.771199	-0.127664
1	-2.404273	-2.892381	-0.797452
1	-4.280380	0.740428	0.563805
1	-4.604794	-4.022793	-0.803437

[(2*E*)-1-[4-(Dimethylamino)phenyl]-3-(4-methoxyphenyl)-2-propen-1-ylidene]malononitrile (3g)

6	1.802152	0.537797	0.032180
6	1.711336	-0.528630	0.946673
6	2.856218	0.495689	-0.898569
6	2.624015	-1.572402	0.945570
1	0.928540	-0.519280	1.699065
6	3.763772	-0.551255	-0.925930
1	2.957156	1.290461	-1.630562
6	3.677809	-1.619961	-0.000114
1	2.522986	-2.349195	1.693652
1	4.548332	-0.535056	-1.672278
7	4.578495	-2.664335	-0.021723
6	5.732609	-2.608267	-0.905876
1	6.379115	-1.744219	-0.693685
1	6.323865	-3.516524	-0.779080
1	5.425936	-2.554189	-1.958076
6	4.526348	-3.686359	1.010755
1	3.556124	-4.198915	1.013118
1	5.295708	-4.434396	0.813104
1	4.697733	-3.275683	2.017229
6	0.844264	1.660059	0.073149
6	1.293536	2.976318	0.040321
6	2.674280	3.340495	0.088562
6	0.379941	4.075730	-0.006103
7	3.787222	3.682661	0.134068
7	-0.371441	4.965953	-0.038212
6	-0.581494	1.410808	0.157566
1	-1.198644	2.272635	0.395468
6	-1.177910	0.218250	-0.101989
1	-0.545842	-0.615983	-0.398206
6	-2.600882	-0.078291	-0.051462
6	-3.040690	-1.359149	-0.429575
6	-3.584556	0.851966	0.358897
6	-4.387030	-1.715305	-0.412143

1	-2.307017	-2.095450	-0.749325
6	-4.924143	0.513683	0.382849
1	-3.293551	1.852074	0.664878
6	-5.340886	-0.774217	-0.003547
1	-4.679431	-2.714045	-0.714718
1	-5.679066	1.226947	0.697876
8	-6.678219	-1.001251	0.057407

{(2*E*)-1,3-Bis|4-(dimethylamino)phenyl]-2-propen-1-ylidene}malononitrile (3h)

6	2.151068	0.535617	0.027519
6	2.053768	-0.521212	0.951426
6	3.204145	0.478203	-0.902659
6	2.958871	-1.572181	0.958579
1	1.271139	-0.499444	1.703788
6	4.104678	-0.575699	-0.921217
1	3.311431	1.267341	-1.639939
6	4.010579	-1.636268	0.012346
1	2.852250	-2.341430	1.713718
1	4.890193	-0.570121	-1.666795
7	4.902581	-2.690464	-0.002900
6	6.066191	-2.640160	-0.874447
1	6.720042	-1.783709	-0.652314
1	6.646661	-3.555558	-0.747813
1	5.769831	-2.577560	-1.928919
6	4.854683	-3.690924	1.050288
1	3.879572	-4.193158	1.074772
1	5.613207	-4.451133	0.856425
1	5.043303	-3.263847	2.047199
6	1.198807	1.665126	0.058188
6	1.663727	2.978317	0.030480
6	3.047181	3.326790	0.094673
6	0.762103	4.086301	-0.025404
7	4.163810	3.655915	0.152114
7	0.018820	4.983338	-0.065821
6	-0.224875	1.426106	0.127536
1	-0.840305	2.294815	0.344245
6	-0.828716	0.231237	-0.122359
1	-0.197123	-0.610211	-0.399477
6	-2.247625	-0.056693	-0.084648
6	-2.700409	-1.342125	-0.446599
6	-3.235732	0.877919	0.295747
6	-4.042084	-1.684897	-0.440174
1	-1.970565	-2.091485	-0.745307
6	-4.579563	0.554349	0.309989
1	-2.946145	1.882424	0.589811
6	-5.028630	-0.741287	-0.060311
1	-4.326619	-2.688700	-0.731481
1	-5.292245	1.312690	0.610822
7	-6.366421	-1.064797	-0.048104

[(2*E*)-1-|4-(Dimethylamino)phenyl]-5-(trimethylsilyl)-2-penten-4-yn-1-ylidene]malononitrile (8)

6	1.816510	0.541126	0.050465
6	1.782223	-0.573397	0.912109
6	2.891543	0.619152	-0.855356
6	2.768115	-1.547411	0.885501
1	0.984387	-0.657256	1.643748
6	3.872066	-0.357710	-0.909075
1	2.948516	1.450542	-1.550335
6	3.844586	-1.472811	-0.033987
1	2.707438	-2.366024	1.592049
1	4.666327	-0.252373	-1.63762
7	4.820302	-2.443170	-0.078465
6	5.964180	-2.284875	-0.963597
1	6.536419	-1.373656	-0.739033
1	6.629471	-3.141302	-0.844876
1	5.655563	-2.243144	-2.016471
6	4.795823	-3.545481	0.869915
1	3.865443	-4.122356	0.788626
1	5.626069	-4.220169	0.655915
1	4.894239	-3.201211	1.909913
6	0.780600	1.587103	0.113741
6	1.120161	2.934040	0.128036
6	2.467330	3.405642	0.209459
6	0.124834	3.961562	0.093506
7	3.547538	3.835027	0.285049
7	-0.684872	4.798717	0.069392
6	-0.628196	1.229000	0.161253
1	-1.328950	2.016868	0.422949
6	-1.125634	0.004362	-0.155016
1	-0.448095	-0.787813	-0.467732
6	-2.502116	-0.310192	-0.123181
6	-3.687077	-0.610936	-0.107348
14	-5.496297	-1.026039	-0.086726
6	-6.409387	0.236349	-1.168526
1	-7.485284	0.025097	-1.179879
1	-6.269105	1.255147	-0.791855
1	-6.049165	0.207422	-2.202464
6	-6.111520	-0.933611	1.705657
1	-7.181358	-1.168603	1.754978
1	-5.580236	-1.645787	2.346139
1	-5.966593	0.068647	2.122808

{(2*E*)-3-Chloro-1-|4-(dimethylamino)phenyl]-2-propen-1-ylidene}malononitrile (9)

6	0.047588	0.223206	-0.041162
6	-0.580156	-0.749320	-0.847213
6	-0.782244	0.994910	0.796410
6	-1.953219	-0.932612	-0.834280
1	0.018029	-1.346258	-1.528791
6	-2.153245	0.807372	0.836877
1	-0.341501	1.738813	1.451580
6	-2.786359	-0.159062	0.013840
1	-2.383405	-1.672877	-1.497433
1	-2.738013	1.415978	1.515315
7	-4.148851	-0.339202	0.039272
6	-4.983113	0.517589	0.869188
1	-4.874146	1.577171	0.600460
1	-6.028957	0.239525	0.732389
1	-4.741373	0.408287	1.934954
6	-4.772453	-1.323620	-0.831768
1	-4.388819	-2.333874	-0.637290
1	-5.847705	-1.333392	-0.648526
1	-4.610148	-1.094571	-1.894583
6	1.502787	0.431280	-0.093287
6	2.058318	1.700248	-0.146064
6	1.283364	2.894975	-0.278761
6	3.474719	1.902230	-0.105592
7	0.693794	3.892286	-0.397056
7	4.627868	2.063404	-0.077859
6	2.411680	-0.714940	-0.090687
1	3.442851	-0.540100	-0.383473
6	2.050408	-1.941082	0.309872
1	1.070911	-2.224138	0.669889
17	3.194362	-3.297472	0.317104

{(2*E*)-3-Cyclohexyl-1-[4-(dimethylamino)phenyl]-2-propen-1-ylidene}malononitrile (10)

6	-1.188892	0.627300	-0.077232
6	-1.189960	-0.491891	-0.932563
6	-2.246390	0.727980	0.846204
6	-2.192959	-1.447414	-0.884717
1	-0.405431	-0.593788	-1.675967
6	-3.242953	-0.230837	0.922172
1	-2.277402	1.563488	1.537755
6	-3.250433	-1.350465	0.053662
1	-2.159800	-2.269439	-1.589282
1	-4.023109	-0.105942	1.662791
7	-4.241211	-2.305256	0.123266
6	-5.376931	-2.108869	1.011070
1	-5.941837	-1.197503	0.767620
1	-6.051660	-2.961551	0.922290
1	-5.058281	-2.042625	2.059231
6	-4.270598	-3.395113	-0.838897
1	-3.347459	-3.987085	-0.798017
1	-5.102299	-4.059923	-0.600764
1	-4.401782	-3.038038	-1.871252
6	-0.135181	1.653280	-0.162018
6	-0.449680	3.004101	-0.161171
6	-1.788158	3.505997	-0.207686
6	0.568181	4.010704	-0.150395

7	-2.860077	3.959438	-0.255067
7	1.397308	4.829022	-0.144872
6	1.270314	1.265024	-0.249364
1	1.965579	2.047731	-0.546235
6	1.767753	0.052502	0.065538
1	1.092359	-0.730844	0.408505
6	3.219887	-0.316458	-0.004103
6	3.742092	-0.775827	1.379463
6	3.458398	-1.425799	-1.059295
1	3.794189	0.570193	-0.310072
6	5.215741	-1.206202	1.321196
1	3.128778	-1.620646	1.727733
1	3.607603	0.031287	2.109760
6	4.933530	-1.851756	-1.113645
1	2.834611	-2.297045	-0.808462
1	3.125613	-1.073786	-2.043578
6	5.446399	-2.295799	0.264073

{1-[4-(Dimethylamino)phenyl]-2-tricyclo[3.3.1.1^{3,7}]dec-2-ylideneethylidene}malononitrile (11)

6	-1.201544	0.823944	-0.190379
6	-1.359205	-0.229462	-1.113657
6	-2.181317	0.943504	0.814957
6	-2.434084	-1.100971	-1.055273
1	-0.633754	-0.343501	-1.912968
6	-3.248097	0.064506	0.901689
1	-2.094296	1.724394	1.562578
6	-3.413150	-0.985216	-0.036330
1	-2.518855	-1.870651	-1.812866
1	-3.960369	0.197583	1.706643
7	-4.474717	-1.858418	0.043718
6	-5.525138	-1.638688	1.026346
1	-6.025305	-0.669537	0.888080
1	-6.274681	-2.425492	0.930148
1	-5.130193	-1.675754	2.049745
6	-4.655676	-2.880401	-0.974753
1	-3.782420	-3.542295	-1.033952
1	-5.520430	-3.493502	-0.716720
1	-4.826586	-2.449948	-1.972561
6	-0.075251	1.758952	-0.319380
6	-0.237232	3.124395	-0.133175
6	-1.497980	3.762680	0.085222
6	0.884192	4.011588	-0.192201
7	-2.504431	4.323659	0.257697
7	1.796405	4.734596	-0.243577
6	1.248919	1.282690	-0.737898
1	1.793878	1.969634	-1.384376
6	1.906942	0.163320	-0.357897
6	1.475097	-0.859444	0.674504
6	3.293556	-0.128998	-0.901151

DCE-**1** (AB‡)

6	1.032888	-1.389785	-0.523283
6	3.906952	0.335568	0.515384
6	3.208944	-0.778054	1.012962
6	2.258649	-1.622716	-0.492771
1	2.356817	-0.587571	1.655253
1	3.792637	-1.652615	1.287685
1	3.038259	-2.056582	-1.094297
6	-0.280957	-0.944759	-0.365849
6	-0.620404	0.412872	-0.611413
6	-1.321119	-1.821554	0.035361
6	-1.915722	0.862224	-0.467043
1	0.163858	1.109583	-0.891293
6	-2.618534	-1.377391	0.180929
1	-1.085907	-2.864137	0.226796
6	-2.960003	-0.018165	-0.068539
1	-2.124453	1.908263	-0.652789
1	-3.379690	-2.083185	0.489532
7	-4.246857	0.427765	0.074708
6	-5.298956	-0.486103	0.499210
1	-5.093420	-0.907662	1.492039
1	-6.243557	0.055900	0.551532
1	-5.422715	-1.316067	-0.208666
6	-4.572767	1.826415	-0.175702
1	-4.342748	2.115020	-1.209368
1	-5.639922	1.978994	-0.011910
1	-4.024764	2.496719	0.499181
6	5.193632	0.183055	-0.067633
6	3.238427	1.582863	0.385653
7	2.639289	2.579582	0.280069
7	6.250342	0.023583	-0.537248

ν_i = -360.2721

DCE-**1** (AB‡) (PCM)

6	-0.895676	-1.163265	0.739364
6	-4.118810	0.243248	-0.515908
6	-3.169598	-0.700330	-0.900318
6	-2.100829	-1.438923	0.816662
1	-2.286736	-0.361964	-1.429758
1	-3.496651	-1.712801	-1.116334
1	-2.894859	-1.899375	1.381766
6	0.428761	-0.777760	0.504634
6	0.916729	0.481188	0.942714
6	1.335174	-1.640120	-0.166203
6	2.224563	0.858769	0.723170
1	0.243947	1.159717	1.463868
6	2.643913	-1.269390	-0.391897
1	0.986483	-2.612288	-0.509953
6	3.135692	-0.004660	0.046515
1	2.548529	1.830612	1.077494
1	3.295515	-1.962194	-0.911888
7	4.430247	0.365081	-0.171829
6	5.348830	-0.533492	-0.864802
1	5.008013	-0.748509	-1.885776
1	6.329881	-0.061875	-0.925280
1	5.458944	-1.484849	-0.329211
6	4.912326	1.668559	0.275369
1	4.830980	1.774693	1.364707
1	5.962132	1.772932	0.000418
1	4.351930	2.486673	-0.194774
6	-5.399145	-0.149798	-0.037850
6	-3.811110	1.631379	-0.487814
7	-3.557802	2.770637	-0.474287
7	-6.450021	-0.480462	0.347961

ν_i = -339.0770

TCE-**1** (AB‡)

6	-0.694606	-0.904754	0.913106
6	-3.483150	0.792276	-0.340305
6	-2.892398	-0.475602	-0.607883
6	-1.941919	-1.023629	0.971560
1	-2.055185	-0.452902	-1.299883
1	-2.697527	-1.246506	1.706554
6	0.635376	-0.632513	0.624461
6	1.104069	0.711046	0.554325
6	1.576759	-1.674437	0.398643
6	2.423445	0.990691	0.281761
1	0.396254	1.522912	0.691229
6	2.896964	-1.398599	0.125334
1	1.240804	-2.705518	0.448817
6	3.367840	-0.053949	0.061232
1	2.732395	2.026655	0.224464
1	3.579044	-2.222943	-0.040317
7	4.676943	0.223488	-0.207403
6	5.628034	-0.857507	-0.443824
1	5.343251	-1.461328	-1.314774
1	6.612668	-0.430732	-0.634842
1	5.707216	-1.520025	0.427179
6	5.139998	1.606273	-0.273855
1	4.979714	2.128652	0.677376
1	6.208559	1.614141	-0.489038
1	4.627371	2.164734	-1.067071
6	-4.751669	0.918008	0.277981
6	-2.660718	1.939457	-0.467858
7	-1.927902	2.843978	-0.566983
7	-5.796569	1.014103	0.789514
6	-3.753484	-1.618051	-0.821893
7	-4.415590	-2.557198	-0.993185

ν_i = -347.9235

TCNE-**1** ($AB^{‡}$)

6	0.551199	-0.765557	-1.108016
6	3.342455	0.862497	0.187435
6	2.797050	-0.462871	0.378771
6	1.807028	-0.870918	-1.166566
1	2.534427	-1.016251	-1.950337
6	-0.773151	-0.530869	-0.809398
6	-1.254600	0.803356	-0.635915
6	-1.705472	-1.600139	-0.661242
6	-2.572516	1.047136	-0.340803
1	-0.552331	1.628132	-0.706695
6	-3.023008	-1.358813	-0.362150
1	-1.357014	-2.620139	-0.787414
6	-3.504968	-0.024221	-0.191756
1	-2.891847	2.071328	-0.197791
1	-3.696848	-2.198738	-0.251936
7	-4.808904	0.217425	0.110335
6	-5.745127	-0.888974	0.296602
1	-5.432807	-1.542986	1.119725
1	-6.728705	-0.486007	0.536618
1	-5.836509	-1.491972	-0.614778
6	-5.286534	1.587209	0.292089
1	-5.134523	2.184090	-0.614770
1	-6.354115	1.565376	0.509673
1	-4.775729	2.082392	1.126807
6	4.572499	1.044862	-0.484470
6	2.498796	1.977984	0.395471
7	1.758364	2.870109	0.541992
7	5.586821	1.192790	-1.044442
6	1.824899	-0.595833	1.458462
6	3.759416	-1.559193	0.390352
7	1.034334	-0.709361	2.300110
7	4.500557	-2.452271	0.377391

ν_i = -314.5575

2f-1 ($AB^{‡}$)

6	-0.132899	-0.059921	-1.147866
6	2.292426	1.823665	0.368245
6	2.040724	0.407651	0.335740
6	1.109225	0.117420	-1.238894
1	1.270393	0.128279	1.049347
1	1.811529	0.237927	-2.048222
6	-1.471460	-0.155568	-0.789070
6	-2.197059	0.994164	-0.363869
6	-2.171118	-1.391694	-0.847855
6	-3.531093	0.911732	-0.032265
1	-1.673310	1.940765	-0.271068
6	-3.504536	-1.47836	-0.513896
1	-1.638217	-2.280866	-1.170712
6	-4.232585	-0.325659	-0.099992
1	-4.038336	1.808594	0.300407
1	-3.996743	-2.440969	-0.574961
7	-5.558144	-0.406281	0.227210
6	-6.252882	-1.686757	0.179598
1	-5.798647	-2.417956	0.860744
1	-7.290169	-1.541697	0.482332
1	-6.250073	-2.110049	-0.833210
6	-6.288297	0.786272	0.642346
1	-6.271789	1.557603	-0.137648
1	-7.328169	0.519428	0.832668
1	-5.871940	1.216555	1.562323
6	3.416761	2.439631	-0.228523
6	1.234791	2.660956	0.799926
7	0.315403	3.297701	1.142662
7	4.345398	2.945057	-0.727948
6	3.140330	-0.611183	0.303225
6	4.232165	-0.542849	-0.577142
6	3.058330	-1.698961	1.186690
6	5.220288	-1.526061	-0.554125
1	4.322658	0.283062	-1.274073
6	4.048770	-2.679441	1.211237
1	**2.213123**	**-1.77112**	**1.867196**
6	**5.13501**	**-2.595898**	**0.339121**
1	**6.061492**	**-1.452696**	**-1.237882**
1	**3.97001**	**-3.507819**	**1.91021**
1	**5.908235**	**-3.359229**	**0.353299**

ν_i = -321.8833

DCE-**1** (B)

6	1.060019	-1.272077	-0.443189
6	3.924578	0.286331	0.460575
6	3.204914	-0.956542	0.842728
6	2.335882	-1.44709	-0.390339
1	2.53471	-0.793206	1.687646
1	3.905647	-1.758048	1.092167
1	2.924556	-1.869229	-1.202764
6	-0.246117	-0.87096	-0.30743
6	-0.621726	0.493892	-0.528674
6	-1.287763	-1.786949	0.03919
6	-1.930073	0.899934	-0.421151
1	0.155178	1.217808	-0.754042
6	-2.594307	-1.376739	0.157876
1	-1.031691	-2.828021	0.209869
6	-2.964397	-0.018638	-0.074888
1	-2.162447	1.94484	-0.584493
1	-3.34739	-2.106856	0.427491
7	-4.264454	0.3893	0.036909
6	-5.304116	-0.556679	0.424119
1	-5.107858	-0.989228	1.413655
1	-6.261768	-0.03751	0.465827
1	-5.393098	-1.376239	-0.30041
6	-4.623035	1.783668	-0.19925
1	-4.354357	2.099479	-1.214901
1	-5.700872	1.899199	-0.083206
1	-4.128075	2.454938	0.514233
6	5.190163	0.212959	-0.147998
6	3.215555	1.501756	0.462671
7	2.56067	2.473591	0.472266
7	6.248071	0.106379	-0.640105

DCE-**1** (B) (PCM)

6	0.907345	-0.920596	-0.322972
6	4.219463	0.152438	0.381199
6	3.166256	-0.844354	0.782755
6	2.173571	-1.160292	-0.373345
1	2.601435	-0.482696	1.645623
1	3.622621	-1.801791	1.062593
1	2.616493	-1.609144	-1.267813
6	-0.408223	-0.618834	-0.235700
6	-0.908429	0.671303	-0.640976
6	-1.362880	-1.580427	0.257138
6	-2.236407	0.971848	-0.562085
1	-0.205814	1.410690	-1.020630
6	-2.690305	-1.279754	0.344076
1	-1.004621	-2.560933	0.565601
6	-3.183442	0.009578	-0.063423
1	-2.568452	1.953158	-0.879943
1	-3.372008	-2.031623	0.723931
7	-4.490816	0.306471	0.018553
6	-5.455177	-0.673681	0.534404
1	-5.213722	-0.952901	1.565599
1	-6.449975	-0.230649	0.519688
1	-5.466269	-1.575228	-0.087560
6	-4.992392	1.621625	-0.400783
1	-4.771794	1.804138	-1.457908
1	-6.072508	1.647130	-0.263473
1	-4.545619	2.420234	0.201244
6	5.325163	-0.257334	-0.371022
6	4.027516	1.517980	0.614614
7	3.858523	2.661525	0.835141
7	6.251990	-0.631905	-0.992298

DCE-**1** ($BC^{‡}$)

6	-1.813815	0.000164	-1.349237
6	-2.795677	-0.000042	0.606952
6	-3.944187	-0.000419	-0.421603

6	-3.102581	0.000069	-1.648003
1	-4.587124	0.883805	-0.332242
1	-4.586123	-0.885405	-0.332561
1	-3.479472	-0.000090	-2.676270
6	-0.458199	0.000202	-1.034974
6	0.252485	-1.217691	-0.845538
6	0.252555	1.218017	-0.845362
6	1.575916	-1.216707	-0.461179
1	-0.267427	-2.159338	-0.982911
6	1.575979	1.216898	-0.461014
1	-0.267288	2.159719	-0.982608
6	2.281530	0.000053	-0.250346
1	2.070407	-2.167895	-0.309539
1	2.070533	2.168036	-0.309281
7	3.595628	-0.000051	0.140639
6	4.282900	1.257031	0.404174
1	3.800375	1.824047	1.211607
1	5.310075	1.046225	0.703555
1	4.315473	1.892097	-0.490397
6	4.282678	-1.257318	0.403928
1	4.314882	-1.892310	-0.490708
1	5.309974	-1.046787	0.703077
1	3.800202	-1.824300	1.211418
6	-2.406356	-1.214005	1.215396
6	-2.406470	1.214083	1.215138
7	-2.031194	2.238380	1.637274
7	-2.030866	-2.238301	1.637355

ν_i = -325.8545

DCE-**1** ($BC^{\ddagger}$) (PCM)

6	-1.475544	-0.000415	1.292744
6	-3.271274	0.000315	-0.420215
6	-3.831900	0.000017	1.011928
6	-2.631866	-0.000017	1.908968
1	-4.464083	-0.879505	1.194091
1	-4.464478	0.879183	1.194509
1	-2.685804	0.000314	3.005198
6	-0.165539	-0.000410	0.920289
6	0.544838	1.228555	0.698957
6	0.545099	-1.229324	0.699534
6	1.855863	1.230371	0.310404
1	0.021885	2.170877	0.850639
6	1.856151	-1.231070	0.311060
1	0.022361	-2.171694	0.851698
6	2.565135	-0.000319	0.100637
1	2.353411	2.181587	0.162026
1	2.353882	-2.182309	0.163243
7	3.858117	-0.000260	-0.282265
6	4.576059	-1.260349	-0.498944
1	4.103870	-1.850673	-1.292262
1	5.599458	-1.036797	-0.797928
1	4.606049	-1.858564	0.418659
6	4.575612	1.259896	-0.500063
1	4.606166	1.858565	0.417231
1	5.598833	1.036408	-0.799712
1	4.102709	1.849706	-1.293333
6	-3.129832	1.205615	-1.121171
6	-3.133170	-1.204254	-1.123067
7	-3.005895	-2.225301	-1.690632
7	-2.999657	2.227166	-1.687164

ν_i = -205.3808

DCE-**1** (C)

6	-1.685003	0.882791	-0.006606
6	-2.888838	-0.097826	0.008586
6	-3.789770	1.217322	0.008781
6	-2.483652	1.970485	-0.006267
1	-4.410550	1.310966	0.906704
1	-4.425498	1.301300	-0.879589
1	-2.279426	3.035876	-0.014322
6	-0.265513	0.588072	-0.015188
6	0.213461	-0.733079	-0.023249
6	0.690117	1.621722	-0.011536
6	1.571395	-1.015305	-0.030507
1	-0.486163	-1.564199	-0.021599
6	2.048753	1.356265	-0.018368
1	0.359652	2.657314	0.000444
6	2.533382	0.023098	-0.034713
1	1.883891	-2.052166	-0.031622
1	2.740769	2.189542	-0.009694
7	3.885843	-0.248530	-0.056746
6	4.848225	0.835415	0.048370
1	4.753806	1.388247	0.995061
1	5.857408	0.423871	-0.004762
1	4.736423	1.551674	-0.775980
6	4.350056	-1.623832	0.024867
1	3.967541	-2.224098	-0.810532
1	5.439827	-1.637306	-0.027475
1	4.045650	-2.112330	0.962455
6	-3.040369	-0.928141	-1.192821
6	-3.019365	-0.914310	1.221892
7	-3.115319	-1.531892	2.200220
7	-3.153467	-1.557400	-2.161837

DCE-**1** (C) (PCM)

6	-1.686050	0.881418	-0.000266
6	-2.892845	-0.097977	0.007107
6	-3.791112	1.221604	0.014600
6	-2.483181	1.971068	0.006971
1	-4.413469	1.309557	0.912811
1	-4.425640	1.312124	-0.874745
1	-2.277582	3.038988	0.006422
6	-0.266872	0.582102	-0.010515
6	0.215641	-0.738984	-0.017601
6	0.688146	1.619187	-0.009338
6	1.574978	-1.019930	-0.025808
1	-0.477954	-1.578185	-0.013727
6	2.047666	1.355585	-0.017343
1	0.358099	2.657104	0.001322
6	2.537523	0.021547	-0.032890
1	1.885762	-2.058544	-0.025563
1	2.735099	2.194049	-0.010744
7	3.886543	-0.246176	-0.056816
6	4.850255	0.840983	0.043174
1	4.758863	1.391232	0.991102
1	5.858822	0.429320	-0.016448
1	4.730590	1.557565	-0.779311
6	4.357268	-1.621662	0.024395
1	3.970481	-2.224579	-0.806959
1	5.446559	-1.630012	-0.034385
1	4.059314	-2.107597	0.965093
6	-3.043473	-0.920369	-1.198516
6	-3.026857	-0.922917	1.212882
7	-3.120958	-1.544892	2.188642
7	-3.150652	-1.540496	-2.174109

TCE-**1** (C)

6	-1.247619	-0.589440	-0.353476
6	-2.369799	0.477138	-0.234387
6	-3.366684	-0.735153	-0.592692
6	-2.112625	-1.585622	-0.639040
1	-3.877993	-0.572459	-1.554799
1	-2.004477	-2.645426	-0.852953
6	0.181535	-0.418282	-0.218498
6	0.759113	0.830478	0.079811
6	1.052498	-1.516044	-0.382840
6	2.130690	0.984519	0.210262
1	0.133394	1.711175	0.213697
6	2.422674	-1.378883	-0.253876
1	0.645585	-2.499050	-0.616019
6	3.009537	-0.118447	0.047387
1	2.518905	1.970153	0.440161
1	3.044310	-2.256823	-0.388922
7	4.367819	0.023103	0.173270
6	5.243774	-1.131632	0.024666
1	5.153602	-1.582385	-0.972686
1	6.278397	-0.813958	0.159390
1	5.024658	-1.907110	0.771305
6	4.941897	1.321677	0.499234

1	4.583166	1.693283	1.468904
1	6.027300	1.229096	0.552130
1	4.700997	2.072972	-0.264716
6	-2.542491	1.059714	1.101046
6	-2.355686	1.531912	-1.254730
7	-2.332988	2.340570	-2.086521
7	-2.661519	1.500159	2.167832
6	-4.367694	-1.062050	0.421429
7	-5.159392	-1.352229	1.219524

TCNE-**1** (C)

6	-0.906137	-0.526631	-0.000419
6	-1.979469	0.590185	0.000425
6	-3.053985	-0.645874	-0.000488
6	-1.811107	-1.527068	-0.001566
1	-1.758035	-2.608295	-0.002927
6	0.530049	-0.392223	-0.000050
6	1.155818	0.868847	0.000460
6	1.360720	-1.531487	-0.000400
6	2.534305	0.993407	0.000644
1	0.557027	1.774978	0.000736
6	2.738002	-1.423088	-0.000255
1	0.913914	-2.522242	-0.000755
6	3.371998	-0.150904	0.000286
1	2.964004	1.987099	0.001119
1	3.331230	-2.329071	-0.000605
7	4.739927	-0.036070	0.000545
6	5.576051	-1.227490	-0.000899
1	5.401138	-1.845629	-0.891758
1	6.624684	-0.928212	0.000248
1	5.400073	-1.848233	0.887890
6	5.362922	1.279753	-0.000306
1	5.084338	1.861096	0.888847
1	6.447132	1.162244	-0.000037
1	5.084590	1.860017	-0.890275
6	-2.014612	1.427947	1.203473
6	-2.014726	1.429379	-1.201690
7	-2.010062	2.087944	-2.157012
7	-2.009347	2.085196	2.159699
6	-3.892177	-0.729263	-1.204320
6	-3.891591	-0.731176	1.203616
7	-4.535281	-0.837585	-2.164127
7	-4.534729	-0.840862	2.163245

2f-1 (C)

6	-0.165516	-0.028026	-0.691018
6	-1.177702	1.034850	-0.196191
6	-2.261091	0.212488	-1.095646
6	-1.095510	-0.700601	-1.398700
1	-2.555656	0.846675	-1.940892
1	-1.052718	-1.593593	-2.014218
6	1.257378	-0.124002	-0.428648
6	1.910322	0.767259	0.440318
6	2.041639	-1.119415	-1.041984
6	3.271116	0.673806	0.691113
1	1.346712	1.552720	0.935493
6	3.400541	-1.226621	-0.800871
1	1.575443	-1.820956	-1.729219
6	4.058839	-0.332530	0.082318
1	3.722975	1.389386	1.366721
1	3.958033	-2.006863	-1.304573
7	5.410009	-0.441761	0.338429
6	6.209810	-1.422504	-0.376020
1	6.214424	-1.247535	-1.462364
1	7.239955	-1.371627	-0.020003
1	5.845378	-2.442441	-0.197585
6	6.072332	0.550559	1.169364
1	5.641555	0.578073	2.178550
1	7.127776	0.290844	1.264761
1	6.005638	1.562493	0.743140
6	-1.431371	1.033405	1.246449
6	-0.940548	2.401499	-0.674311
7	-0.757439	3.467615	-1.096786
7	-1.609892	1.011235	2.393361
6	-3.496977	-0.328134	-0.422733
6	-4.728837	0.312181	-0.614737
6	-3.446356	-1.463866	0.396650
6	-5.884644	-0.168351	-0.000307
1	-4.781457	1.192059	-1.252393
6	-4.601505	-1.946892	1.010458
1	-2.497364	-1.969281	0.553757
6	-5.823207	-1.300547	0.814144
1	-6.832117	0.339143	-0.160072
1	-4.546497	-2.828164	1.643737
1	-6.723092	-1.677911	1.292251

DCE-**1** (CD‡)

6	-1.687134	0.741760	-0.029391
6	-2.745030	-0.283768	0.135843
6	-3.712671	1.633770	0.359943
6	-2.410390	1.906725	-0.155908
1	-3.843935	1.340982	1.395604
1	-4.616141	2.035016	-0.106920
1	-2.116125	2.825938	-0.657413
6	-0.260203	0.492556	-0.043531
6	0.270817	-0.779381	-0.336926
6	0.658347	1.526720	0.230246
6	1.635044	-1.013478	-0.348650
1	-0.400666	-1.597964	-0.579338
6	2.024755	1.312452	0.211754
1	0.283838	2.514510	0.486203
6	2.557500	0.027944	-0.074548
1	1.989088	-2.008943	-0.586273
1	2.686178	2.139640	0.439133
7	3.914660	-0.196842	-0.085689
6	4.839427	0.894746	0.174542
1	4.707482	1.312347	1.182562
1	5.862234	0.524073	0.095098
1	4.718237	1.710451	-0.551086
6	4.431981	-1.531849	-0.343349
1	4.159964	-1.888701	-1.346343
1	5.520576	-1.513089	-0.276221
1	4.059232	-2.259223	0.390305
6	-3.524171	-0.691987	-1.002717
6	-2.637500	-1.275171	1.172056
7	-2.590946	-2.014587	2.071705
7	-4.131514	-1.060181	-1.926229

ν_i = -575.7733

DCE-**1** (CD‡) (PCM)

6	-1.682984	0.754345	-0.015127
6	-2.749811	-0.276095	0.133570
6	-3.727021	1.620283	0.327450
6	-2.409355	1.915050	-0.146055
1	-3.892536	1.340461	1.363547
1	-4.619898	2.002197	-0.177693
1	-2.111764	2.848976	-0.623319
6	-0.260355	0.498100	-0.035671
6	0.267308	-0.780549	-0.315939
6	0.663283	1.535618	0.223767
6	1.630627	-1.020247	-0.325399
1	-0.403068	-1.604098	-0.556068
6	2.027966	1.315698	0.208749
1	0.295476	2.532191	0.463491
6	2.558993	0.022939	-0.060967
1	1.978337	-2.020481	-0.557444
1	2.689652	2.147409	0.423339
7	3.909854	-0.204842	-0.067076
6	4.842236	0.893055	0.156599
1	4.708093	1.341986	1.149775
1	5.862353	0.512967	0.091791
1	4.723800	1.684085	-0.595880
6	4.428484	-1.540797	-0.332602
1	4.163928	-1.887936	-1.340855
1	5.516030	-1.523539	-0.253216
1	4.045413	-2.270684	0.392281
6	-3.480490	-0.705500	-1.024583
6	-2.670706	-1.257385	1.179542
7	-2.651979	-1.989319	2.087016
7	-4.055714	-1.084498	-1.965619

ν_i = -598.3719

TCE-**1** (CD‡)

6	1.229817	-0.413405	0.104631
6	2.162979	0.752491	0.206725
6	3.350353	-0.971813	0.576772
6	2.084242	-1.485226	0.099010
1	3.459889	-0.626969	1.606048
1	1.911218	-2.505075	-0.242546
6	-0.207822	-0.323046	0.035327
6	-0.862193	0.861962	-0.368324
6	-1.019423	-1.431741	0.370465
6	-2.241024	0.946737	-0.426665
1	-0.278997	1.731680	-0.667133
6	-2.397217	-1.365726	0.310023
1	-0.552819	-2.356353	0.706876
6	-3.057795	-0.167600	-0.087516
1	-2.688274	1.877891	-0.755293
1	-2.970187	-2.242897	0.588301
7	-4.421684	-0.094077	-0.143932
6	-5.237698	-1.263141	0.165154
1	-5.093205	-1.594231	1.202000
1	-6.289587	-1.007820	0.033464
1	-5.003892	-2.103931	-0.500610
6	-5.076037	1.151318	-0.529185
1	-4.818949	1.443435	-1.556152
1	-6.156812	1.018223	-0.473210
1	-4.797792	1.973571	0.142228
6	2.842751	1.211282	-0.970149
6	1.949193	1.759590	1.206468
7	1.826897	2.522594	2.078945
7	3.384252	1.588660	-1.930354
6	4.586307	-1.346555	-0.039173
7	5.587793	-1.602647	-0.576851

ν_i = -436.8606

TCNE-**1** (CD‡)

6	-0.926443	-0.298280	-0.217302
6	-1.814792	0.878772	0.041020
6	-3.117638	-0.917802	-0.022769
6	-1.785153	-1.324395	-0.477346
1	-1.586049	-2.272214	-0.968813
6	0.517659	-0.249699	-0.176782
6	1.222732	0.958589	-0.358507
6	1.277864	-1.418348	0.044784
6	2.603556	1.004860	-0.321606
1	0.676456	1.877038	-0.553889
6	2.657976	-1.389760	0.078329
1	0.766384	-2.360749	0.220918
6	3.368699	-0.171227	-0.101888
1	3.095896	1.956301	-0.478075
1	3.193772	-2.311929	0.265430
7	4.738315	-0.134154	-0.065618
6	5.502369	-1.358146	0.133656
1	5.279814	-2.101138	-0.642864
1	6.566763	-1.126977	0.082168
1	5.299317	-1.811832	1.113275
6	5.441352	1.134874	-0.199413
1	5.140477	1.846307	0.580443
1	6.513475	0.961224	-0.102469
1	5.259173	1.598776	-1.178005
6	-1.656379	1.656979	1.228104
6	-2.399710	1.562904	-1.071809
7	-2.847939	2.130210	-1.985467
7	-1.570992	2.239724	2.234163
6	-4.239972	-1.097682	-0.894550
6	-3.437416	-0.869276	1.374309
7	-5.121132	-1.210833	-1.648117
7	-3.697353	-0.863375	2.509682

ν_i = -283.3932

2f-1 (CD‡)

6	-0.113115	0.001047	-0.253624
6	-0.883814	1.267799	-0.090307
6	-2.281552	-0.204971	-0.890012
6	-1.078370	-0.927695	-0.513479
1	-2.244299	0.370682	-1.811523
1	-1.014420	-2.009944	-0.422174
6	1.330672	-0.124953	-0.145434
6	2.109981	0.833475	0.529328
6	2.008552	-1.222776	-0.711018
6	3.485724	0.709369	0.637100
1	1.625151	1.688133	0.992341
6	3.381139	-1.367184	-0.604306
1	1.443792	-1.965879	-1.268158
6	4.165048	-0.401047	0.077606
1	4.035653	1.475591	1.169420
1	3.852732	-2.223959	-1.070094
7	5.531940	-0.537187	0.191217
6	6.206962	-1.664696	-0.429457
1	6.098542	-1.664686	-1.524259
1	7.271419	-1.618418	-0.194486
1	5.821599	-2.620007	-0.049912
6	6.320261	0.522555	0.799580
1	6.034717	0.687041	1.847082
1	7.374056	0.240579	0.781034
1	6.212364	1.476332	0.263570
6	-1.586140	1.489177	1.136701
6	-0.509329	2.444878	-0.816434
7	-0.247233	3.369612	-1.476929
7	-2.151319	1.647393	2.144527
6	-3.613493	-0.509378	-0.407797
6	-4.745620	-0.058194	-1.119434
6	-3.806698	-1.239730	0.783118
6	-6.026987	-0.357336	-0.673889
1	-4.604145	0.521218	-2.028610
6	-5.091008	-1.540851	1.224743
1	-2.941144	-1.548766	1.361142
6	-6.201312	-1.103002	0.497491
1	-6.891643	-0.010710	-1.232609
1	-5.229772	-2.102851	2.143781
1	-7.203729	-1.332011	0.848881

ν_i = -296.9255

DCE-**1** (D)

6	-0.304403	-0.298630	-0.124545
6	0.514923	-1.366772	0.300163
6	0.353202	0.880398	-0.535300
6	1.893601	-1.262013	0.351844
1	0.052172	-2.292475	0.629697
6	1.731264	0.994977	-0.506827
1	-0.221156	1.717423	-0.914488
6	2.548936	-0.069198	-0.047626
1	2.466572	-2.108903	0.709228
1	2.178660	1.918430	-0.853084
7	3.916863	0.048007	0.000061
6	4.559838	1.289351	-0.405035
1	4.210287	2.139699	0.195043
1	5.637354	1.196736	-0.263173
1	4.375088	1.518657	-1.463541
6	4.731331	-1.068283	0.454934
1	4.598836	-1.954313	-0.180852
1	5.783242	-0.782157	0.418756
1	4.492285	-1.351013	1.489194
6	-1.760180	-0.463034	-0.153182
6	-2.647814	0.580355	0.048761
6	-2.254039	-1.825887	-0.436852
1	-1.664806	-2.383422	-1.162481
6	-3.298212	-2.425457	0.148960
1	-3.898220	-1.944008	0.914174
1	-3.578764	-3.438650	-0.124196
6	-2.252166	1.881362	0.498503
6	-4.060983	0.458438	-0.154807
7	-1.982681	2.949329	0.877566
7	-5.214658	0.421287	-0.310229

DCE-**1** (D) (PCM)

6	-0.303464	-0.313686	-0.122504

6	0.529607	-1.387672	0.276841
6	0.345335	0.881608	-0.516910
6	1.904332	-1.270746	0.327034
1	0.080780	-2.327279	0.591079
6	1.719902	1.008109	-0.493576
1	-0.235126	1.714564	-0.902375
6	2.550748	-0.060601	-0.052296
1	2.483322	-2.122237	0.665964
1	2.156971	1.938055	-0.839186
7	3.908889	0.065647	-0.007253
6	4.547267	1.318278	-0.399025
1	4.192000	2.156228	0.213703
1	5.624783	1.227363	-0.259364
1	4.356897	1.556620	-1.453782
6	4.740206	-1.056449	0.416745
1	4.610942	-1.924857	-0.242025
1	5.787767	-0.756021	0.382791
1	4.505315	-1.364179	1.443743
6	-1.746119	-0.482504	-0.145859
6	-2.642518	0.570232	0.037532
6	-2.257194	-1.844164	-0.395172
1	-1.698525	-2.428936	-1.126721
6	-3.289262	-2.409508	0.245952
1	-3.843111	-1.899038	1.029578
1	-3.593375	-3.427620	0.015758
6	-2.269436	1.852749	0.542477
6	-4.040688	0.464900	-0.237974
7	-2.032699	2.906799	0.981845
7	-5.184895	0.460991	-0.462987

DCE-**1** ($DE^{\ddagger}$)

6	1.718968	1.125014	0.089533
6	2.554091	-0.017580	-0.021359
6	1.907857	-1.272356	-0.154751
6	0.529180	-1.364255	-0.173297
6	-0.314107	-0.230879	-0.067654
6	0.342458	1.018438	0.064869
7	3.921093	0.089108	0.001635
6	4.553387	1.393895	0.139079
6	-1.760826	-0.407602	-0.110194
6	-2.734031	0.575994	-0.065678
6	-2.516834	1.985078	0.044336
7	-2.391037	3.139879	0.135680
6	-2.286272	-1.801923	-0.269974
6	-2.566657	-2.621023	0.743116
6	4.749881	-1.101429	-0.119049
6	-4.122437	0.227209	-0.152036
7	-5.259907	-0.010384	-0.229888
1	0.083395	-2.347519	-0.267750
1	-0.227022	1.932908	0.154421
1	2.489015	-2.182339	-0.241490
1	2.154028	2.111173	0.196144
1	4.266306	1.885721	1.077738
1	5.636646	1.267508	0.141865
1	4.290829	2.061707	-0.692102
1	4.576758	-1.621461	-1.070826
1	5.800600	-0.812019	-0.078766
1	4.561310	-1.810749	0.697870
1	-2.462280	-2.126146	-1.296403
1	-2.415422	-2.327750	1.778848
1	-2.973149	-3.612748	0.566823

ν_i = -89.1228

DCE-**1** ($DE^{\ddagger}$) (PCM)

6	1.709708	1.067535	0.345880
6	2.552050	-0.027575	-0.003337
6	1.910889	-1.253482	-0.338676
6	0.536155	-1.358200	-0.340569
6	-0.312746	-0.260260	-0.037033
6	0.336382	0.951118	0.320725
7	3.909045	0.091500	-0.004515
6	4.541161	1.357396	0.357259
6	-1.746632	-0.435683	-0.084040
6	-2.708539	0.571543	-0.095372
6	-2.459412	1.974596	-0.168084
7	-2.323642	3.130240	-0.247515
6	-2.274710	-1.832343	-0.180480
6	-2.702411	-2.540433	0.865028
6	4.750662	-1.055610	-0.333400
6	-4.103498	0.258757	-0.116600
7	-5.254301	0.072709	-0.140716
1	0.099800	-2.318988	-0.597358
1	-0.240678	1.815092	0.626194
1	2.495302	-2.129518	-0.595734
1	2.138515	2.015275	0.651200
1	4.312834	1.641252	1.392762
1	5.622307	1.254882	0.261539
1	4.214179	2.168731	-0.304506
1	4.535928	-1.431297	-1.341498
1	5.796785	-0.750599	-0.299534
1	4.608391	-1.877408	0.380207
1	-2.302601	-2.260745	-1.186183
1	-2.684113	-2.143534	1.878045
1	-3.088712	-3.548446	0.736297

ν_i = -77.7614

DCE-**1** (E)

6	-2.430915	0.015780	0.029348
6	-1.801250	1.064127	-0.687804
6	-0.425091	1.219827	-0.664050
6	0.411590	0.334814	0.046031
6	-0.215849	-0.710262	0.752265
6	-1.591533	-0.864565	0.757688
6	1.873017	0.493020	0.028638
6	2.472165	1.822769	0.186963
6	1.852598	2.891706	0.711587
7	-3.797731	-0.138534	0.023369
6	-4.630642	0.759717	-0.760353
6	-4.405829	-1.275523	0.697928
6	2.721085	-0.590198	-0.135501
6	4.144095	-0.447456	-0.061940
7	5.301792	-0.331818	-0.006838
6	2.268674	-1.917069	-0.421020
7	1.946884	-3.009380	-0.665407
1	0.018637	2.025485	-1.240269
1	0.384340	-1.401828	1.333921
1	-2.390701	1.756031	-1.276867
1	-2.017840	-1.675705	1.334952
1	-4.203964	-1.259724	1.777229
1	-5.487134	-1.237651	0.559130
1	-4.043380	-2.231949	0.296474
1	-4.413335	0.692910	-1.836175
1	-5.678967	0.498475	-0.609698
1	-4.496654	1.804017	-0.449484
1	3.515126	1.915290	-0.106105
1	0.827515	2.855653	1.065739
1	2.377059	3.837001	0.814606

DCE-**1** (E) (PCM)

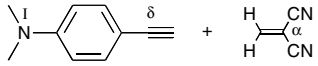
6	-2.435158	-0.007666	0.014012
6	-1.816644	1.072186	-0.674302
6	-0.444674	1.240355	-0.652746
6	0.407881	0.335758	0.023227
6	-0.209125	-0.738878	0.704077
6	-1.581281	-0.902946	0.717021
6	1.856449	0.507010	0.005039
6	2.446318	1.844826	0.117676
6	1.843678	2.896299	0.696734
7	-3.791568	-0.175476	0.005287
6	-4.647514	0.783449	-0.684031
6	-4.399113	-1.301891	0.705091
6	2.722911	-0.578610	-0.122961
6	4.136881	-0.431602	0.005074
7	5.294289	-0.332941	0.107428
6	2.300265	-1.903330	-0.441453
7	2.015800	-2.997247	-0.727898
1	-0.014916	2.067352	-1.211926
1	0.397148	-1.430496	1.283965
1	-2.413234	1.781013	-1.237300
1	-1.996417	-1.724268	1.290252

1	-4.215336	-1.254834	1.786889
1	-5.477094	-1.283376	0.541749
1	-4.013763	-2.259175	0.331972
1	-4.428224	0.819495	-1.759178
1	-5.688899	0.484986	-0.559743
1	-4.529792	1.795219	-0.274614
1	3.462656	1.965786	-0.256667
1	0.851200	2.833204	1.133224
1	2.351774	3.854989	0.762911

ESI 6. Computational data from B3LYP/6-31G(d) including the SCF (E_{SCF}) energy and zero-point ($H_{0\,K}$), thermal ($H_{298\,K}$) and free-energy ($G_{298\,K}$) corrected energies (Hartrees).

Entry	E_{SCF}	$H_{0\,K}$	$H_{298\,K}$	$G_{298\,K}$
1	-442.362121	-442.179205	-442.167351	-442.215779
1 (PCM)	-442.371235	-442.189028	-442.177139	-442.225795
3b	-1141.062224	-1140.739814	-1140.714887	-1140.797076
3c	-1049.886010	-1049.556911	-1049.532507	-1049.612870
3d	-1012.707631	-1012.379147	-1012.354584	-1012.434944
3e	-949.099860	-948.790250	-948.766360	-948.846487
3f	-936.562713	-936.242654	-936.220337	-936.295508
3g	-1051.087348	-1050.734604	-1050.709690	-1050.790743
3h	-1070.534404	-1070.141071	-1070.114191	-1070.200401
8	-904.702260	-904.350458	-904.322792	-904.410683
9	-719.824768	-719.595699	-719.576716	-719.643846
10	-940.185374	-939.795190	-939.771503	-939.849681
11	-1055.716323	-1055.281288	-1055.257473	-1055.334588
DCE	-263.062682	-263.012878	-263.006333	-263.041351
DCE (PCM)	-263.074597	-263.024856	-263.018340	-263.053307
DCE-**1** ($AB^{‡}$)	-705.414455	-705.179530	-705.161434	-705.227095
DCE-**1** ($AB^{‡}$) (PCM)	-705.438648	-705.205066	-705.186778	-705.253630
DCE-**1** (B)	-705.420608	-705.184251	-705.166119	-705.231823
DCE-**1** (B) (PCM)	-705.457662	-705.220870	-705.202844	-705.268933
DCE-**1** ($BC^{‡}$)	-705.419116	-705.182523	-705.165236	-705.227760
DCE-**1** ($BC^{‡}$) (PCM)	-705.451389	-705.215394	-705.197942	-705.262327
DCE-**1** (C)	-705.475990	-705.237332	-705.220055	-705.282875
DCE-**1** (C) (PCM)	-705.492075	-705.254145	-705.236876	-705.299493
DCE-**1** ($CD^{‡}$)	-705.432100	-705.195701	-705.178519	-705.240718
DCE-**1** ($CD^{‡}$) (PCM)	-705.451808	-705.216047	-705.198913	-705.260718
DCE-**1** (D)	-705.494804	-705.256573	-705.238789	-705.302215
DCE-**1** (D) (PCM)	-705.513918	-705.276273	-705.258572	-705.321440
DCE-**1** ($DE^{‡}$)	-705.490230	-705.252496	-705.235305	-705.297864
DCE-**1** ($DE^{‡}$) (PCM)	-705.509283	-705.272260	-705.255108	-705.317196
DCE-**1** (E)	-705.498380	-705.260057	-705.242309	-705.305591
DCE-**1** (E) (PCM)	-705.516681	-705.278903	-705.261263	-705.323907
TCE	-355.295391	-355.246922	-355.238663	-355.279072
TCE-**1** ($AB^{‡}$)	-797.646110	-797.412555	-797.392745	-797.462351
TCE-**1** (C)	-797.706399	-797.469444	-797.450299	-797.517557
TCE-**1** ($CD^{‡}$) --> *trans*	-797.673151	-797.438141	-797.419126	-797.485967
TCE-**1** ($CD^{‡}$) --> *cis*	-797.666241	-797.431231	-797.412320	-797.478578
2f	-494.128412	-493.996498	-493.985566	-494.033139
2f-1 ($AB^{‡}$)	-936.465838	-936.149414	-936.126784	-936.203417
2f-1 (C)	-936.527974	-936.208432	-936.186412	-936.261033
2f-1 ($CD^{‡}$) --> *trans*	-936.504234	-936.186200	-936.164454	-936.237965
2f-1 ($CD^{‡}$) --> *cis*	-936.490690	-936.173157	-936.151317	-936.224990
TCNE	-447.518338	-447.471682	-447.461584	-447.505951
TCNE-**1** ($AB^{‡}$)	-889.867706	-889.636375	-889.614704	-889.688244
TCNE-**1** ($CD^{‡}$)	-889.899067	-889.665844	-889.645010	-889.715800

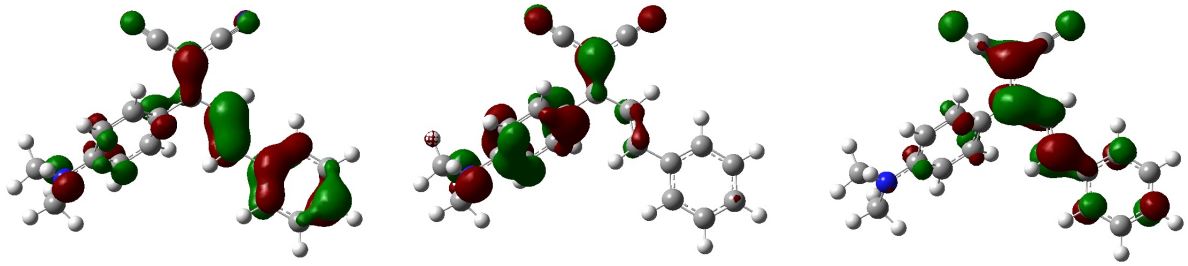
ESI 7. APT Charges for selected points along the reaction coordinate involving reaction of DMAA with DCE from gas-phase calculations and with PCM solvation in acetonitrile.



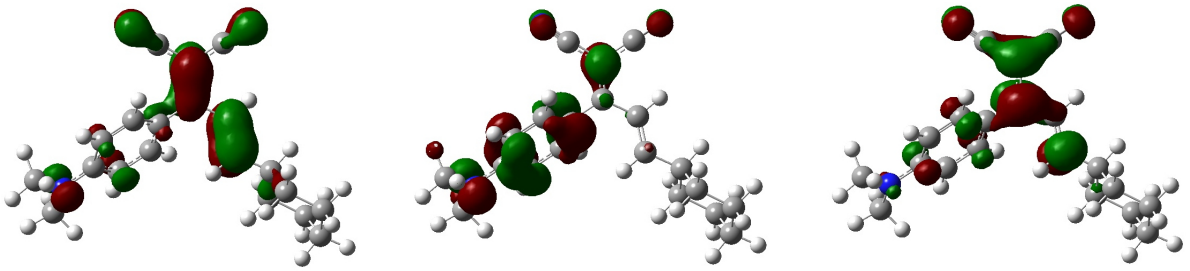
	APT Charges		
Entry	α	δ	I
1	---	0.20	-1.00
1 (PCM)	---	0.30	-1.30
DCE	0.22	---	---
DCE (PCM)	0.14	---	---
DCE-**1** ($AB^{\ddagger}$)	-0.48	0.77	-1.21
DCE-**1** ($AB^{\ddagger}$) (PCM)	-0.08	1.54	-1.62
DCE-**1** (B)	-0.13	0.13	-1.54
DCE-**1** (B) (PCM)	-0.04	1.50	-1.64
DCE-**1** ($BC^{\ddagger}$)	-0.57	0.67	-1.10
DCE-**1** ($BC^{\ddagger}$) (PCM)	-1.40	1.65	-1.52
DCE-**1** (C)	0.17	0.47	-1.00
DCE-**1** (C) (PCM)	0.15	0.62	-1.32
DCE-**1** ($CD^{\ddagger}$)	0.08	0.51	-1.00
DCE-**1** ($CD^{\ddagger}$) (PCM)	-0.03	0.84	-1.46

ESI 8. Representative molecular orbital pictures of **3f**: HOMO-1 (a), HOMO (b) and LUMO (c) and **10**: HOMO-1 (d), HOMO (e) and LUMO (f).

(a) (b) (c)



(d) (e) (f)



ESI 8. Calculated B3LYP/6-31G(d) orbital energies of selected molecules **2h**, **3b**, **3c**, **3f**, **3g**, **3h**, **10** and **11**.

Compound	HOMO-1	HOMO	LUMO	LUMO+1
		(eV)		
2h	–7.43	–5.79	–2.31	–0.53
3b	–6.70	–5.82	–3.25	–2.21
3c	–6.49	–5.73	–3.01	–1.67
3f	–6.19	–5.58	–2.58	–0.78
3g	–5.81	–5.49	–2.42	–0.60
3h	–5.39	–5.24	–2.21	–0.42
10	–6.54	–5.58	–2.29	–0.37
11	–6.41	–5.54	–2.17	–0.37

ESI 9. References.

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