Supplementary Information (SI) for Physical Chemistry Chemical Physics.

A Redefinition of Global Conceptual Density Functional Theory Reactivity Indexes by means of the Cubic Expansions of the Energy

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Table S1. Descriptors obtained using I_{HOMO} and A_{LUMO} for the electrophiles.

Molecule	ω_q	ω_{GCV}^{+}	ω_{CDP}^{+}	$\Delta\omega_{GCV,a}^{\pm}$	$\Delta\omega_{CDP,a}^{\pm}$	$\Delta\omega_{GCV,g}^{\pm}$	$\Delta\omega_{CDP,g}^{\pm}$	ω_{c,α^*}	$\Delta\omega_{\beta^*,a}^{\pm}$	$\Delta\omega_{\beta^*,g}^{\pm}$
(ani)2CH+	5.79	7.74	2.34	11.96	6.56	11.19	5.02	3.87	3.87	3.11
(dfp)(mfp)CH+	7.88	11.09	3.62	16.17	8.70	15.35	7.06	4.63	4.63	3.79
(dfp)PhCH+	7.52	10.46	3.36	15.46	8.35	14.63	6.69	4.57	4.57	3.84
(dma)2CH+	4.81	6.29	1.83	9.98	5.52	9.28	4.11	3.37	3.37	2.56
(dpa)2CH+	4.71	6.22	1.84	9.76	5.38	9.09	4.05	3.24	3.24	2.52
(ftol)2CH+	6.97	9.64	3.07	14.34	7.76	13.55	6.18	4.31	4.31	3.63
(fur)(ani)CH+	5.68	7.59	2.29	11.74	6.44	10.98	4.92	3.81	3.81	3.06
(fur)2CH+	5.62	7.51	2.26	11.62	6.37	10.87	4.87	3.77	3.77	3.02
(ind)2CH+	4.59	5.97	1.72	9.53	5.28	8.84	3.90	3.25	3.25	2.43
(jul)2CH+	4.37	5.63	1.60	9.08	5.05	8.39	3.69	3.14	3.14	2.30
(lil)2CH+	4.38	5.62	1.59	9.10	5.07	8.41	3.69	3.16	3.16	2.29
(mfa)2CH+	5.28	7.04	2.11	10.93	6.00	10.21	4.57	3.57	3.57	2.84
(mfp)2CH+	7.58	10.60	3.42	15.57	8.40	14.76	6.77	4.55	4.55	3.80
(mfp)PhCH+	7.23	9.97	3.16	14.86	8.05	14.04	6.40	4.49	4.49	3.78
(mor)2CH+	4.94	6.51	1.92	10.22	5.63	9.52	4.24	3.40	3.40	2.64
(mpa)2CH+	4.62	5.97	1.71	9.59	5.33	8.89	3.91	3.30	3.30	2.44
(pcp)2CH+	7.22	10.11	3.27	14.83	8.00	14.06	6.45	4.33	4.33	3.60
(pfa)2CH+	5.09	6.72	1.99	10.53	5.80	9.82	4.37	3.49	3.49	2.73
(pfp)2CH+	7.01	9.63	3.03	14.44	7.84	13.61	6.19	4.42	4.42	3.70
(pyr)2CH+	4.57	5.91	1.69	9.49	5.27	8.79	3.87	3.27	3.27	2.41
(tfm)PhCH+	7.35	10.13	3.21	15.12	8.19	14.27	6.50	4.58	4.58	3.85
(thq)2CH+	4.54	5.88	1.68	9.42	5.23	8.73	3.84	3.24	3.24	2.40
(tol)2CH+	6.38	8.62	2.64	13.17	7.19	12.36	5.57	4.18	4.18	3.43
(ani)(Ph)CH+	6.22	8.35	2.54	12.85	7.03	12.04	5.41	4.13	4.13	3.35
(ani)(pop)CH+	5.74	7.67	2.31	11.87	6.51	11.11	4.98	3.85	3.85	3.09
(ani)(tol)CH	6.05	8.11	2.46	12.49	6.84	11.70	5.25	4.02	4.02	3.25
Benzhydrylium ion	6.88	9.36	2.90	14.19	7.73	13.34	6.04	4.43	4.43	3.68
(pfp)(Ph)CH+	6.94	9.48	2.96	14.30	7.78	13.47	6.11	4.42	4.42	3.69
(pop)(Ph)CH+	6.16	8.30	2.54	12.71	6.94	11.92	5.37	4.04	4.04	3.31
(tol)(Ph)CH+	6.61	8.96	2.76	13.64	7.44	12.81	5.78	4.30	4.30	3.55

Table S2. Descriptors obtained using I^+ and A^- for the electrophiles.

Molecule	ω_q	ω_{GCV}^{+}	ω_{CDP}^{+}	$\Delta\omega_{GCV,a}^{\pm}$	$\Delta\omega_{CDP,a}^{\pm}$	$\Delta\omega_{GCV,g}^{\pm}$	$\Delta\omega_{CDP,g}^{\pm}$	ω_{c,α^*}	$\Delta\omega_{\beta^*,a}^{\pm}$	$\Delta\omega_{\beta^*,g}^{\pm}$
(ani)2CH+	6.25	8.62	2.73	12.86	6.97	12.14	5.53	4.51	4.55	3.48
(dfp)(mfp)CH+	8.29	11.88	3.98	16.97	9.07	16.19	7.51	5.54	5.60	4.26
(dfp)PhCH+	7.92	11.23	3.71	16.23	8.71	15.44	7.13	5.41	5.47	4.22
(dma)2CH+	5.37	7.38	2.32	11.06	6.00	10.43	4.74	3.91	3.94	3.01
(dpa)2CH+	5.69	8.12	2.70	11.66	6.24	11.11	5.14	3.84	3.88	2.98
(ftol)2CH+	7.49	10.63	3.52	15.35	8.23	14.60	6.75	5.11	5.16	3.98
(fur)(ani)CH+	6.17	8.52	2.70	12.68	6.87	11.98	5.46	4.44	4.48	3.44
(fur)2CH+	6.12	8.47	2.70	12.59	6.82	11.90	5.43	4.40	4.43	3.41
(ind)2CH+	5.18	7.11	2.23	10.66	5.79	10.05	4.57	3.77	3.80	2.90
(jul)2CH+	5.07	7.00	2.22	10.43	5.65	9.85	4.49	3.66	3.69	2.83
(lil)2CH+	4.98	6.78	2.11	10.25	5.58	9.65	4.37	3.66	3.69	2.79
(mfa)2CH+	5.94	8.31	2.69	12.20	6.57	11.56	5.30	4.18	4.21	3.26
(mfp)2CH+	7.96	11.31	3.75	16.31	8.74	15.52	7.17	5.42	5.48	4.22
(mfp)PhCH+	7.58	10.65	3.46	15.56	8.38	14.76	6.79	5.29	5.34	4.14
(mor)2CH+	5.63	7.86	2.53	11.55	6.23	10.95	5.02	3.97	4.01	3.10
(mpa)2CH+	5.33	7.36	2.34	10.97	5.94	10.36	4.72	3.84	3.88	2.97
(pcp)2CH+	7.77	11.14	3.74	15.90	8.50	15.17	7.04	5.19	5.25	3.98
(pfa)2CH+	5.90	8.30	2.71	12.10	6.51	11.49	5.28	4.10	4.14	3.21
(pfp)2CH+	7.34	10.25	3.30	15.08	8.14	14.29	6.55	5.18	5.23	4.05
(pyr)2CH+	5.19	7.11	2.23	10.69	5.80	10.07	4.58	3.79	3.82	2.90
(tfm)PhCH+	7.64	10.63	3.41	15.71	8.49	14.86	6.80	5.44	5.48	4.23
(thq)2CH+	5.16	7.09	2.23	10.63	5.77	10.03	4.56	3.76	3.79	2.89
(tol)2CH+	6.85	9.50	3.04	14.07	7.61	13.31	6.08	4.89	4.93	3.80
(ani)(Ph)CH+	6.61	9.09	2.87	13.60	7.38	12.83	5.84	4.79	4.83	3.69
(ani)(pop)CH+	6.30	8.74	2.79	12.96	7.01	12.25	5.60	4.50	4.54	3.50
(ani)(tol)CH	6.50	8.97	2.85	13.37	7.24	12.63	5.76	4.68	4.72	3.62
Benzhydrylium ion	7.22	10.01	3.19	14.85	8.04	14.04	6.41	5.17	5.22	4.01
(pfp)(Ph)CH+	7.28	10.12	3.24	14.95	8.08	14.15	6.47	5.18	5.22	4.03
(pop)(Ph)CH+	6.62	9.15	2.91	13.61	7.37	12.86	5.86	4.76	4.80	3.68
(tol)(Ph)CH+	7.02	9.73	3.10	14.43	7.81	13.64	6.23	5.02	5.07	3.90

Table S3. Descriptors obtained using I_{HOMO} and A_{LUMO} for the nucleophiles.

Molecule	ω_q	ω_{GCV}^{+}	ω_{CDP}^{+}	$\Delta\omega_{GCV,a}^{\pm}$	$\Delta\omega_{CDP,a}^{\pm}$	$\Delta\omega_{GCV,g}^{\pm}$	$\Delta\omega_{CDP,g}^{\pm}$	ω_{c,α^*}	$\Delta\omega_{\beta^*,a}^{\pm}$	$\Delta\omega_{\beta^*,g}^{\pm}$
1-hexene	0.78	4.21	4.09	2.20	2.08	0.91	0.52	1.45	0.17	1.23
1-methyl-4-vinyl-benzene	0.79	3.98	3.74	2.12	1.88	1.02	0.31	1.31	0.16	1.14
1-methylcyclopentene	0.68	3.76	3.68	1.96	1.87	0.77	0.51	1.30	0.16	1.15
1,3-dimethoxybenzene	0.68	3.68	3.57	1.92	1.82	0.78	0.46	1.26	0.15	1.09
2-chloropropene	0.80	4.28	4.13	2.25	2.09	0.96	0.49	1.46	0.17	1.24
2-methyl-pent-1-ene	0.75	4.07	3.94	2.13	2.00	0.88	0.50	1.39	0.17	1.18
2-methyl-furan	0.66	3.66	3.57	1.91	1.82	0.75	0.49	1.27	0.15	1.11
2,3-dimethyl-but-1-ene	0.76	4.10	3.96	2.15	2.01	0.90	0.49	1.40	0.17	1.16
2,3,3-trimethyl-but-1-ene	0.77	4.12	3.97	2.16	2.02	0.91	0.48	1.40	0.17	1.18
2,4,4-trimethyl-pent-1-ene	0.76	4.08	3.93	2.14	2.00	0.90	0.48	1.39	0.17	1.17
furan	0.69	3.83	3.75	1.99	1.91	0.77	0.53	1.33	0.16	1.18
isobutylene	0.75	4.08	3.95	2.14	2.01	0.88	0.50	1.40	0.17	1.19
N-methylpyrrole	0.65	3.57	3.47	1.86	1.76	0.75	0.46	1.23	0.15	1.07
norbornene	0.74	3.98	3.85	2.08	1.96	0.86	0.48	1.36	0.16	1.15
styrene	0.86	4.21	3.91	2.27	1.96	1.16	0.25	1.36	0.16	1.18

Table S4. Descriptors obtained using I^+ and A^- for the nucleophiles.

Molecule	ω_q	ω_{GCV}^{+}	ω_{CDP}^{+}	$\Delta\omega_{GCV,a}^{\pm}$	$\Delta\omega_{CDP,a}^{\pm}$	$\Delta\omega_{GCV,g}^{\pm}$	$\Delta\omega_{CDP,g}^{\pm}$	ω_{c,α^*}	$\Delta\omega_{\beta^*,a}^{\pm}$	$\Delta\omega_{\beta^*,g}^{\pm}$
1-hexene	0.86	4.51	4.31	2.38	2.18	1.06	0.46	1.40	0.07	1.36
1-methyl-4-vinyl-benzene	0.79	4.00	3.76	2.13	1.89	1.03	0.31	1.24	0.06	1.22
1-methylcyclopentene	0.75	4.00	3.85	2.10	1.95	0.91	0.45	1.24	0.06	1.23
1,3-dimethoxybenzene	0.74	3.85	3.68	2.04	1.86	0.91	0.39	1.19	0.06	1.16
2-chloropropene	0.91	4.67	4.42	2.48	2.23	1.17	0.40	1.45	0.07	1.40
2-methyl-pent-1-ene	0.83	4.32	4.12	2.28	2.08	1.02	0.43	1.34	0.06	1.30
2-methyl-furan	0.75	3.96	3.79	2.08	1.92	0.92	0.42	1.23	0.06	1.21
2,3-dimethyl-but-1-ene	0.83	4.34	4.13	2.30	2.09	1.04	0.42	1.35	0.06	1.28
2,3,3-trimethyl-but-1-ene	0.83	4.33	4.12	2.29	2.08	1.04	0.42	1.34	0.06	1.27
2,4,4-trimethyl-pent-1-ene	0.82	4.26	4.06	2.25	2.05	1.01	0.42	1.32	0.06	1.27
furan	0.79	4.19	4.02	2.21	2.04	0.97	0.45	1.30	0.06	1.28
isobutylene	0.84	4.39	4.19	2.32	2.12	1.04	0.44	1.36	0.06	1.32
N-methylpyrrole	0.75	3.87	3.68	2.05	1.86	0.94	0.36	1.20	0.06	1.09
norbornene	0.80	4.20	4.01	2.22	2.03	0.99	0.42	1.30	0.06	1.26
styrene	0.85	4.23	3.94	2.27	1.98	1.15	0.27	1.31	0.06	1.30

Nucleophiles

Equilibrium Geometries and Cartesian Coordinates

1-hexene

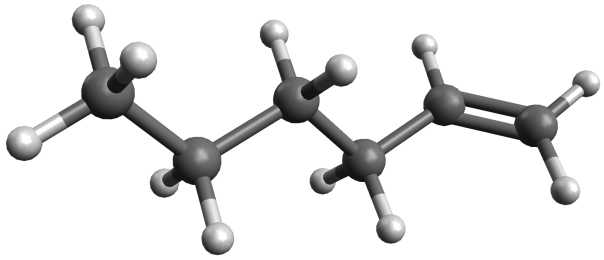

Figure S1. Model of 1- Hexene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

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1_HEXENE

18

C  3.061858   -0.194695  -0.442199
C  2.034592   -0.188829  0.397043
C  0.771926   0.598570   0.211552
C  -0.469025  -0.293547  0.102510
C  -1.765409  0.499545   -0.045784
C  -2.997351  -0.393695  -0.159791
H  3.945251   -0.795508  -0.256514
H  3.055832   0.406795   -1.347052
H  2.079684   -0.809277  1.291623
H  0.642185   1.279233   1.063119
H  0.855718   1.225313   -0.683261
H  -0.350018  -0.967757  -0.753937
H  -0.535433  -0.934459  0.990906
H  -1.876457  1.172034   0.813103
H  -1.694567  1.142617   -0.930928
H  -3.911237  0.196182   -0.265542
H  -2.923094  -1.054406  -1.028826
H  -3.107412  -1.024863  0.727323
```

1-methyl-4-vinyl-benzene

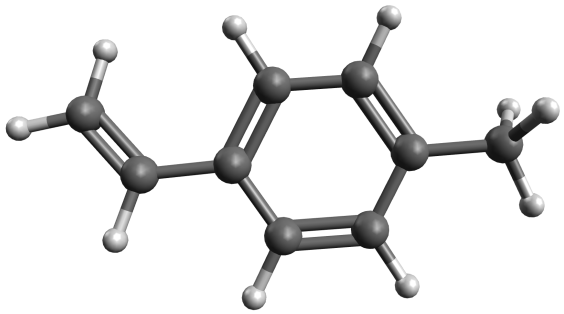

Figure S2. Model of 1-methyl-4-vinyl-benzene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

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1_METHYL_4_VINYL_BENZENE

19

C  3.281192   -0.246218  0.038729
C  1.785856   -0.071144  0.011883
C  1.199362   1.189799   0.027631
C  -0.181982  1.336118   -0.002832
C  -1.026646  0.227115   -0.043503
C  -0.434475  -1.040813  -0.068132
C  0.941200   -1.183508  -0.038806
C  -2.485377  0.432083   -0.059990
C  -3.426116  -0.493907  0.106421
H  3.589819   -0.852962  0.894789
H  3.632720   -0.752499  -0.865014
H  3.793184   0.715520   0.105647
H  1.829348   2.072944   0.062858
H  -0.613831  2.332050   0.010293
H  -1.055948  -1.927653  -0.122440
H  1.374393   -2.178994  -0.061218
H  -2.798949  1.462521   -0.214354
H  -3.192389  -1.538106  0.285610
H  -4.476436  -0.229981  0.075420
```

1-methylcyclopentene

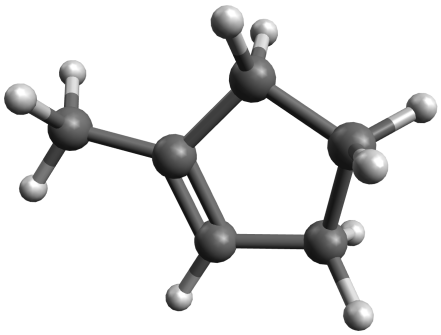

Figure S3. Model of 1-methylcyclopentene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

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1_METHYLCYCLOPENTENE

15

C  -2.245976  0.029267   -0.041467
C  -0.753172  0.075333   -0.001790
C  0.025266   1.154208   -0.024798
C  1.488746   0.813274   0.091712
C  1.507274   -0.708795  -0.167564
C  0.072851   -1.184816  0.133629
H  -2.678220  1.029440   -0.111701
H  -2.595111  -0.558220  -0.897483
H  -2.643256  -0.454289  0.857879
H  -0.341600  2.174002   -0.075269
H  2.115500   1.363717   -0.616090
H  1.860241   1.057753   1.095411
H  1.731503   -0.890012  -1.222328
H  2.262796   -1.231535  0.422078
H  -0.022336  -1.583213  1.152763
H  -0.259454  -1.978471  -0.543596
```

2-chloropropene

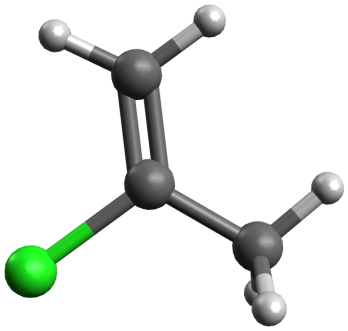

Figure S4. Model of 2-chloropropene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Chloride = Green balls.

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2_CHLOROPROPENE

8

Cl 1.303949   -0.092361  -0.000057
C  -0.443568  0.139450   0.000736
C  -0.938009  1.366356   0.000003
C  -1.219522  -1.137112  -0.000103
H  -0.304212  2.242921   -0.000986
H  -2.012482  1.508006   -0.000220
H  -0.977811  -1.734885  0.882346
H  -2.289759  -0.924117  -0.001135
H  -0.976270  -1.733956  -0.882853
```

2-methyl-pent-1-ene

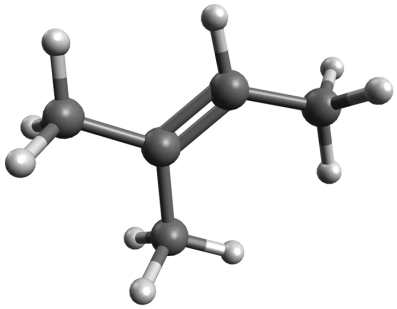

Figure S5. Model of 2-methyl-pent-1-ene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

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2_METHYL_PENT_1_ENE

18

C  1.638927   -1.286517  0.040509
C  1.160377   0.139396   0.097426
C  1.952368   1.159669   -0.220194
C  -0.268836  0.352055   0.531110
C  -1.305407  -0.229959  -0.438290
C  -2.737172  0.063023   0.000243
H  1.468246   -1.789622  0.998511
H  1.094197   -1.855947  -0.719310
H  2.703205   -1.342952  -0.194171
H  2.980237   1.005610   -0.532816
H  1.599170   2.185004   -0.175844
H  -0.416238  -0.106081  1.518706
H  -0.455801  1.424196   0.651176
H  -1.128014  0.186085   -1.436028
H  -1.167598  -1.312889  -0.523415
H  -2.916960  1.140751   0.059071
H  -3.462762  -0.359108  -0.699379
H  -2.939224  -0.361043  0.988680
```

2-methyl-furan

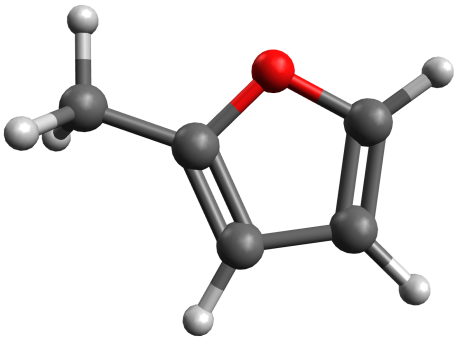

Figure S6. Model of 2-methylfuran Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

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2_METHYLFURAN

12

C  -2.117490  -0.014130  0.000071
C  -0.632568  0.105760   -0.000116
O  0.072172   -1.053797  -0.000119
C  1.388639   -0.731683  0.000137
C  1.544201   0.611706   -0.000017
C  0.222070   1.160199   0.000010
H  -2.399996  -1.067380  -0.004064
H  -2.553176  0.454064   0.886029
H  -2.553820  0.461249   -0.881702
H  2.076026   -1.560503  0.000195
H  2.479136   1.149075   -0.000058
H  -0.054662  2.202757   0.000035
```

1,3-dimethoxybenzene

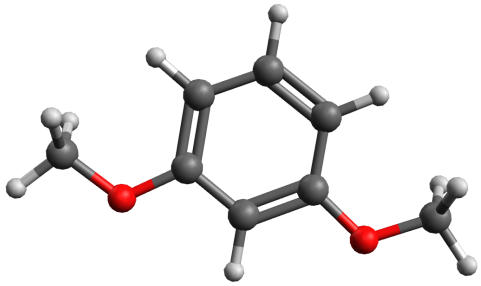

Figure S7. Model of 1,3-dimethoxybenzene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
13_DIMETHOXYBENZENE

20

C  -3.575079  -0.351288  0.000180
O  -2.320757  -0.995132  -0.000497
C  -1.205526  -0.224567  0.000031
C  -0.000000  -0.916595  -0.000158
C  1.205525   -0.224572  -0.000186
C  1.214106   1.172996   0.000135
C  0.000003   1.845657   0.000314
C  -1.214104  1.172998   0.000248
O  2.320756   -0.995134  -0.000138
C  3.575077   -0.351288  0.000013
H  -3.709453  0.267925   0.894592
H  -3.709972  0.268785   -0.893567
H  -4.319827  -1.145350  0.000021
H  -0.000004  -1.998717  -0.000364
H  2.138245   1.734016   0.000232
H  0.000003   2.930040   0.000375
H  -2.138240  1.734023   0.000199
H  4.319826   -1.145348  -0.000043
H  3.709745   0.268460   -0.893989
H  3.709674   0.268252   0.894170
```

2,3-dimethyl-but-1-ene

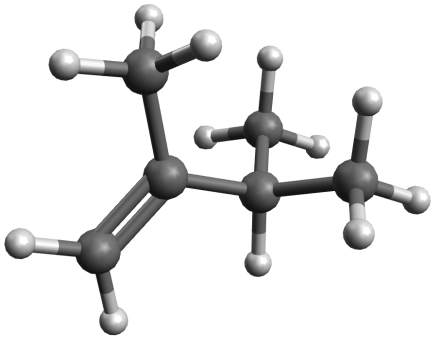

Figure S8. Model of 2,3-dimethyl-but-1-ene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
23_DIMETHYL_BUT_1_ENE

18

C  -1.177452  1.341255   -0.011272
C  -0.813212  -0.119878  0.001022
C  -1.746620  -1.067703  0.008920
C  0.661808   -0.476730  0.004223
C  1.372432   0.016889   -1.262066
C  1.372442   0.039564   1.261441
H  -0.772805  1.858183   0.864444
H  -0.771926  1.843695   -0.894964
H  -2.260188  1.476563   -0.012896
H  -2.804533  -0.824912  0.006678
H  -1.483596  -2.120869  0.017907
H  0.723236   -1.570463  0.014050
H  2.403543   -0.346740  -1.286888
H  0.863600   -0.337077  -2.162284
H  1.409580   1.109909   -1.298856
H  0.863528   -0.298080  2.167859
H  2.403506   -0.323667  1.292834
H  1.409666   1.133070   1.278505
```

2,3,3-trimethyl-but-1-ene

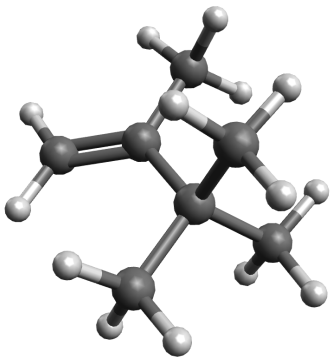

Figure S9. Model of 2,3,3-trimethyl-but-1-ene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
233_TRIMETHYL_BUT_1_ENE

21

C  0.888290   -1.877551  0.000000
C  -0.271624  -0.911305  0.000000
C  -1.517908  -1.379690  0.000000
C  0.063889   0.582953   0.000000
C  -1.194502  1.458161   0.000000
C  0.888290   0.927632   1.254440
C  0.888290   0.927632   -1.254440
H  0.531744   -2.908677  0.000000
H  1.524314   -1.743433  -0.879662
H  1.524314   -1.743433  0.879662
H  -2.388850  -0.736866  0.000000
H  -1.708034  -2.448146  0.000000
H  -1.808475  1.278910   0.886825
H  -0.908874  2.513833   0.000000
H  -1.808475  1.278910   -0.886825
H  1.853425   0.415522   1.263422
H  1.087376   2.002991   1.288617
H  0.346187   0.652439   2.163674
H  0.346187   0.652439   -2.163674
H  1.087376   2.002991   -1.288617
H  1.853425   0.415522   -1.263422
```

2,4,4-trimethyl-pent-1-ene

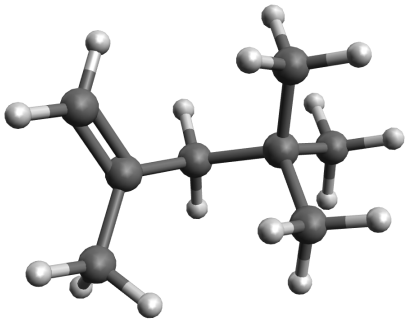

Figure S10. Model of 2,4,4-trimethyl-pent-1-ene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
244_TRIMETHYL_PENT_1_ENE

24

C  2.264115   1.147949   0.029966
C  1.518528   -0.129764  -0.250196
C  2.043479   -1.318607  0.037355
C  0.166755   0.003507   -0.917475
C  -1.074158  0.021295   0.015671
C  -0.952388  1.110047   1.087587
C  -2.303445  0.309363   -0.855945
C  -1.252773  -1.338849  0.698596
H  3.202934   0.960428   0.554601
H  2.493621   1.661545   -0.910361
H  1.665692   1.840556   0.627984
H  1.523271   -2.240072  -0.203558
H  3.012847   -1.411024  0.516489
H  0.155709   0.927244   -1.508883
H  0.033727   -0.820976  -1.626351
H  -0.792680  2.095137   0.637254
H  -1.868173  1.159795   1.684570
H  -0.122889  0.904556   1.769876
H  -2.412826  -0.443866  -1.642601
H  -3.217325  0.301385   -0.254046
H  -2.225136  1.289982   -1.336066
H  -0.397459  -1.579550  1.334309
H  -2.150327  -1.336215  1.324771
H  -1.361661  -2.138561  -0.041342
```

Furan

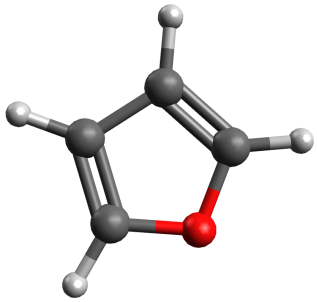

Figure S11. Model of Furan Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
FURAN

9

O  -0.000000  1.152160   -0.000062
C  -1.086840  0.347157   0.000041
C  -0.715997  -0.954691  0.000059
C  0.715997   -0.954691  0.000066
C  1.086840   0.347157   -0.000102
H  -2.041538  0.845487   0.000060
H  -1.373723  -1.808922  0.000123
H  1.373723   -1.808922  0.000123
H  2.041538   0.845487   -0.000197
```

Isobutylene

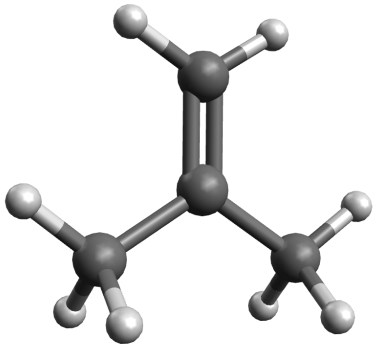

Figure S12. Model of Isobutylene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls

```
ISOBUTYLENE

12

C  0.000000   1.271850   -0.677582
C  0.000000   0.000000   0.125344
C  -0.000000  -1.271850  -0.677582
C  0.000000   0.000000   1.454809
H  -0.879481  1.316946   -1.329216
H  0.000065   2.156052   -0.037905
H  0.879354   1.316843   -1.329374
H  0.879481   -1.316946  -1.329216
H  -0.000065  -2.156052  -0.037905
H  -0.879354  -1.316843  -1.329374
H  -0.000029  0.925445   2.021529
H  0.000029   -0.925445  2.021529
```

N-methylpyrrole

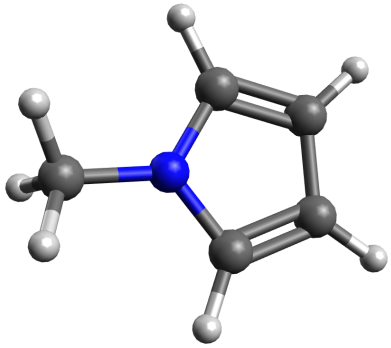

Figure S13. Model of N-methylpyrrole Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
N_METHYLPYRROLE

13

C  -2.065628  -0.000006  0.025080
N  -0.621072  0.000018   -0.036943
C  0.173505   -1.113716  -0.013259
C  1.484805   -0.709490  0.014549
C  1.484834   0.709453   0.014578
C  0.173549   1.113721   -0.013262
H  -2.422268  -0.002163  1.059053
H  -2.452624  0.885277   -0.481173
H  -2.452922  -0.882963  -0.485025
H  -0.261749  -2.100937  -0.021956
H  2.346148   -1.359074  0.021782
H  2.346200   1.359007   0.021814
H  -0.261670  2.100956   -0.022018
```

Norbornene

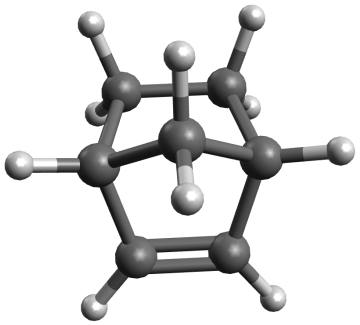

Figure S14. Model of Norbornene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls

```
NORBORNENE

17

C  -0.085184  1.122765   0.323140
C  -1.273652  0.666559   -0.502944
C  -1.273727  -0.666461  -0.502919
C  -0.085271  -1.122763  0.323126
C  1.182314   -0.777182  -0.517830
C  1.182389   0.777106   -0.517798
C  -0.035901  -0.000009  1.375959
H  -0.117106  2.148649   0.688379
H  -1.916689  1.321518   -1.077416
H  -1.916828  -1.321370  -1.077376
H  -0.117263  -2.148651  0.688350
H  2.078874   -1.172962  -0.033493
H  1.130919   -1.201187  -1.522077
H  1.131050   1.201156   -1.522028
H  2.078975   1.172786   -0.033426
H  0.885730   -0.000050  1.966222
H  -0.903469  0.000020   2.038465
```

Styrene

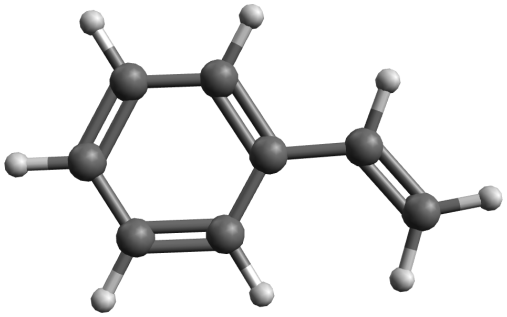

Figure S15. Model of Styrene Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls

```
STYRENE

16

C  2.961096   0.336441   -0.000098
C  1.951543   -0.529798  0.000115
C  0.510238   -0.220885  -0.000088
C  -0.405474  -1.276100  -0.000015
C  -1.774160  -1.040651  -0.000013
C  -2.254365  0.261779   -0.000025
C  -1.354926  1.323639   -0.000035
C  0.010383   1.085771   0.000153
H  3.987486   -0.010236  -0.000154
H  2.811724   1.410869   -0.000399
H  2.186548   -1.592135  0.000407
H  -0.036218  -2.296885  0.000012
H  -2.465054  -1.876146  -0.000098
H  -3.321658  0.451298   -0.000065
H  -1.721710  2.344023   -0.000002
H  0.692867   1.928035   0.000340
```

Electrophiles

Equilibrium Geometries and Cartesian Coordinates

(Ani)2CH+

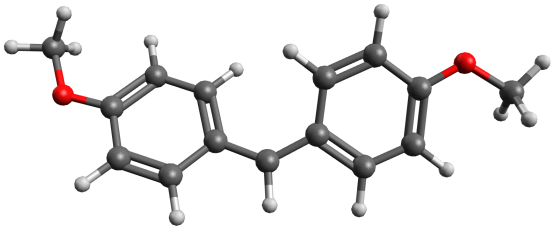

Figure S16. Model of (Ani)2CH+ Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
ANI_2CH

32

C  -6.177620  -0.476894  -0.235495
O  -4.962596  -1.139260  0.123915
C  -3.817869  -0.489761  0.088099
C  -3.676492  0.860117   -0.286458
C  -2.428244  1.429987   -0.272096
C  -1.267971  0.686525   0.062934
C  -0.028666  1.347367   -0.005482
H  -0.098019  2.433377   -0.051862
C  1.285218   0.847509   -0.022841
C  2.348065   1.757958   0.241708
C  3.646763   1.342020   0.283184
C  3.959721   -0.007549  0.013554
O  5.238339   -0.317107  0.068709
C  5.669553   -1.654323  -0.193642
C  2.933461   -0.917061  -0.319260
C  1.629294   -0.493154  -0.332102
C  -1.446438  -0.663624  0.479001
C  -2.685091  -1.233999  0.492457
H  -6.956445  -1.225901  -0.125913
H  -6.136609  -0.135416  -1.272474
H  -6.372488  0.359975   0.439213
H  -4.535016  1.451886   -0.571334
H  -2.321870  2.471898   -0.554399
H  2.114614   2.797645   0.443572
H  4.458839   2.021272   0.507211
H  6.747638   -1.639387  -0.062728
H  5.427007   -1.941925  -1.219417
H  5.220430   -2.350034  0.519045
H  3.166984   -1.937359  -0.589925
```

```
H  0.862812   -1.186569  -0.652239
H  -0.604909  -1.229998  0.855256
H  -2.841011  -2.249239  0.833630
```

Ani(Ph)CH+

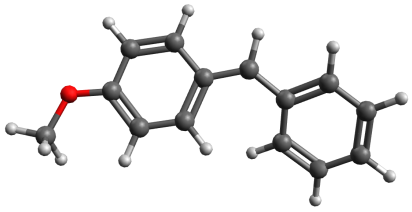

Figure S17. Model of Ani(Ph)CH+ Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
ANI_PH_CH

28

C  -4.889156  -1.412320  0.220077
O  -4.360040  -0.109146  -0.058472
C  -3.071204  0.115328   -0.018899
C  -2.675383  1.443950   -0.308833
C  -1.356407  1.774399   -0.285409
C  -0.347931  0.794196   -0.018147
C  0.982920   1.192697   -0.056640
H  1.143198   2.269832   -0.080736
C  2.179267   0.412363   -0.060863
C  3.361147   1.031878   0.398088
C  4.544307   0.322348   0.462920
C  4.580926   -0.997838  0.021062
C  3.437260   -1.608327  -0.492882
C  2.243622   -0.916100  -0.533497
C  -0.777793  -0.524666  0.314561
C  -2.101952  -0.861124  0.317239
H  -5.963307  -1.315765  0.094347
H  -4.660697  -1.703383  1.247403
H  -4.495640  -2.142562  -0.489891
H  -3.446715  2.168823   -0.533675
H  -1.054580  2.792781   -0.503966
H  3.329520   2.064535   0.728014
H  5.442070   0.795730   0.839677
H  5.513822   -1.548430  0.052054
H  3.490294   -2.618780  -0.878347
H  1.377254   -1.371359  -0.996209
H  -0.050171  -1.259531  0.633283
H  -2.402462  -1.859425  0.603165
```

Ani(pop)CH+

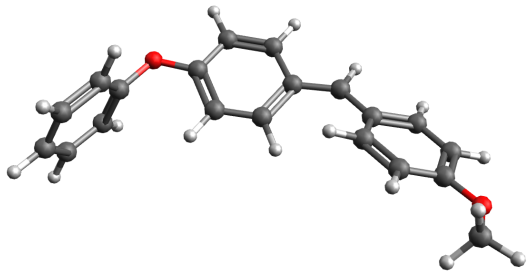

Figure S18. Model of Ani(pop)CH+ Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
ANI_POP_CH

39

C  -6.249959  2.757959   0.214615
O  -6.233786  1.384906   -0.180970
C  -5.121818  0.683297   -0.102491
C  -5.220753  -0.663467  -0.512464
C  -4.122684  -1.471540  -0.457429
C  -2.856019  -0.973629  -0.038685
C  -1.762801  -1.858245  -0.050113
H  -2.034001  -2.911129  -0.116478
C  -0.379734  -1.613822  0.009324
C  0.475917   -2.706148  0.325695
C  1.826450   -2.539992  0.444952
C  2.394045   -1.273909  0.203437
O  3.711252   -1.201581  0.326131
C  4.368889   0.017117   0.106377
C  4.872236   0.279969   -1.155350
C  5.562593   1.469270   -1.357239
C  5.738087   2.363873   -0.307745
C  5.228513   2.071774   0.952332
C  4.535847   0.886684   1.169911
C  1.581672   -0.187047  -0.178224
C  0.225586   -0.360369  -0.269660
C  -2.792312  0.370379   0.408346
C  -3.895731  1.184969   0.382633
H  -7.264624  3.098382   0.029606
H  -5.549273  3.340515   -0.388213
H  -6.017386  2.854342   1.277853
H  -6.181966  -1.026060  -0.852520
```

H	-4.206599	-2.507377	-0.767507
H	0.040858	-3.683218	0.505218
H	2.483628	-3.358380	0.708359
H	4.734951	-0.438783	-1.954088
H	5.969853	1.691402	-2.336063
H	6.282146	3.286306	-0.469690
H	5.376630	2.762984	1.773108
H	4.143573	0.630690	2.146776
H	2.035028	0.764199	-0.422509
H	-0.379290	0.461540	-0.629883
H	-1.877688	0.749985	0.844789
H	-3.823710	2.195282	0.760641

Ani(tol)CH+

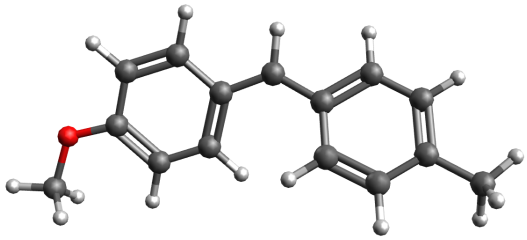

Figure S19. Model of Ani(tol)CH+ Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
ANI_TOL_CH

31

C  -5.235640  -1.637001  -0.195905
O  -4.794792  -0.301218  0.072382
C  -3.520271  0.005478   0.022966
C  -3.207339  1.356222   0.302046
C  -1.910528  1.769750   0.267410
C  -0.845315  0.855929   -0.000250
C  0.461637   1.344695   0.026248
H  0.543874   2.430853   0.024040
C  1.705333   0.659861   0.050555
C  2.853073   1.375279   -0.357011
C  4.086984   0.763042   -0.404185
C  4.239849   -0.566748  0.002400
C  5.578496   -1.237516  -0.020440
C  3.112474   -1.264139  0.468001
C  1.871140   -0.674245  0.492230
C  -1.191784  -0.486777  -0.321030
C  -2.493672  -0.907301  -0.313522
H  -6.313229  -1.613862  -0.063847
H  -4.789788  -2.336548  0.514416
H  -4.994918  -1.919141  -1.223182
H  -4.020695  2.033323   0.527743
H  -1.673812  2.807025   0.477319
H  2.753968   2.410809   -0.664304
H  4.951430   1.320663   -0.744476
H  6.358310   -0.575778  -0.396155
H  5.545571   -2.128908  -0.653083
H  5.857061   -1.565214  0.984930
H  3.231965   -2.277822  0.833591
H  1.035545   -1.213128  0.920123
```

```
  H  -0.422597  -1.177001  -0.641578
  H  -2.730973  -1.924677  -0.591669
```

Benzhydrylium ion

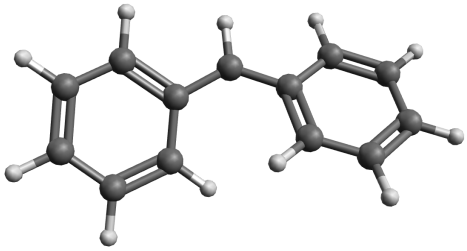

Figure S20. Model of Benzhydrylium ion Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
BENZHYDRYLIUM ION

24

C  0.000026   -1.035422  -0.000512
H  -0.000075  -2.124848  -0.000746
C  -1.279655  -0.441447  0.044838
C  -2.387143  -1.256110  -0.302299
C  -3.660192  -0.728958  -0.331147
C  -3.860024  0.601104   0.037123
C  -2.792186  1.406204   0.441958
C  -1.512217  0.898503   0.446794
C  1.279670   -0.441538  -0.045383
C  1.512433   0.898320   -0.447465
C  2.792367   1.406076   -0.441927
C  3.859997   0.601057   -0.036408
C  3.659986   -0.728988  0.331851
C  2.386963   -1.256159  0.302433
H  -2.220744  -2.292199  -0.576037
H  -4.500783  -1.345840  -0.621696
H  -4.863814  1.010317   0.034563
H  -2.975412  2.421349   0.770358
H  -0.696357  1.501071   0.823960
H  0.696710   1.500777   -0.825132
H  2.975748   2.421188   -0.770341
H  4.863763   1.010326   -0.033231
H  4.500438   -1.345790  0.622968
H  2.220372   -2.292214  0.576195
```

(Dfp)(mfp)CH+

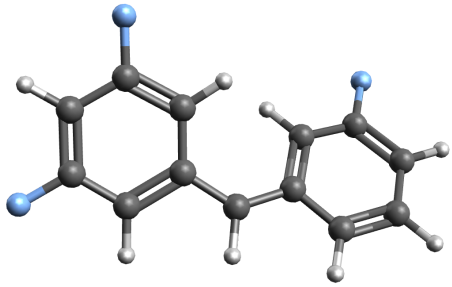

Figure S21. Model of Benzhydrylium ion Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
DFP_MFP_CH

24

F  -3.556555  2.023709   0.818489
C  -3.212617  0.824780   0.374073
C  -4.215084  -0.039742  -0.068711
C  -3.887235  -1.321445  -0.497320
C  -2.569781  -1.734188  -0.478889
C  -1.544768  -0.839076  -0.078297
C  -0.221493  -1.315677  -0.145082
H  -0.127451  -2.397175  -0.228334
C  1.010349   -0.612968  -0.120311
C  2.160956   -1.363797  0.209916
C  3.376343   -0.718203  0.294232
F  4.454067   -1.403830  0.634823
C  3.505435   0.633232   0.007062
C  2.370762   1.345282   -0.366331
F  2.501228   2.624015   -0.679011
C  1.126344   0.760055   -0.432426
C  -1.890750  0.458337   0.377881
H  -5.244300  0.299467   -0.045172
H  -4.668130  -1.995017  -0.825304
H  -2.308895  -2.736254  -0.798851
H  2.102986   -2.423391  0.426535
H  4.473253   1.118308   0.048232
H  0.291099   1.342993   -0.793802
H  -1.157989  1.136467   0.793192
```

(Dfp)PhCH+

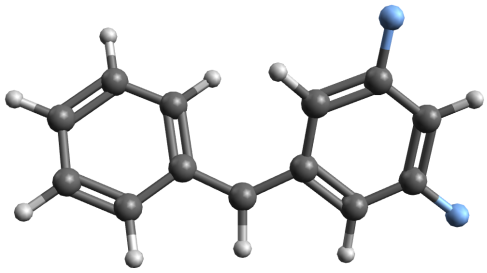

Figure S22. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
DFP_PH_CH

24

F  -2.447666  2.621080   -0.439414
C  -2.214115  1.332871   -0.242143
C  -3.289121  0.496586   0.033682
C  -3.046631  -0.859464  0.198541
F  -4.066606  -1.664424  0.446034
C  -1.777917  -1.389019  0.087735
C  -0.692863  -0.516163  -0.141250
C  0.601284   -1.103479  -0.201840
H  0.606608   -2.171538  -0.414641
C  1.866739   -0.522568  -0.029804
C  2.990523   -1.270245  -0.477346
C  4.258692   -0.741865  -0.391425
C  4.438808   0.514663   0.188625
C  3.356852   1.244725   0.691877
C  2.082004   0.740252   0.587476
C  -0.921851  0.863618   -0.328978
H  -4.296194  0.891027   0.092989
H  -1.632129  -2.455507  0.207361
H  2.836241   -2.249340  -0.917375
H  5.110913   -1.300527  -0.756097
H  5.439647   0.922593   0.274354
H  3.527849   2.195354   1.180559
H  1.254061   1.273138   1.036026
H  -0.132967  1.545432   -0.613658
```

(Dma)2CH+

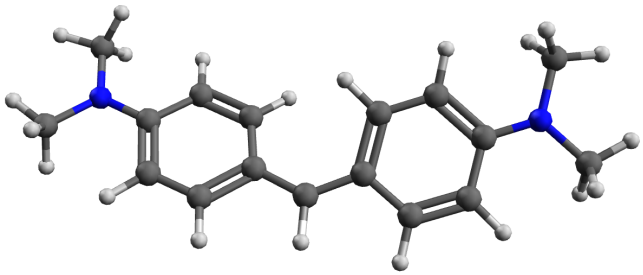

Figure S23. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
DMA_2CH

40

C  -5.435716  2.034838   -0.301049
N  -5.184578  0.628636   -0.007142
C  -6.318038  -0.238202  0.295590
C  -3.936981  0.134639   -0.037613
C  -3.676254  -1.237262  0.247825
C  -2.401010  -1.720150  0.223557
C  -1.278217  -0.889768  -0.044734
C  -0.000001  -1.467158  0.000087
H  0.000008   -2.556496  0.000136
C  1.278219   -0.889762  0.044842
C  2.400996   -1.720161  -0.223428
C  3.676246   -1.237281  -0.247758
C  3.936988   0.134631   0.037583
C  2.824357   0.958183   0.388308
C  1.553782   0.463023   0.385321
N  5.184585   0.628646   0.007020
C  6.318000   -0.238159  -0.295963
C  5.435734   2.034767   0.301271
C  -1.553768  0.462998   -0.385311
C  -2.824336  0.958168   -0.388357
H  -6.491433  2.245028   -0.150872
H  -5.183387  2.276632   -1.337835
H  -4.863823  2.683173   0.367652
H  -7.231832  0.349339   0.264978
H  -6.225936  -0.672592  1.294835
H  -6.406723  -1.043865  -0.438488
H  -4.488472  -1.910303  0.480602
```

```
H  -2.234051  -2.769136  0.444749
H  2.234031   -2.769163  -0.444541
H  4.488444   -1.910364  -0.480477
H  2.985054   1.982231   0.693232
H  0.750755   1.107371   0.718564
H  6.407205   -1.043518  0.438394
H  7.231730   0.349523   -0.266122
H  6.225406   -0.672963  -1.294978
H  4.863951   2.683270   -0.367368
H  6.491477   2.244963   0.151277
H  5.183284   2.276349   1.338077
H  -0.750728  1.107311   -0.718591
H  -2.985025  1.982186   -0.693385
```

(Dpa)2CH+

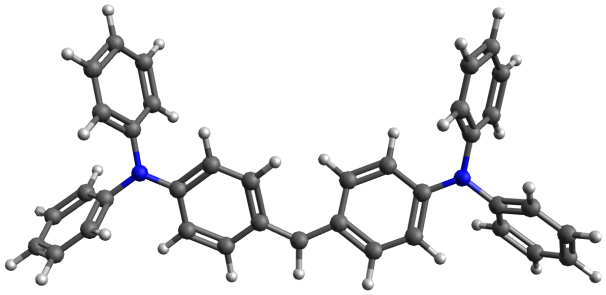

Figure S24. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
DPA_2CH

68

C  0.000046   -2.086799  0.000098
H  0.000044   -3.175977  -0.000068
C  1.277961   -1.508535  -0.043185
C  2.401050   -2.339204  0.225239
C  3.676576   -1.855781  0.247542
C  3.927265   -0.485399  -0.030975
C  2.820851   0.344629   -0.368406
C  1.551187   -0.152631  -0.376032
N  5.186650   0.014340   -0.008511
C  6.339726   -0.841282  0.022904
C  6.591789   -1.700629  -1.041536
C  7.719349   -2.510055  -1.014187
C  8.594856   -2.450148  0.063859
C  8.342280   -1.579508  1.117655
C  7.212782   -0.772479  1.101832
C  5.440559   1.426975   -0.013972
C  6.189286   1.983668   -1.044215
C  6.460016   3.345143   -1.032596
C  5.983640   4.144784   -0.000122
C  5.239578   3.580421   1.029441
C  4.971334   2.218289   1.029744
C  -1.277874  -1.508538  0.043386
C  -1.551188  -0.152727  0.376544
C  -2.820863  0.344499   0.368892
C  -3.927233  -0.485457  0.031109
C  -3.676465  -1.855771  -0.247705
C  -2.400927  -2.339163  -0.225342
```

```
N  -5.186619  0.014295   0.008589
C  -5.440537  1.426927   0.013963
C  -4.971221  2.218222   -1.029730
C  -5.239505  3.580344   -1.029509
C  -5.983710  4.144724   -0.000059
C  -6.460189  3.345102   1.032381
C  -6.189418  1.983637   1.044085
C  -6.339721  -0.841300  -0.022912
C  -7.212623  -0.772544  -1.101968
C  -8.342154  -1.579524  -1.117886
C  -8.594923  -2.450059  -0.064051
C  -7.719582  -2.509901  1.014133
C  -6.591989  -1.700523  1.041578
H  2.233258   -3.385509  0.457998
H  4.501545   -2.511442  0.489345
H  3.002384   1.369189   -0.663789
H  0.749243   0.488892   -0.717292
H  5.906887   -1.731045  -1.881601
H  7.919541   -3.179998  -1.841739
H  9.477439   -3.078122  0.080050
H  9.025701   -1.528671  1.956659
H  7.008738   -0.086150  1.915403
H  6.561463   1.350392   -1.841054
H  7.044385   3.782050   -1.833361
H  6.198444   5.206583   0.005789
H  4.877930   4.198901   1.842180
H  4.403386   1.764584   1.834273
H  -0.749314  0.488712   0.718133
H  -3.002462  1.368969   0.664543
H  -4.501372  -2.511402  -0.489786
H  -2.233086  -3.385416  -0.458310
H  -4.403178  1.764509   -1.834187
H  -4.877782  4.198802   -1.842231
H  -6.198547  5.206516   -0.006036
H  -7.044673  3.782016   1.833058
H  -6.561678  1.350383   1.840903
H  -7.008430  -0.086292  -1.915566
H  -9.025449  -1.528730  -1.956994
H  -9.477532  -3.077995  -0.080313
H  -7.919934  -3.179753  1.841720
H  -5.907225  -1.730880  1.881757
```

(Ftol)2CH+

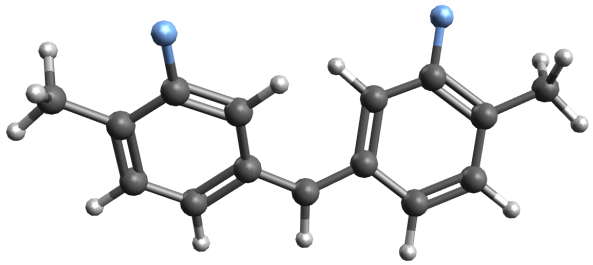

Figure S25. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
FTOL_2CH

30

C  -5.286783  -0.652287  0.126648
C  -3.913919  -0.069195  0.094347
C  -3.653679  1.266699   0.412113
C  -2.375868  1.778509   0.340619
C  -1.282568  0.947837   -0.005408
C  -0.000024  1.533782   -0.000093
H  -0.000037  2.622511   0.000027
C  1.282623   0.947858   0.005376
C  2.375903   1.778539   -0.340595
C  3.653728   1.266691   -0.412048
C  3.913906   -0.069212  -0.094352
C  5.286775   -0.652337  -0.126602
C  2.824216   -0.866744  0.296596
F  3.069894   -2.127201  0.645985
C  1.539199   -0.402299  0.351550
C  -1.539233  -0.402292  -0.351618
C  -2.824240  -0.866730  -0.296654
F  -3.069926  -2.127198  -0.645954
H  -6.024817  0.086999   0.433547
H  -5.322660  -1.499890  0.816507
H  -5.558242  -1.039676  -0.859152
H  -4.477666  1.907359   0.701608
H  -2.198327  2.820895   0.579271
H  2.198437   2.820949   -0.579160
H  4.477733   1.907379   -0.701438
H  6.024733   0.086788   -0.434089
H  5.322509   -1.500338  -0.815964
```

```
H  5.558455   -1.039071  0.859394
H  0.765660   -1.058623  0.725438
H  -0.765705  -1.058616  -0.725558
```

(Fur)2CH+

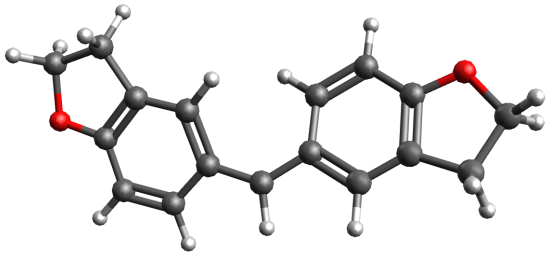

Figure S26. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
FUR_2CH

34

C  -5.799382  -0.396878  0.150568
C  -5.035672  0.872084   0.582429
C  -3.618262  0.521264   0.214821
C  -2.453573  1.228934   0.241331
C  -1.226134  0.594293   -0.116964
C  -0.049003  1.360292   -0.034421
H  -0.213718  2.434987   0.028124
C  1.303086   0.977318   -0.015941
C  2.268568   1.993153   -0.269829
C  3.613352   1.727610   -0.331726
C  4.010998   0.410253   -0.085871
O  5.264142   0.012836   -0.086247
C  5.311893   -1.428316  0.128065
C  3.893269   -1.849579  0.557443
C  3.095542   -0.613576  0.234482
C  1.760924   -0.343533  0.274926
C  -1.263754  -0.751883  -0.577088
C  -2.434796  -1.464565  -0.632407
C  -3.604536  -0.817817  -0.215155
O  -4.791190  -1.383579  -0.221079
H  -6.420301  -0.240310  -0.731127
H  -6.398336  -0.842351  0.941861
H  -5.129274  1.053294   1.655285
H  -5.395090  1.758202   0.057795
H  -2.442155  2.265128   0.562837
H  1.921624   3.004566   -0.451311
H  4.346352   2.493300   -0.546312
H  6.077037   -1.609850  0.879085
```

```
H  5.616525   -1.875386  -0.818585
H  3.845686   -2.073990  1.625687
H  3.550514   -2.728836  0.011075
H  1.060227   -1.104969  0.592869
H  -0.360884  -1.206218  -0.963009
H  -2.476928  -2.475944  -1.013630
```

(Fur)(ani)CH+

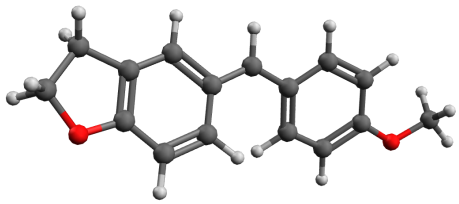

Figure S27. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
FUR_ANI_CH

33

C  -6.476060  -0.033011  -0.165584
O  -5.340910  -0.825542  0.187905
C  -4.128975  -0.311080  0.123812
C  -3.840921  1.007242   -0.275387
C  -2.535070  1.431618   -0.289795
C  -1.462409  0.566397   0.038625
C  -0.153847  1.080680   -0.060291
H  -0.099550  2.167710   -0.103058
C  1.088683   0.431768   -0.112342
C  1.248267   -0.949795  -0.424168
C  2.481883   -1.546279  -0.449905
C  3.592887   -0.744758  -0.154577
O  4.827417   -1.190440  -0.146363
C  5.744704   -0.080335  0.091928
C  4.871637   1.157117   0.387049
C  3.485544   0.630832   0.124525
C  2.257633   1.220129   0.121969
C  -1.786014  -0.746726  0.480767
C  -3.081970  -1.172065  0.523656
H  -7.334872  -0.684428  -0.032106
H  -6.413136  0.285612   -1.208857
H  -6.562451  0.831722   0.496700
H  -4.630907  1.689108   -0.557243
H  -2.316357  2.450397   -0.591326
H  0.384113   -1.531025  -0.716996
H  2.614860   -2.585821  -0.717519
H  6.344443   0.024692   -0.811438
H  6.384731   -0.375841  0.920513
```

```
  H  5.126461   1.995347   -0.262743
  H  4.978129   1.487533   1.422270
  H  2.150697   2.279945   0.328164
  H  -1.008614  -1.399809  0.854585
  H  -3.345432  -2.157698  0.885010
```

(Ind)2CH+

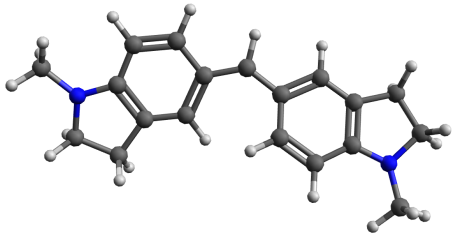

Figure S28. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
IND_2CH

48

C  5.539017   2.145490   -0.434296
N  5.032453   0.855455   -0.024645
C  5.938949   -0.277288  0.200200
C  5.007109   -1.434640  0.614427
C  3.637131   -0.914341  0.253886
C  2.422657   -1.517539  0.237094
C  1.242638   -0.770807  -0.081524
C  0.010572   -1.444647  -0.054248
H  0.096755   -2.530346  -0.040242
C  -1.310826  -0.973377  -0.038798
C  -2.341654  -1.912213  -0.325056
C  -3.665875  -1.566963  -0.386867
C  -4.008580  -0.227524  -0.113162
N  -5.222342  0.328993   -0.081304
C  -6.475933  -0.371683  -0.247665
C  -5.185095  1.693772   0.456541
C  -3.683730  2.046423   0.506735
C  -3.007661  0.724642   0.234506
C  -1.699607  0.369374   0.273584
C  1.401952   0.590997   -0.458651
C  2.624925   1.209439   -0.473688
C  3.757028   0.460417   -0.088429
H  6.474929   2.342175   0.089697
H  4.831326   2.930703   -0.166902
H  5.725439   2.180375   -1.513528
H  6.670695   -0.021165  0.968662
H  6.480131   -0.498153  -0.726809
H  5.071113   -1.623207  1.689006
```

```
H  5.255055   -2.362346  0.098316
H  2.328580   -2.568306  0.492423
H  -2.059914  -2.941629  -0.520083
H  -4.421477  -2.307999  -0.611072
H  -6.378167  -1.143379  -1.011702
H  -7.236818  0.336105   -0.577922
H  -6.805596  -0.832485  0.690027
H  -5.644186  1.703438   1.451174
H  -5.758397  2.362996   -0.188124
H  -3.397897  2.471542   1.469443
H  -3.426202  2.773242   -0.267381
H  -0.958402  1.085707   0.604368
H  0.544219   1.142442   -0.820611
H  2.719931   2.231962   -0.814626
```

(Jul)2CH+

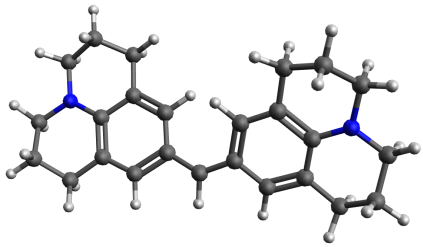

Figure S29. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
JUL_2CH

56

C  -5.979991  -1.530146  1.109474
C  -6.344836  -0.366826  0.206097
N  -5.188660  0.485570   -0.075339
C  -5.507097  1.859095   -0.467925
C  -4.331614  2.796193   -0.263987
C  -3.112759  2.237494   -0.984106
C  -2.838644  0.829044   -0.523296
C  -1.567686  0.331229   -0.500792
C  -1.280909  -1.009397  -0.133358
C  0.001991   -1.573494  -0.071526
H  0.011271   -2.662554  -0.046114
C  1.276035   -0.985475  -0.036319
C  1.539681   0.374249   0.270413
C  2.802461   0.895452   0.276924
C  3.029022   2.349328   0.613152
C  4.428783   2.566834   1.167877
C  5.442025   1.959015   0.215330
N  5.175025   0.539035   -0.010837
C  6.330947   -0.282391  -0.372487
C  6.119483   -1.738741  -0.001426
C  4.839707   -2.242061  -0.652555
C  3.682769   -1.334528  -0.317606
C  2.403292   -1.810993  -0.284390
C  3.918924   0.048043   -0.029016
C  -2.394633  -1.842148  0.151357
C  -3.681696  -1.385732  0.169849
C  -4.830935  -2.309268  0.486524
C  -3.935742  -0.009038  -0.131420
H  -6.856215  -2.166014  1.246651
```

```
H  -5.689000  -1.150607  2.093573
H  -7.104156  0.259042   0.678490
H  -6.764781  -0.731674  -0.740338
H  -6.358843  2.181516   0.134192
H  -5.827818  1.868665   -1.517869
H  -4.123648  2.895723   0.805667
H  -4.593762  3.785475   -0.643054
H  -2.234677  2.863134   -0.811928
H  -3.297334  2.238243   -2.064947
H  -0.766179  0.972725   -0.846166
H  0.724608   1.019382   0.574910
H  2.270920   2.684716   1.324259
H  2.903324   2.952601   -0.293875
H  4.525451   2.094461   2.150014
H  4.639739   3.630594   1.290014
H  6.449456   2.041268   0.626166
H  5.435748   2.491880   -0.744534
H  7.197163   0.122756   0.153327
H  6.525922   -0.184375  -1.448337
H  6.051692   -1.830763  1.086739
H  6.981388   -2.322291  -0.329394
H  4.613690   -3.261530  -0.333302
H  4.973634   -2.272442  -1.740250
H  2.239174   -2.864945  -0.490235
H  -2.213111  -2.885407  0.393433
H  -4.493586  -3.106396  1.151876
H  -5.176092  -2.789865  -0.436454
```

(Lil)2CH+

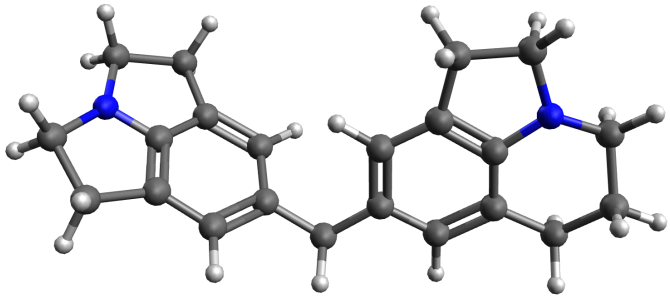

Figure S30. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
LIL_2CH

47

C  3.55941  -2.19451  -0.35952
C  3.65824  -0.66223  -0.23798
N  2.4529  -0.17678   0.40289
C  2.23657   1.14473   0.94536
C  0.72045   1.1899   1.29777
C  0.18089  -0.00535   0.57979
C -1.13623  -0.42062   0.38147
C -1.37064  -1.61135  -0.36113
C -2.75525  -2.14572  -0.65383
H -2.84861  -3.14187  -0.16909
C -3.89963  -1.24696  -0.26538
C -4.05718   0.02442  -0.91153
C -5.13817   0.83123  -0.52826
C -5.65712   2.19232  -0.93221
N -6.97707   1.16587   0.74692
C -7.78715   0.5507   1.76687
C -7.06005  -0.83416   2.01509
C -5.89209  -0.79574   1.05603
C -4.83974  -1.66544   0.73418
C -5.95933   0.3672   0.41124
C -0.26527  -2.3511  -0.85657
C  1.04994  -1.92339  -0.60232
C  2.27795  -2.64716  -1.10763
C  1.2167  -0.74771   0.11423
H  3.50761  -2.59514   0.67766
H  4.46182  -2.62198  -0.84603
```

```
H  3.75402  -0.20238  -1.24517
H  4.54751  -0.3934   0.37124
H  2.45124   1.87052   0.13011
H  2.876   1.3654   1.82605
H  0.27582   2.15407   0.97114
H  0.53829   1.02003   2.38061
H -1.94141   0.17725   0.7847
H -3.36464   0.35964  -1.67299
H -8.8214   0.40294   1.38965
H -7.78361   1.17994   2.68221
H -7.72608  -1.68791   1.76765
H -6.69114  -0.91294   3.0598
H -4.74859  -2.62101   1.23416
H -0.42979  -3.25792  -1.42628
H  2.36041  -2.45389  -2.19841
H  2.17472  -3.7425  -0.95072
C -6.93682   2.385  -0.0193
H -5.92822   2.19062  -2.00933
H -4.8915   2.96866  -0.72037
H -6.82156   3.25503   0.66156
H -7.85974   2.47756  -0.63042
```

(Mfa)2CH+

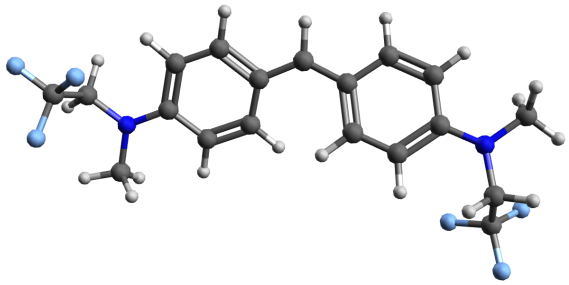

Figure S31. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls; Fluorine = Light blue.

```
MFA_2CH

46

C  4.799790   -2.428132  0.795325
N  4.818829   -0.967828  0.719497
C  6.118265   -0.329228  0.760703
C  6.755233   -0.191328  -0.616009
F  6.903846   -1.384728  -1.204539
F  6.010862   0.567233   -1.431939
F  7.957400   0.373415   -0.503333
C  3.667673   -0.264110  0.633985
C  3.649618   1.146380   0.452245
C  2.466493   1.822535   0.390674
C  1.209501   1.162220   0.453696
C  0.044862   1.936556   0.334180
H  0.201854   3.007486   0.456618
C  -1.287901  1.570846   0.085172
C  -2.305622  2.527135   0.340490
C  -3.630524  2.240408   0.176104
C  -4.043092  0.970177   -0.312600
C  -3.025278  0.026744   -0.634264
C  -1.707394  0.318897   -0.439588
N  -5.357075  0.702236   -0.488878
C  -6.375990  1.662892   -0.066942
C  -5.827736  -0.528639  -1.088898
C  -6.104136  -1.620024  -0.063217
F  -4.996431  -1.955669  0.613297
F  -7.015829  -1.224894  0.833154
F  -6.563032  -2.711574  -0.676204
```

```
C  1.237587   -0.240610  0.673580
C  2.413296   -0.928028  0.762485
H  5.817245   -2.797620  0.699799
H  4.218760   -2.849223  -0.026923
H  4.389589   -2.770474  1.749861
H  6.791901   -0.927131  1.375636
H  6.063228   0.658230   1.217016
H  4.567429   1.699112   0.322777
H  2.487179   2.897321   0.245344
H  -2.023935  3.509594   0.704315
H  -4.361856  3.001097   0.405547
H  -3.281181  -0.946736  -1.023894
H  -0.970727  -0.410696  -0.748653
H  -6.335560  2.572714   -0.672280
H  -6.254477  1.917478   0.987650
H  -7.356468  1.209242   -0.184000
H  -5.120199  -0.914007  -1.821852
H  -6.760054  -0.334529  -1.619976
H  0.314835   -0.777939  0.848942
H  2.380942   -1.986956  0.973091
```

(Mfp)2CH+

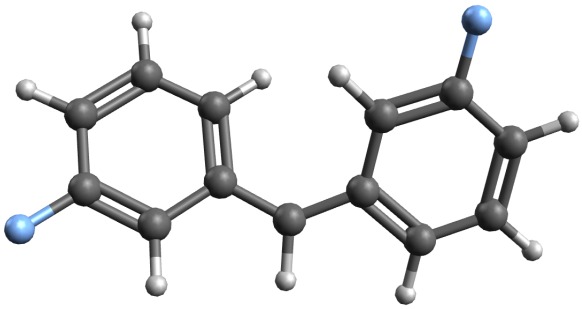

Figure S32. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
MFP_2CH

24

F  4.736503   -0.782129  -0.600814
C  3.599074   -0.225917  -0.212670
C  3.608757   1.090776   0.237398
C  2.424622   1.683684   0.670508
C  1.236651   0.983615   0.622222
C  1.222150   -0.347590  0.137940
C  0.051759   -1.134445  0.047215
C  -1.306164  -0.748128  0.017264
C  -2.266974  -1.748525  0.304865
C  -3.610681  -1.431383  0.349869
C  -4.025783  -0.136963  0.057497
C  -3.083295  0.835517   -0.275895
F  -3.505278  2.050898   -0.593988
C  -1.738409  0.562454   -0.301571
C  2.439582   -0.963340  -0.243306
H  -1.939151  -2.759232  0.518341
H  -4.344151  -2.189144  0.592682
H  -5.075978  0.130776   0.056168
H  0.222693   -2.208500  -0.008842
H  2.468108   -1.990097  -0.588715
H  4.549233   1.628560   0.265586
H  2.445630   2.693181   1.060343
H  0.335879   1.428236   1.022551
H  -1.051035  1.328769   -0.632927
```

(Mfp)PhCH+

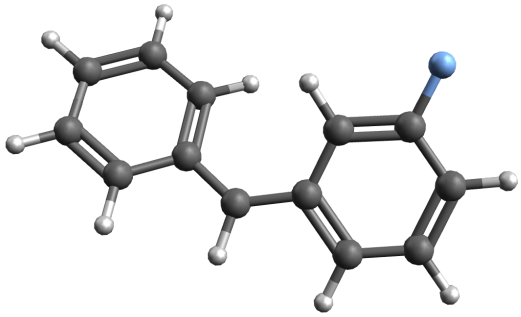

Figure S33. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
MFP_PH_CH

24

F  -3.030605  2.170528   -0.450808
C  -2.662184  0.922266   -0.196000
C  -3.640144  -0.012051  0.139897
C  -3.280072  -1.335633  0.365294
C  -1.956866  -1.718138  0.251666
C  -0.958856  -0.758219  -0.037663
C  0.381718   -1.214145  -0.080342
H  0.491485   -2.290666  -0.203922
C  1.591284   -0.500299  0.012301
C  2.770294   -1.164100  -0.418456
C  3.982920   -0.510817  -0.408189
C  4.053939   0.793760   0.080493
C  2.917950   1.447493   0.567140
C  1.696067   0.815626   0.535397
C  -1.334552  0.582512   -0.287434
H  2.703228   -2.182061  -0.786339
H  4.876172   -1.009556  -0.761487
H  5.011433   1.301413   0.107355
H  3.005085   2.441932   0.985865
H  -0.623187  1.326824   -0.618059
H  -4.674066  0.308007   0.193335
H  -4.040957  -2.065190  0.610276
H  -1.674385  -2.752011  0.412494
H  0.831650   1.297009   0.973129
```

(Mor)2CH+

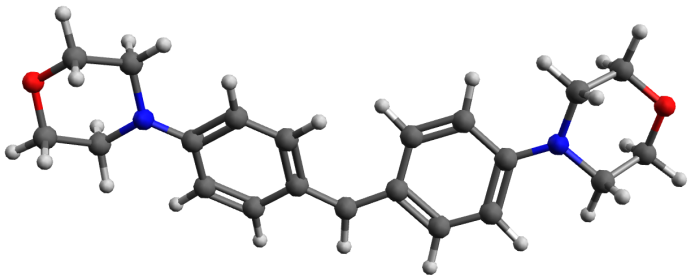

Figure S34. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls; Nitrogen = Blue balls.

```
MOR_2CH

50

C  6.718987   -2.045269  0.533664
C  5.506792   -1.699938  -0.320801
N  5.198263   -0.269137  -0.227364
C  6.372371   0.564115   -0.500149
C  7.552370   0.101635   0.351192
O  7.827750   -1.263375  0.165518
C  3.945722   0.221859   -0.156967
C  3.660737   1.592305   -0.430113
C  2.388573   2.076716   -0.344362
C  1.278061   1.251734   -0.020936
C  -0.000050  1.829633   0.000090
H  -0.000066  2.918854   -0.000105
C  -1.278138  1.251689   0.021292
C  -2.388701  2.076752   0.344402
C  -3.660847  1.592336   0.430214
C  -3.945788  0.221803   0.157393
C  -2.841028  -0.597624  -0.231740
C  -1.573213  -0.102044  -0.296884
N  -5.198349  -0.269134  0.227683
C  -5.506996  -1.699892  0.321363
C  -6.718583  -2.045432  -0.533863
O  -7.827570  -1.263415  -0.166568
C  -7.552086  0.101550   -0.352382
C  -6.372573  0.564262   0.499532
C  1.573197   -0.101890  0.297679
C  2.841014   -0.597459  0.232560
```

```
H  6.994887   -3.088217  0.378067
H  6.479462   -1.896750  1.597268
H  4.658940   -2.305523  -0.016239
H  5.727421   -1.930258  -1.370091
H  6.167137   1.602399   -0.252595
H  6.625829   0.497290   -1.564806
H  7.337659   0.306997   1.410644
H  8.447159   0.653157   0.062837
H  4.445520   2.266250   -0.738107
H  2.213497   3.122532   -0.574147
H  -2.213633  3.122629   0.573918
H  -4.445684  2.266303   0.738021
H  -3.003433  -1.618967  -0.541666
H  -0.791188  -0.748142  -0.674038
H  -5.728515  -1.929812  1.370553
H  -4.658884  -2.305608  0.017795
H  -6.994621  -3.088337  -0.378227
H  -6.478385  -1.897129  -1.597340
H  -8.447044  0.653138   -0.064680
H  -7.336745  0.306679   -1.411752
H  -6.626633  0.497797   1.564063
H  -6.167151  1.602451   0.251732
H  0.791238   -0.747872  0.675157
H  3.003459   -1.618702  0.542788
```

(Mpa)2CH+

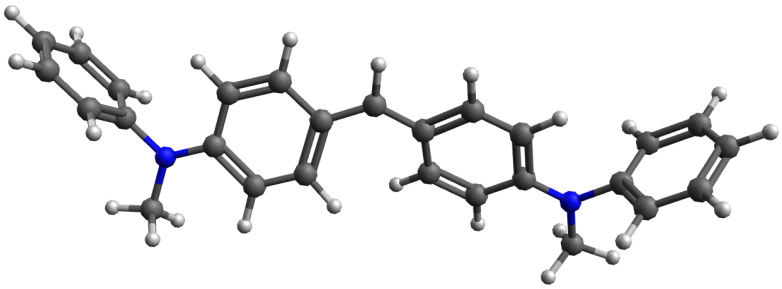

Figure S35. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
MPA_2CH

54

C  -5.431869  -2.431398  0.592448
N  -5.169497  -1.027729  0.284961
C  -6.311244  -0.185793  0.051820
C  -6.897166  0.485943   1.117975
C  -8.013494  1.281284   0.892497
C  -8.536810  1.400227   -0.389759
C  -7.945326  0.724301   -1.450646
C  -6.828464  -0.072523  -1.232913
C  -3.920340  -0.529935  0.247540
C  -3.684190  0.840597   -0.060063
C  -2.412215  1.326876   -0.103412
C  -1.273666  0.499621   0.112354
C  -0.000016  1.077943   0.000214
H  -0.000020  2.167349   0.000485
C  1.273631   0.499683   -0.112235
C  1.525655   -0.851317  -0.473556
C  2.793817   -1.351219  -0.544094
C  3.920322   -0.529804  -0.247752
C  3.684145   0.840558   0.060580
C  2.412167   1.326819   0.104076
N  5.169482   -1.027585  -0.285302
C  5.431914   -2.431105  -0.593368
C  6.311240   -0.185749  -0.051839
C  6.896384   0.487397   -1.117540
C  8.012718   1.282643   -0.891789
```

```
C  8.536848   1.400064   0.390278
C  7.946156   0.722721   1.450701
C  6.829263   -0.073990  1.232697
C  -1.525659  -0.851575  0.472985
C  -2.793812  -1.351510  0.543377
H  -6.501184  -2.604132  0.497483
H  -5.129591  -2.676986  1.614927
H  -4.909690  -3.089772  -0.106756
H  -6.476958  0.385181   2.112233
H  -8.475487  1.806643   1.719670
H  -9.408515  2.019903   -0.562475
H  -8.353713  0.816378   -2.449848
H  -6.354842  -0.603356  -2.050890
H  -4.523403  1.494138   -0.254052
H  -2.259074  2.374645   -0.339890
H  0.703586   -1.490295  -0.768832
H  2.938533   -2.374344  -0.860942
H  4.523328   1.494000   0.255034
H  2.259014   2.374458   0.341120
H  4.909798   -3.089817  0.105564
H  6.501245   -2.603821  -0.498572
H  5.129593   -2.676295  -1.615936
H  6.475560   0.387781   -2.111655
H  8.474102   1.809102   -1.718603
H  9.408569   2.019658   0.563201
H  8.355165   0.813622   2.449755
H  6.356231   -0.605891  2.050322
H  -0.703564  -1.490706  0.767850
H  -2.938530  -2.374782  0.859748
```

(Pcp)2CH+

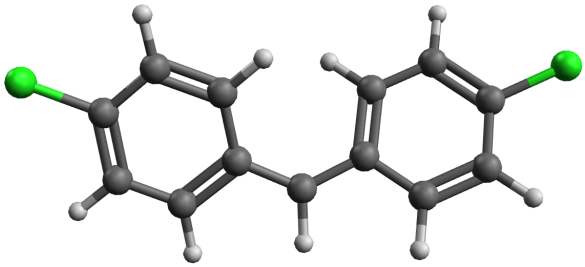

Figure S36. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Chloride = Green balls.

```
PCP_2CH

24

Cl -5.447724  -0.910686  -0.007971
C  -3.861950  -0.264053  -0.025565
C  -3.662994  1.073306   0.330504
C  -2.389476  1.588314   0.297189
C  -1.278931  0.772534   -0.039505
C  -0.000031  1.364231   -0.000293
H  0.000069   2.453370   -0.000194
C  1.278921   0.772436   0.039109
C  2.389538   1.588316   -0.297057
C  3.663094   1.073343   -0.330129
C  3.861933   -0.264095  0.025630
Cl 5.447770   -0.910650  0.008512
C  2.795259   -1.079813  0.425843
C  1.520623   -0.569708  0.430109
C  -1.520766  -0.569466  -0.430904
C  -2.795361  -1.079622  -0.426340
H  -4.506989  1.688240   0.613460
H  -2.227378  2.626934   0.563282
H  2.227559   2.627022   -0.562870
H  4.507157   1.688440   -0.612531
H  2.988647   -2.094874  0.746902
H  0.710913   -1.183286  0.802416
H  -0.711085  -1.182854  -0.803622
H  -2.988831  -2.094607  -0.747585
```

(Pfa)2CH+

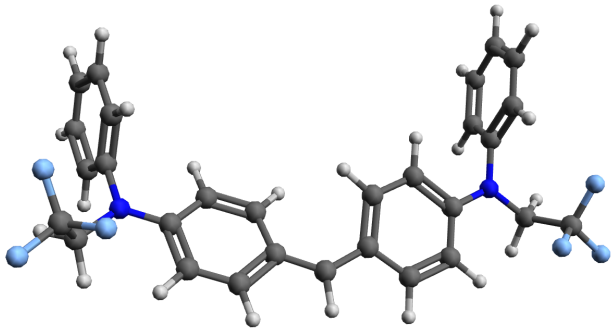

Figure S37. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls; Fluorine = Light blue.

```
PFA_2CH

60

F  7.855065   -2.223646  -1.084576
C  6.823854   -1.376895  -1.104384
F  7.199811   -0.274290  -1.757852
F  5.833851   -1.942543  -1.811918
C  6.392964   -1.068679  0.324241
N  5.230796   -0.203248  0.405492
C  5.491826   1.212248   0.483412
C  5.875149   1.766896   1.698565
C  6.138546   3.128489   1.773381
C  6.011271   3.924673   0.641065
C  5.623595   3.361334   -0.569128
C  5.364306   1.999701   -0.653383
C  3.960163   -0.677454  0.454935
C  3.662967   -2.057717  0.308749
C  2.373504   -2.499016  0.394726
C  1.279131   -1.613575  0.581335
C  -0.014709  -2.157873  0.605820
H  -0.043708  -3.240187  0.725145
C  -1.278046  -1.553872  0.504625
C  -2.416382  -2.322710  0.865463
C  -3.681660  -1.810229  0.838643
C  -3.906281  -0.476472  0.406640
C  -2.783070  0.277961   -0.037055
C  -1.522988  -0.241339  0.017182
N  -5.144581  0.078254   0.394433
```

```
C  -6.311662  -0.589459  0.940777
C  -7.066620  -1.436100  -0.076622
F  -7.564808  -0.693852  -1.069133
F  -6.277736  -2.368466  -0.632310
F  -8.079947  -2.058355  0.529129
C  -5.347983  1.414859   -0.106930
C  -5.359920  2.479574   0.785998
C  -5.566860  3.767169   0.308339
C  -5.752889  3.982573   -1.052330
C  -5.735450  2.911572   -1.938125
C  -5.534704  1.620375   -1.467621
C  1.593669   -0.239327  0.763898
C  2.878378   0.214152   0.706026
H  7.231298   -0.570983  0.812268
H  6.221152   -2.012484  0.842218
H  5.960926   1.136169   2.576633
H  6.440795   3.566862   2.716739
H  6.219043   4.986224   0.701157
H  5.532351   3.980643   -1.453201
H  5.075563   1.543470   -1.592477
H  4.443411   -2.772463  0.097012
H  2.175905   -3.558996  0.275380
H  -2.275262  -3.348193  1.190001
H  -4.507878  -2.451886  1.103808
H  -2.936976  1.269852   -0.438008
H  -0.707926  0.347587   -0.381935
H  -7.005128  0.168418   1.306020
H  -6.042793  -1.227049  1.783630
H  -5.205173  2.297795   1.843877
H  -5.581351  4.601550   0.999059
H  -5.915867  4.987512   -1.422768
H  -5.886728  3.078902   -2.997607
H  -5.530704  0.774516   -2.144071
H  0.812766   0.462904   1.024466
H  3.086063   1.260003   0.883662
```

(Pfp)2CH+

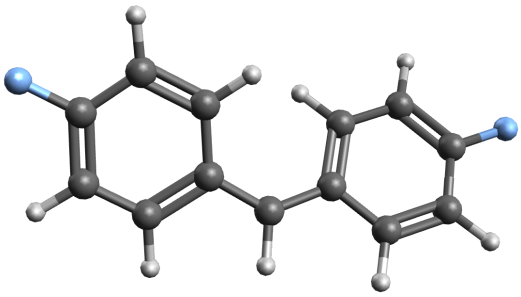

Figure S38. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
PFP_2CH

24

F  -5.062848  -0.914486  -0.015434
C  -3.846171  -0.421099  -0.026009
C  -3.663290  0.913712   0.328971
C  -2.388527  1.423497   0.295374
C  -1.279232  0.602176   -0.039097
C  -0.000003  1.192005   0.000080
H  0.000031   2.281164   -0.000010
C  1.279200   0.602134   0.039303
C  2.388448   1.423453   -0.295392
C  3.663229   0.913725   -0.329121
C  3.846190   -0.421066  0.025898
F  5.062868   -0.914442  0.015291
C  2.796069   -1.250876  0.424332
C  1.521889   -0.741848  0.428946
C  -1.521838  -0.741834  -0.428794
C  -2.795997  -1.250919  -0.424290
H  -4.518659  1.516291   0.604959
H  -2.221829  2.462071   0.558331
H  2.221701   2.462028   -0.558328
H  4.518527   1.516358   -0.605198
H  3.011694   -2.262512  0.742664
H  0.711716   -1.355449  0.800016
H  -0.711589  -1.355371  -0.799780
H  -3.011561  -2.262585  -0.742569
```

Pfp(Ph)CH+

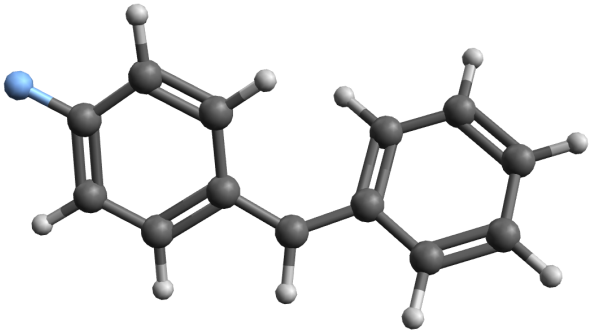

Figure S39. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
PFP_PH_CH

24

F  -4.685929  -0.743430  -0.037096
C  -3.446034  -0.313874  -0.036198
C  -3.199044  1.011103   0.319811
C  -1.900235  1.454376   0.298448
C  -0.830504  0.575772   -0.025423
C  0.474317   1.096235   0.025360
H  0.533401   2.183775   0.042774
C  1.724748   0.434673   0.054396
C  2.866432   1.190687   -0.308655
C  4.111316   0.599461   -0.352620
C  4.249527   -0.737581  0.016670
C  3.147441   -1.485522  0.437716
C  1.894603   -0.913241  0.456731
C  -1.138302  -0.755863  -0.416596
C  -2.436449  -1.198280  -0.423249
H  -4.025588  1.656335   0.587004
H  -1.681826  2.482984   0.562697
H  2.750132   2.233526   -0.582648
H  4.977656   1.173235   -0.655702
H  5.231166   -1.197010  0.002568
H  3.282494   -2.507627  0.767975
H  1.056145   -1.473837  0.849039
H  -0.355615  -1.410098  -0.776636
H  -2.701517  -2.198088  -0.741548
```

Pop(Ph)CH+

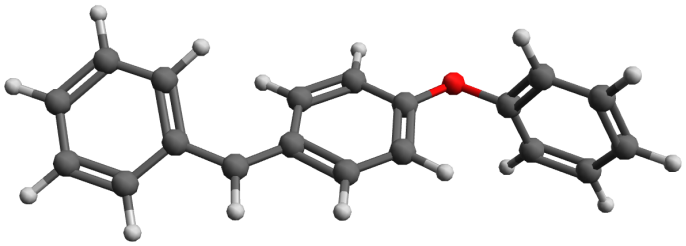

Figure S40. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Oxygen = Red balls.

```
PFP_PH_CH

35

C  2.439993   1.072039   0.129378
H  2.413258   2.149568   0.286064
C  3.749821   0.501482   0.143488
C  4.834950   1.357876   -0.139097
C  6.124036   0.864088   -0.183991
C  6.357904   -0.478088  0.104354
C  5.305035   -1.326708  0.444680
C  4.010205   -0.848392  0.462566
C  1.201671   0.471331   -0.060723
C  1.015386   -0.856672  -0.559518
C  -0.232344  -1.383210  -0.689267
C  -1.365927  -0.614661  -0.327065
O  -2.526410  -1.216957  -0.474116
C  -3.720128  -0.538331  -0.163378
C  -4.367800  0.154133   -1.170021
C  -5.567924  0.785826   -0.865591
C  -6.091709  0.712142   0.420044
C  -5.421830  0.001621   1.409485
C  -4.220675  -0.636005  1.122090
C  -1.221210  0.714892   0.126317
C  0.034589   1.241220   0.230238
H  4.648134   2.405313   -0.349435
H  6.949733   1.521050   -0.426165
H  7.371368   -0.861584  0.089031
H  5.504969   -2.356639  0.712384
H  3.206387   -1.494846  0.790711
H  1.869439   -1.429466  -0.895550
H  -0.397054  -2.375226  -1.089344
```

```
H  -3.947462  0.185624   -2.167891
H  -6.096155  1.330116   -1.638745
H  -7.029724  1.202539   0.649302
H  -5.836320  -0.064785  2.407918
H  -3.688354  -1.207435  1.872796
H  -2.095670  1.300897   0.374180
H  0.154472   2.263038   0.573743
```

(Pyr)2CH+

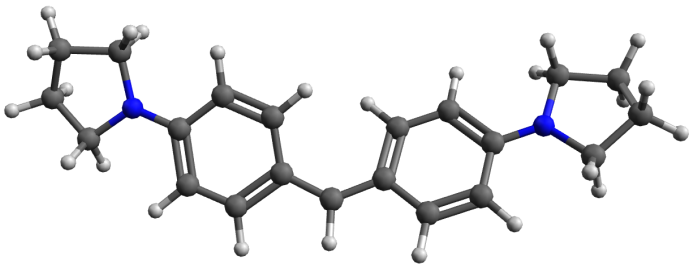

Figure S41. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Nitrogen = Blue balls.

```
PYR_2CH

48

C  -7.060300  -1.699245  -0.503625
C  -7.446031  -0.646295  0.535635
C  -6.358081  0.413400   0.378093
N  -5.179951  -0.359650  -0.035283
C  -5.535589  -1.731384  -0.420438
C  -3.936917  0.127023   -0.055006
C  -3.676813  1.497683   0.237939
C  -2.401199  1.977921   0.217239
C  -1.278673  1.144635   -0.048496
C  0.000012   1.720300   0.000169
H  -0.000154  2.809726   0.000129
C  1.278740   1.144714   0.048694
C  2.401212   1.977941   -0.217348
C  3.676818   1.497673   -0.238029
C  3.936913   0.127066   0.055132
C  2.826183   -0.701099  0.400512
C  1.555156   -0.208625  0.389949
N  5.179944   -0.359636  0.035273
C  6.358002   0.413331   -0.378453
C  7.445889   -0.646413  -0.536101
C  7.060384   -1.699191  0.503416
C  5.535651   -1.731305  0.420605
C  -1.555133  -0.208759  -0.389539
C  -2.826167  -0.701213  -0.400152
H  -7.371355  -1.377849  -1.501151
H  -7.501816  -2.676468  -0.310807
H  -7.406043  -1.073555  1.541136
```

```
H  -8.443488  -0.235689  0.382304
H  -6.158008  0.948200   1.308836
H  -6.615952  1.145976   -0.395456
H  -5.185957  -2.436393  0.342497
H  -5.073639  -1.995624  -1.374053
H  -4.495804  2.169248   0.454429
H  -2.232000  3.027593   0.433873
H  2.231974   3.027564   -0.434164
H  4.495814   2.169175   -0.454712
H  2.992227   -1.730302  0.687110
H  0.750139   -0.856647  0.710775
H  6.616051   1.145996   0.394953
H  6.157739   0.948022   -1.309217
H  8.443396   -0.235813  -0.383084
H  7.405638   -1.073829  -1.541526
H  7.371693   -1.377644  1.500814
H  7.501835   -2.676453  0.310644
H  5.073930   -1.995351  1.374385
H  5.185810   -2.436449  -0.342107
H  -0.750120  -0.856894  -0.710163
H  -2.992204  -1.730474  -0.686550
```

(Tfm)PhCH+

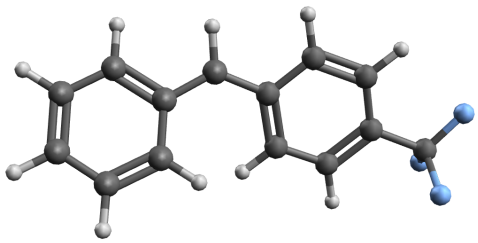

Figure S42. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls; Fluorine = Light blue.

```
TFM_PH_CH

27

F  4.011472   1.359728   -0.814227
C  3.840642   0.316845   0.001694
F  4.627931   -0.673203  -0.412290
F  4.230176   0.681653   1.224983
C  2.379669   -0.092881  0.019139
C  1.998610   -1.376989  -0.355046
C  0.662909   -1.723541  -0.308557
C  -0.314232  -0.771328  0.058906
C  -1.670253  -1.186003  0.028104
H  -1.819492  -2.264798  0.053866
C  -2.849079  -0.422302  -0.032225
C  -4.065557  -1.074750  0.303246
C  -5.251614  -0.375144  0.316835
C  -5.257753  0.969785   -0.054539
C  -4.083279  1.619014   -0.447619
C  -2.887698  0.938591   -0.438106
C  0.103453   0.518753   0.466548
C  1.438951   0.847941   0.448175
H  2.744588   -2.097263  -0.663117
H  0.357492   -2.725994  -0.586683
H  -4.047847  -2.123169  0.579994
H  -6.173986  -0.866724  0.597896
H  -6.194487  1.515453   -0.063543
H  -4.120714  2.649133   -0.778166
H  -1.991603  1.420672   -0.806309
H  -0.614784  1.225994   0.859614
H  1.766016   1.825139   0.780927
```

(Thq)2CH +

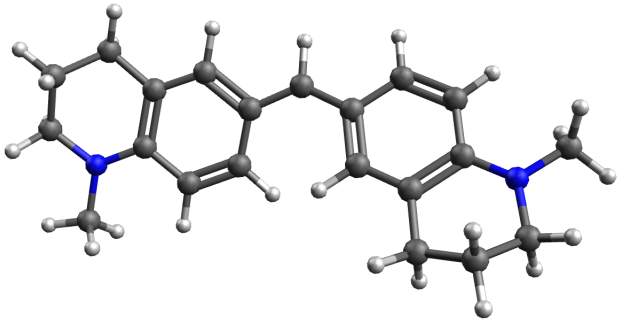

Figure S43. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls

```
THQ_2CH

48

C  -6.379011  -1.007645  -0.543583
N  -5.364011  -0.041265  -0.148341
C  -5.840556  1.305165   0.184762
C  -4.864040  2.047075   1.078354
C  -3.478313  2.026930   0.446828
C  -3.057041  0.606686   0.173943
C  -1.744248  0.234593   0.194837
C  -1.315910  -1.099106  -0.055626
C  0.018607   -1.531528  -0.075091
H  0.137673   -2.612387  -0.009048
C  1.227198   -0.823283  -0.164705
C  1.353890   0.524407   -0.589287
C  2.568910   1.143978   -0.634640
C  3.760094   0.462842   -0.249098
N  4.947025   1.093252   -0.263812
C  5.067330   2.455553   -0.763550
C  6.191817   0.437087   0.151174
C  5.937165   -0.732178  1.084422
C  4.920221   -1.676814  0.456731
C  3.663547   -0.918613  0.120604
C  2.434645   -1.511238  0.143186
C  -2.333746  -2.066403  -0.262015
C  -3.654163  -1.726298  -0.306001
C  -4.064189  -0.378559  -0.104785
H  -7.318150  -0.480489  -0.700588
```

H	-6.533493	-1.767376	0.229089
H	-6.108336	-1.498276	-1.481052
H	-6.802494	1.195981	0.689633
H	-6.015816	1.863649	-0.743136
H	-4.832269	1.570424	2.062847
H	-5.217658	3.069843	1.218609
H	-2.745328	2.515058	1.092396
H	-3.500651	2.588549	-0.494795
H	-1.012322	0.983809	0.471109
H	0.486334	1.063374	-0.946151
H	2.622443	2.163492	-0.988600
H	4.523387	3.161980	-0.129749
H	4.698375	2.535485	-1.789608
H	6.118742	2.735371	-0.762018
H	6.806971	1.188169	0.650751
H	6.735872	0.105151	-0.741862
H	5.559999	-0.362367	2.042729
H	6.882123	-1.242662	1.277458
H	4.688983	-2.506251	1.127626
H	5.341710	-2.111807	-0.457179
H	2.372727	-2.556968	0.430780
H	-2.051564	-3.103446	-0.410278
H	-4.391602	-2.498111	-0.472652

(Tol)2CH+

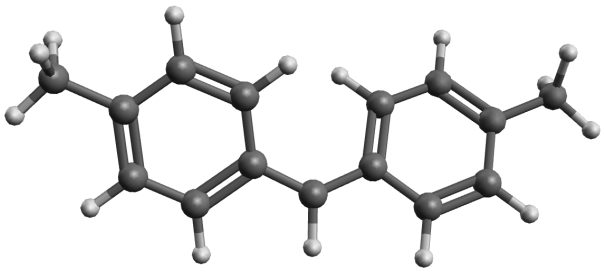

Figure S44. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
TOL_2CH

30

C  -5.278815  -0.979580  -0.013914
C  -3.896837  -0.407958  -0.022983
C  -3.662615  0.929825   0.320234
C  -2.388293  1.447661   0.287583
C  -1.279726  0.628143   -0.040329
C  -0.000003  1.217234   -0.000019
H  0.000017   2.306589   -0.000028
C  1.279725   0.628148   0.040300
C  2.388296   1.447666   -0.287571
C  3.662623   0.929827   -0.320209
C  3.896841   -0.407947  0.023031
C  5.278814   -0.979598  0.013887
C  2.808521   -1.211724  0.410586
C  1.528988   -0.716569  0.419702
C  -1.528995  -0.716586  -0.419697
C  -2.808524  -1.211739  -0.410550
H  -6.022042  -0.246659  0.297681
H  -5.328084  -1.836453  0.664089
H  -5.544539  -1.343326  -1.010546
H  -4.495845  1.563500   0.599206
H  -2.221763  2.487946   0.545636
H  2.221789   2.487948   -0.545645
H  4.495851   1.563501   -0.599185
H  6.022175   -0.246374  -0.296675
H  5.328278   -1.835712  -0.665071
H  5.544178   -1.344467  1.010195
H  2.992462   -2.232497  0.725772
```

```
H  0.720117   -1.336143  0.784040
H  -0.720122  -1.336150  -0.784047
H  -2.992475  -2.232513  -0.725732
```

Tol(Ph)CH +

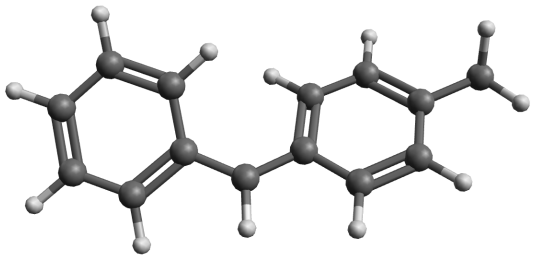

Figure S45. Model of Equilibrium Geometry, 3D View. Hydrogen = White balls; Carbon = Black balls.

```
TOL_PH_CH

27
C  -4.877691  -0.761905  -0.040469
C  -3.464470  -0.276305  -0.034479
C  -3.153216  1.045734   0.313830
C  -1.850753  1.484062   0.295388
C  -0.789213  0.596639   -0.023714
C  0.518262   1.102830   0.031860
H  0.588591   2.189615   0.057977
C  1.765022   0.428119   0.055772
C  2.912290   1.172690   -0.308467
C  4.151985   0.569710   -0.355177
C  4.278726   -0.768675  0.012093
C  3.170115   -1.505659  0.433212
C  1.922301   -0.920883  0.454910
C  -1.117333  -0.732149  -0.409218
C  -2.423595  -1.146956  -0.412827
H  -5.578931  0.013993   0.263771
H  -4.984737  -1.615410  0.635350
H  -5.152938  -1.109641  -1.040373
H  -3.949688  1.727882   0.585425
H  -1.622217  2.511365   0.557830
H  2.805628   2.217057   -0.580597
H  5.022966   1.136061   -0.659061
H  5.255866   -1.237436  -0.004398
H  3.294894   -2.529991  0.760720
H  1.077997   -1.474132  0.844795
H  -0.343767  -1.399115  -0.766361
H  -2.668245  -2.153756  -0.731357
```