Supporting Information

The Solvation of Carbenes: π and Ylidic Complexes of *p*-Nitrophenylchlorocarbene

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1. Figures S-1 – S-22

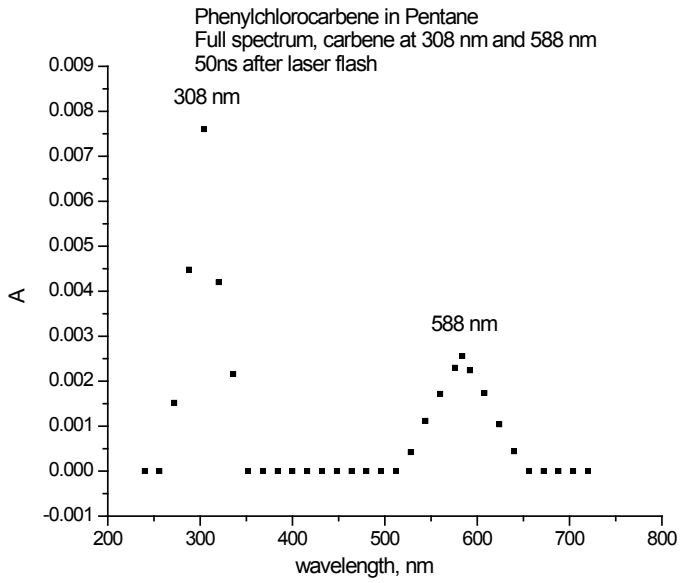

Figure S-1. LFP-UV spectrum of PCC (**2**) in pentane.

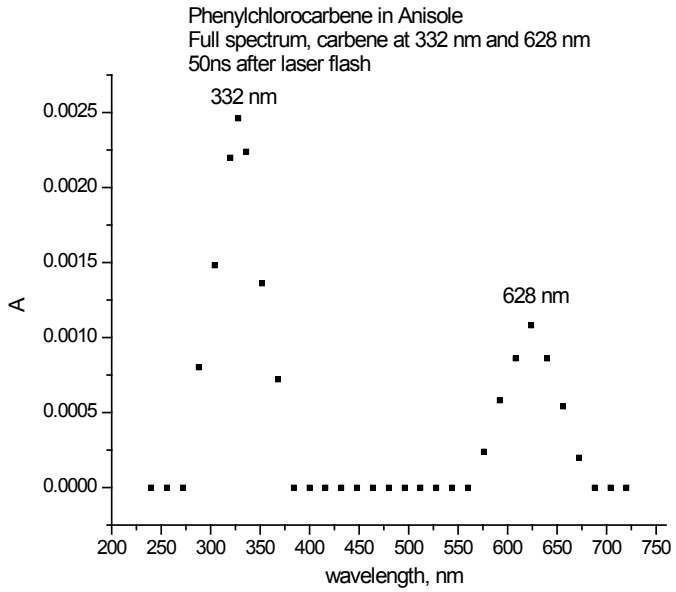

Figure S-2. LFP-UV spectrum of PCC (**2**) in anisole.

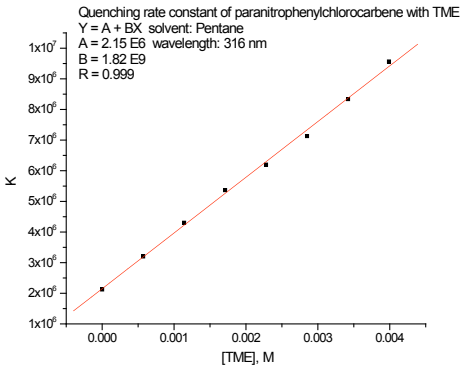

Figure S-3. Determination of the rate constant for addition of PNPCC to TME; k_{obs} for the disappearance of PNPCC at 316 nm vs [TME] in pentane.

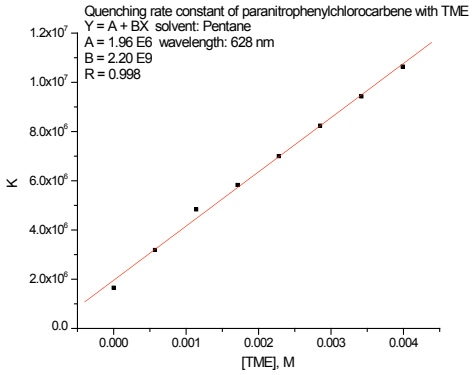

Figure S-4. Determination of the rate constant for the addition of PNPCC to TME; k_{obs} for the disappearance of PNPCC at 628 nm vs [TME] in pentane.

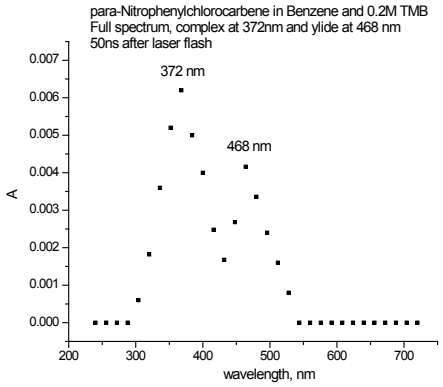

Figure S-5a. LFP-UV spectrum of PNPCC with 0.2 M TMB in benzene 50 ns after the laser pulse.

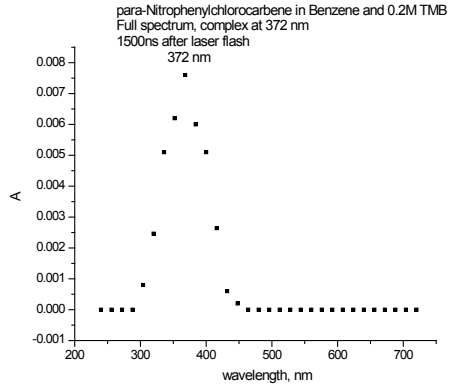

Figure S-5b. LFP-UV spectrum of PNPCC with 0.2 M TMB in benzene 1500 ns after the laser pulse.

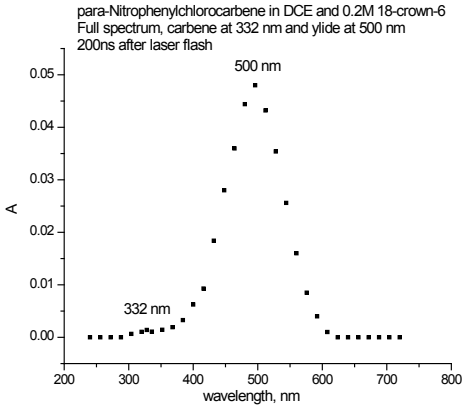

Figure S-6. LFP-UV spectrum of PNPCC with 0.2 M 18-crown-6 in DCE 200 ns after the laser pulse. Note the decrease in the signal at 332 nm.

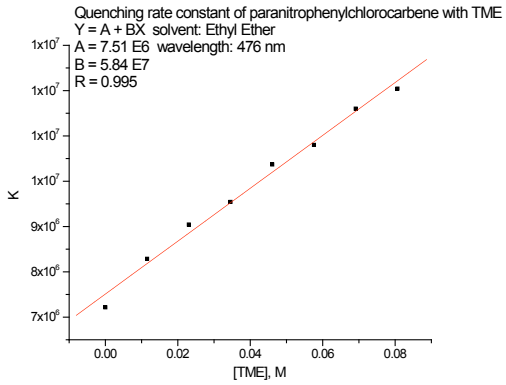

Figure S-7. Determination of the rate constant for addition of PNPCC to TME in diethyl ether; k_{obs} for the disappearance of *O*-ylide at 476 nm vs [TME].

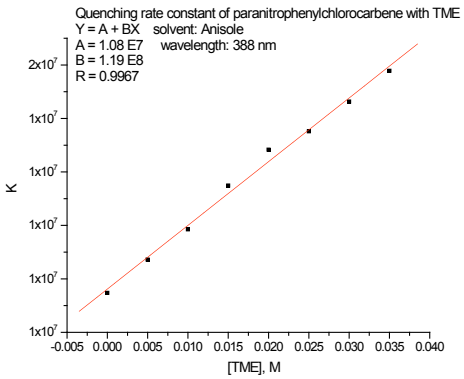

Figure S-8. Determination of the rate constant for addition of PNPCC to TME in anisole; k_{obs} for the disappearance of π-complex at 388 nm vs [TME].

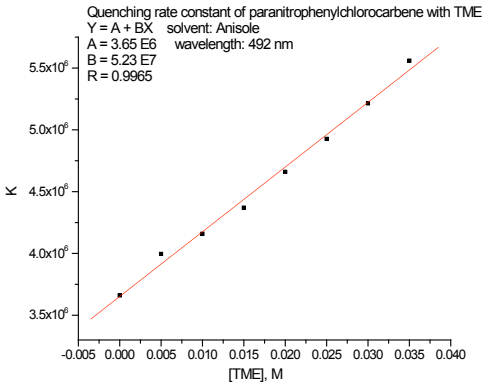

Figure S-9. Determination of the rate constant for addition of PNPCC to TME in anisole; k_{obs} for the disappearance of *O*-ylide at 492 nm vs [TME].

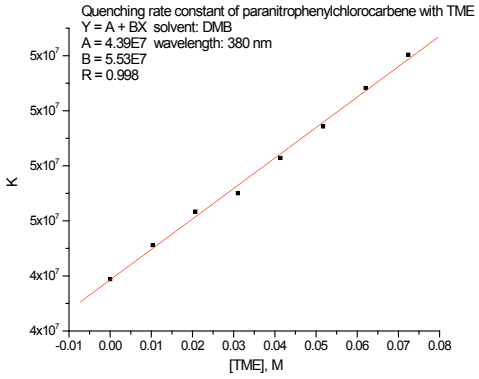

Figure S-10. Determination of the rate constant for addition of PNPCC to TME in 1,3-DMB; k_{obs} for disappearance of π-complex at 380 nm vs [TME].

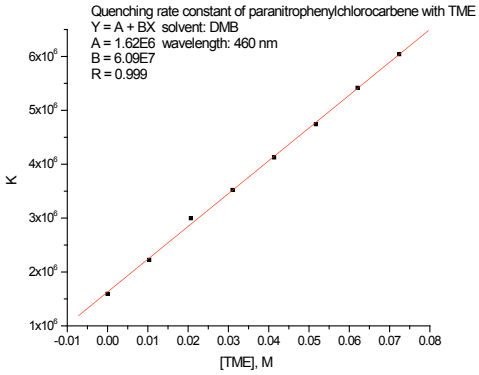

Figure S-11. Determination of the rate constant for addition of PNPCC to TME in 1,3-DMB; k_{obs} for the disappearance of *O*-ylide at 460 nm vs [TME].

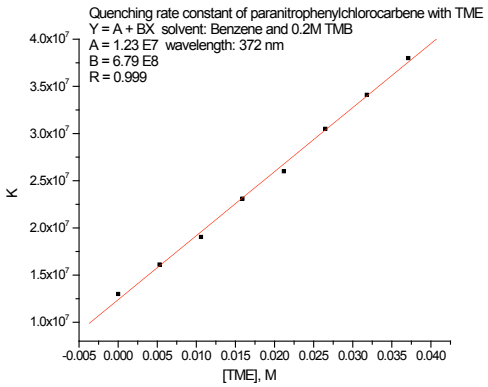

Figure S-12. Determination of the rate constant for addition of PNPCC to TME with 0.2 M TMB in benzene; k_{obs} for disappearance of π-complex at 372 nm vs [TME].

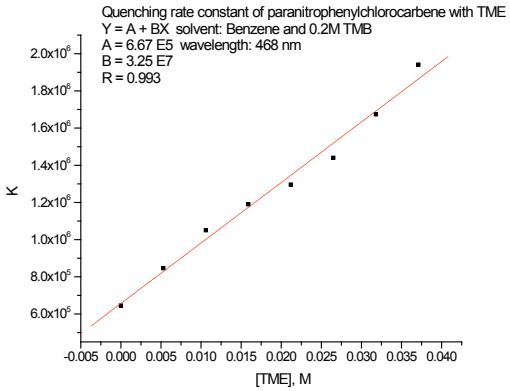

Figure S-13. Determination of the rate constant for addition of PNPCC to TME with 0.2 M TMB in benzene; k_{obs} for disappearance of *O*-ylide at 468 nm vs [TME].

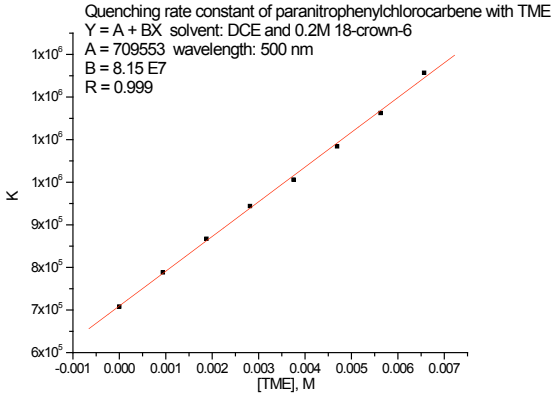

Figure S-14. Determination of the rate constant for addition of PNPCC to TME with 0.2 M 18-crown-6 in DCE; k_{obs} for disappearance of *O*-ylide at 500 nm vs [TME].

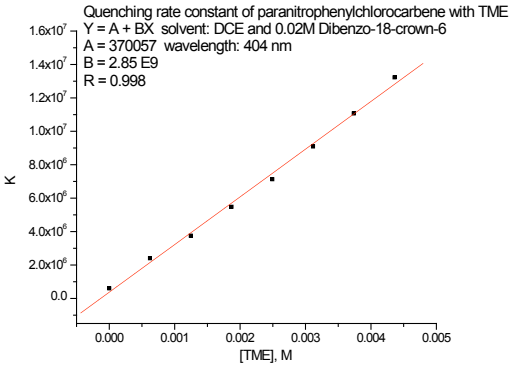

Figure S-15. Determination of the rate constant for addition of PNPCC to TME with 0.02 M dibenzo-18-crown-6 in DCE; k_{obs} for disappearance of π-complex at 404 nm vs [TME].

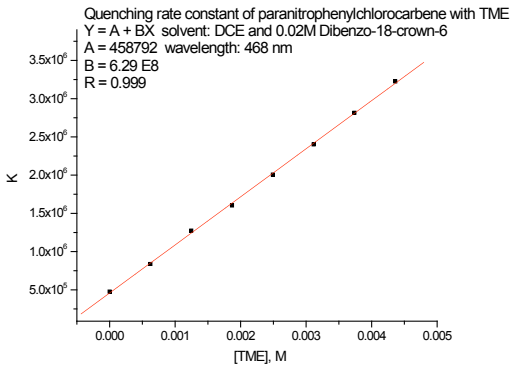

Figure S-16. Determination of the rate constant for addition of PNPCC to TME with 0.02 M dibenzo-18-crown-6 in DCE; k_{obs} for disappearance of *O*-ylide at 468 nm vs [TME]

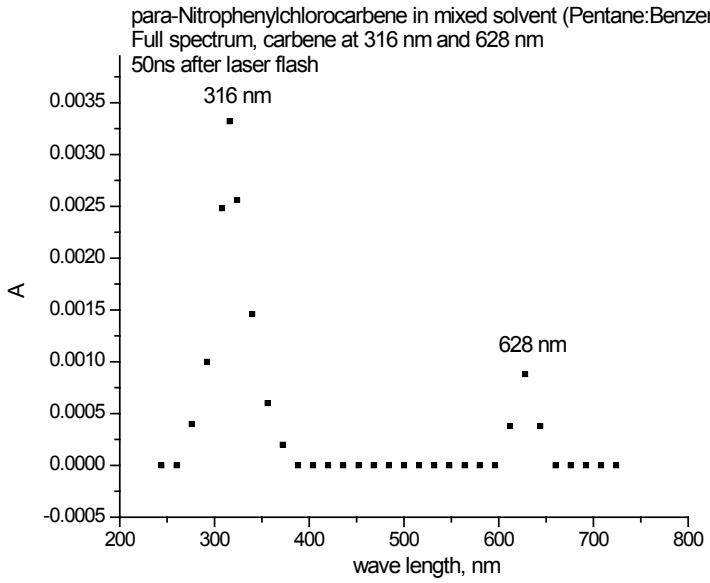

Figure S-17. LFP-UV spectrum of PNPCC in 9:1 pentane-benzene.

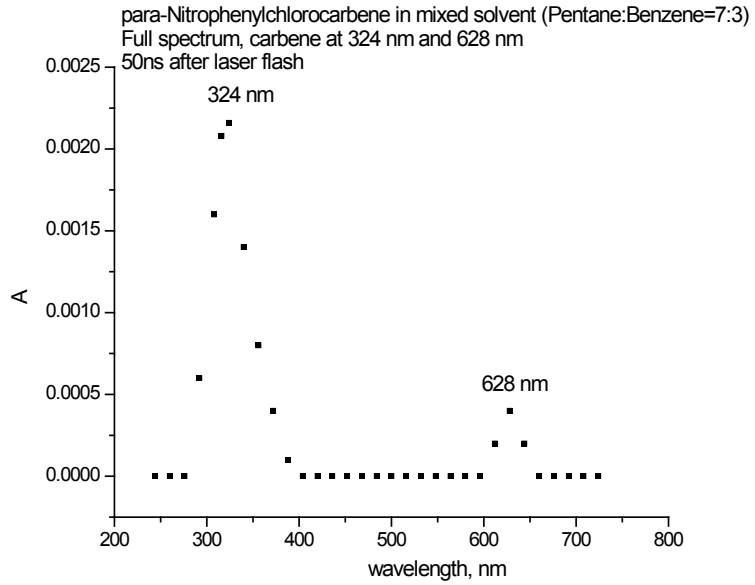

Figure S-18. LFP-UV spectrum of PNPCC in 7:3 pentane-benzene.

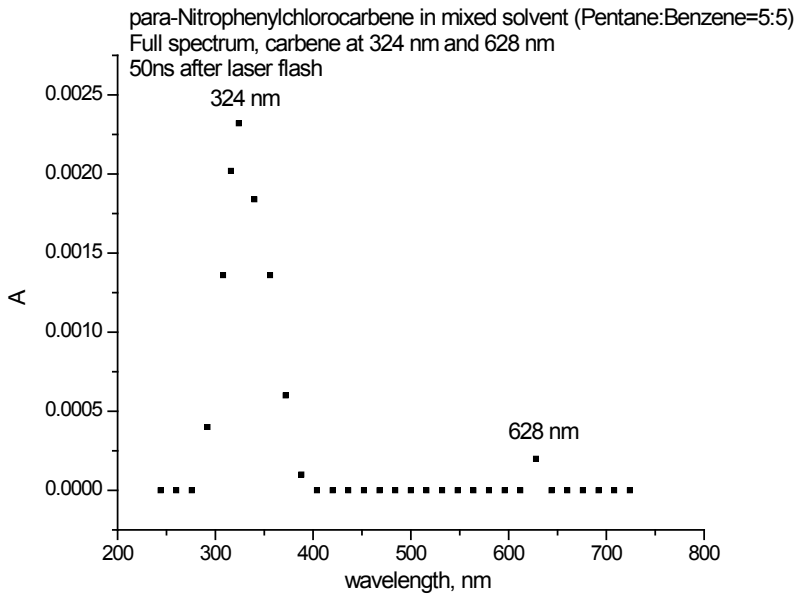

Figure S-19. LFP-UV spectrum of PNPCC in 1:1 pentane-benzene.

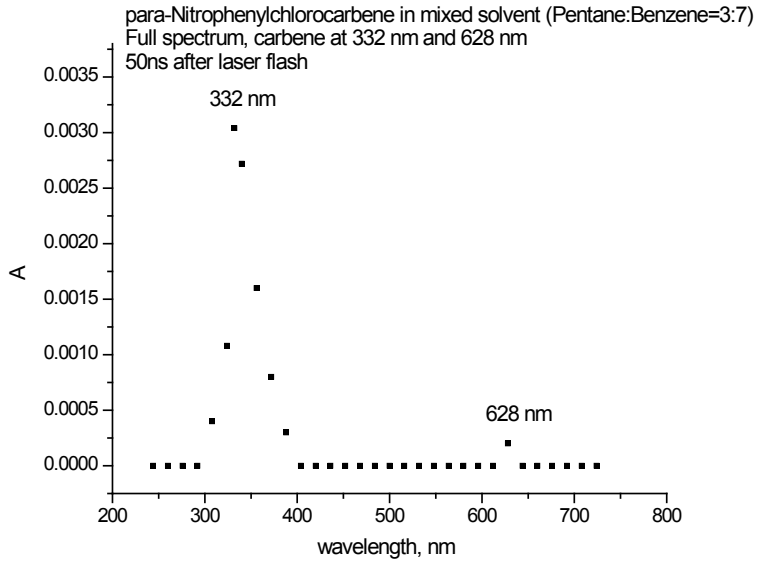

Figure S-20. LFP-UV spectrum of PNPCC in 3:7 pentane-benzene.

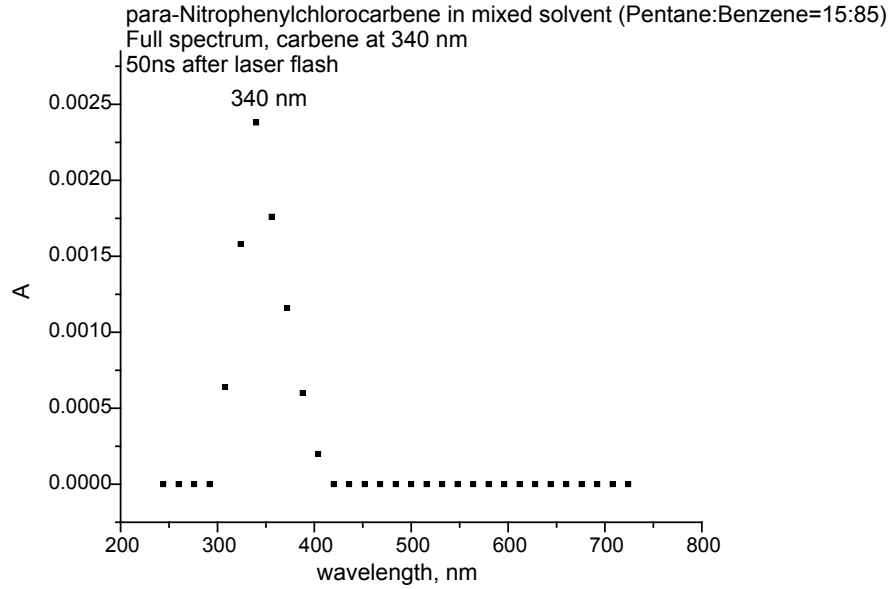

Figure S-21. LFP-UV spectrum of PNPCC in 15:85 pentane-benzene.

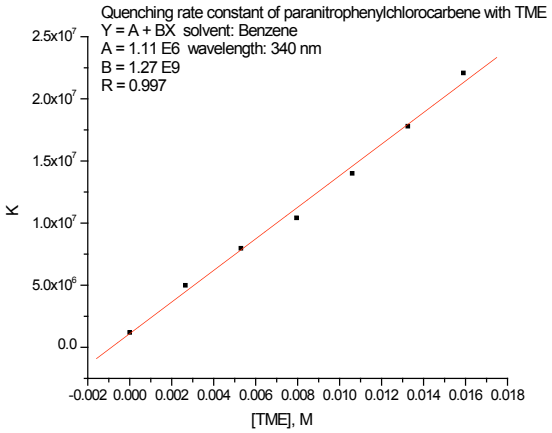

Figure S-22. Determination of the rate constant for addition of PNPCC to TME in benzene; k_{obs} for disappearance of PNPCC at 340 nm vs [TME].

2. Complete Reference 17

(1) Gaussian 03, Revision B.03: Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Montgomery, J.A.; Jr,; Vreven, T.; Kudin, K.N.; Burant, J.C.; Millam, J.M.; Iyengar, S.S; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Zakrzewski, V.G.; Dapprich, S.; Daniels, A.D.; Strain, M..C.; Farkas, O.; Malick, D.K.; Rabuck, A.D.; Raghavachari, K.; Foresman, J.B.; Ortiz, J.V.; Cui, Q.; Baboul, A.G.; Clifford, S.; Cioslowski, J.; Stefanov, B.B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox, D.J.; Keith, T.; Al-Laham, M.A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P.M.W.; Johnson, B.; Chen, W.; Wong, M.W.; Gonzalez, C.; and Pople, J.A. Gaussian, Inc., Pittsburgh, PA, 2003.

3. Optimized geometries (Å) and absolute energies (a.u.) for PNPCC, Diethyl Ether, THF, PNPCC:Ether (8), and PNPCC:THF (9) (PBE/6-311+G(d)). Electronic excitation energies (eV, nm) and oscillator strengths for PNPCC, PNPCC:Ether, and PNPCC:THF (B3LYP/6-311+G(d)//PBE/6-311+G(d) with CPCM solvent correction).

PNPCC, *p*-nitrophenylchlorocarbene

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0 1

C	0	-1.45729	0.	-0.62848
C	0	-1.47648	0.	0.76641
C	0	-0.25301	0.	1.43795
C	0	0.98066	0.	0.77104
C	0	0.98498	0.	-0.61817
C	0	-0.23416	0.	-1.34695
H	0	-2.38636	0.	-1.20403
H	0	-2.40777	0.	1.3343
H	0	1.90411	0.	1.35248
H	0	1.93506	0.	-1.15791
C	0	-0.44089	0.	-2.8002
N	0	-0.25616	0.	2.93425
O	0	0.83911	0.	3.50092
O	0	-1.35333	0.	3.49631
Cl	0	1.07288	0.	-3.66659

SCF Done: E(RPBE-PBE) = -933.761161706 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -933.667716
Sum of electronic and thermal Energies= -933.658133
Sum of electronic and thermal Enthalpies= -933.657189
Sum of electronic and thermal Free Energies= -933.704765

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A" 1.4749 eV 840.66 nm f=0.0017
43 -> 44 0.62867
43 -> 45 -0.12412

Excited State 2: Singlet-A" 3.2718 eV 378.95 nm f=0.0022
43 -> 44 0.18270
43 -> 45 0.66582

Excited State 3: Singlet-A' 3.4110 eV 363.48 nm f=0.0399
41 -> 46 0.12802
42 -> 44 0.66992

Excited State 4: Singlet-A" 3.5693 eV 347.36 nm f=0.0000

40 -> 44 0.62759
40 -> 45 0.27720

Excited State 5: Singlet-A' 3.9117 eV 316.95 nm f=0.6022
41 -> 44 0.64794

Excited State 6: Singlet-A" 3.9919 eV 310.59 nm f=0.0001
39 -> 44 0.63901
39 -> 45 0.26136

Excited State 7: Singlet-A" 4.4058 eV 281.41 nm f=0.0000
43 -> 46 0.70327

Excited State 8: Singlet-A" 4.5717 eV 271.20 nm f=0.0005
37 -> 44 0.66836
37 -> 45 -0.13379
40 -> 45 -0.10495

Excited State 9: Singlet-A' 4.6921 eV 264.24 nm f=0.0100
42 -> 45 0.69347

Diethyl Ether

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0 1
C,0,-0.4653910767,-0.0123399454,1.3353478895
O,0,-0.6683116749,-0.0042922361,-0.0776036407
C,0,0.446904268,-0.4812944465,-0.8284503053
H,0,-1.470183106,0.126604454,1.7648908293
H,0,1.3118339755,0.2047083335,-0.7283474768
H,0,-0.1036972874,-1.012816176,1.6537906914
H,0,0.7643209849,-1.4703700833,-0.4340252053
C,0,0.0308957818,-0.5922482229,-2.2844472861
H,0,-0.2781836702,0.3880029157,-2.6778068611
H,0,0.8689548805,-0.9596979635,-2.8974440407
H,0,-0.8135074634,-1.2886070332,-2.3979973815
C,0,0.4753434598,1.0793112131,1.8422288589
H,0,1.5098657387,0.9377623791,1.4935864098
H,0,0.132713594,2.0721420099,1.5117672688
H,0,0.4978611552,1.0760374631,2.9443399492

SCF Done: E(RPBE-PBE) = -233.401209348 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -233.268276

Sum of electronic and thermal Energies= -233.261381
Sum of electronic and thermal Enthalpies= -233.260437
Sum of electronic and thermal Free Energies= -233.298622

THF
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0 1
C,0,-1.1323331456,-0.4694101337,0.1622201147
O,0,0.0010436696,-1.2092919547,-0.3017050213
C,0,1.1338470222,-0.4671545216,0.1601586018
C,0,0.7759475831,1.0187656388,-0.0505972952
C,0,-0.7785803917,1.0164505506,-0.0533056165
H,0,-2.0080756165,-0.8147447946,-0.4053919797
H,0,-1.3036675648,-0.6820177054,1.2384381123
H,0,1.3092529464,-0.6818775946,1.2352658314
H,0,2.0086707767,-0.8089304012,-0.4110189632
H,0,1.1975702958,1.656390684,0.7412013151
H,0,1.1684446676,1.3827294772,-1.0117625944
H,0,-1.205226556,1.6565205078,0.733821765
H,0,-1.1686047143,1.3743562597,-1.0177681449

SCF Done: E(RPBE-PBE) = -232.204704777 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -232.090936
Sum of electronic and thermal Energies= -232.085945
Sum of electronic and thermal Enthalpies= -232.085001
Sum of electronic and thermal Free Energies= -232.119552

PNPCC:Ether ylide, 8
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0 1
C,0,2.2639568319,-0.7000933003,1.6358529739
O,0,2.1646691172,-0.6184295093,0.0964728533
C,0,3.3815041201,-1.0526075581,-0.6521040978
H,0,1.2787990267,-0.3263491156,1.9383663933
H,0,3.9956970814,-0.1518391384,-0.7922180528
C,0,1.3663636967,0.4088634537,-0.5744335546
C,0,-0.0304884237,0.2679215919,-0.318403351
C,0,-0.6091694288,-1.0140553831,-0.0442139999
C,0,-0.9312979721,1.3718075186,-0.4328564617
C,0,-1.9768012454,-1.1752965551,0.1040034185
H,0,0.0346422103,-1.8941720542,0.0304659669

C,0,-2.2994094413,1.2056876315,-0.2922292532
H,0,-0.5319909826,2.3669114719,-0.6372352824
C,0,-2.8313959103,-0.0665518762,-0.0200127567
H,0,-2.4089945107,-2.1550642837,0.3150116468
H,0,-2.9785282559,2.0559133651,-0.3760311168
N,0,-4.2629398346,-0.2363855175,0.1446183891
O,0,-4.9907837745,0.7676064203,0.0249901035
O,0,-4.6926363878,-1.378900741,0.3991913463
Cl,0,2.1290237388,2.0183983615,-0.3536051638
H,0,2.319573049,-1.7813200284,1.8257995621
H,0,3.890640954,-1.7452747653,0.0329243586
C,0,2.9808097437,-1.7097201722,-1.9493182651
H,0,2.4046918936,-1.0136265789,-2.5730502341
H,0,3.8963938301,-1.9963206831,-2.4913422285
H,0,2.3841911612,-2.6175569274,-1.7785032866
C,0,3.4172505386,0.0729660337,2.2280284765
H,0,4.3973237108,-0.2855087105,1.8802611577
H,0,3.3374903793,1.1487444405,2.0327063732
H,0,3.3893190405,-0.0783481818,3.3206906059

SCF Done: E(RPBE-PBE) = -1167.17887663 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -1166.949097
Sum of electronic and thermal Energies= -1166.931987
Sum of electronic and thermal Enthalpies= -1166.931043
Sum of electronic and thermal Free Energies= -1166.995181

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8023 eV 442.44 nm f=0.5307
64 -> 65 0.58113

Excited State 2: Singlet-A 3.7706 eV 328.82 nm f=0.0025
63 -> 65 0.16253
64 -> 66 0.66927

Excited State 3: Singlet-A 3.9168 eV 316.54 nm f=0.0000
61 -> 65 0.68099

PNPCC:THF ylide, 9

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0 1
C,0,2.3025495253,0.0220976583,-1.5444474548
O,0,2.1701745375,0.0123188115,-0.0010461098

C,0,3.5378286504,0.0872804004,0.6151820553
C,0,4.4916991907,0.1164007323,-0.5701351045
C,0,3.6486926794,0.6769113722,-1.7354164104
H,0,2.2598273682,-1.0337879914,-1.8431227784
H,0,1.4207243978,0.5746179899,-1.8851042802
H,0,3.5226741828,1.0094559686,1.2105013889
H,0,3.6257420725,-0.7884503134,1.2666350758
H,0,5.3751791832,0.7354126756,-0.3592875833
H,0,4.8377830452,-0.9014885177,-0.8069384881
H,0,3.5633422548,1.7732947223,-1.6726608326
H,0,4.0838043166,0.4272775923,-2.714977362
C,0,1.1762474409,-0.7967005182,0.6971358181
C,0,-0.1515914281,-0.3118387513,0.4712281038
C,0,-0.3935316505,1.0829227555,0.2598666549
C,0,-1.2941279374,-1.1620227312,0.5617249367
C,0,-1.6792510088,1.5856218736,0.1449055269
H,0,0.4496677792,1.7776921518,0.2196541625
C,0,-2.5801644867,-0.6563131965,0.4531740022
H,0,-1.1514112266,-2.2329850441,0.7178333569
C,0,-2.7803567116,0.7179942843,0.2408576085
H,0,-1.8568077672,2.6503721867,-0.0160194311
H,0,-3.4487272226,-1.3141105846,0.5160896447
N,0,-4.1276978968,1.2454907236,0.1124066583
O,0,-5.0808117428,0.4497777446,0.2074468989
O,0,-4.2610129121,2.4682831813,-0.088751811
Cl,0,1.5245483678,-2.5301704163,0.3573473103

SCF Done: E(RPBE-PBE) = -1165.98822253 A.U. after 2 cycles
Sum of electronic and zero-point Energies= -1165.777413
Sum of electronic and thermal Energies= -1165.762417
Sum of electronic and thermal Enthalpies= -1165.761473
Sum of electronic and thermal Free Energies= -1165.821010

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5643 eV 483.50 nm f=0.6547
63 -> 64 -0.60815

Excited State 2: Singlet-A 3.8113 eV 325.31 nm f=0.0015
62 -> 64 -0.28863
63 -> 65 -0.63371

Excited State 3: Singlet-A 3.9382 eV 314.83 nm f=0.0003
60 -> 64 0.67835

4. Optimized geometries (Å) and absolute energies (a.u.) for Anisole and PNPCC:Anisole complexes 10a-10c. Electronic excitation energies (eV, nm) and oscillator strengths for PNPCC:Anisole complexes 10a-10c (B3LYP/6-311+G(d)//PBE/6-311+G(d) with CPCM solvent correction)

Anisole
---
0 1
C,0,-0.3530704728,0.0000013347,-1.0046618898
C,0,-0.3535161077,0.0000005689,0.39976568
C,0,0.8668498711,-0.0000010482,1.100080868
C,0,2.0722502102,-0.000001794,0.400007232
C,0,2.0832912361,-0.000001154,-1.0034044949
C,0,0.869077304,0.0000004536,-1.6935819158
H,0,-1.2874898316,0.0000028229,-1.5692574237
H,0,0.8421145636,-0.000001619,2.1928695025
H,0,3.0143193177,-0.0000030456,0.9560167895
H,0,3.0301534646,-0.000001991,-1.5493853301
H,0,0.860739334,0.0000009779,-2.7876114658
O,0,-1.4836860093,0.0000016197,1.1769285121
C,0,-2.7429449177,0.0000000564,0.5120722941
H,0,-3.4988745071,-0.0000005814,1.3066919223
H,0,-2.8715499203,0.900890242,-0.1132093499
H,0,-2.8715470862,-0.9008902668,-0.1132093834

SCF Done: E(RPBE-PBE) = -346.410850929 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -346.281723
Sum of electronic and thermal Energies= -346.274656
Sum of electronic and thermal Enthalpies= -346.273711
Sum of electronic and thermal Free Energies= -346.312895

***p*-Nitrophenylchlorocarbene:Anisole complex, 10a**
---
0 1
O,0,-1.7008289048,-0.6666374495,1.1106952943
C,0,-2.5539413781,-1.4781321709,1.9846488104
H,0,-3.1628688037,-2.1602660001,1.3783415469
H,0,-1.8605000544,-2.0439360375,2.6124891258
H,0,-3.1707683118,-0.7810383451,2.5649719414
C,0,-0.7070146271,-1.6227756554,0.2938985842
Cl,0,-1.5678136315,-2.107142348,-1.1883156416
C,0,-1.6376423493,1.6400518045,0.3692961383
C,0,-2.2214287778,2.7206721958,-0.3016581516
C,0,-3.4914741719,2.5967322677,-0.8780659281

C,0,-4.1837868303,1.3837628902,-0.7930596322
C,0,-3.6141585392,0.286633108,-0.135280107
C,0,-2.3554282906,0.4477452513,0.4419113362
H,0,-0.6480776257,1.7189056117,0.8199985998
H,0,-1.6762158965,3.6656429165,-0.3656185917
H,0,-3.9413960507,3.4468152201,-1.3970389791
H,0,-5.1711087858,1.2787558943,-1.2499714811
H,0,-4.1431429555,-0.6660916067,-0.087137225
C,0,0.5573644884,-0.9475044007,0.1399276037
C,0,1.3803601603,-1.157562994,-1.0033479983
C,0,1.1223117891,-0.2039091184,1.2221355595
C,0,2.674266573,-0.6563442822,-1.0642623272
H,0,0.9869306874,-1.7226342014,-1.8500102734
C,0,2.4060689819,0.3107403786,1.1558048691
H,0,0.5385686053,-0.0527979165,2.1338656933
C,0,3.1879833651,0.0840946033,0.0092386329
H,0,3.2951949743,-0.8105062748,-1.9484373578
H,0,2.8305030647,0.8808745335,1.9839407025
N,0,4.5377309877,0.6287034396,-0.0637456192
O,0,5.2110708372,0.3872813108,-1.0810163677
O,0,4.9435972692,1.3095497359,0.8959544735

SCF Done: E(RPBE-PBE) = -1280.17262887 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -1279.947699
Sum of electronic and thermal Energies= -1279.929949
Sum of electronic and thermal Enthalpies= -1279.929005
Sum of electronic and thermal Free Energies= -1279.995354

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4860 eV 498.73 nm f=0.5316
72 -> 73 0.61736

Excited State 2: Singlet-A 3.6121 eV 343.25 nm f=0.0261
72 -> 74 0.66678
72 -> 76 0.11703

Excited State 3: Singlet-A 3.8051 eV 325.84 nm f=0.0066
69 -> 73 0.13767
71 -> 73 0.59754
72 -> 74 0.10656
72 -> 76 -0.30651

Excited State 4: Singlet-A 3.8943 eV 318.37 nm f=0.0001
67 -> 73 0.67607

Excited State 5: Singlet-A 3.9281 eV 315.63 nm f=0.0065
72 -> 75 0.69949

Excited State 6: Singlet-A 3.9939 eV 310.43 nm f=0.0309
71 -> 73 0.29322
72 -> 76 0.59956

***p*-Nitrophenylchlorocarbene:Anisole complex, 10b**

---

0 1
C,0,-1.0257773611,1.773747474,-1.2809094302
C,0,-2.1591032538,1.2117047693,-0.6623694747
C,0,-2.5714254165,1.6809764289,0.5969054798
C,0,-1.8434749118,2.7030920141,1.2242104057
C,0,-0.7164738059,3.2629270304,0.6149941444
C,0,-0.3148563524,2.7908253966,-0.6446275386
H,0,-0.7263316606,1.398884872,-2.2631822284
H,0,-3.4445587229,1.2583020141,1.0970572813
H,0,-2.1727219828,3.0632694347,2.2034586198
H,0,-0.1609866006,4.0646876965,1.1085272968
H,0,0.5604722153,3.2224114285,-1.1390030542
C,0,-4.00208296,-0.3124101639,-0.830581996
H,0,-4.3438153074,-1.0555092364,-1.5608616753
H,0,-3.8423808106,-0.8059182685,0.142595614
H,0,-4.7624286979,0.4808853855,-0.7286845839
C,0,4.0592713478,-0.4424334051,-0.3568980417
O,0,-2.781285525,0.2115950744,-1.3604371529
Cl,0,4.3680880097,1.2482571775,-0.0681946887
C,0,2.6732652282,-0.7968012013,-0.0707003626
C,0,2.2892050729,-2.0455085548,-0.6297740037
C,0,1.7393058285,-0.0907372076,0.7341023089
C,0,1.0037206789,-2.5479486917,-0.4470039744
H,0,3.0290911957,-2.5944556019,-1.2175253475
C,0,0.4705264734,-0.6075866454,0.9667115295
H,0,2.0224108344,0.866133876,1.1778930495
C,0,0.1230868742,-1.8237572962,0.3627964506
H,0,0.6806152156,-3.4896540894,-0.8925159532
H,0,-0.2608775174,-0.0783280364,1.5792729449
N,0,-1.2421013644,-2.3683987676,0.5931736589
O,0,-1.5913169126,-3.3403930958,-0.0828806018
O,0,-1.938947491,-1.8098057041,1.4481838985

SCF Done: E(RPBE-PBE) = -1280.17834016 A.U. after 3 cycles
Sum of electronic and zero-point Energies= -1279.954886
Sum of electronic and thermal Energies= -1279.936006
Sum of electronic and thermal Enthalpies= -1279.935061
Sum of electronic and thermal Free Energies= -1280.008131

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.6809 eV 737.60 nm f=0.0079
71 -> 73 0.62631
71 -> 74 0.14408

Excited State 2: Singlet-A 1.8123 eV 684.12 nm f=0.0055
72 -> 73 0.70301

Excited State 3: Singlet-A 2.5974 eV 477.34 nm f=0.0038
70 -> 73 0.70463

Excited State 4: Singlet-A 3.1328 eV 395.77 nm f=0.0095
72 -> 74 0.70336

Excited State 5: Singlet-A 3.2451 eV 382.07 nm f=0.0331
68 -> 75 0.11286
69 -> 73 0.66581

Excited State 6: Singlet-A 3.3405 eV 371.15 nm f=0.0168
71 -> 73 -0.19618
71 -> 74 0.65393

Excited State 7: Singlet-A 3.6031 eV 344.11 nm f=0.1119
66 -> 73 0.43618
66 -> 74 -0.20022
67 -> 73 -0.23950
67 -> 74 0.10777
68 -> 73 0.38944

Excited State 8: Singlet-A 3.8192 eV 324.64 nm f=0.3886
66 -> 73 -0.33105
66 -> 74 0.13810
67 -> 73 0.16097
68 -> 73 0.51285

Excited State 9: Singlet-A 3.9272 eV 315.71 nm f=0.0060
70 -> 74 0.69637

Excited State 10: Singlet-A 4.0927 eV 302.94 nm f=0.0029
64 -> 73 0.59173
64 -> 74 -0.24707
66 -> 73 -0.10983
67 -> 73 -0.21127

***p*-Nitrophenylchlorocarbene:Anisole complex, 10c**

---

0 1
C,0,2.7879203867,1.0105566796,0.1207932467
C,0,2.4638176153,1.7911999813,-1.0074076536
C,0,1.3355048709,2.6077222781,-0.9885156389
C,0,0.5127823066,2.6671244427,0.1507248651
C,0,0.8395570782,1.8957854649,1.2675351072
C,0,1.9661456881,1.0596805493,1.262991106
H,0,1.0952027986,3.2111246543,-1.8689538321
H,0,-0.3670378518,3.3156104887,0.1629438529
H,0,0.2118035097,1.9343445042,2.1626689482
H,0,2.1958349227,0.4598638164,2.1444046062
C,0,0.9981523019,-1.9171143576,0.3280062133
H,0,3.116637932,1.7395881791,-1.8826752307
C,0,-0.325365022,-1.3436825282,0.1073401184
C,0,-0.7693711578,-0.6253932714,-1.0339324819
C,0,-1.205444534,-1.4832662004,1.2126550343
C,0,-2.046972792,-0.0792741593,-1.0735193788
H,0,-0.0873950737,-0.4765586998,-1.8736575295
C,0,-2.5038605434,-0.9840040997,1.1625172587
H,0,-0.8417709549,-2.0061866331,2.100802529
C,0,-2.8997613241,-0.2813177822,0.0192254738
H,0,-2.4020286699,0.4919461595,-1.9326924216
H,0,-3.202795807,-1.106102457,1.9910439388
N,0,-4.2721847631,0.2931659803,-0.0289638751
O,0,-5.0116639716,0.0807974016,0.9370987399
O,0,-4.5816570452,0.943899738,-1.0320239548
Cl,0,1.7768054771,-2.3248562735,-1.1784590716
O,0,3.9116929682,0.2453411541,0.0082090611
C,0,4.2452282116,-0.6104292794,1.1067717373
H,0,3.4277814737,-1.3223765285,1.3115874849
H,0,5.1434780457,-1.1542720256,0.7911802872
H,0,4.4729157782,-0.0224193264,2.0125178952

SCF Done: E(RPBE-PBE) = -1280.17873446 A.U. after 2 cycles
Sum of electronic and zero-point Energies= -1279.955299
Sum of electronic and thermal Energies= -1279.936537
Sum of electronic and thermal Enthalpies= -1279.935593
Sum of electronic and thermal Free Energies= -1280.007119

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.6356 eV 758.02 nm f=0.0216
71 -> 73 -0.38013
72 -> 73 -0.51223
Excited State 2: Singlet-A 1.9423 eV 638.32 nm f=0.0381
71 -> 73 -0.50320
72 -> 73 0.45263

Excited State 3: Singlet-A 2.6226 eV 472.75 nm f=0.0379
70 -> 73 -0.69550

Excited State 4: Singlet-A 3.0494 eV 406.58 nm f=0.0148
71 -> 74 0.12935
72 -> 74 0.67651

Excited State 5: Singlet-A 3.2587 eV 380.48 nm f=0.0291
68 -> 75 0.10476
69 -> 73 -0.66361

Excited State 6: Singlet-A 3.3972 eV 364.96 nm f=0.0166
71 -> 73 0.16130
71 -> 74 -0.64369
72 -> 74 0.16266

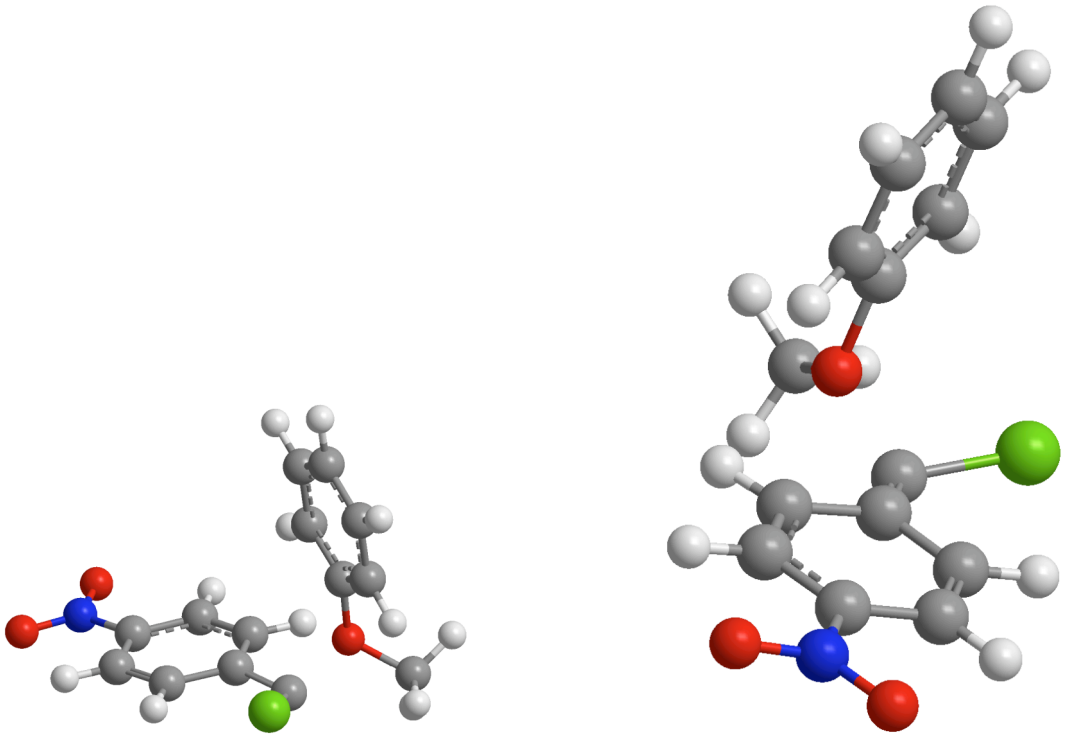
Excited State 7: Singlet-A 3.6728 eV 337.58 nm f=0.0537
66 -> 73 0.18092
67 -> 73 -0.53429
67 -> 74 0.24252
68 -> 73 0.28354

Excited State 8: Singlet-A 3.7631 eV 329.48 nm f=0.3554
67 -> 73 -0.24614
67 -> 74 0.12358
68 -> 73 -0.57978

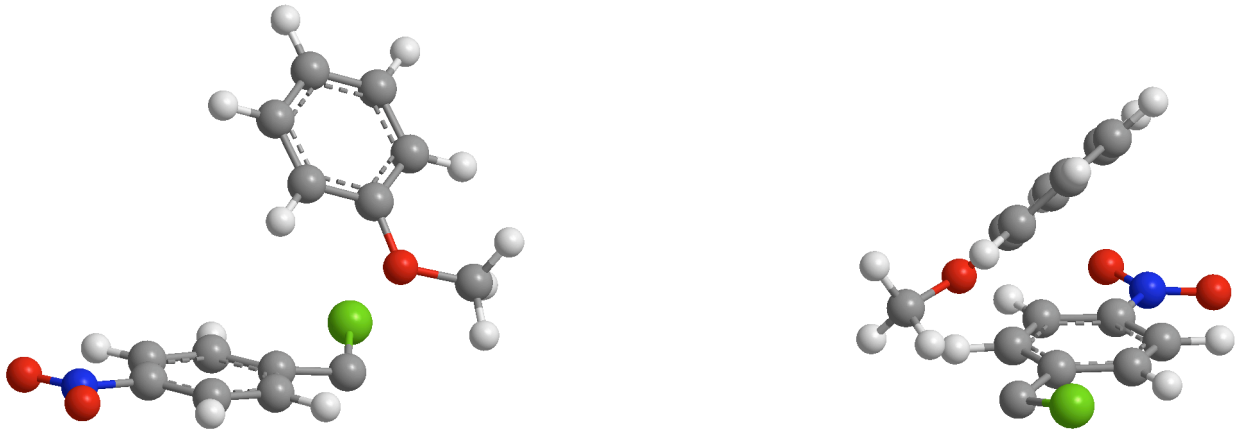
Excited State 9: Singlet-A 3.9375 eV 314.88 nm f=0.0180
70 -> 74 -0.69723

Excited State 10: Singlet-A 4.1354 eV 299.81 nm f=0.0002
64 -> 73 0.63130
64 -> 74 -0.27588

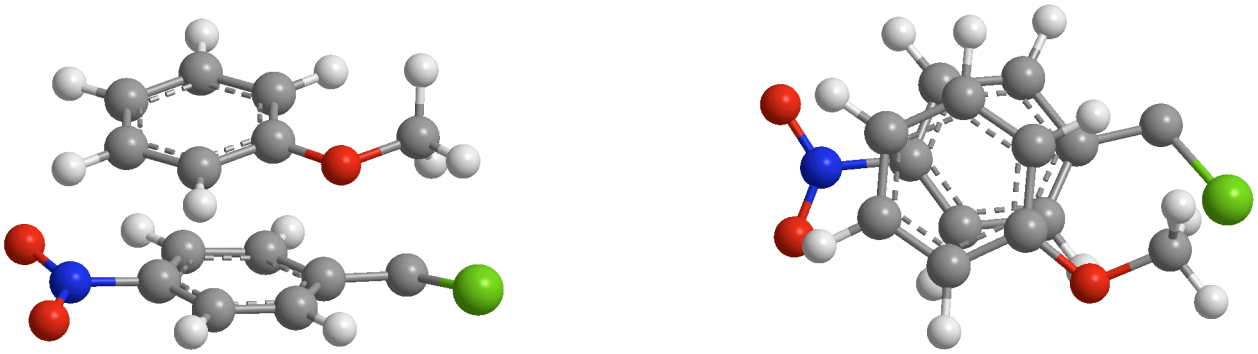
5. **Additional PNPCC:Anisole complexes; structures and energetics**



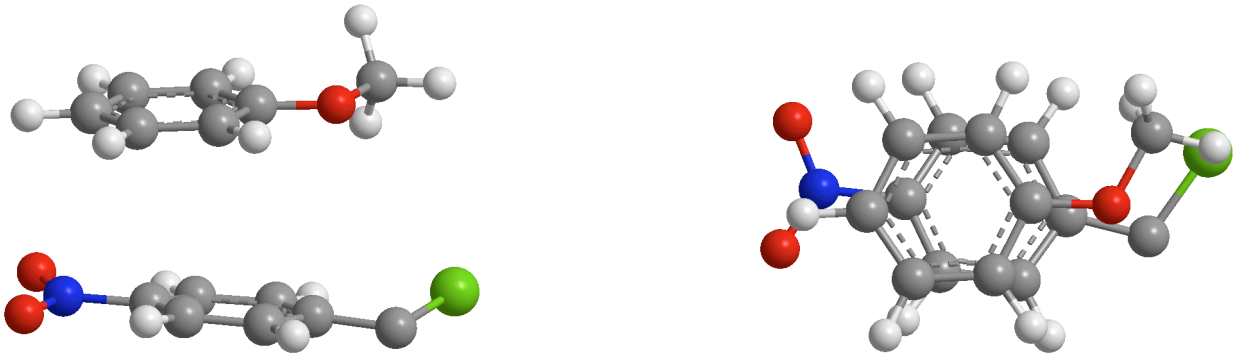
PNPCC:Anisole complex **A** (**10a**); two different side views



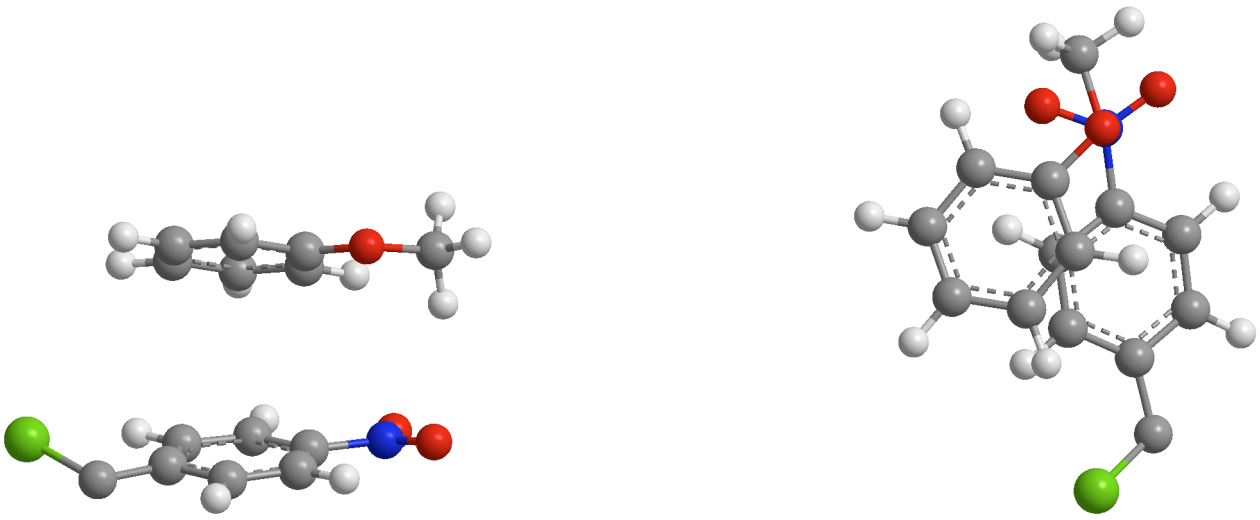
PNPCC:Anisole complex **B**; two different side views



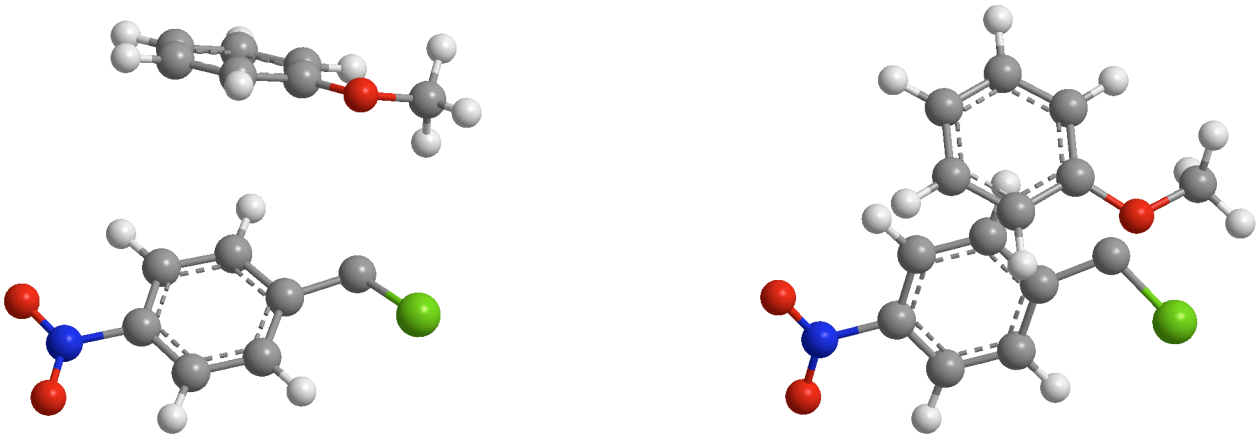
PNPCC:Anisole complex **C**; side view (left) and top view (right)



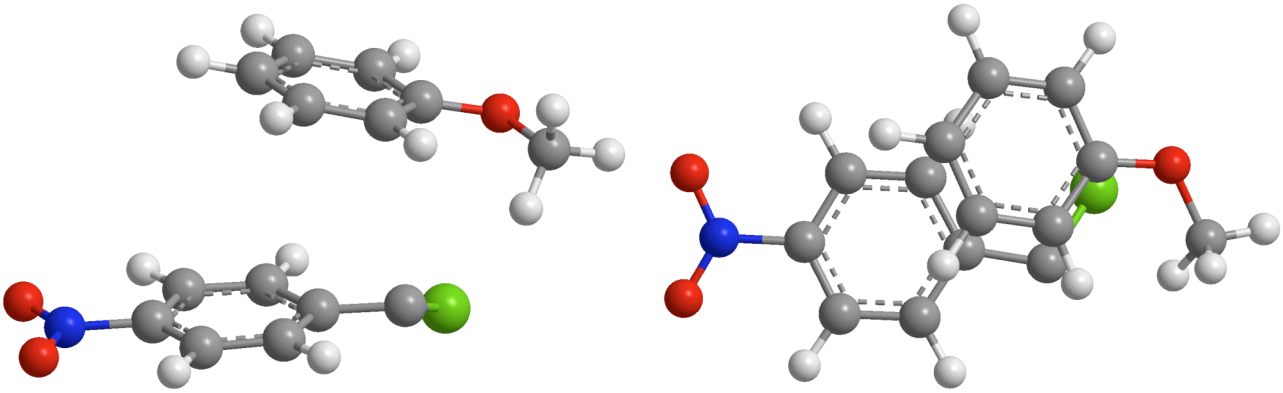
PNPCC:Anisole complex **D**; side view (left) and top view (right)



PNPCC:Anisole complex **E** (**10b**) ; side view (left) and top view (right)



PNPCC:Anisole complex **F**; side view (left) and top view (right)



PNPCC:Anisole complex **G** (**10c**); side view (left) and top view (right)

Computed energetics for 1:1 PNPCC:Anisole complex formation (PBE/6-311+G(d), kcal/mol)[a]

Structure	ΔE	ΔH^{b}	$\Delta G^{b,c}$
A 10a	-0.39	1.19	14.00
B	-3.58	-2.27	7.96
C	-3.67	-2.31	7.22
D	-3.49	-2.19	6.70
E 10b	-3.97	-2.61	5.98
F	-3.95	-2.58	4.62
G 10c	-4.20	-2.94	4.72

[a] Energies are in kcal/mol, relative to the energies of separated reactants. [b] T = 298.15 K. [c] The free energy differences were computed using a reference state of 1 M concentration for each species participating in the reaction, and T = 298.15 K.

Computed transition energies and oscillator strengths [TD-B3LYP/6-311+G(d)//PBE/6-311+G(d), CPCM model with MK radii]

Structure	Medium	λ_1	f_1	λ_2	f_2	λ_3	f_3
A 10a	THF	498.7	0.5316	343.2	0.0261	325.8	0.0066
B	THF	728.3	0.0378	582.3	0.0476	442.1	0.0098
		386.3	0.0297	372.4	0.0310	357.1	0.0381
		336.4	0.0159	325.1	0.4395	298.6	0.0002
C	THF	741.3	0.0043	699.2	0.0163	490.6	0.0009
				400.1	0.0018	381.5	0.0294
		366.0	0.0106	343.4	0.1231	321.8	0.3715
D	THF	736.0	0.0066	493.4	0.0092	404.4	0.0034
				380.2	0.0265	369.1	0.0137
		342.8	0.1416	326.3	0.2684	322.7	0.0499
E 10b	THF	737.6	0.0079	684.1	0.0055	477.3	0.0038
				395.8	0.0095	382.1	0.0331
		371.2	0.0168	344.1	0.1119	324.6	0.3886
F	THF	776.9	0.0039	676.4	0.0024	469.4	0.0089
		391.9	0.0030	379.9	0.0346	368.6	0.0103
		337.6	0.0223	325.9	0.4932	307.1	0.0067
G 10c	THF	758.0	0.0216	638.3	0.0381	472.8	0.0379
		406.6	0.0148	380.5	0.0291	365.0	0.0166
		337.6	0.0537	329.5	0.3554	314.9	0.0180

6. Optimized geometries (Å) and absolute energies (a.u.) for Benzene and PNPCC:Benzene complexes 15a-15c. Electronic excitation energies (eV, nm) and oscillator strengths for PNPCC:Benzene complexes 15a-15c (B3LYP/6-311+G(d)//PBE/6-311+G(d) with CPCM solvent correction)

Benzene
---
0 1
C,0,0.1263400081,0.6813785978,1.21717622
C,0,0.7735731765,1.1653887623,0.0734170095
C,0,0.6467981036,0.4842803562,-1.1439952339
C,0,-0.124629779,-0.6824816715,-1.2167703067
C,0,-0.7719040029,-1.1664839871,-0.0728923888
C,0,-0.6486294453,-0.4831467194,1.1434759414
H,0,0.2213674183,1.2155156147,2.1671919796
H,0,1.377702894,2.0756703637,0.1302584055
H,0,1.1519176193,0.8627853835,-2.0375159153
H,0,-0.2224620545,-1.2150267229,-2.1673734845
H,0,-1.3774649091,-2.0758097622,-0.1303146437
H,0,-1.1603493346,-0.8567469067,2.0352862092

SCF Done: E(RPBE-PBE) = -231.984325914 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -231.886800
Sum of electronic and thermal Energies= -231.882258
Sum of electronic and thermal Enthalpies= -231.881314
Sum of electronic and thermal Free Energies= -231.914341

PNPCC:Benzene complex, 15a
---
0 1
C,0,-1.4307362118,1.6770190763,1.6217073106
C,0,-0.5905808256,2.5437191163,0.9110745171
C,0,-0.9103689599,2.9064672563,-0.4041740002
C,0,-2.0667382352,2.3977946731,-1.0101048761
C,0,-2.9054634617,1.5280034167,-0.3004466609
C,0,-2.5890930848,1.1702811203,1.0169982202
H,0,-1.1849373267,1.399582794,2.6509925126
H,0,-0.2593810984,3.5912695585,-0.9560465226
H,0,-2.318677913,2.6840383139,-2.0356469603
H,0,-3.8080377688,1.1305157249,-0.773225577
H,0,-3.248672799,0.4980241571,1.5736589362
C,0,3.4076420763,-0.1980996997,0.7670041852
H,0,0.3118529548,2.9409911884,1.384897201
C,0,2.0885202334,-0.6303827041,0.3140878579
C,0,1.3847157997,-0.2289480137,-0.8530184453

C,0,1.4459734044,-1.502298577,1.2330998615
C,0,0.0967388585,-0.6875833347,-1.0972625908
H,0,1.8578719479,0.4601644992,-1.5561327494
C,0,0.1635903448,-1.9867607158,0.9880468108
H,0,1.9895028114,-1.7819344567,2.1391717742
C,0,-0.4884572713,-1.562743086,-0.1732617922
H,0,-0.4677356141,-0.3804883205,-1.9785087759
H,0,-0.34480606,-2.6586923282,1.6807554463
N,0,-1.8741387197,-2.0451396827,-0.4310850214
O,0,-2.4660161704,-2.5911852245,0.5045617036
O,0,-2.336794298,-1.8647189815,-1.5603101363
Cl,0,4.3164717441,0.5600546546,-0.5146373565

SCF Done: E(RPBE-PBE) = -1165.74977145 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -1165.558080
Sum of electronic and thermal Energies= -1165.542611
Sum of electronic and thermal Enthalpies= -1165.541667
Sum of electronic and thermal Free Energies= -1165.605519

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.5216 eV 814.85 nm f=0.0067
64 -> 65 0.62469
64 -> 66 -0.13115

Excited State 2: Singlet-A 2.4697 eV 502.02 nm f=0.0145
62 -> 65 0.32878
63 -> 65 0.62203

Excited State 3: Singlet-A 2.4736 eV 501.22 nm f=0.0004
62 -> 65 0.62449
63 -> 65 -0.32924

Excited State 4: Singlet-A 3.2792 eV 378.10 nm f=0.0083
64 -> 65 0.18692
64 -> 66 0.66425

Excited State 5: Singlet-A 3.3814 eV 366.67 nm f=0.0314
60 -> 67 0.12004
61 -> 65 0.66922

Excited State 6: Singlet-A 3.5594 eV 348.32 nm f=0.0462
59 -> 65 -0.56531
59 -> 66 -0.26766
60 -> 65 0.26429

Excited State 7: Singlet-A 3.8290 eV 323.80 nm f=0.0010
62 -> 66 0.23786
63 -> 66 0.65944

Excited State 8: Singlet-A 3.8422 eV 322.69 nm f=0.3707
59 -> 65 0.22675
60 -> 65 0.51568
62 -> 66 0.34189

Excited State 9: Singlet-A 3.8525 eV 321.82 nm f=0.0985
59 -> 65 0.14605
60 -> 65 0.27941
62 -> 66 -0.56929
63 -> 66 0.23881

Excited State 10: Singlet-A 4.0198 eV 308.44 nm f=0.0011
58 -> 65 0.62850
58 -> 66 0.26311

Excited State 11: Singlet-A 4.4862 eV 276.37 nm f=0.0074
64 -> 67 0.70103

Excited State 12: Singlet-A 4.6349 eV 267.50 nm f=0.0050
61 -> 66 0.69265

Excited State 13: Singlet-A 4.6603 eV 266.04 nm f=0.0322
54 -> 65 -0.65737
54 -> 66 0.12634
59 -> 66 0.12780

Excited State 14: Singlet-A 4.8907 eV 253.51 nm f=0.0082
55 -> 65 0.42599
56 -> 65 -0.12645
57 -> 65 0.52124

Excited State 15: Singlet-A 4.9307 eV 251.45 nm f=0.0005
55 -> 65 0.12760
56 -> 65 0.69190

PNPCC:Benzene complex, 15b

---

0 1
C,0,-1.7643994983,-2.6861312304,-0.5764808638
C,0,-1.1249264815,-2.5489400037,0.6627875967
C,0,-1.5900772659,-1.6071442881,1.5895788359
C,0,-2.6914517428,-0.7990239239,1.2761200722
C,0,-3.3270375169,-0.932163245,0.0343889297
C,0,-2.8646327141,-1.8775436424,-0.8908390894
H,0,-1.4055117283,-3.4272323516,-1.2969729021
H,0,-1.0956918572,-1.5051680469,2.5602311423

H,0,-3.0570492726,-0.0657790159,2.0010844379
H,0,-4.1847335306,-0.2995513149,-0.2110906478
H,0,-3.366612602,-1.9866643529,-1.8568889383
C,0,3.2383303978,-0.9227155284,-0.6436193658
H,0,-0.2656601809,-3.1803932067,0.9067697404
C,0,2.1151552465,-0.0172936941,-0.420870341
C,0,1.9286619135,0.9082108606,0.6425364264
C,0,1.0777342147,-0.1766823836,-1.3764638061
C,0,0.7525483047,1.6382082095,0.7451768818
H,0,2.7132052094,1.0315148955,1.3929840332
C,0,-0.0827651342,0.5924275332,-1.3161311422
H,0,1.218441111,-0.9186950355,-2.1660882885
C,0,-0.2271825535,1.4765945808,-0.246088742
H,0,0.5749057219,2.335536262,1.5655674561
H,0,-0.8830785362,0.4927763553,-2.0496719011
N,0,-1.4844082801,2.2684354124,-0.1385190275
O,0,-2.2170579042,2.3072943494,-1.1297728416
O,0,-1.7074292709,2.8306092862,0.9380874636
Cl,0,4.6411057651,-0.4556141545,0.2809776312

SCF Done: E(RPBE-PBE) = -1165.74983157 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -1165.558047
Sum of electronic and thermal Energies= -1165.541700
Sum of electronic and thermal Enthalpies= -1165.540755
Sum of electronic and thermal Free Energies= -1165.607530

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.5308 eV 809.92 nm f=0.0068
64 -> 65 0.62511
64 -> 66 0.13172

Excited State 2: Singlet-A 2.4815 eV 499.62 nm f=0.0083
62 -> 65 0.24301
63 -> 65 0.66168

Excited State 3: Singlet-A 2.4968 eV 496.58 nm f=0.0097
62 -> 65 0.66241
63 -> 65 -0.24037

Excited State 4: Singlet-A 3.2767 eV 378.38 nm f=0.0114
64 -> 65 -0.18677
64 -> 66 0.66186

Excited State 5: Singlet-A 3.3762 eV 367.23 nm f=0.0345
60 -> 67 0.11545
61 -> 65 0.66746

Excited State 6: Singlet-A 3.5496 eV 349.29 nm f=0.0693
59 -> 65 0.50489

59 -> 66 -0.24497
60 -> 65 0.37207

Excited State 7: Singlet-A 3.8404 eV 322.84 nm f=0.0012
63 -> 66 0.70095

Excited State 8: Singlet-A 3.8593 eV 321.26 nm f=0.0345
60 -> 65 -0.16606
62 -> 66 0.67178

Excited State 9: Singlet-A 3.8975 eV 318.11 nm f=0.4240
59 -> 65 0.33974
59 -> 66 -0.12101
60 -> 65 -0.50347
62 -> 66 -0.21329

Excited State 10: Singlet-A 4.0303 eV 307.63 nm f=0.0005
57 -> 65 -0.11190
58 -> 65 0.62425
58 -> 66 -0.26336

Excited State 11: Singlet-A 4.4909 eV 276.08 nm f=0.0079
64 -> 67 0.69944

Excited State 12: Singlet-A 4.6114 eV 268.87 nm f=0.0153
54 -> 65 -0.19030
61 -> 66 0.65933

Excited State 13: Singlet-A 4.6478 eV 266.76 nm f=0.0138
54 -> 65 -0.61821
54 -> 66 -0.12373
60 -> 66 0.15887
61 -> 66 -0.20883

Excited State 14: Singlet-A 4.9000 eV 253.03 nm f=0.0079
55 -> 65 -0.42285
57 -> 65 0.53118

PNPCC:Benzene complex, 15c

---

0 1
C,0,2.9539841858,1.264613053,0.5143751409
C,0,2.7993082303,1.8605496009,-0.7442419452
C,0,1.6757405877,2.6543099114,-1.0104162952
C,0,0.7073916943,2.852803185,-0.0168209515
C,0,0.8632208439,2.2579169832,1.2419243232

C,0,1.9856412128,1.4628538859,1.507412471
H,0,3.8301032432,0.6441534947,0.7233672824
H,0,1.5572838733,3.1251824136,-1.9909586565
H,0,-0.1673033293,3.4769335342,-0.2226899128
H,0,0.1090756488,2.4165560442,2.0184479242
H,0,2.1072084906,0.9932376369,2.4875638701
C,0,1.5616236413,-2.1512015223,0.6850376995
H,0,3.558990423,1.7103343932,-1.5172404345
C,0,0.284971059,-1.5642971795,0.3012608596
C,0,-0.0069896866,-0.8410463373,-0.8857437339
C,0,-0.7150698305,-1.6690641707,1.3044351117
C,0,-1.2515349443,-0.2495889126,-1.0631970939
H,0,0.7658174074,-0.7213666802,-1.6477534521
C,0,-1.9829369466,-1.127843408,1.1114393013
H,0,-0.4645006935,-2.1936114123,2.2298624422
C,0,-2.2238702853,-0.4160214638,-0.068349935
H,0,-1.4911226995,0.3298959682,-1.9559790917
H,0,-2.7718255482,-1.2186608652,1.859157419
N,0,-3.5611390724,0.2113300764,-0.2655343338
O,0,-4.4005261228,0.0502960692,0.6253292384
O,0,-3.7413529765,0.849549625,-1.3071213658
Cl,0,2.5364941714,-2.543801904,-0.7019641029

SCF Done: E(RPBE-PBE) = -1165.74929054 A.U. after 1 cycles
Sum of electronic and zero-point Energies= -1165.557783
Sum of electronic and thermal Energies= -1165.541334
Sum of electronic and thermal Enthalpies= -1165.540390
Sum of electronic and thermal Free Energies= -1165.608595

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.5672 eV 791.13 nm f=0.0124
64 -> 65 0.61833
64 -> 66 -0.13423

Excited State 2: Singlet-A 2.4994 eV 496.05 nm f=0.0259
62 -> 65 -0.20674
63 -> 65 0.66891

Excited State 3: Singlet-A 2.5066 eV 494.62 nm f=0.0018
62 -> 65 0.67473
63 -> 65 0.20595

Excited State 4: Singlet-A 3.2608 eV 380.23 nm f=0.0180
64 -> 65 0.18962
64 -> 66 0.65812

Excited State 5: Singlet-A 3.3583 eV 369.19 nm f=0.0325
60 -> 67 0.11358

61 -> 65 0.66639

Excited State 6: Singlet-A 3.5765 eV 346.66 nm f=0.0010
59 -> 65 0.62000
59 -> 66 0.28416

Excited State 7: Singlet-A 3.7899 eV 327.14 nm f=0.4311
60 -> 65 0.63740
63 -> 66 -0.10527

Excited State 8: Singlet-A 3.8777 eV 319.74 nm f=0.0366
62 -> 66 -0.12560
63 -> 66 0.68322

Excited State 9: Singlet-A 3.9036 eV 317.62 nm f=0.0006
62 -> 66 0.69370
63 -> 66 0.12704

Excited State 10: Singlet-A 4.0265 eV 307.92 nm f=0.0001
58 -> 65 0.63417
58 -> 66 0.27245

Excited State 11: Singlet-A 4.5083 eV 275.01 nm f=0.0137
61 -> 66 0.10960
64 -> 67 0.69155

Excited State 12: Singlet-A 4.5806 eV 270.67 nm f=0.0043
61 -> 66 0.68402
64 -> 67 -0.10805

Excited State 13: Singlet-A 4.7325 eV 261.99 nm f=0.0457
54 -> 65 -0.62038
54 -> 66 0.12221
59 -> 66 -0.11268
60 -> 66 -0.21561

7. Optimized geometries and electronic excitation energies for diazoalkane isomer of diazirine 3 and PNPCC: 3 *N*-ylide

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(p-NO2Ph)C(N2)Cl diazo-alkane species

---

0 1
N,0,2.0578681621,-2.3373368565,-0.4733891146
C,0,0.8931800652,-1.8784171388,-0.8580107385
Cl,0,0.1055192707,-2.8423416566,-2.0805884838
C,0,0.3293642524,-0.6665523207,-0.2966517841
C,0,-0.9312292287,-0.1920778322,-0.7293656844
C,0,-1.4732295407,0.9710772183,-0.1910629546
C,0,-0.761969465,1.6736522896,0.7861437349
C,0,0.4881491497,1.2276881887,1.2335439995
C,0,1.0287440698,0.0670429188,0.6961330814
H,0,-1.4868616387,-0.7401254537,-1.4920064297
H,0,-2.4446192725,1.3440225609,-0.519156762
N,0,-1.3361918824,2.9053825429,1.3555813582
H,0,1.0195043827,1.7974551812,1.997168531
H,0,2.005002768,-0.2731111101,1.0515597102
N,0,3.082270142,-2.7373191557,-0.1325399846
O,0,-2.4421184487,3.2707529908,0.9359629554
O,0,-0.6769483774,3.499497175,2.2190989742

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9815 eV 625.72 nm f=0.0000
50 -> 52 0.67916

Excited State 2: Singlet-A 3.0279 eV 409.47 nm f=0.5189
50 -> 51 0.65086

Excited State 3: Singlet-A 3.7739 eV 328.53 nm f=0.0000
48 -> 51 0.67205
48 -> 53 0.14159

(pNO2-Ph)C(Cl)N=N-C(NO2Ph)(Cl), pbe/6-311+G(d) geometry

pNO2phenyl-chloro-carbene:[pNO2phenyl-chloro-diazirine] N-ylide

---

0 1
N,0,-0.0896709148,-2.2090387272,0.0065854473
N,0,0.894797138,-3.1100329762,0.0914262254
C,0,1.0188640312,-1.9019146745,0.8729418484
C,0,-1.2436069791,-1.9714576797,-0.5694134215
C,0,-2.0280406614,-0.763114308,-0.3686541221
Cl,0,-1.7849953033,-3.2482141152,-1.6238291548
Cl,0,0.6564493366,-2.0208232053,2.6371034604
C,0,-3.2425436646,-0.5720931032,-1.0685565682
C,0,-3.9987607919,0.582413133,-0.885626139
C,0,-3.5464523776,1.5600592064,0.0034339479
C,0,-2.3514120909,1.4007322186,0.714416489
C,0,-1.5994465855,0.2475511696,0.5290691614
H,0,-3.5947782053,-1.335960393,-1.7629031916
H,0,-4.9352235401,0.7354663558,-1.4237670143
H,0,-2.029143966,2.1814096595,1.4048648658
H,0,-0.6766476725,0.131156276,1.0984898533
N,0,-4.3467424489,2.7879427222,0.2004909099
O,0,-3.9119916482,3.630935806,0.9943646583
O,0,-5.3986766175,2.8931162212,-0.4407221938
C,0,1.9901294488,-0.8232587599,0.4867402937
C,0,2.5503226237,-0.8875942133,-0.8038807936
C,0,2.3547375919,0.2209634895,1.3529813586
C,0,3.4574589068,0.0818133612,-1.2281140895
H,0,2.2807639503,-1.7124713724,-1.4675905414
C,0,3.2602796237,1.1983854736,0.9356012676
H,0,1.9424518764,0.2656348963,2.3623149526
C,0,3.7967042515,1.1139057556,-0.349783788
H,0,3.9076695664,0.0467675529,-2.2210635759
H,0,3.5573923944,2.0168573088,1.5926074863
N,0,4.7654909286,2.1532180074,-0.7968920923
O,0,5.2248909917,2.046182251,-1.9372073587
O,0,5.042811543,3.0512412926,0.0027121279

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7022 eV 458.83 nm f=0.0486
93 -> 94 0.49003
93 -> 95 0.49399

Excited State 2: Singlet-A 2.9600 eV 418.87 nm f=0.5019
93 -> 94 -0.43567
93 -> 95 0.47576
93 -> 96 0.11346

Excited State 3: Singlet-A 3.7196 eV 333.33 nm f=0.0000

88 -> 94	0.54985
88 -> 95	-0.34805
88 -> 96	-0.21633