Supporting information

Role of Donor-Acceptor Orientation on Solvent-Dependent Three-Photon Activity in Through-Space Charge-Transfer Systems - Case Study of [2, 2]-Paracyclophane Derivatives

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Contents

A) Optimized Cartesian Coordinates of PCP1

i) In gas phase

Atomic Symbol	X	Y	Z
C	1.02085208	1.36653810	-0.88694507
C	1.30141810	1.47920811	0.47393604
C	0.27648302	1.19556509	1.40240111
C	-1.02072508	1.36724711	0.88605407
C	-1.30127910	1.47886111	-0.47491604
C	-0.27634702	1.19446509	-1.40314211
H	1.82649014	1.31546210	-1.60797512
H	-1.82638814	1.31666910	1.60709112
C	1.01725908	-1.87207914	-0.99937108
C	1.31544510	-1.83507514	0.37441503
C	0.33494503	-1.66698513	1.36252510
C	-1.01737008	-1.87114114	1.00070508
C	-1.31555110	-1.83523614	-0.37310803
C	-0.33502703	-1.66800613	-1.36134910
H	2.35343218	-1.85746614	0.69040105
H	-2.35354918	-1.85765414	-0.68906105
C	-0.38676803	0.52473204	-2.76804921
H	-1.10481509	1.00079807	-3.44390926
H	0.58663304	0.62169405	-3.25420125
C	-0.72973506	-1.03525808	-2.68394121
H	-1.80464014	-1.17398509	-2.83363422
H	-0.24234102	-1.48562512	-3.55055727
C	0.38690003	0.52672904	2.76775621
H	1.10499909	1.00318708	3.44328826
H	-0.58647404	0.62409605	3.25387825
C	0.72974106	-1.03334808	2.68466521
H	0.24233602	-1.48309911	3.55159327
H	1.80463814	-1.17206709	2.83440922
N	2.69177921	1.91606815	0.91695607
N	-2.69165121	1.91529614	-0.91832707
N	-2.00612415	-1.94009515	2.01348415
N	2.00596815	-1.94208515	-2.01212915
C	2.53114119	3.13373624	1.81553714
H	1.92791115	2.86768522	2.68046621
H	3.52289527	3.45761426	2.13520116
H	2.04161916	3.92187030	1.24328010
C	3.47171726	0.85171406	1.66637512
H	2.97459723	0.62795205	2.60438720
H	3.52966527	-0.03838500	1.04420108
H	4.47062934	1.24327010	1.86395014
C	3.55712127	2.35317318	-0.24887302
H	3.02787423	3.10651324	-0.83099406
H	4.47083034	2.78035721	0.16422901
H	3.80844329	1.49008012	-0.86398806
C	-3.55700027	2.35338718	0.24711702
H	-3.02779823	3.10728824	0.82855206
H	-4.47074634	2.78012121	-0.16635701
H	-3.80821429	1.49081312	0.86299706
C	-2.53104019	3.13217524	-1.81798814
H	-1.92793115	2.86535022	-2.68276321

H	-3.52281027	3.45585127	-2.13782216
H	-2.04139116	3.92077230	-1.24647909
C	-3.47155626	0.85027807	-1.66685313
H	-2.97439423	0.62570705	-2.60465420
H	-3.52955327	-0.03930400	-1.04394208
H	-4.47045734	1.24166710	-1.86481814
C	1.87179815	-3.08422523	-2.94107423
H	0.82573606	-3.26237925	-3.18792424
H	2.42006518	-2.87031822	-3.86352030
H	2.27431317	-4.00915630	-2.50088719
C	3.39733626	-1.79937014	-1.60390012
H	3.54229227	-0.85628306	-1.06374108
H	3.75990729	-2.62363620	-0.96708808
H	4.02509631	-1.77082214	-2.49888819
C	-3.39743126	-1.79742114	1.60503912
H	-3.54213327	-0.85473307	1.06410708
H	-3.76013429	-2.62211320	0.96885507
H	-4.02524231	-1.76801914	2.49996119
C	-1.87224814	-3.08149324	2.94338922
H	-0.82623606	-3.25963525	3.19047224
H	-2.42054818	-2.86672222	3.86561430
H	-2.27489517	-4.00671630	2.50393919

ii) In MeCN solvent

Atomic Symbol	X	Y	Z
C	-1.01448373	1.37756129	0.89255785
C	-1.30287658	1.49386771	-0.46517740
C	-0.28501479	1.20043148	-1.39681766
C	1.01441927	1.37748597	-0.89276768
C	1.30281074	1.49392359	0.46496756
C	0.28495010	1.20057198	1.39662303
H	-1.81548984	1.34675222	1.61905584
H	1.81541725	1.34660235	-1.61926687
C	-0.99480983	-1.89174609	1.01783198
C	-1.32242817	-1.84365142	-0.34878541
C	-0.36121410	-1.67263571	-1.35626036
C	0.99493174	-1.89175752	-1.01769687
C	1.32254628	-1.84345549	0.34891798
C	0.36131491	-1.67244670	1.35637582
H	-2.36717600	-1.83663884	-0.64149882
H	2.36729231	-1.83629729	0.64163292
C	0.40935568	0.52557146	2.75591604
H	1.12283473	1.00619007	3.43180463
H	-0.56487158	0.60636081	3.24297170
C	0.78014343	-1.02390030	2.66527127
H	1.86175407	-1.13791552	2.77865990
H	0.33021750	-1.48408691	3.54775342
C	-0.40939261	0.52525024	-2.75603010
H	-1.12287500	1.00575488	-3.43199450

H	0.56483524	0.60602852	-3.24308620
C	-0.78010213	-1.02423656	-2.66521088
H	-0.33015616	-1.48448960	-3.54764752
H	-1.86170451	-1.13834236	-2.77858507
N	-2.68049202	1.95994425	-0.89830670
N	2.68037966	1.96008603	0.89817449
N	1.96410839	-2.00263023	-2.04960771
N	-1.96398567	-2.00258697	2.04975235
C	-2.48745691	3.17713950	-1.79128717
H	-1.90759897	2.89355210	-2.66572397
H	-3.47131649	3.53668910	-2.09237550
H	-1.95954188	3.93881066	-1.21913376
C	-3.48812222	0.92082071	-1.64975357
H	-3.00706975	0.69992009	-2.59638825
H	-3.56813461	0.02445196	-1.03954334
H	-4.47844448	1.33696279	-1.83299684
C	-3.52650942	2.41796639	0.27264633
H	-2.97420008	3.15994742	0.84612796
H	-4.43082885	2.86317107	-0.13913005
H	-3.79493088	1.56507234	0.89341361
C	3.52656091	2.41812431	-0.27266150
H	2.97417028	3.15980928	-0.84644690
H	4.43061913	2.86371744	0.13926834
H	3.79544869	1.56520128	-0.89318066
C	2.48715686	3.17731351	1.79106514
H	1.90722600	2.89372639	2.66545425
H	3.47096027	3.53695034	2.09223592
H	1.95924613	3.93891247	1.21881126
C	3.48792391	0.92105048	1.64984320
H	3.00665890	0.70015498	2.59637646
H	3.56815289	0.02465224	1.03970475
H	4.47816896	1.33727623	1.83330755
C	-1.76836418	-3.14985050	2.95081347
H	-0.71656630	-3.26456745	3.21135625
H	-2.34019683	-2.99170652	3.87107123
H	-2.10838117	-4.09238223	2.48949077
C	-3.36746331	-1.90673763	1.66774443
H	-3.56502965	-0.96854109	1.14410274
H	-3.70546457	-2.74039743	1.02800051
H	-3.97647631	-1.91397620	2.57636805
C	3.36758196	-1.90661896	-1.66764030
H	3.56505107	-0.96835008	-1.14409635
H	3.70567346	-2.74017850	-1.02781566
H	3.97658295	-1.91388682	-2.57627193
C	1.76857815	-3.14996512	-2.95059651
H	0.71677566	-3.26484620	-3.21104713
H	2.34031689	-2.99179083	-3.87090728
H	2.10876316	-4.09242441	-2.48925072

iii) In THF solvent

Atomic Symbol	X	Y	Z

C	-1.01311172	1.38647921	0.89386693
C	-1.30479150	1.49844598	-0.46358307
C	-0.28731679	1.20930969	-1.39712305
C	1.01293349	1.38643834	-0.89414733
C	1.30460209	1.49869389	0.46327313
C	0.28715383	1.20961635	1.39687262
H	-1.81209678	1.35573471	1.62225888
H	1.81190515	1.35568862	-1.62254986
C	-1.00023311	-1.88375544	1.01315184
C	-1.32006649	-1.83618150	-0.35536427
C	-0.35395434	-1.66372510	-1.35776486
C	1.00048363	-1.88387936	-1.01281541
C	1.32031065	-1.83596266	0.35569150
C	0.35417978	-1.66339792	1.35805356
H	-2.36285284	-1.83759697	-0.65503596
H	2.36309462	-1.83721203	0.65537042
C	0.40953208	0.53678648	2.75746722
H	1.12783860	1.01401837	3.43088538
H	-0.56260923	0.62667112	3.24696762
C	0.76727842	-1.01704672	2.66972186
H	1.84681569	-1.13961470	2.79374233
H	0.30504354	-1.47214628	3.54816209
C	-0.40959884	0.53620780	-2.75759156
H	-1.12797479	1.01320703	-3.43109900
H	0.56252960	0.62614231	-3.24710949
C	-0.76712574	-1.01766351	-2.66955577
H	-0.30481726	-1.47285678	-3.54790730
H	-1.84664414	-1.14040086	-2.79356864
N	-2.68988467	1.94888653	-0.89421340
N	2.68963555	1.94938617	0.89384851
N	1.97463813	-1.99666940	-2.03900807
N	-1.97437670	-1.99636218	2.03937222
C	-2.51482092	3.16973069	-1.78583719
H	-1.92417090	2.89668648	-2.65656582
H	-3.50280186	3.51223206	-2.09404170
H	-2.00605476	3.94223794	-1.21077661
C	-3.48590065	0.90161466	-1.64810024
H	-3.00205831	0.68847761	-2.59514373
H	-3.55525885	0.00244240	-1.04076986
H	-4.48118352	1.30683521	-1.82965403
C	-3.54079022	2.39277386	0.27881658
H	-2.99892623	3.14340346	0.85138396
H	-4.45343984	2.82330504	-0.13043010
H	-3.79422317	1.53535206	0.90038729
C	3.54051882	2.39328514	-0.27919017
H	2.99855496	3.14374611	-0.85188243
H	4.45306447	2.82404011	0.13005761
H	3.79415679	1.53583261	-0.90064214
C	2.51437864	3.17028760	1.78534628
H	1.92379994	2.89722388	2.65611690
H	3.50230793	3.51298938	2.09349059
H	2.00545897	3.94264710	1.21022226

C	3.48580344	0.90232547	1.64787169
H	3.00202617	0.68927658	2.59496787
H	3.55524841	0.00306937	1.04067641
H	4.48104328	1.30770169	1.82932264
C	-1.78134668	-3.14178753	2.94490232
H	-0.73053211	-3.25556546	3.20926056
H	-2.35670485	-2.98097795	3.86236235
H	-2.11885545	-4.08494952	2.48435232
C	-3.37543446	-1.90647559	1.64790449
H	-3.57229375	-0.96683320	1.12540119
H	-3.70570427	-2.73926785	1.00341561
H	-3.99113780	-1.91881266	2.55181021
C	3.37568994	-1.90662987	-1.64756635
H	3.57251740	-0.96686476	-1.12527602
H	3.70599848	-2.73926340	-1.00289076
H	3.99139371	-1.91914896	-2.55147079
C	1.78167803	-3.14230758	-2.94428162
H	0.73086663	-3.25624668	-3.20857713
H	2.35699086	-2.98164893	-3.86179648
H	2.11929107	-4.08533644	-2.48353607

B) Optimized Coordinates of PCP2

i) In Gas phase

Atomic Symbol	X	Y	Z
C	-0.79892606	1.39593211	1.19147109
C	0.60968305	1.30959010	1.26335310
C	1.25272410	1.63593212	0.05403600
C	0.54371004	1.47755812	-1.13992709
C	-0.83001907	1.20771909	-1.21033409
C	-1.51962911	1.44791911	0.00261800
H	-1.31877610	1.33272910	2.13842317
H	1.08063308	1.47889611	-2.08243316
C	-0.34809803	-1.76849614	1.27057010
C	1.01993808	-1.54212312	1.09084808
C	1.56807612	-1.79974214	-0.19177001
C	0.66743905	-1.78666814	-1.27291210
C	-0.71615806	-1.66697613	-1.10122708
C	-1.24133910	-1.90038015	0.19605101
H	-0.73213705	-1.74267213	2.28501517
H	1.04946608	-1.78149614	-2.28832117
C	-1.32482410	0.48194704	-2.45544719
H	-2.23703517	0.90494707	-2.88794722
H	-0.55721604	0.60822505	-3.22408125
C	-1.55198112	-1.08720208	-2.23178917
H	-2.61274020	-1.25713910	-2.05146816
H	-1.31809610	-1.56471912	-3.18962325
C	1.79334214	-0.80973206	2.17791017
H	1.81775814	-1.35597510	3.12885824

H	2.83422322	-0.68908605	1.86615314
C	1.18325209	0.61663105	2.50124319
H	1.92627115	1.19846709	3.05083323
H	0.34952403	0.48258404	3.19603424
N	-3.00155123	1.78368014	0.03117000
N	2.68181120	2.13828616	-0.07102901
N	2.97250023	-1.93304915	-0.36616903
N	-2.63574420	-2.13012616	0.38524503
C	3.55535227	1.22123609	-0.90988907
H	3.52800827	0.21431602	-0.48097404
H	3.18188124	1.20873409	-1.93235015
H	4.56809335	1.62775412	-0.90317207
C	2.62557320	3.50912127	-0.73122405
H	2.03915115	4.17558732	-0.09794801
H	3.64652028	3.88059630	-0.83109306
H	2.16499317	3.42308826	-1.71329413
C	3.37906426	2.33829318	1.25541909
H	4.31908833	2.85330722	1.05678108
H	2.75219921	2.95096323	1.90142914
H	3.58663327	1.37090510	1.70478113
C	-3.50560627	2.05457416	1.43305111
H	-2.89335022	2.82379921	1.90174414
H	-4.53287434	2.40831118	1.34885810
H	-3.48731827	1.13006809	2.00933215
C	-3.19045924	3.06764623	-0.76212106
H	-2.61454720	3.86164329	-0.28581202
H	-2.84163022	2.90986222	-1.78104014
H	-4.25289432	3.31689425	-0.76332006
C	-3.10452824	-2.16436816	1.77281114
H	-4.18981832	-2.29573217	1.77261714
H	-2.66514720	-2.98784823	2.35709318
H	-2.87404722	-1.22339309	2.28498518
C	-3.15086324	-3.31616425	-0.33853103
H	-4.24454232	-3.29511325	-0.33040803
H	-2.81104622	-3.31777325	-1.37399011
H	-2.81445921	-4.25076632	0.13331801
C	3.43712526	-2.12592316	-1.74412613
H	4.52825035	-2.18535116	-1.73911513
H	3.04714123	-3.04980923	-2.19793017
H	3.14702424	-1.28371610	-2.37956218
C	3.60517227	-2.94676023	0.50951404
H	4.69118236	-2.82729722	0.46568204
H	3.28750125	-2.82706022	1.54451912
H	3.35069326	-3.96720930	0.18869601
C	-3.90356930	0.70528706	-0.55797904
H	-3.81179129	0.71929106	-1.63999213
H	-3.60176927	-0.27003402	-0.16035201
H	-4.93081538	0.95057307	-0.28517202

ii) In MeCN solvent

Atomic Symbol	X	Y	Z

C	-0.78908061	1.37532382	1.18980565
C	0.61644726	1.28538917	1.26199917
C	1.26254992	1.60975522	0.05404220
C	0.56123835	1.43694028	-1.14079050
C	-0.81222715	1.17099563	-1.20866870
C	-1.50322857	1.42756663	-0.00152803
H	-1.31271867	1.32380806	2.13498532
H	1.09911171	1.43728448	-2.08196101
C	-0.35317833	-1.80477588	1.28293742
C	1.01335982	-1.57213690	1.09641009
C	1.55207005	-1.82330487	-0.19095066
C	0.64699495	-1.81849014	-1.26763941
C	-0.73597923	-1.70455539	-1.08935845
C	-1.25131417	-1.94000563	0.21145428
H	-0.73665150	-1.75634919	2.29654803
H	1.02472294	-1.78332689	-2.28383609
C	-1.31364103	0.44349103	-2.44837576
H	-2.21578188	0.87904915	-2.88843118
H	-0.53668308	0.54426209	-3.21043336
C	-1.57659137	-1.11334460	-2.21124523
H	-2.63731009	-1.25582181	-2.00847916
H	-1.36994854	-1.60557213	-3.16823184
C	1.79450382	-0.83183685	2.17359248
H	1.82971413	-1.37765968	3.12452255
H	2.83026179	-0.70674194	1.84831917
C	1.18576826	0.59190403	2.49896017
H	1.93355256	1.16845757	3.04646146
H	0.35045670	0.45772319	3.19118302
N	-2.97111991	1.80182791	0.01734936
N	2.67249828	2.15236163	-0.06036098
N	2.95719956	-1.93901065	-0.37643744
N	-2.64253821	-2.17159586	0.40935135
C	3.58043579	1.26637279	-0.89014877
H	3.58255646	0.26475541	-0.45613827
H	3.21613842	1.23974798	-1.91492679
H	4.57844232	1.70452846	-0.87327760
C	2.57338107	3.51924262	-0.72393116
H	1.95101861	4.15950066	-0.09966929
H	3.58158886	3.92512154	-0.80577297
H	2.13191978	3.41127686	-1.71187015
C	3.34540668	2.37671410	1.27270170
H	4.26777958	2.92363792	1.08279498
H	2.68772582	2.96628440	1.90832672
H	3.58288041	1.41766343	1.72442173
C	-3.46892469	2.11708358	1.41131620
H	-2.83195712	2.87481468	1.86335419
H	-4.48248858	2.50127830	1.31079115
H	-3.48287173	1.20741407	2.00851973
C	-3.11754928	3.07575606	-0.79968663
H	-2.51309417	3.85537341	-0.33715564
H	-2.77501194	2.88718927	-1.81456516
H	-4.17087769	3.35619810	-0.80182624

C	-3.10965067	-2.21753904	1.79441959
H	-4.19748420	-2.32766056	1.78972561
H	-2.68240121	-3.06157218	2.36157138
H	-2.86563153	-1.29271488	2.32291683
C	-3.17402559	-3.32872245	-0.33298341
H	-4.26774888	-3.29133995	-0.32130825
H	-2.83938977	-3.31397879	-1.37006979
H	-2.85247468	-4.28170482	0.11821650
C	3.42118880	-2.08520068	-1.75597017
H	4.51428335	-2.10315620	-1.75451996
H	3.06167593	-3.01450732	-2.22809510
H	3.09754826	-1.24170858	-2.37027396
C	3.60651461	-2.94916543	0.47783858
H	4.69114887	-2.81392306	0.42882414
H	3.29505053	-2.84359997	1.51654379
H	3.36662426	-3.97331342	0.14873143
C	-3.89839748	0.74108438	-0.55408073
H	-3.79473331	0.72247887	-1.63463697
H	-3.63622917	-0.22847288	-0.12514784
H	-4.91917253	1.02614511	-0.29956331

iii) In THF solvent

Atomic Symbol	X	Y	Z
C	-0.78936335	1.37766208	1.18652185
C	0.61665564	1.29033438	1.25968941
C	1.26246452	1.61690462	0.05215640
C	0.56047669	1.44574494	-1.14291581
C	-0.81254079	1.17583847	-1.21232026
C	-1.50478996	1.42758656	-0.00445853
H	-1.31261850	1.32085641	2.13156934
H	1.09907565	1.44741287	-2.08383733
C	-0.35126862	-1.79529997	1.28272703
C	1.01537442	-1.56602962	1.09458223
C	1.55334879	-1.81922983	-0.19256051
C	0.64711675	-1.81391943	-1.26812060
C	-0.73541322	-1.69853721	-1.08861502
C	-1.25075071	-1.92965164	0.21273884
H	-0.73256222	-1.74776043	2.29725681
H	1.02282280	-1.78467344	-2.28539190
C	-1.30897782	0.44538628	-2.45296313
H	-2.20670751	0.88212130	-2.90098747
H	-0.52683108	0.54211491	-3.21034867
C	-1.57427202	-1.11086865	-2.21316263
H	-2.63550249	-1.25343288	-2.01359298
H	-1.36511794	-1.60504538	-3.16845964
C	1.79668364	-0.82660413	2.17180114
H	1.83164402	-1.37225000	3.12276504
H	2.83275770	-0.70108222	1.84761914
C	1.18524931	0.59591337	2.49715632

H	1.92909992	1.17387974	3.04865726
H	0.34812079	0.45809872	3.18653933
N	-2.97631234	1.79173320	0.01641920
N	2.67556287	2.15283251	-0.06221288
N	2.95812196	-1.93785744	-0.37866892
N	-2.64313742	-2.15569151	0.41238826
C	3.58092636	1.26152602	-0.89064699
H	3.57314733	0.25692613	-0.46219651
H	3.22293721	1.24377125	-1.91798884
H	4.58207625	1.69241856	-0.86652677
C	2.58659609	3.52014062	-0.72638100
H	1.97365403	4.16780960	-0.10027532
H	3.59801814	3.91753907	-0.81297653
H	2.14000828	3.41628021	-1.71257295
C	3.34690370	2.37397326	1.27224006
H	4.27315984	2.91536538	1.08514034
H	2.68994593	2.96676872	1.90594535
H	3.57768044	1.41369097	1.72466825
C	-3.48216449	2.07770304	1.41394890
H	-2.85476546	2.83375270	1.88245604
H	-4.49928530	2.45389058	1.31799066
H	-3.48935467	1.15690878	1.99431544
C	-3.12889592	3.07879850	-0.77851166
H	-2.53736515	3.85703636	-0.29719056
H	-2.77618971	2.91221447	-1.79379127
H	-4.18467493	3.34985140	-0.78478617
C	-3.10744452	-2.19489721	1.79919241
H	-4.19495237	-2.30779266	1.79741301
H	-2.67789115	-3.03422306	2.37063151
H	-2.86375349	-1.26605670	2.32242103
C	-3.17486549	-3.32000011	-0.32119724
H	-4.26851122	-3.28528429	-0.30496067
H	-2.84380536	-3.31060924	-1.35946874
H	-2.84838242	-4.26836934	0.13465287
C	3.41852464	-2.09673447	-1.75865486
H	4.51139103	-2.12062718	-1.75961665
H	3.05305214	-3.02732434	-2.22259641
H	3.09791076	-1.25638642	-2.37927342
C	3.60554375	-2.94793275	0.47935466
H	4.69051555	-2.81753703	0.42685533
H	3.29676407	-2.83714062	1.51819771
H	3.35991241	-3.97148587	0.15468191
C	-3.89519585	0.73540583	-0.57824298
H	-3.78007853	0.73077569	-1.65783004
H	-3.63416177	-0.23906857	-0.15769475
H	-4.91968368	1.01542439	-0.33210946

C) Optimized coordinate of PCP3

i) In Gas phase

Atomic Symbol	X	Y	Z

C	-0.19598947	1.54045988	1.48995103
C	-1.22124422	1.49228963	0.55259499
C	-0.94078375	1.49109531	-0.81806662
C	0.34933220	1.88732351	-1.18371263
C	1.38276925	1.90927123	-0.24747369
C	1.17255135	1.48792037	1.09343748
H	0.53288707	2.07858231	-2.23199903
C	-0.25348941	-1.78836895	1.17286627
C	-1.40280769	-1.79648730	0.35326346
C	-1.28828162	-1.30825738	-0.97991840
C	-0.00068698	-1.32484333	-1.58146509
C	1.13131492	-1.31477981	-0.73765206
C	0.98520218	-1.38446859	0.64973687
H	2.12400208	-1.20753952	-1.15857920
C	2.18651728	0.65980990	1.88000205
H	3.21047879	0.98771358	1.70712946
H	2.05394830	0.78268100	2.95292546
C	2.11825092	-0.92895431	1.54728567
H	3.07946820	-1.19286530	1.09375786
H	2.08305145	-1.44611929	2.51165443
C	-1.95450472	1.01830465	-1.84217388
H	-2.84386105	1.66057901	-1.84904742
H	-1.50210983	1.09056331	-2.83442003
C	-2.41640829	-0.46322447	-1.57091798
H	-2.86076804	-0.83667499	-2.49970179
H	-3.22645514	-0.44074633	-0.83771763
N	2.76232604	2.39001229	-0.71747098
N	0.11041848	-1.18652256	-2.96317542
C	2.66736358	3.16554519	-2.02328108
H	1.90471365	3.93768109	-1.93063755
H	3.64108013	3.62141605	-2.20247543
H	2.43721064	2.48638894	-2.84174414
C	3.32779779	3.37568504	0.29238384
H	3.45504180	2.89322377	1.25655295
H	4.29437389	3.72456231	-0.07353771
H	2.63384693	4.21203833	0.37743099
C	3.76234515	1.27299203	-0.96502488
H	3.95593650	0.72814258	-0.04716329
H	3.34848044	0.60256250	-1.71491131
H	4.68683629	1.72293147	-1.33041884
C	1.42147490	-1.01707091	-3.57348527
H	1.94770476	-0.16282729	-3.13306996
H	2.06181877	-1.90742758	-3.47687898
H	1.29176712	-0.80463751	-4.63723893
C	-0.83682744	-1.90398586	-3.83319576
H	-1.51305620	-2.51314804	-3.23301460
H	-1.42515314	-1.21473545	-4.45122671
H	-0.29039716	-2.57948206	-4.50100850
H	-2.25296314	1.37243507	0.85439649
H	-0.31534347	-2.08930395	2.21225107
N	-0.58513071	1.70189158	2.96926781
N	-2.67424506	-2.12525081	0.84937716

C	0.23280894	2.82874453	3.57637741
H	-0.05804216	2.93728313	4.62234949
H	1.29170615	2.59457913	3.51263667
H	0.01576833	3.74576859	3.02816275
C	-0.44079248	0.44965590	3.81812515
H	0.60692932	0.21724837	3.97855690
H	-0.92188338	0.63674536	4.77912598
H	-0.92591799	-0.36713935	3.29189306
C	-2.03836759	2.13046760	3.11161365
H	-2.19447993	2.40534406	4.15460959
H	-2.22802060	2.98913442	2.46924861
H	-2.69372936	1.29880938	2.85799648
C	-2.80624264	-2.48160406	2.25748147
H	-3.86413857	-2.64382554	2.47787085
H	-2.25976500	-3.39940324	2.52689232
H	-2.46155235	-1.66990517	2.90642882
C	-3.51775008	-3.00286375	0.01545041
H	-4.57098934	-2.83691521	0.26020115
H	-3.37236768	-2.79269938	-1.04231079
H	-3.28076852	-4.06298111	0.18999069

ii) In MeCN solvent

Atomic Symbol	X	Y	Z
C	-0.36135969	1.46773432	1.26070198
C	-1.26984390	1.18420039	0.24693280
C	-0.83320261	0.99298861	-1.06754648
C	0.45442540	1.44793455	-1.36418310
C	1.36747241	1.71649746	-0.34589447
C	1.04003166	1.47008238	1.01323390
H	0.74059791	1.50739584	-2.40520093
C	-0.04534634	-1.87967918	1.42778389
C	-1.08499999	-2.13010875	0.50835134
C	-0.86432782	-1.83862026	-0.86535093
C	0.47748444	-1.79579667	-1.32009854
C	1.50245461	-1.56692243	-0.38310458
C	1.20503236	-1.43296526	0.97879441
H	2.52111998	-1.41087235	-0.71781517
C	2.02863108	0.88080341	2.01577001
H	3.02449476	1.30814652	1.91928953
H	1.74187024	1.11256782	3.03738926
C	2.17703904	-0.72602692	1.90312886
H	3.20335778	-0.92744977	1.58044698
H	2.08911872	-1.11395619	2.92290320
C	-1.67610609	0.27086290	-2.09998572
H	-2.63272857	0.78346586	-2.25753991
H	-1.14057044	0.28217103	-3.05184006
C	-1.99230154	-1.21997073	-1.68918371
H	-2.25995882	-1.75773970	-2.60543662
H	-2.88765730	-1.21536423	-1.06348330

N	2.72491417	2.30136968	-0.72965479
N	0.71886949	-1.81437835	-2.70929521
C	2.69747726	2.88940951	-2.13076056
H	1.85283763	3.57058050	-2.21688875
H	3.63250004	3.42989035	-2.26884297
H	2.63483920	2.09238504	-2.86761082
C	3.04635647	3.47127219	0.18860720
H	3.14506306	3.12834685	1.21281301
H	3.98665698	3.90885631	-0.14462119
H	2.23708102	4.19567077	0.10958655
C	3.86480051	1.30147049	-0.70781212
H	4.00215266	0.90843832	0.29324428
H	3.63334000	0.49675847	-1.40134657
H	4.76979401	1.81853041	-1.02608084
C	2.06057800	-1.51195550	-3.18688405
H	2.39314281	-0.54166496	-2.81228326
H	2.80680426	-2.27272837	-2.90243821
H	2.03734957	-1.45357838	-4.27869101
C	0.14426582	-2.93608797	-3.46444275
H	-0.81478492	-3.23529700	-3.04598987
H	-0.00475929	-2.64130620	-4.50860751
H	0.81159564	-3.81335709	-3.44619072
H	-2.31839951	1.03341036	0.46365727
H	-0.22291516	-1.96951030	2.49311020
N	-0.91421632	1.84210343	2.63767956
N	-2.37655181	-2.52378721	0.91895583
C	-0.20174158	3.09232826	3.13143493
H	-0.64735499	3.37762791	4.08379407
H	0.85553825	2.88952106	3.26905099
H	-0.34236553	3.87895878	2.39117003
C	-0.82239681	0.75279662	3.68918940
H	0.21225712	0.56737645	3.95558285
H	-1.36892559	1.09166557	4.56912317
H	-1.27410133	-0.14839183	3.28701683
C	-2.38480731	2.22112740	2.55132050
H	-2.66020372	2.64823973	3.51411299
H	-2.52032823	2.95827061	1.76221561
H	-2.98768476	1.33461872	2.36805275
C	-2.63849775	-2.65631935	2.34635078
H	-3.69668421	-2.89441441	2.48424330
H	-2.04506789	-3.45393858	2.82423163
H	-2.44487910	-1.71854206	2.87089415
C	-2.97481776	-3.64388733	0.17819128
H	-4.05760311	-3.64678588	0.33857148
H	-2.78728732	-3.54943645	-0.89028931
H	-2.57206830	-4.61382488	0.51452878

iii) In THF solvent

Atomic Symbol	X	Y	Z
C	-0.36138794	1.46798781	1.25620370

C	-1.26804141	1.18483711	0.24095906
C	-0.83002331	0.99503999	-1.07353260
C	0.45741017	1.45243149	-1.36814658
C	1.36904950	1.72080369	-0.34830555
C	1.04080604	1.47457122	1.01109741
H	0.74479808	1.51157962	-2.40895414
C	-0.04474861	-1.87492328	1.43255036
C	-1.08533328	-2.12645496	0.51424522
C	-0.86572435	-1.83303040	-0.85943117
C	0.47570921	-1.79114213	-1.31602203
C	1.50113685	-1.56053125	-0.37980580
C	1.20510908	-1.42856129	0.98220483
H	2.51977484	-1.40682148	-0.71529807
C	2.02933440	0.88646157	2.01492670
H	3.02525268	1.31388427	1.91759045
H	1.74304280	1.12120141	3.03623216
C	2.17727843	-0.72151798	1.90571189
H	3.20409639	-0.92420812	1.58506402
H	2.08968757	-1.10782006	2.92618355
C	-1.67165583	0.27061708	-2.10538942
H	-2.62499758	0.78659121	-2.27188836
H	-1.13167540	0.27194768	-3.05468130
C	-1.99428369	-1.21496948	-1.68308110
H	-2.26909013	-1.75675290	-2.59467333
H	-2.88709093	-1.20199009	-1.05375618
N	2.72935734	2.30168022	-0.73135128
N	0.71604205	-1.81048362	-2.70440335
C	2.70702418	2.88875490	-2.13328139
H	1.86691502	3.57537176	-2.22141782
H	3.64565152	3.42336797	-2.27206330
H	2.63929463	2.09149436	-2.86952412
C	3.05256381	3.47163627	0.18594051
H	3.14383734	3.13062152	1.21167926
H	3.99657636	3.90454343	-0.14319232
H	2.24744287	4.20053153	0.10142701
C	3.86670195	1.29813909	-0.70724579
H	3.99627334	0.89930362	0.29246537
H	3.63737666	0.49670388	-1.40546418
H	4.77511999	1.81448923	-1.01718465
C	2.05819678	-1.51357172	-3.18394292
H	2.39385284	-0.54193641	-2.81392871
H	2.80259214	-2.27495813	-2.89720025
H	2.03423197	-1.46032167	-4.27593411
C	0.13467200	-2.92770035	-3.46278962
H	-0.82062201	-3.22999802	-3.03843915
H	-0.02220630	-2.62638408	-4.50382877
H	0.80222340	-3.80429086	-3.45425218
H	-2.31703343	1.03279424	0.45519267
H	-0.21938273	-1.97031852	2.49785815
N	-0.91805082	1.83694755	2.63406914
N	-2.37512845	-2.52090947	0.92685157
C	-0.21312515	3.09112638	3.12812962

H	-0.67431357	3.38865540	4.06944214
H	0.84143559	2.88780967	3.28644258
H	-0.33870696	3.87020944	2.37652964
C	-0.81993778	0.74582034	3.68351085
H	0.21584890	0.56610389	3.94937821
H	-1.36936342	1.07803343	4.56432912
H	-1.26409362	-0.15762943	3.27753623
C	-2.39154359	2.20553760	2.54859023
H	-2.67341730	2.61926743	3.51552748
H	-2.53188564	2.95086489	1.76795377
H	-2.98683772	1.31628954	2.35301829
C	-2.62984098	-2.66644846	2.35458537
H	-3.68591688	-2.91127646	2.49549228
H	-2.03026621	-3.46472943	2.82291061
H	-2.43889676	-1.73177155	2.88687010
C	-2.98012216	-3.63487399	0.18023770
H	-4.06270132	-3.63270735	0.34111150
H	-2.79238310	-3.53641690	-0.88761851
H	-2.58139112	-4.60739548	0.51204215

2) One photon data for PCP1, PCP2 and PCP3 in gas phase calculated at BLYP and B3LYP functionals and cc-pVDZ basis set

BLYP Results

Systems	ω_{0f} (eV)	Orbitals	Λ
PCP1	0.78	H-L (0.71)	0.192
PCP2	1.06	H-L (-0.71)	0.211
PCP3	1.02	H-L (0.71)	0.196

B3LYP Results

Systems	ω_{0f} (eV)	Orbitals	Λ
PCP1	1.53	H-L (0.71)	0.195
PCP2	1.80	H-L (-0.71)	0.214
PCP3	1.77	H-L (-0.70)	0.185

3) δ^{3PA} (10^6 a.u.) and one-photon excitation energies (ω_{0f}, in eV) of all the systems in gas phase calculated by varying the μ-parameter of CAMB3LYP functional

System	Gas phase δ^{3PA} and ω_{0f} of all the systems for different μ-parameter of CAMB3LYP functional							
	μ →	0.20	0.25	0.30	0.35	0.40	0.45	0.50
PCP1	δ^{3PA}	8.18	5.41	3.99	3.13	2.57	2.19	1.91

	ω_{0f}	2.06	2.26	2.43	2.56	2.67	2.76	2.83
PCP2	δ^{3PA}	4.02	2.70	2.05	1.64	1.37	1.18	1.05
	ω_{0f}	2.32	2.52	2.68	2.81	2.92	3.00	3.07
PCP	δ^{3PA}	26.19	21.30	17.80	15.20	13.50	12.20	11.30
	ω_{0f}	2.29	2.49	2.65	2.79	2.90	2.99	3.06