Supplementary Information

Fluorescent carborane-vinylstilbene functionalised octasilsesquioxanes: synthesis, structural, thermal and photophysical properties

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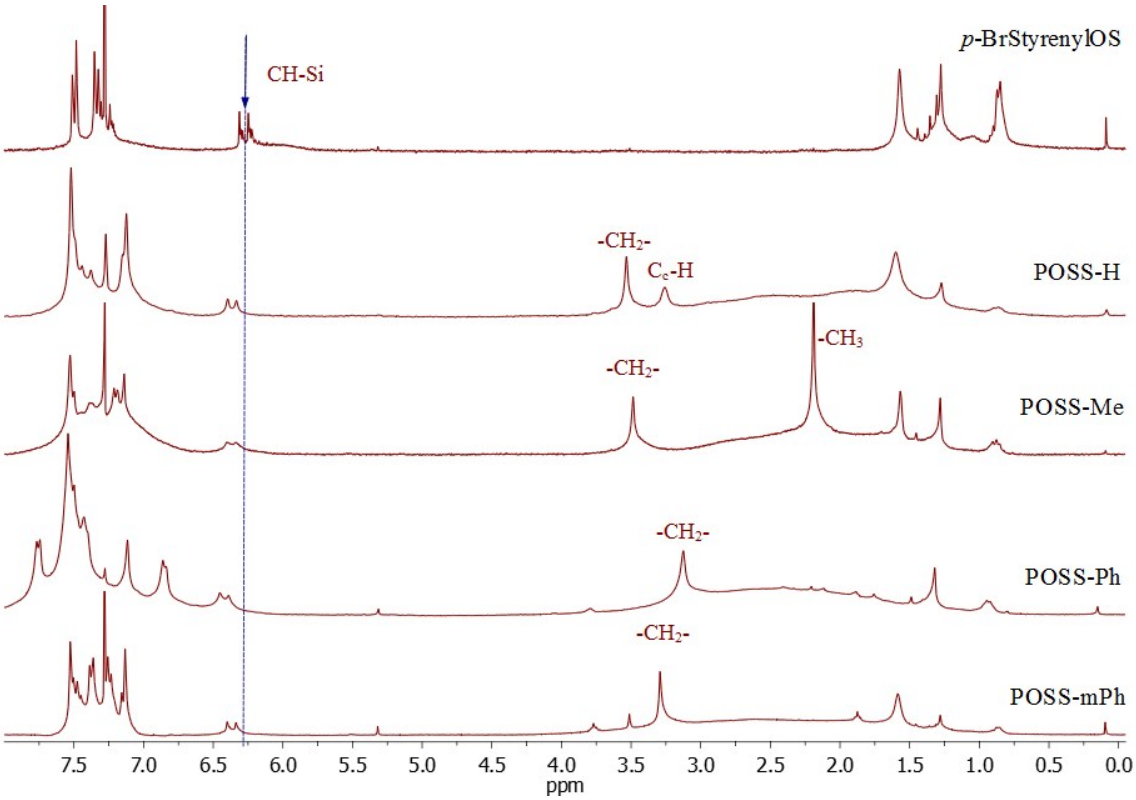

Figure S1. ^{1}H NMR of starting *p*-BrStyrenylOS and final compounds POSS-H, **POSS-Me**, **POSS-Ph** and **POSS-mPh**.

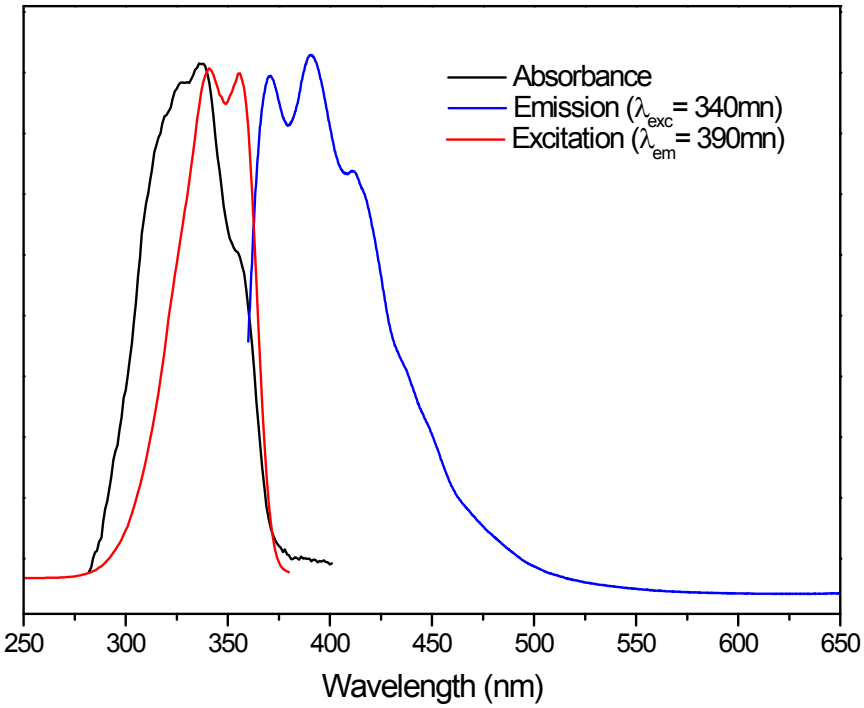

Figure S2. Normalized absorption, excitation and emission of POSS-H in DCM.

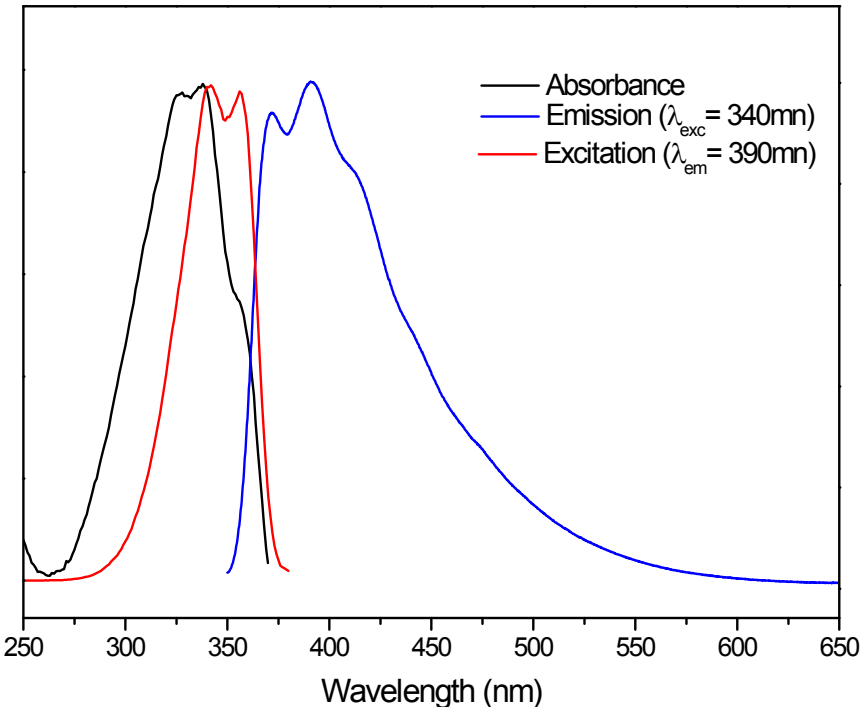

Figure S3. Normalized absorption, excitation and emission of POSS-Me in DCM.

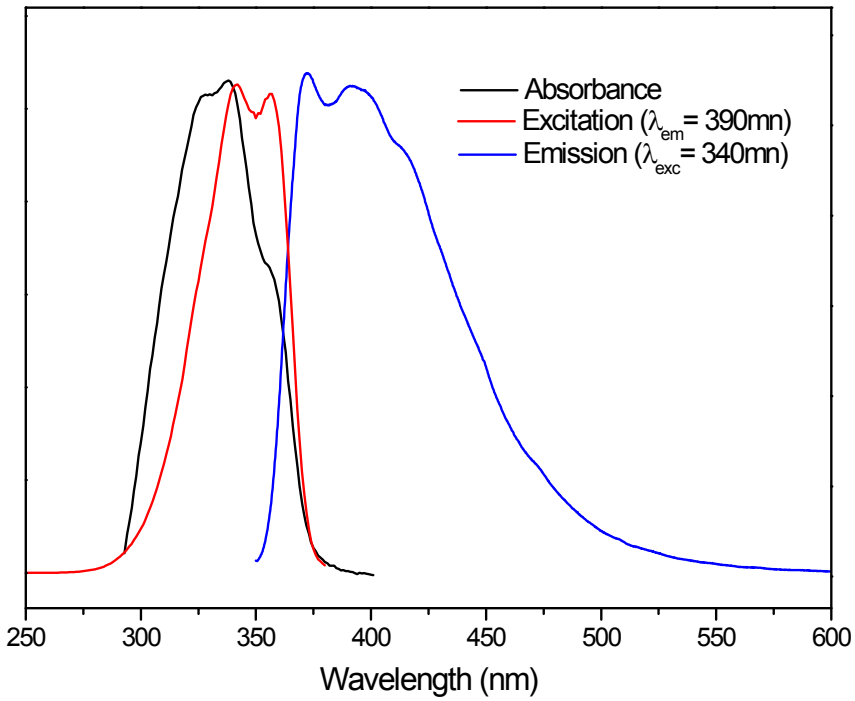

Figure S4. Normalized absorption, excitation and emission of POSS-Ph in DCM.

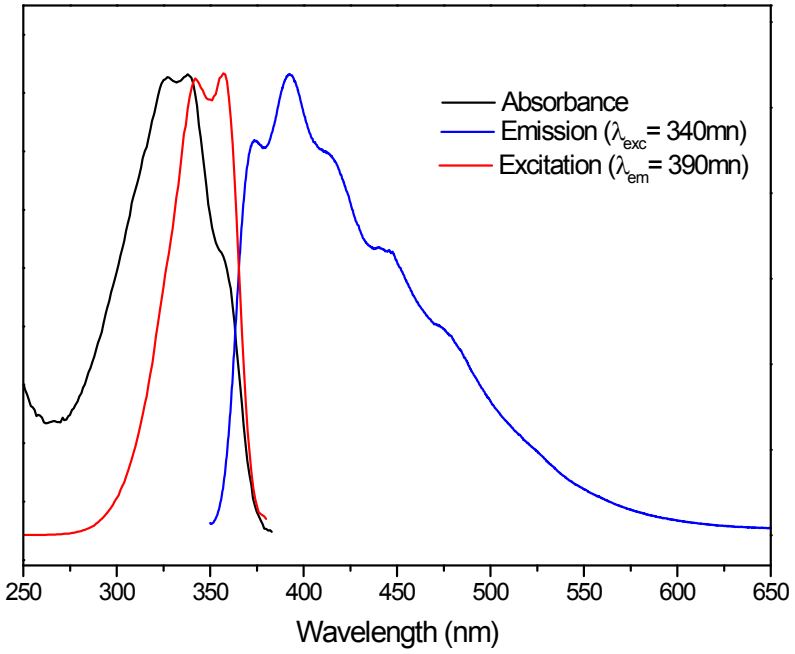

Figure S5. Normalized absorption, excitation and emission of POSS-mPh in DCM.

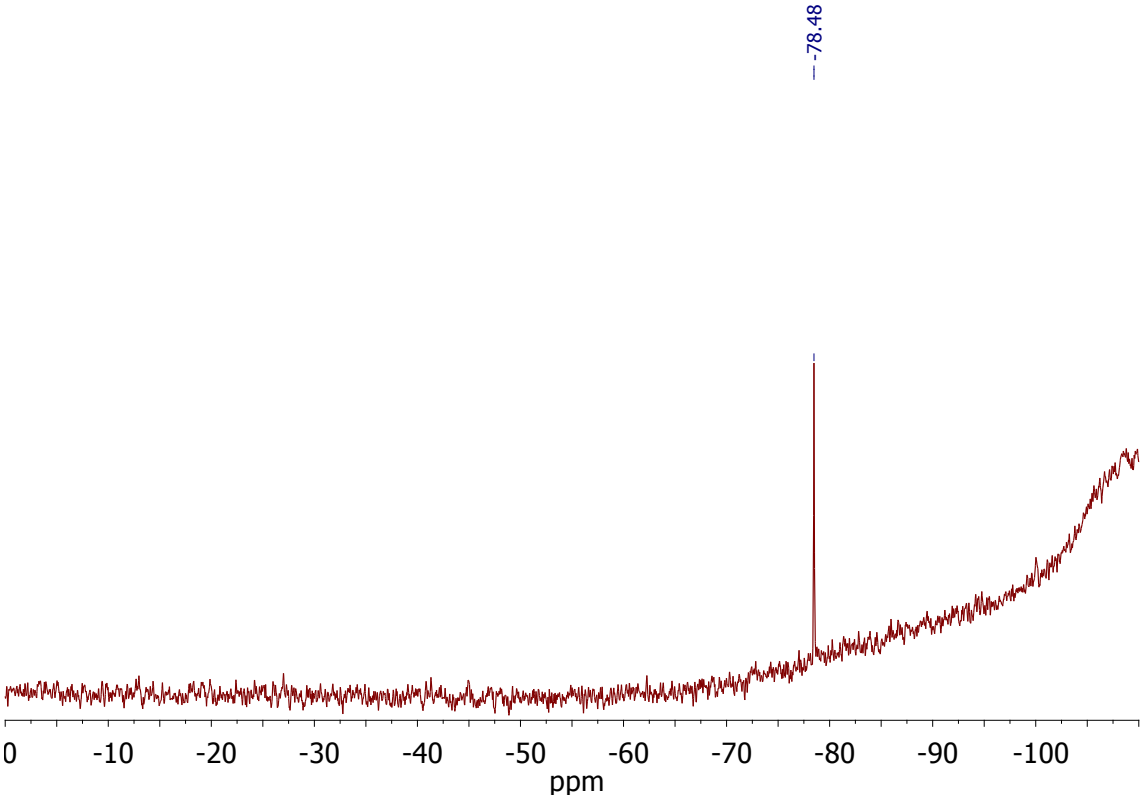

Figure S6. ^{29}Si NMR of starting *p*-BrStyrenylOS.

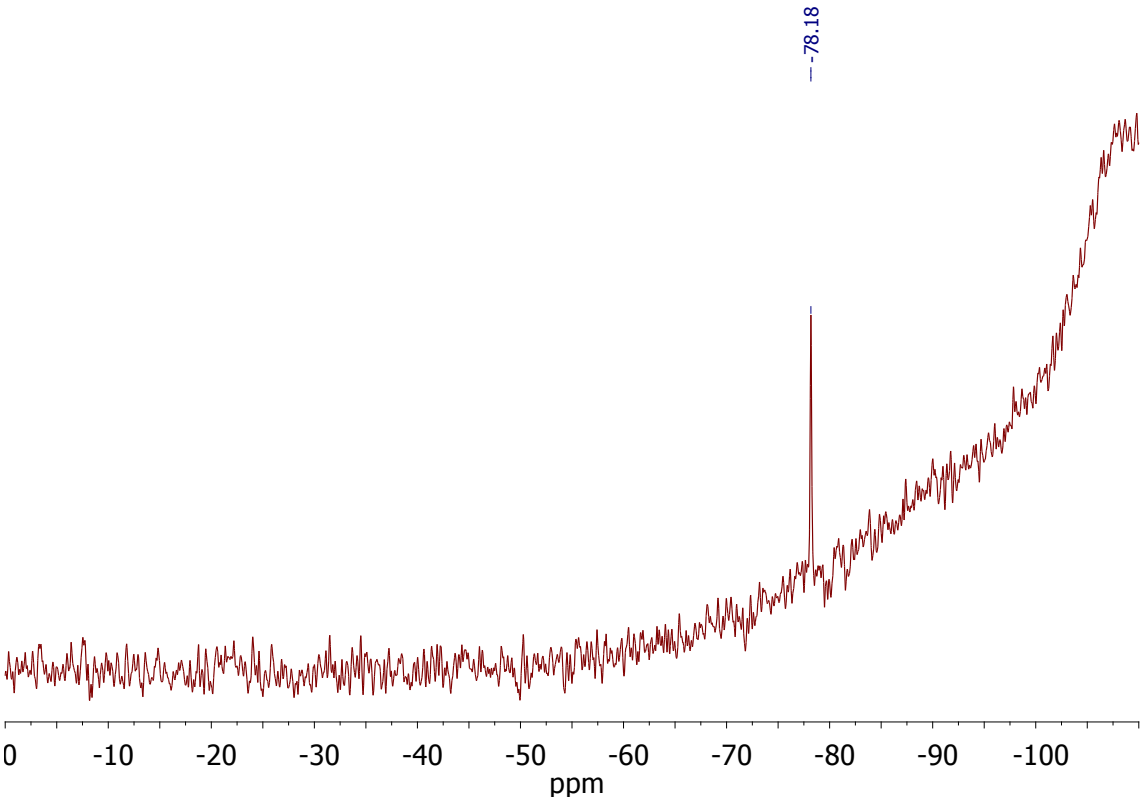

Figure S7. ^{29}Si NMR of **POSS-H**.

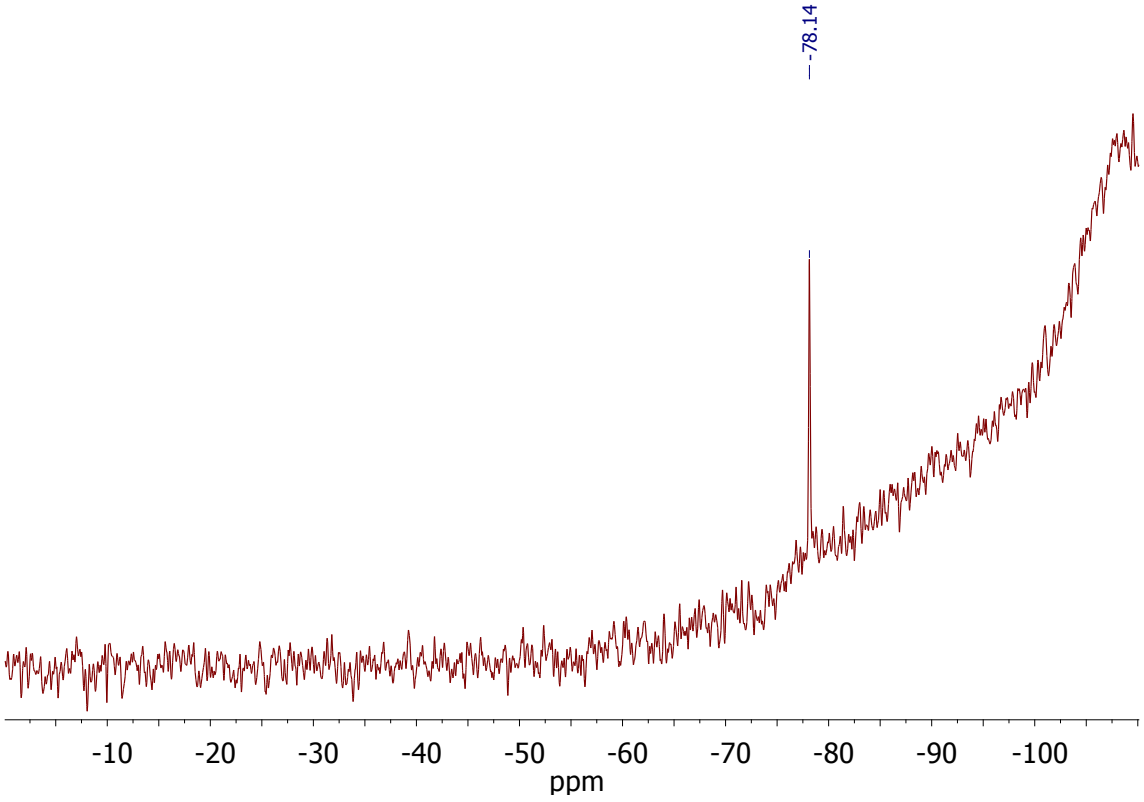

Figure S8. ^{29}Si NMR of **POSS-Me**.

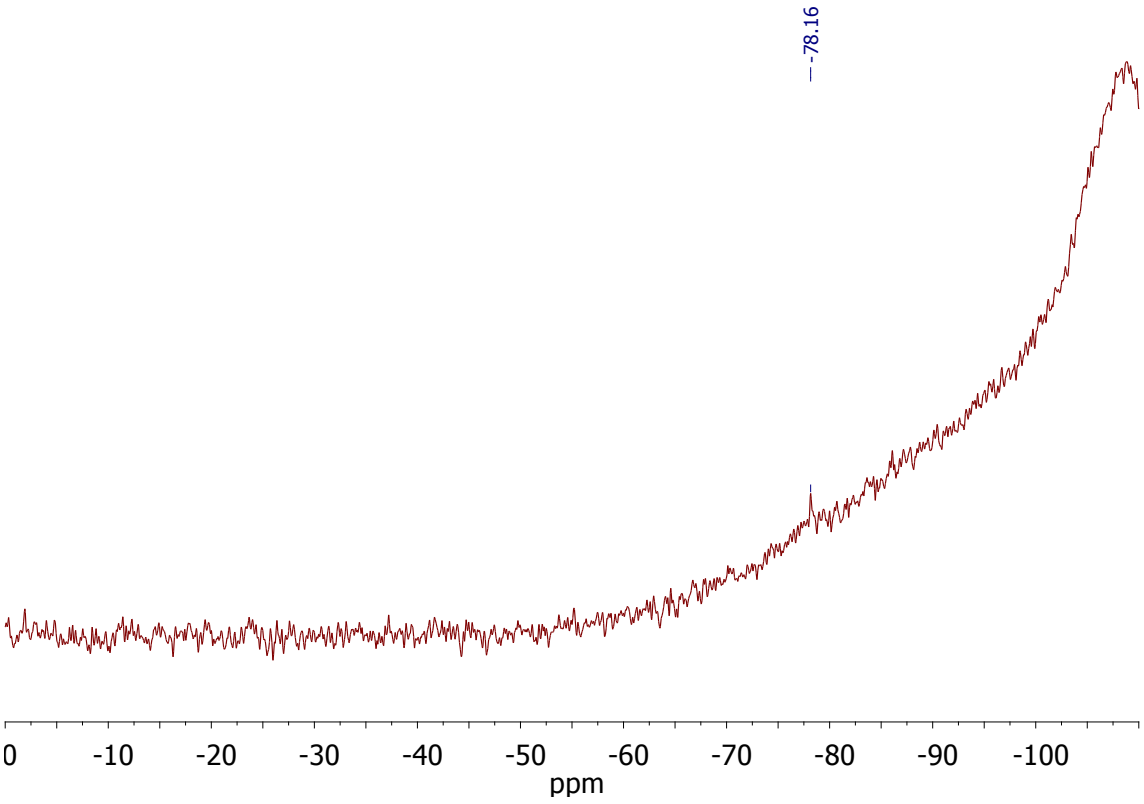

Figure S9. ^{29}Si NMR of **POSS-Ph**.

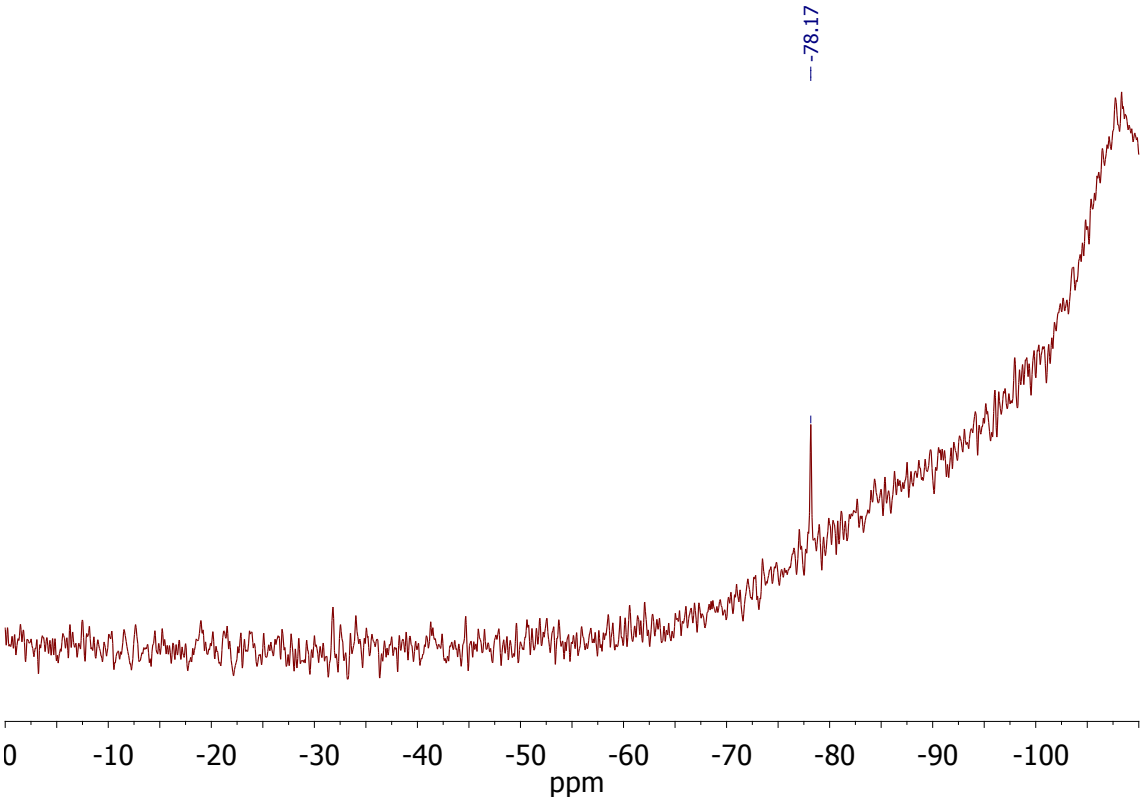

Figure S10. ^{29}Si NMR of **POSS-mPh**.

Cartesian Coordinates of the DFT-optimized POSS-H

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Si	-1.56931500	1.60146200	-1.59586100
O	0.01874000	1.87867100	-1.91673700
Si	1.60407800	1.57059300	-1.59111400
O	1.86049900	1.88581000	0.00281100
Si	-1.60407800	1.57059300	1.59111400
O	-0.01874000	1.87867100	1.91673700
O	1.90878200	0.01609400	1.89169300
Si	1.60407800	-1.57059300	1.59111400
O	-1.86049900	-1.88581000	0.00281100
Si	-1.60407800	-1.57059300	-1.59111400
O	-0.01874000	-1.87867100	-1.91673700
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Si	-1.56931500	-1.60146200	1.59586100
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H	2.65872900	3.70272400	-2.45332700
C	-2.69643900	2.62775100	2.62579300
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C	2.61468600	2.68440900	2.65280700
H	3.69018900	2.66999500	2.48033300
C	2.69643900	-2.62775100	2.62579300
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H	15.76438300	10.61055500	-11.67240400
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C	-4.22836500	-4.56048400	4.48142200
C	-2.77792700	-5.81536800	6.48269000
H	-1.05929700	-4.84608000	5.64881700
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C	-4.16402100	-6.03134800	6.42015700
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H	-5.94399800	-5.51763800	5.29748600
C	-4.79116000	-6.89626100	7.41701900
C	-6.08953700	-7.24456900	7.49364000
H	-4.10308800	-7.28422300	8.16491000
C	-6.71486800	-8.09344200	8.50869500

H	-6.77612700	-6.87527200	6.73524600
C	-8.07660700	-8.41555200	8.38221700
C	-6.03508900	-8.59924000	9.63130500
C	-8.72679600	-9.20520700	9.32258300
H	-8.63433400	-8.03447300	7.53181200
C	-6.68605900	-9.38757000	10.56815300
H	-4.98795900	-8.36401800	9.78610700
C	-8.04164800	-9.70985500	10.43002800
H	-9.78119200	-9.42916800	9.19288300
H	-6.13264800	-9.75201200	11.42830600
C	-8.75473200	-10.54690600	11.46889400
C	-8.78086000	-12.06827700	11.21341900
H	-9.78930200	-10.21016300	11.55602500
H	-8.29211700	-10.37802200	12.44511700
B	-9.84965800	-12.79223200	10.09924000
B	-7.31494900	-12.95077600	11.44118200
B	-8.08786500	-12.83892900	9.84909400
B	-10.17800100	-12.89326100	11.83843000
B	-10.35329000	-14.33382700	10.84205600
B	-9.05766100	-14.30741400	9.60768500
H	-10.52392600	-12.07009100	9.44874600
C	-8.62611900	-13.04550900	12.53644300
B	-7.80676300	-14.48823700	12.19229600
B	-7.47827000	-14.39985900	10.44735800
H	-6.36371200	-12.33833500	11.77678600
H	-7.58412200	-12.15564600	9.03071100
B	-9.57115400	-14.45093000	12.43538100
H	-10.97211800	-12.22825400	12.40499300
B	-8.88125900	-15.33257700	11.05571900
H	-11.43009000	-14.78651600	10.64634400
H	-9.21852800	-14.74950500	8.52040300
H	-8.48527600	-12.52815700	13.47472200
H	-7.10386800	-14.93723400	13.03052500
H	-6.51594900	-14.90310900	9.97491400
H	-10.03895800	-14.87287700	13.43598700
H	-8.91318300	-16.51605700	11.01576700
C	2.83973200	4.33912200	4.55058200
C	2.13248600	4.99311600	5.56970200
C	4.22836500	4.56048400	4.48142200
C	2.77792700	5.81536800	6.48269000
H	1.05929700	4.84608000	5.64881700
C	4.87185500	5.38136400	5.38837600
H	4.81241100	4.08283800	3.70202200
C	4.16402100	6.03134800	6.42015700
H	2.20003500	6.30195400	7.26313200
H	5.94399800	5.51763800	5.29748600
C	4.79116000	6.89626100	7.41701900
C	6.08953700	7.24456900	7.49364000
H	4.10308800	7.28422300	8.16491000
C	6.71486800	8.09344200	8.50869500
H	6.77612700	6.87527200	6.73524600
C	8.07660700	8.41555200	8.38221700
C	6.03508900	8.59924000	9.63130500
C	8.72679600	9.20520700	9.32258300
H	8.63433400	8.03447300	7.53181200
C	6.68605900	9.38757000	10.56815300
H	4.98795900	8.36401800	9.78610700
C	8.04164800	9.70985500	10.43002800
H	9.78119200	9.42916800	9.19288300
H	6.13264800	9.75201200	11.42830600
C	8.75473200	10.54690600	11.46889400
C	8.78086000	12.06827700	11.21341900
H	9.78930200	10.21016300	11.55602500
H	8.29211700	10.37802200	12.44511700
B	9.84965800	12.79223200	10.09924000
B	7.31494900	12.95077600	11.44118200
B	8.08786500	12.83892900	9.84909400

B	10.17800100	12.89326100	11.83843000
B	10.35329000	14.33382700	10.84205600
B	9.05766100	14.30741400	9.60768500
H	10.52392600	12.07009100	9.44874600
C	8.62611900	13.04550900	12.53644300
B	7.80676300	14.48823700	12.19229600
B	7.47827000	14.39985900	10.44735800
H	6.36371200	12.33833500	11.77678600
H	7.58412200	12.15564600	9.03071100
B	9.57115400	14.45093000	12.43538100
H	10.97211800	12.22825400	12.40499300
B	8.88125900	15.33257700	11.05571900
H	11.43009000	14.78651600	10.64634400
H	9.21852800	14.74950500	8.52040300
H	8.48527600	12.52815700	13.47472200
H	7.10386800	14.93723400	13.03052500
H	6.51594900	14.90310900	9.97491400
H	10.03895800	14.87287700	13.43598700
H	8.91318300	16.51605700	11.01576700
C	4.45284000	-2.88401500	4.42368600
C	5.21364400	-2.18724100	5.37351900
C	4.62848800	-4.27902200	4.35091200
C	6.10242900	-2.84736000	6.21074600
H	5.10373000	-1.10972400	5.45408200
C	5.51364800	-4.93730600	5.18335300
H	4.06798200	-4.85599700	3.62318600
C	6.27697100	-4.23892200	6.14144700
H	6.67593400	-2.27647500	6.93526300
H	5.62131300	-6.01177200	5.08255200
C	7.22935500	-4.88011400	7.04542200
C	7.48545500	-6.19733200	7.15618300
H	7.77015300	-4.18794200	7.68711800
C	8.44687500	-6.83747300	8.05467200
H	6.93361000	-6.89139300	6.52644600
C	8.52452300	-8.24022900	8.07827800
C	9.30993900	-6.13021400	8.91079000
C	9.41722600	-8.90499400	8.90942200
H	7.86797600	-8.81782800	7.43430800
C	10.20199500	-6.79606700	9.73804300
H	9.28960400	-5.04624500	8.93193200
C	10.27899600	-8.19406800	9.74794400
H	9.44599600	-9.99030200	8.90097100
H	10.85151800	-6.21820100	10.38857300
C	11.25312100	-8.91722700	10.65137100
C	12.62753800	-9.24817900	10.03149800
H	10.80918100	-9.85704900	10.98461800
H	11.42333200	-8.32017100	11.55147400
B	12.86473200	-10.59323400	9.00990000
B	13.71586000	-7.94411700	9.72480400
B	13.06080700	-8.93080200	8.40418900
B	13.41172600	-10.64945700	10.69489500
B	14.47674400	-11.23593100	9.42123600
B	14.26553200	-10.17156300	7.99843900
H	11.90742200	-11.22372100	8.71786800
C	13.95191900	-9.05863500	11.00102800
B	15.32930300	-8.57374800	10.14178400
B	14.79034100	-8.51939700	8.44809200
H	13.34912100	-6.85831400	10.00489100
H	12.24378900	-8.45245900	7.70162700
B	15.13901400	-10.24176600	10.73908000
H	12.84001900	-11.21217300	11.56121900
B	15.67334500	-9.94899200	9.06975000
H	14.71536700	-12.39315900	9.33963100
H	14.35715900	-10.58040000	6.89022000
H	13.74509300	-8.67962000	11.99174100
H	16.08245700	-7.83584200	10.67697400
H	15.25659100	-7.75018500	7.67771100

H	15.76438300	-10.61055500	11.67240400
H	16.78287100	-10.19582900	8.73622800
C	-4.45284000	2.88401500	4.42368600
C	-5.21364400	2.18724100	5.37351900
C	-4.62848800	4.27902200	4.35091200
C	-6.10242900	2.84736000	6.21074600
H	-5.10373000	1.10972400	5.45408200
C	-5.51364800	4.93730600	5.18335300
H	-4.06798200	4.85599700	3.62318600
C	-6.27697100	4.23892200	6.14144700
H	-6.67593400	2.27647500	6.93526300
H	-5.62131300	6.01177200	5.08255200
C	-7.22935500	4.88011400	7.04542200
C	-7.48545500	6.19733200	7.15618300
H	-7.77015300	4.18794200	7.68711800
C	-8.44687500	6.83747300	8.05467200
H	-6.93361000	6.89139300	6.52644600
C	-8.52452300	8.24022900	8.07827800
C	-9.30993900	6.13021400	8.91079000
C	-9.41722600	8.90499400	8.90942200
H	-7.86797600	8.81782800	7.43430800
C	-10.20199500	6.79606700	9.73804300
H	-9.28960400	5.04624500	8.93193200
C	-10.27899600	8.19406800	9.74794400
H	-9.44599600	9.99030200	8.90097100
H	-10.85151800	6.21820100	10.38857300
C	-11.25312100	8.91722700	10.65137100
C	-12.62753800	9.24817900	10.03149800
H	-10.80918100	9.85704900	10.98461800
H	-11.42333200	8.32017100	11.55147400
B	-12.86473200	10.59323400	9.00990000
B	-13.71586000	7.94411700	9.72480400
B	-13.06080700	8.93080200	8.40418900
B	-13.41172600	10.64945700	10.69489500
B	-14.47674400	11.23593100	9.42123600
B	-14.26553200	10.17156300	7.99843900
H	-11.90742200	11.22372100	8.71786800
C	-13.95191900	9.05863500	11.00102800
B	-15.32930300	8.57374800	10.14178400
B	-14.79034100	8.51939700	8.44809200
H	-13.34912100	6.85831400	10.00489100
H	-12.24378900	8.45245900	7.70162700
B	-15.13901400	10.24176600	10.73908000
H	-12.84001900	11.21217300	11.56121900
B	-15.67334500	9.94899200	9.06975000
H	-14.71536700	12.39315900	9.33963100
H	-14.35715900	10.58040000	6.89022000
H	-13.74509300	8.67962000	11.99174100
H	-16.08245700	7.83584200	10.67697400
H	-15.25659100	7.75018500	7.67771100
H	-15.76438300	10.61055500	11.67240400
H	-16.78287100	10.19582900	8.73622800

Excited States of POSS-H (Energies, oscillator strengths and composition) according to the TD-DFT calculations

Excited State 1: Singlet-A 3.3560 eV 369.44 nm f=0.0000 <S**2>=0.000
853 -> 863 -0.24444
854 -> 864 -0.15154
855 -> 862 0.24547
856 -> 861 0.36941
857 -> 866 -0.21868
858 -> 868 -0.15941
859 -> 865 0.21311
860 -> 867 0.22564
860 -> 868 -0.14829
Excited State 2: Singlet-B1 3.3694 eV 367.97 nm f=0.0039 <S**2>=0.000

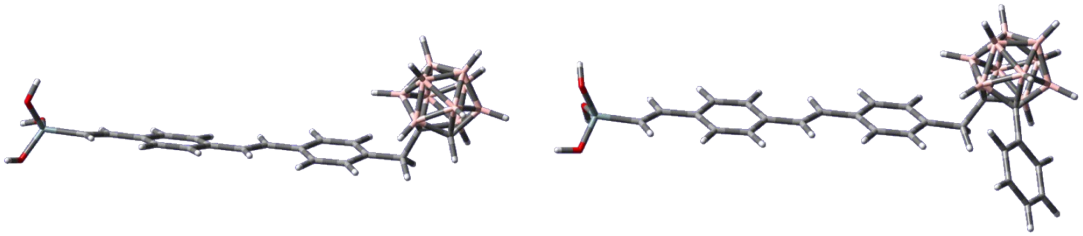
853 -> 866 0.14809
855 -> 865 -0.14835
856 -> 867 0.19620
856 -> 868 -0.13589
857 -> 863 0.24106
859 -> 862 -0.24470
860 -> 861 0.50747
Excited State 3: Singlet-B3 3.3762 eV 367.23 nm f=0.2461 <S**2>=0.000
853 -> 861 -0.22494
854 -> 865 0.10608
855 -> 867 -0.17787
856 -> 863 0.27905
856 -> 865 0.12375
857 -> 868 -0.17520
858 -> 862 0.19958
858 -> 866 -0.11152
859 -> 861 0.36381
860 -> 862 -0.20388
860 -> 866 -0.18097
Excited State 4: Singlet-B2 3.3767 eV 367.18 nm f=0.1237 <S**2>=0.000
853 -> 868 0.16301
854 -> 866 0.13548
855 -> 861 0.24420
856 -> 862 0.27284
856 -> 866 -0.10590
857 -> 861 0.34600
858 -> 863 0.25517
859 -> 867 -0.19465
860 -> 863 0.14251
860 -> 865 -0.19291
Excited State 5: Singlet-B2 3.3880 eV 365.95 nm f=0.0946 <S**2>=0.000
854 -> 866 -0.16504
855 -> 861 -0.14498
856 -> 866 -0.23088
858 -> 863 -0.34281
860 -> 863 0.50769
Excited State 6: Singlet-B3 3.3890 eV 365.84 nm f=0.0495 <S**2>=0.000
853 -> 861 -0.10664
854 -> 865 0.20749
856 -> 865 -0.19968
858 -> 862 0.44112
860 -> 862 0.43742
Excited State 7: Singlet-B1 3.3917 eV 365.55 nm f=0.1835 <S**2>=0.000
854 -> 867 -0.16628
854 -> 868 0.11918
855 -> 863 0.13060
856 -> 868 0.15003
858 -> 861 0.53888
860 -> 864 -0.32383
Excited State 8: Singlet-A 3.3926 eV 365.45 nm f=0.0000 <S**2>=0.000
855 -> 862 -0.12554
855 -> 866 0.27807
859 -> 863 0.59550
859 -> 865 -0.14412
Excited State 9: Singlet-A 3.3932 eV 365.39 nm f=0.0000 <S**2>=0.000
853 -> 863 0.12137
853 -> 865 0.28407
857 -> 862 0.60796
857 -> 866 0.11769
Excited State 10: Singlet-B2 3.3947 eV 365.23 nm f=0.1398 <S**2>=0.000
853 -> 867 0.15082
854 -> 862 -0.24049
856 -> 862 0.33401
857 -> 861 -0.25415
857 -> 864 0.15520
858 -> 863 -0.16099
858 -> 865 -0.25202

860 -> 865 -0.32765
Excited State 11: Singlet-B3 3.3950 eV 365.20 nm f=0.0304 <S**2>=0.000
854 -> 863 0.32149
854 -> 865 -0.10949
856 -> 863 0.38131
858 -> 862 -0.18599
858 -> 866 0.26218
860 -> 862 0.13139
860 -> 866 -0.31180
Excited State 12: Singlet-B3 3.3963 eV 365.06 nm f=0.1732 <S**2>=0.000
853 -> 861 0.24234
854 -> 863 0.10195
855 -> 868 0.24792
857 -> 867 -0.14719
859 -> 861 0.43405
859 -> 864 0.32325
860 -> 866 0.19011
Excited State 13: Singlet-B2 3.3971 eV 364.97 nm f=0.0697 <S**2>=0.000
853 -> 867 -0.18581
854 -> 862 -0.30945
855 -> 861 -0.21262
856 -> 862 0.13135
857 -> 861 0.37254
857 -> 864 -0.27154
858 -> 863 -0.10233
858 -> 865 -0.16491
859 -> 868 -0.12333
860 -> 863 -0.11008
Excited State 14: Singlet-B1 3.3981 eV 364.86 nm f=0.0067 <S**2>=0.000
854 -> 867 0.14790
854 -> 868 0.13479
855 -> 863 0.37181
855 -> 865 -0.16500
858 -> 864 0.29769
859 -> 862 -0.25771
859 -> 866 0.26790
860 -> 861 -0.20188
Excited State 15: Singlet-B1 3.3992 eV 364.75 nm f=0.0047 <S**2>=0.000
853 -> 862 0.49079
853 -> 866 0.12067
855 -> 863 -0.13035
857 -> 863 0.21742
857 -> 865 0.36942
858 -> 864 0.10283
859 -> 866 -0.13191
Excited State 16: Singlet-A 3.4002 eV 364.64 nm f=0.0000 <S**2>=0.000
854 -> 861 0.41712
856 -> 864 0.32445
858 -> 867 -0.21645
858 -> 868 0.19066
860 -> 867 -0.14804
860 -> 868 -0.30995
Excited State 17: Singlet-B1 3.4003 eV 364.63 nm f=0.0032 <S**2>=0.000
853 -> 862 0.19668
854 -> 867 -0.12546
854 -> 868 -0.18194
855 -> 863 0.31829
857 -> 865 0.20973
858 -> 864 -0.30527
859 -> 866 0.32590
860 -> 861 0.20452
Excited State 18: Singlet-A 3.4016 eV 364.48 nm f=0.0000 <S**2>=0.000
854 -> 864 0.35345
856 -> 861 0.36724
858 -> 867 0.26242
858 -> 868 0.26207
860 -> 867 0.19749

860 -> 868 -0.13787
Excited State 19: Singlet-B2 3.4044 eV 364.19 nm f=0.0779 <S**2>=0.000
853 -> 867 -0.10203
854 -> 866 -0.10891
855 -> 861 0.35955
855 -> 864 0.29944
857 -> 864 -0.20809
858 -> 863 -0.16044
859 -> 868 0.40722
Excited State 20: Singlet-B3 3.4044 eV 364.19 nm f=0.1291 <S**2>=0.000
853 -> 861 -0.37944
853 -> 864 0.30060
855 -> 868 0.12817
857 -> 867 0.38273
858 -> 862 -0.11701
859 -> 864 0.20262
Excited State 21: Singlet-B1 3.4258 eV 361.92 nm f=3.4479 <S**2>=0.000
853 -> 862 -0.15429
853 -> 866 0.10841
855 -> 863 0.16572
856 -> 867 -0.19076
856 -> 868 -0.26959
857 -> 863 0.31563
858 -> 861 0.20270
859 -> 862 0.29970
860 -> 864 0.27875
Excited State 22: Singlet-B2 3.4276 eV 361.72 nm f=2.7307 <S**2>=0.000
853 -> 867 -0.18407
853 -> 868 -0.11548
854 -> 862 0.32733
854 -> 866 -0.17991
855 -> 861 0.14453
855 -> 864 -0.10643
856 -> 862 0.11035
857 -> 864 -0.14792
858 -> 863 -0.20603
858 -> 865 0.12552
859 -> 867 -0.11377
859 -> 868 -0.26262
860 -> 863 -0.27539
860 -> 865 -0.13070
Excited State 23: Singlet-B3 3.4278 eV 361.70 nm f=2.7642 <S**2>=0.000
853 -> 861 0.13241
853 -> 864 0.11515
854 -> 863 0.35510
854 -> 865 0.16452
855 -> 868 -0.20790
857 -> 867 0.21844
857 -> 868 0.19449
858 -> 862 0.16040
858 -> 866 0.14478
859 -> 864 -0.14130
860 -> 862 -0.29722
860 -> 866 0.12676
Excited State 24: Singlet-A 3.4355 eV 360.89 nm f=0.0000 <S**2>=0.000
853 -> 865 0.12430
854 -> 864 -0.13942
855 -> 866 0.43824
856 -> 861 -0.22105
856 -> 864 -0.10440
858 -> 868 0.21158
859 -> 863 -0.12271
860 -> 867 0.17070
860 -> 868 -0.30845
Excited State 25: Singlet-B3 3.4362 eV 360.81 nm f=0.0204 <S**2>=0.000
853 -> 861 0.10723
853 -> 864 -0.10047

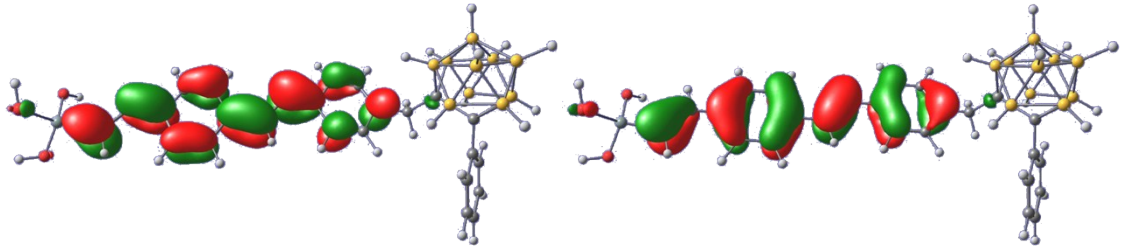
854 -> 865 0.23644
855 -> 868 0.35617
856 -> 863 -0.26800
856 -> 865 -0.11120
857 -> 867 0.22222
858 -> 866 0.16583
859 -> 864 -0.10574
860 -> 866 -0.31089
Excited State 26: Singlet-A 3.4364 eV 360.80 nm f=0.0000 <S**2>=0.000
853 -> 863 0.13412
853 -> 865 0.43494
854 -> 861 0.20207
855 -> 866 -0.12877
856 -> 864 0.15876
857 -> 862 -0.13168
858 -> 867 0.29011
860 -> 867 0.26228
Excited State 27: Singlet-B2 3.4365 eV 360.79 nm f=0.0111 <S**2>=0.000
853 -> 867 0.32938
854 -> 862 -0.14619
854 -> 866 -0.23507
855 -> 861 0.12453
855 -> 864 0.14403
856 -> 862 0.20554
856 -> 866 -0.21181
858 -> 863 0.12318
858 -> 865 0.14973
859 -> 867 0.10620
859 -> 868 -0.23593
860 -> 865 0.27515
Excited State 28: Singlet-B1 3.4367 eV 360.76 nm f=0.0125 <S**2>=0.000
853 -> 862 -0.18394
854 -> 867 0.14370
854 -> 868 0.22011
855 -> 863 -0.22850
856 -> 867 -0.27841
856 -> 868 0.27114
857 -> 865 0.22795
858 -> 864 -0.12319
859 -> 866 0.31189
Excited State 29: Singlet-B1 3.4399 eV 360.43 nm f=0.9830 <S**2>=0.000
853 -> 862 -0.19245
853 -> 866 -0.10832
854 -> 867 0.29503
854 -> 868 -0.15890
855 -> 863 0.13778
856 -> 867 -0.14645
856 -> 868 -0.15099
857 -> 865 0.33200
859 -> 866 -0.25067
860 -> 864 -0.27597
Excited State 30: Singlet-B2 3.4403 eV 360.39 nm f=1.4304 <S**2>=0.000
853 -> 867 0.25371
854 -> 866 0.10475
855 -> 864 -0.20421
856 -> 862 0.20205
856 -> 866 0.32905
857 -> 864 -0.14080
858 -> 863 -0.14745
858 -> 865 0.34212
859 -> 867 -0.16075
859 -> 868 0.18085

DFT-optimized structure of trimethoxysilyl-vinyl-stilbene-carboranes: unsusbtituted and phenyl-substituted compounds:



DFT-calculated frontier MOs of phenyl-substituted trimethoxysilyl-vinyl-stilbene-carborane

LUMO: HOMO:



Excited States of trimethoxysilyl-vinyl-stilbene-carborane **with (Energies, oscillator strengths and composition) according to the TD-DFT calculations**

a) Unsubstituted compound:

Excited State 1: Singlet-A 3.4316 eV 361.30 nm f=1.7196 <S**2>=0.000
115 ->116 0.70599
Excited State 2: Singlet-A 4.2729 eV 290.16 nm f=0.0010 <S**2>=0.000
113 ->116 0.27532
114 ->116 0.41105
115 ->117 0.45904
115 ->119 -0.18275
Excited State 3: Singlet-A 4.3207 eV 286.95 nm f=0.0039 <S**2>=0.000
112 ->116 0.10510
113 ->116 0.49540
114 ->116 -0.21144
115 ->117 -0.22592
115 ->118 0.17573
115 ->119 -0.32550
Excited State 4: Singlet-A 4.3896 eV 282.45 nm f=0.0049 <S**2>=0.000
112 ->116 0.40546
112 ->117 -0.10174
113 ->116 -0.11701
114 ->116 0.16981
114 ->118 0.10660
115 ->118 0.49864
115 ->119 0.10808

a) Ph-substituted compound:

Excited State 1: Singlet-A 3.4267 eV 361.82 nm f=1.7533 <S**2>=0.000
135 ->136 0.70564
Excited State 2: Singlet-A 3.9209 eV 316.22 nm f=0.0022 <S**2>=0.000
135 ->137 0.70216

Excited State 3: Singlet-A 4.2842 eV 289.40 nm f=0.0066 <S**2>=0.000
132 ->136 -0.11341
133 ->136 0.23975
134 ->136 0.41641
135 ->139 0.45712
135 ->141 -0.18737
Excited State 4: Singlet-A 4.3276 eV 286.50 nm f=0.0023 <S**2>=0.000
133 ->136 0.50573
134 ->136 -0.18709
135 ->139 -0.21305
135 ->140 0.19203
135 ->141 -0.33298
Excited State 5: Singlet-A 4.4142 eV 280.88 nm f=0.0046 <S**2>=0.000
132 ->136 0.46152
134 ->136 0.17656
135 ->138 0.23247
135 ->140 0.38919
135 ->141 0.14278
Excited State 6: Singlet-A 4.4863 eV 276.36 nm f=0.0002 <S**2>=0.000
132 ->136 -0.15803
135 ->138 0.65973
135 ->140 -0.14315