

Supporting Information for manuscript

Phthalocyanine- and subphthalocyanine-based functional nanocarbon materials: electronic structures and optical properties

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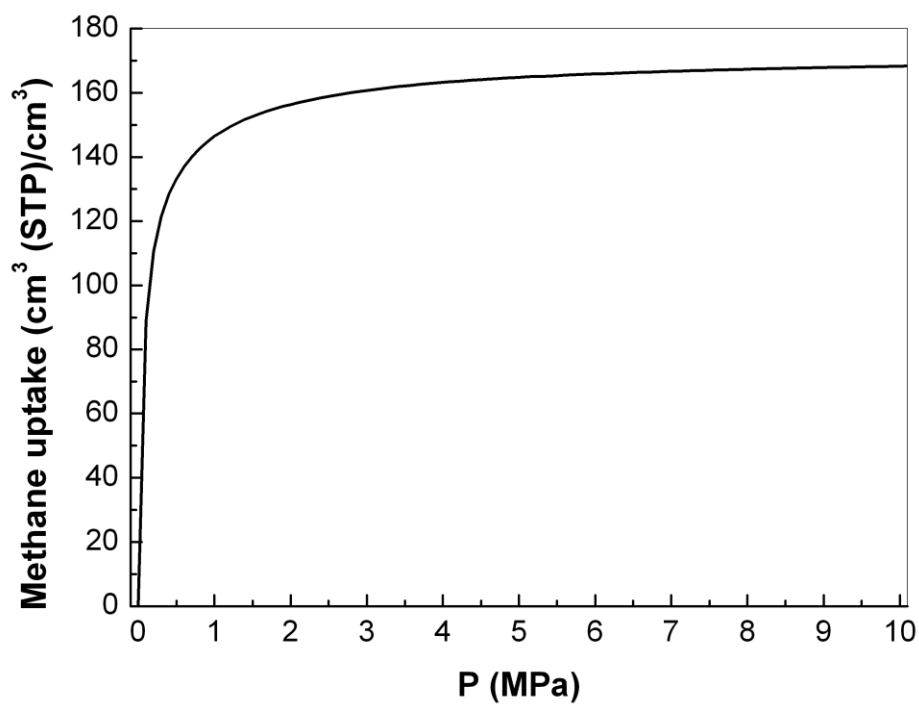


Figure S1. Adsorption isotherm of CH₄ in gas clathrate hydrate at T=298 K.

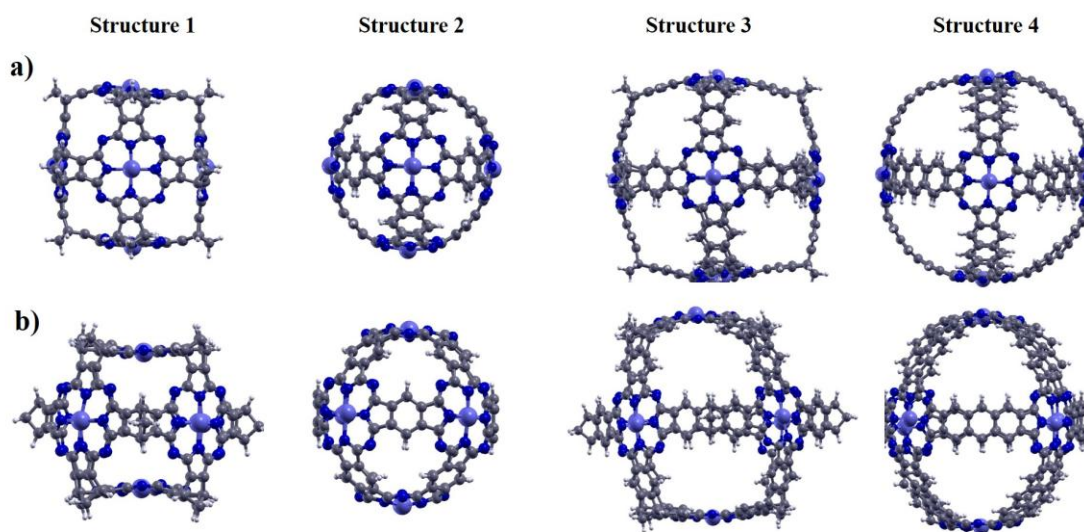


Figure S2. Structures of the nanocages 1-4 after *ab initio* MD simulations: (a)-(b) perspective views.

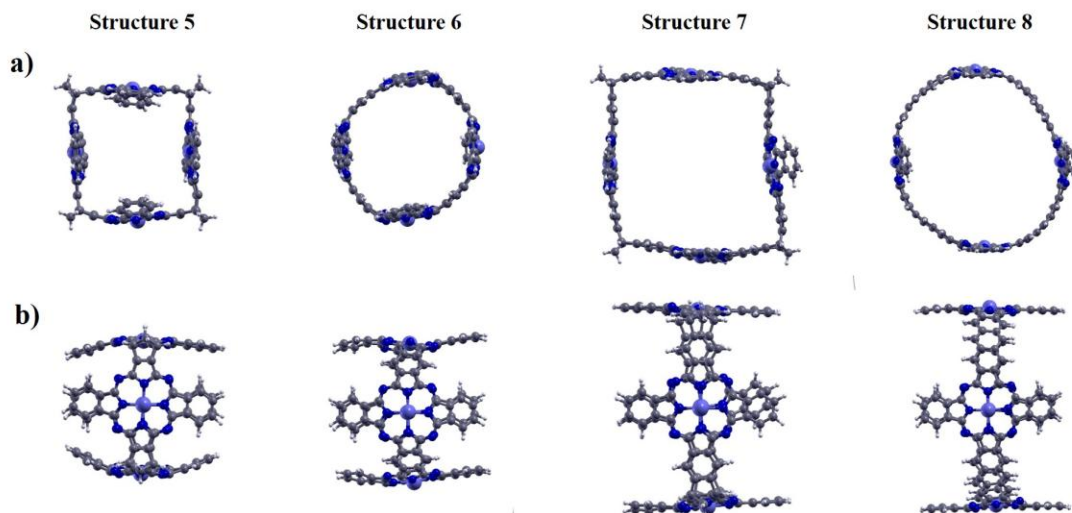


Figure S3. Structure of the nanobarrels **5-8** after *ab initio* MD simulations: (a)-(b) perspective views.

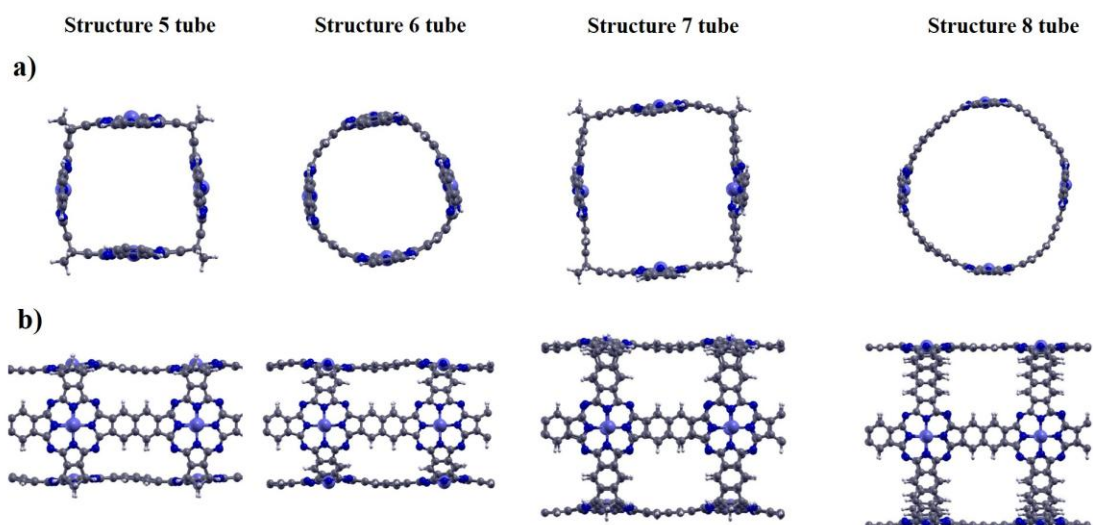


Figure S4. Structures of the nanotubes **5t-8t** after *ab initio* MD simulations: (a)-(b) perspective views.

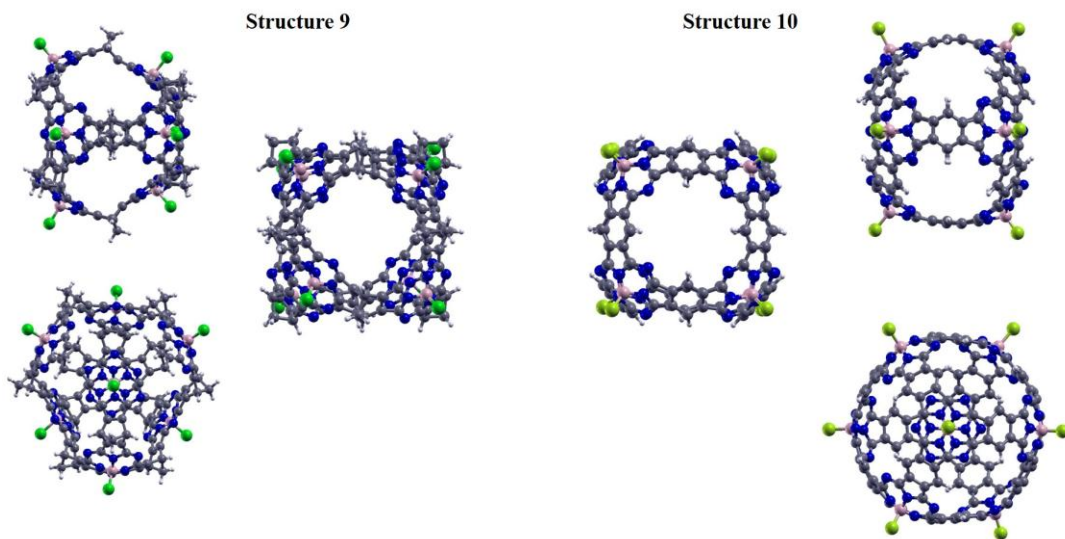


Figure S5. Perspective views of nanocages **9-10** after *ab initio* MD simulations.

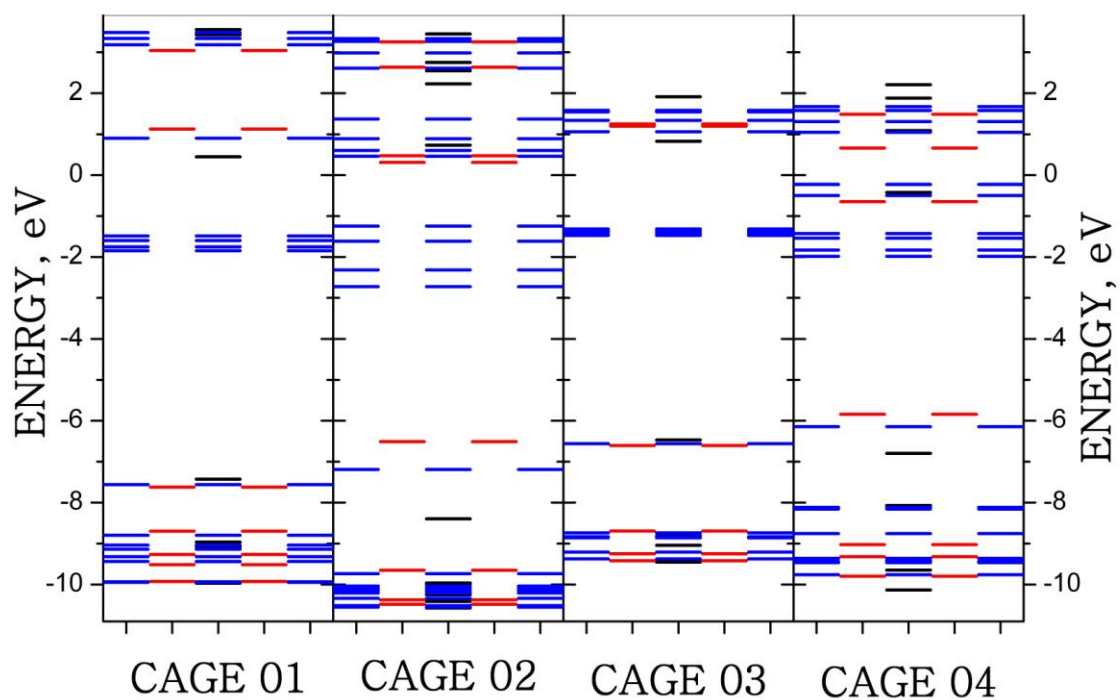


Figure S6: DFT predicted energy diagram for nanostructures **1 - 4**.

Cube_n structure, MOs

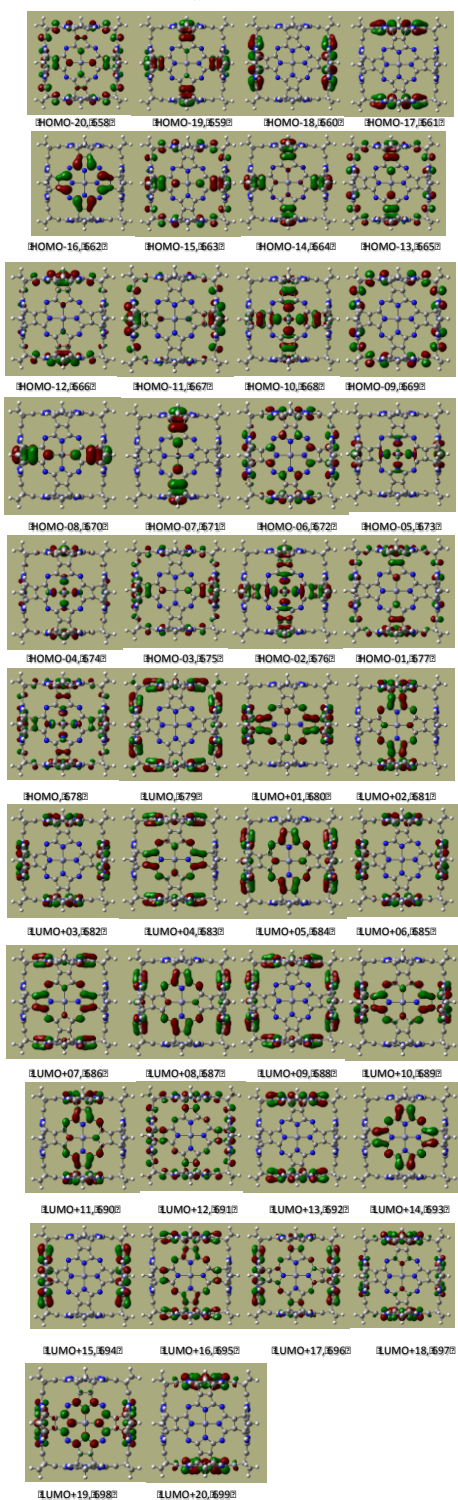


Figure S7. DFT predicted MOs for nanostructure 1.

Cube_h Structure 2, MOs

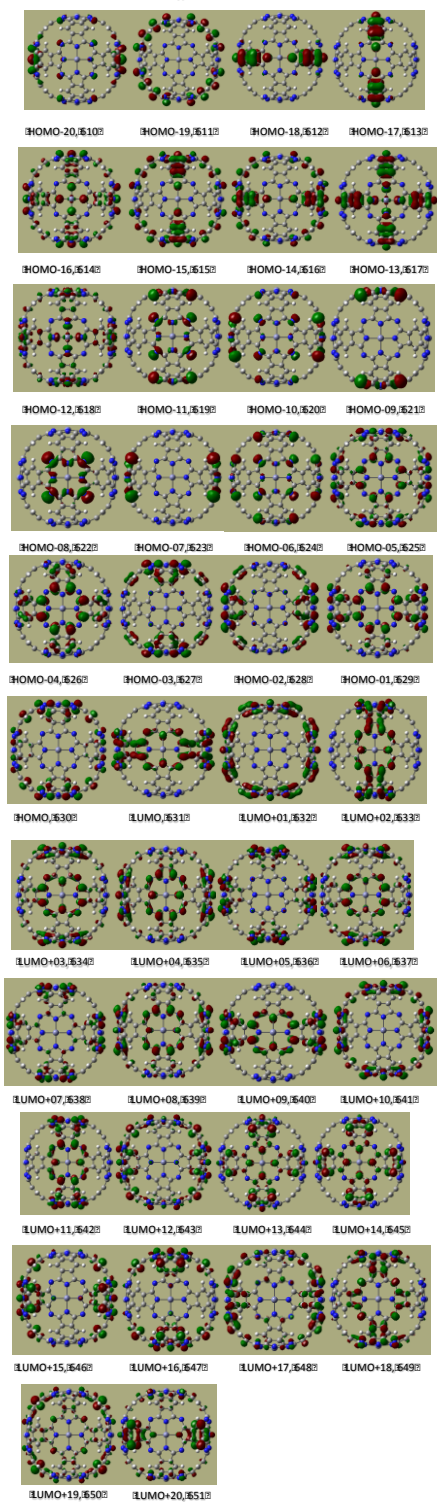


Figure S8. DFT predicted MOs for nanostructure 2.

Cube_h structure MOs

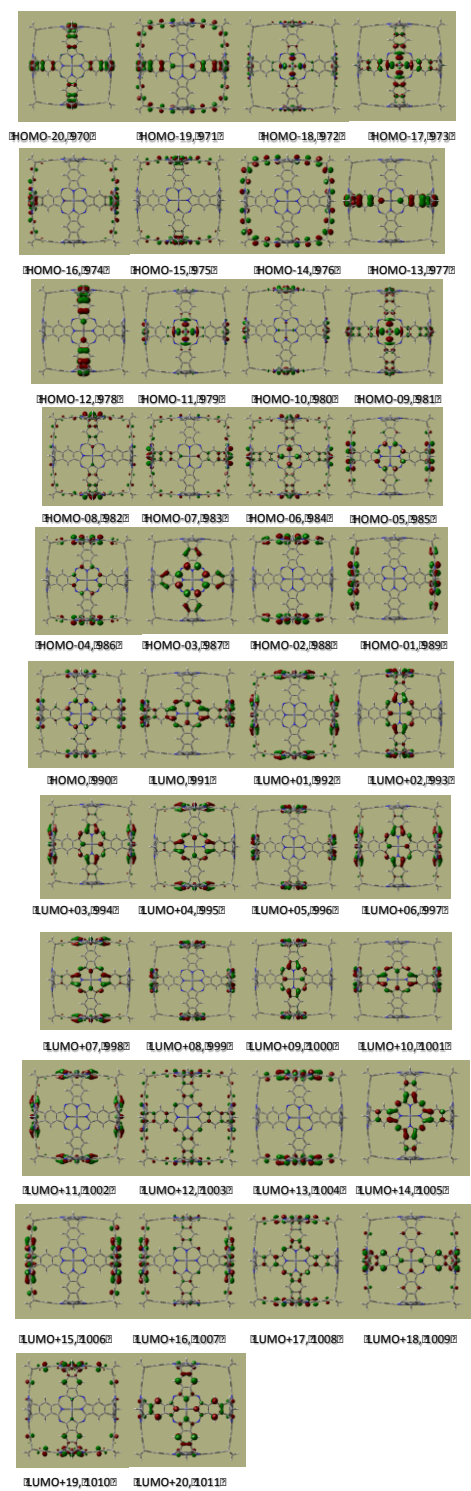


Figure S9. DFT predicted MOs for nanostructure 3.

Cube_h structure, MOs

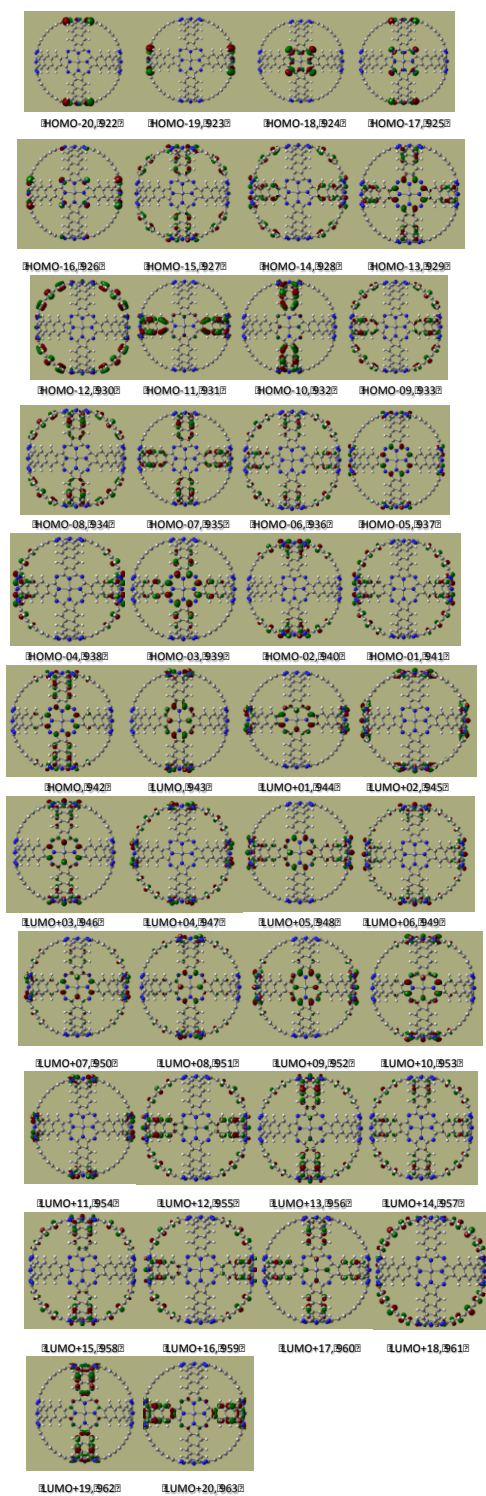


Figure S10. DFT predicted MOs for nanostructure 4.

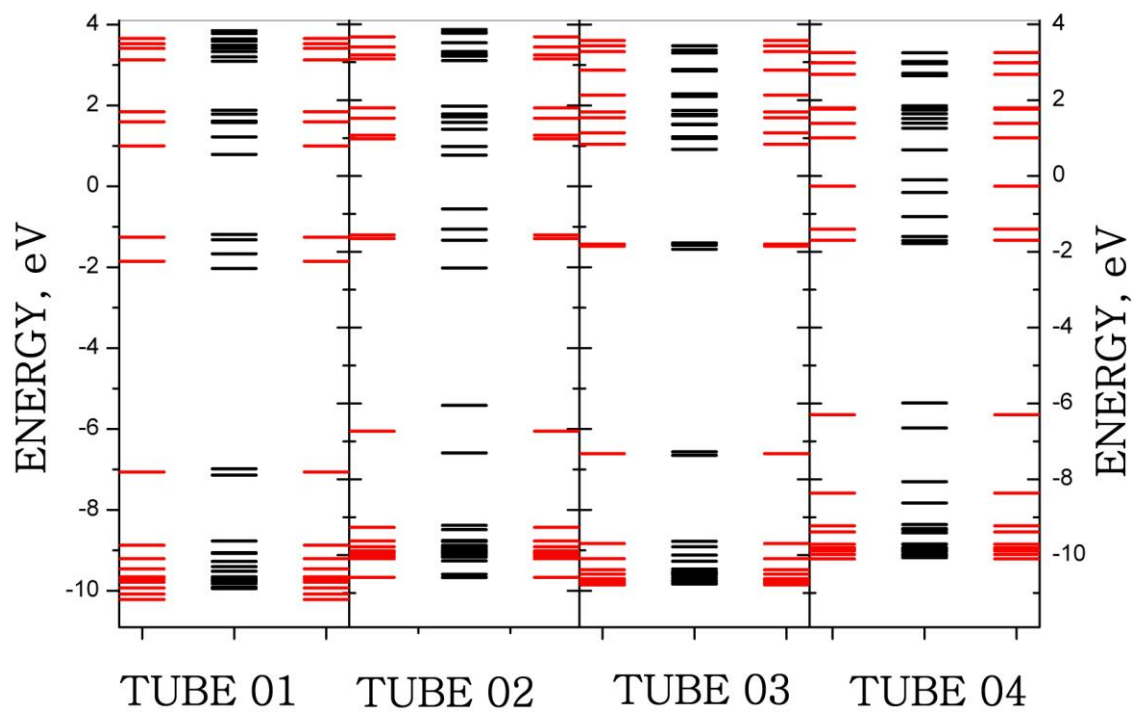


Figure S11. DFT predicted energy diagram for nanostructures 5-8.

Tube_{4h} Structure 7, MOs

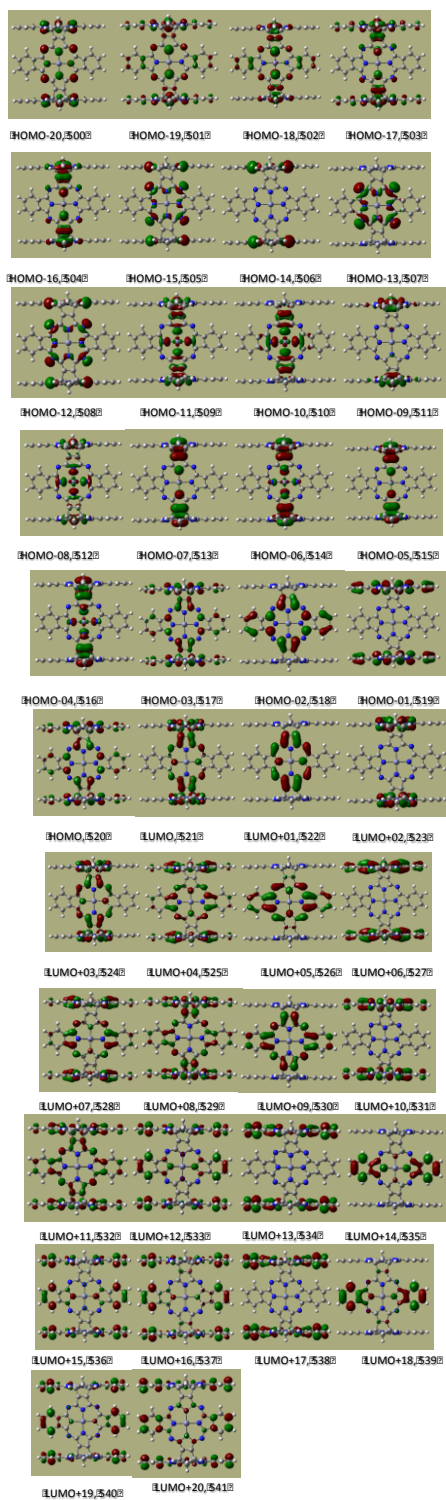


Figure S12. DFT predicted MOs of nanostructure 5.

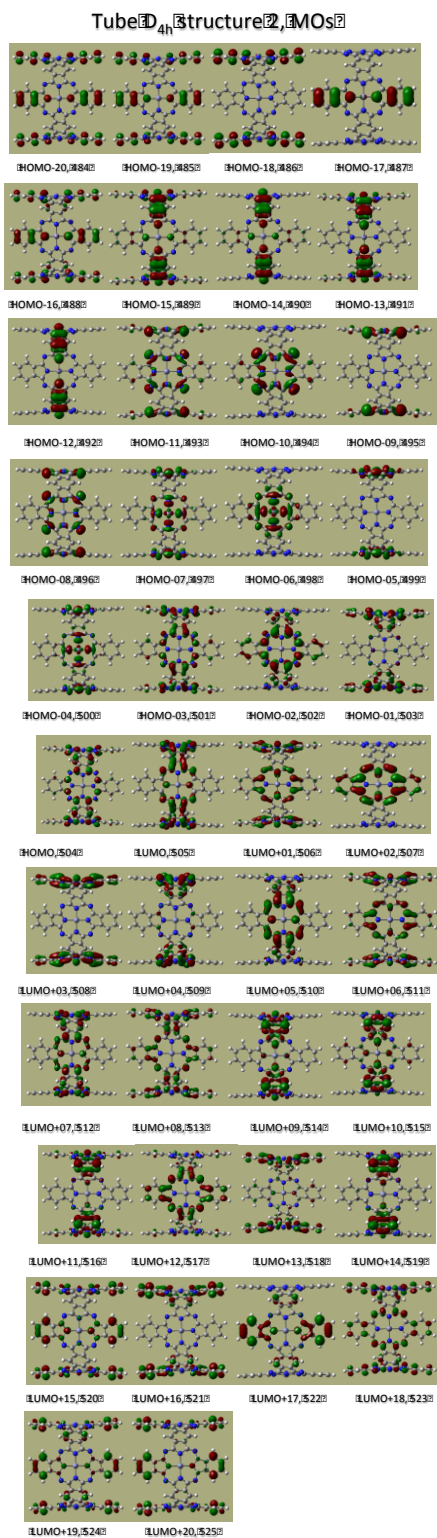


Figure S13. DFT predicted MOs of nanostructure 6.

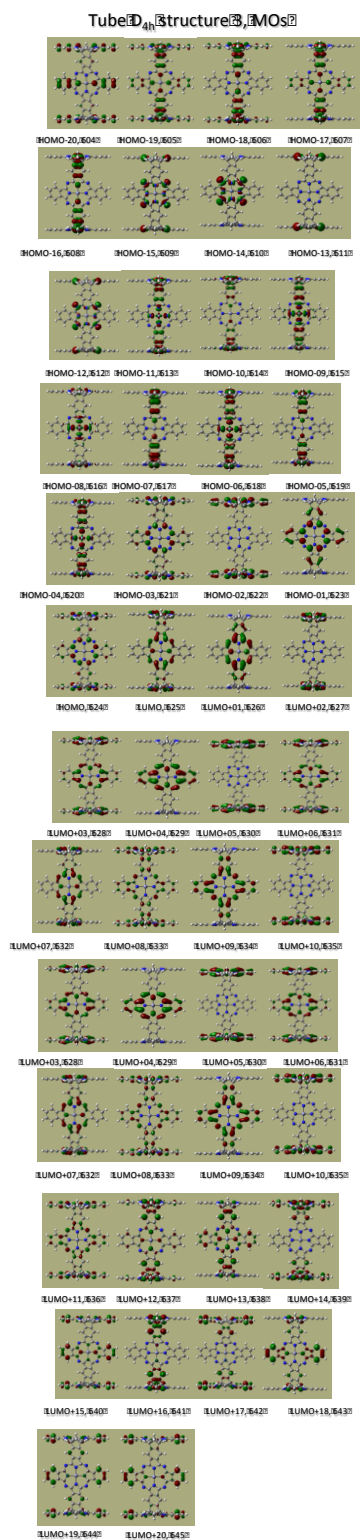


Figure S14. DFT predicted MOs of nanostructure 7.

Tube 41 structure MOs

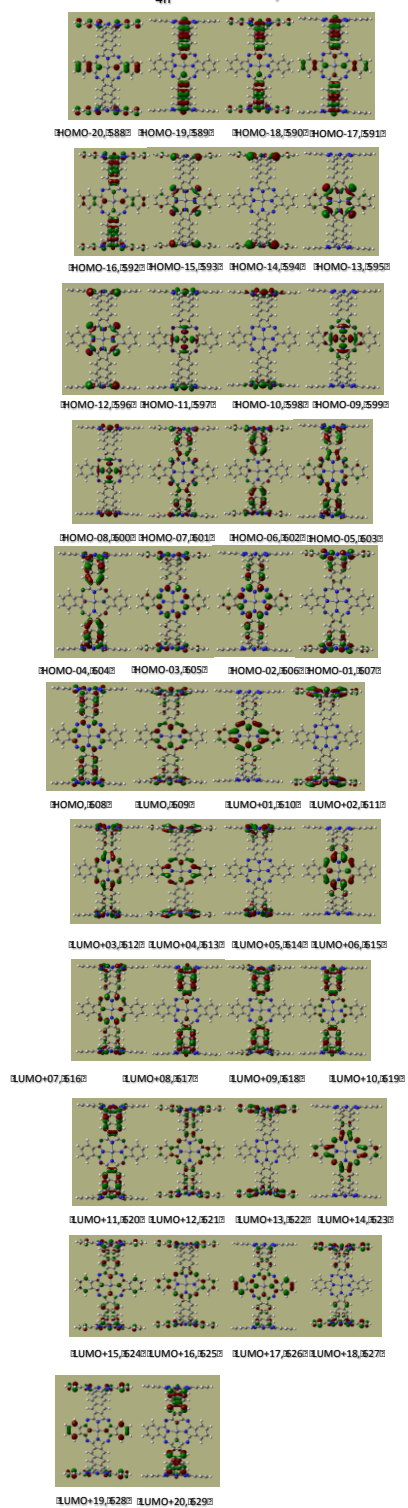


Figure S15. DFT predicted MOs of nanostructure 8.

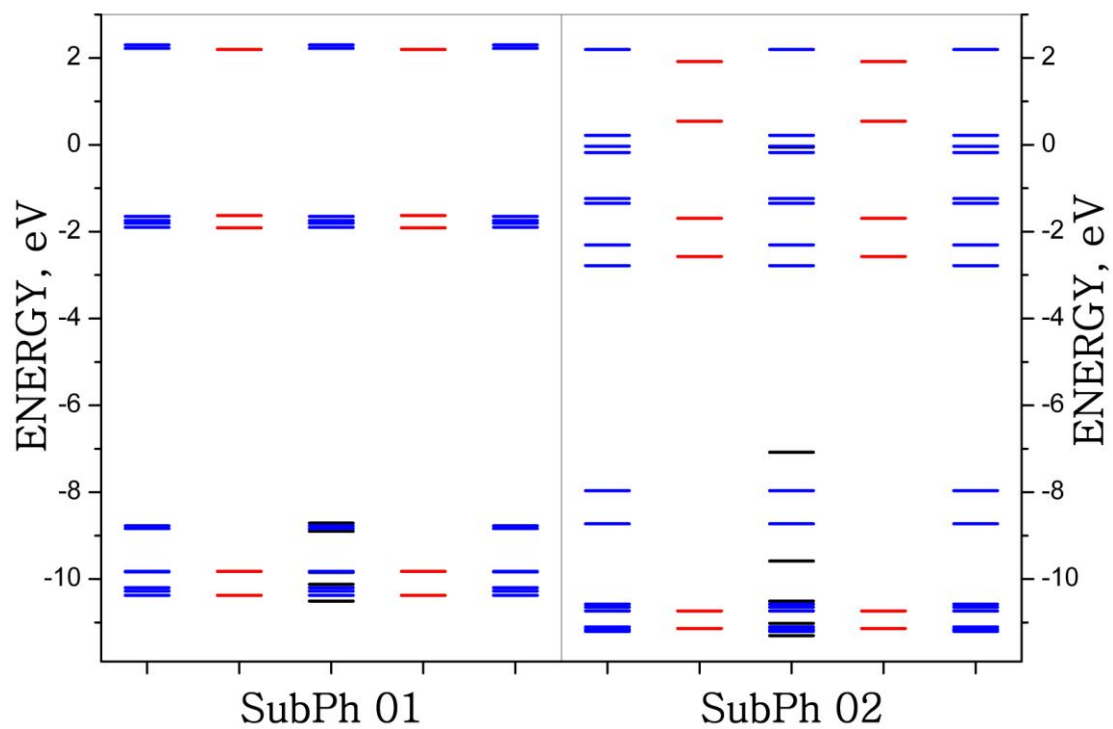


Figure S16. DFT predicted energy diagram of nanostructures **9** and **10**.

SubPh₁₀ Structure MOs

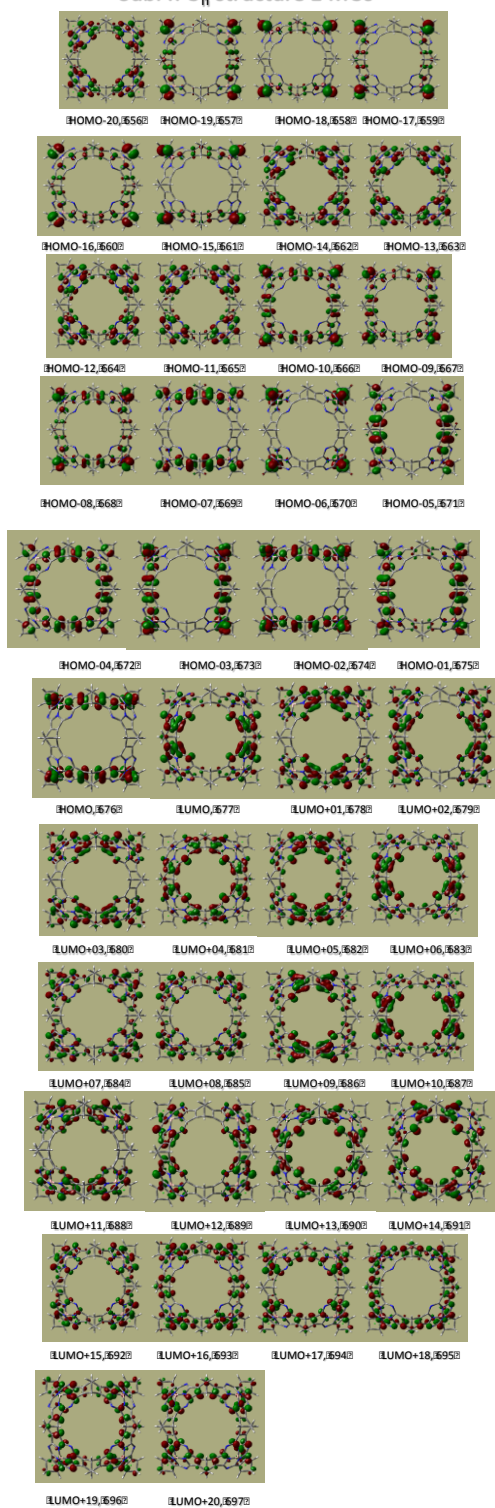


Figure S17. DFT predicted MOs for nanostructure 9.

SubPh_n structure 2, MOs

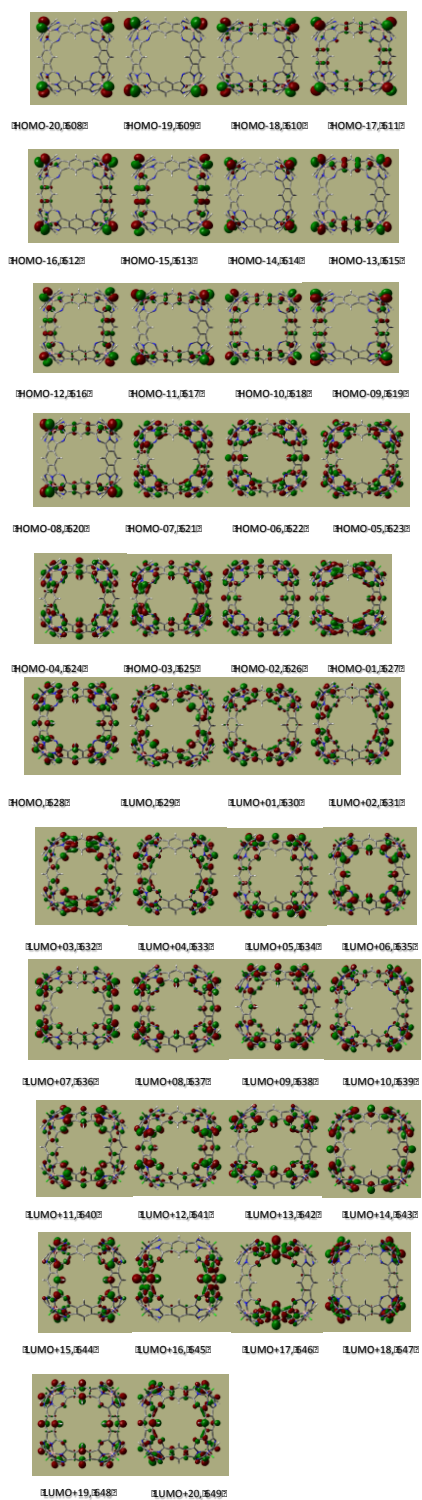


Figure S18. DFT predicted MOs for nanostructure 10.

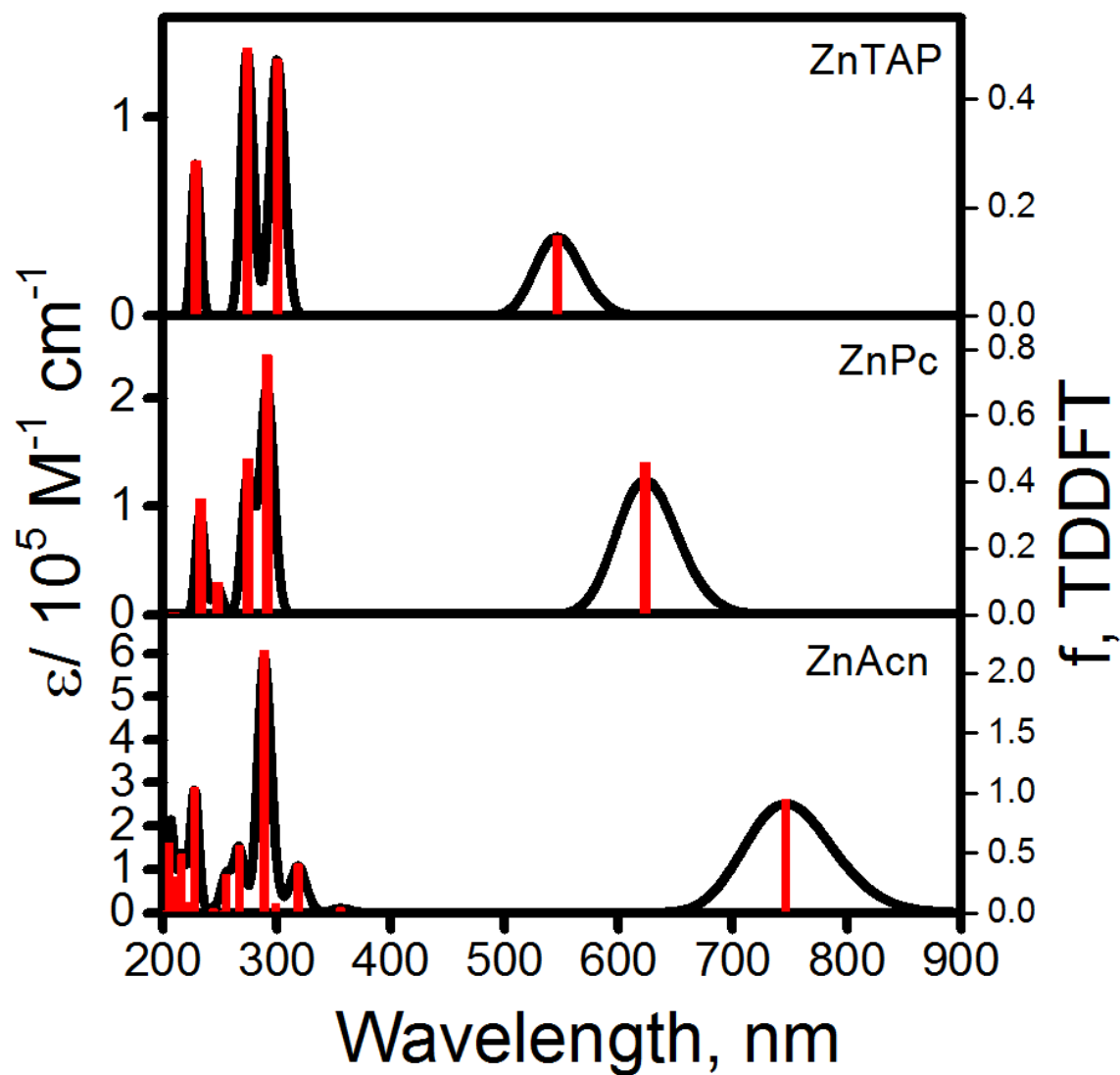


Figure S19. TDDFT-predicted UV-vis spectra of monomeric building blocks of ZnTAP, ZnPc, and ZnAcN.

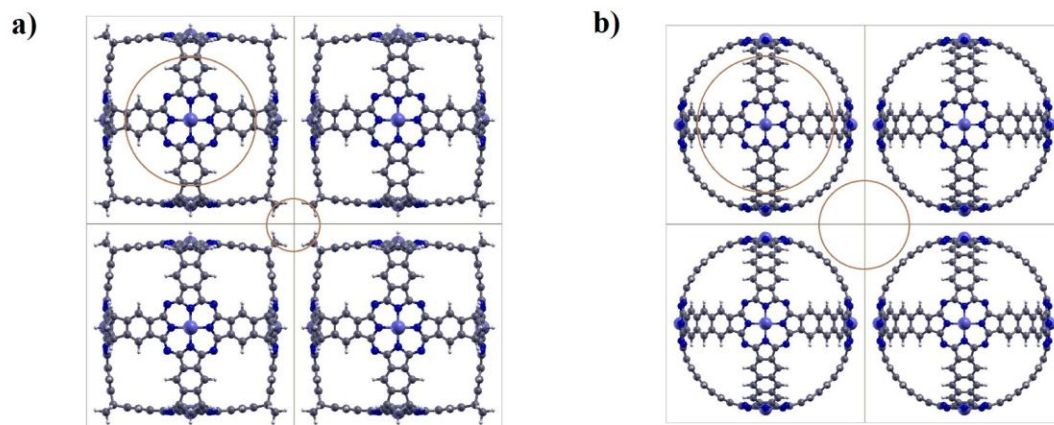


Figure S20. Periodic structures of molecular crystals: (a) 3 and (b) 4 cages used for adsorption calculations. The brown cycles show the adsorption spaces due to crystal formation.

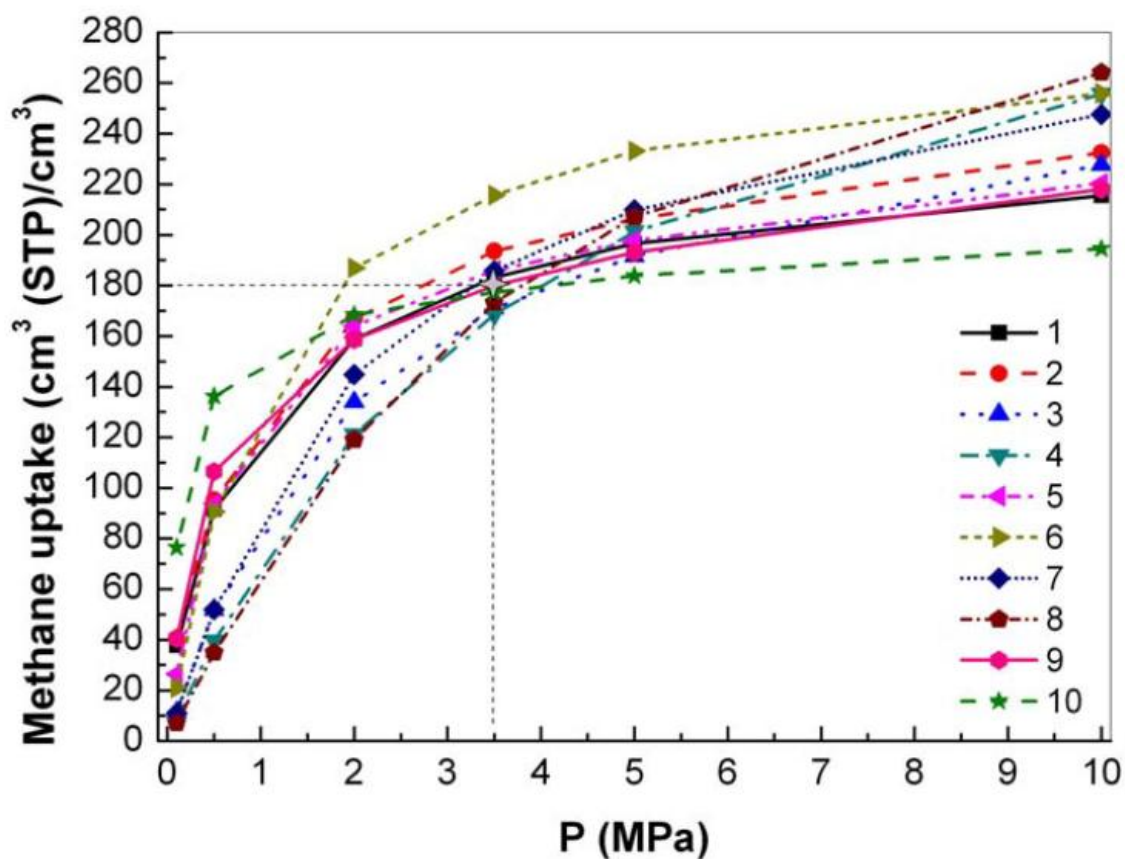


Figure S21. Methane adsorption isotherms for nanocages 1 - 10.

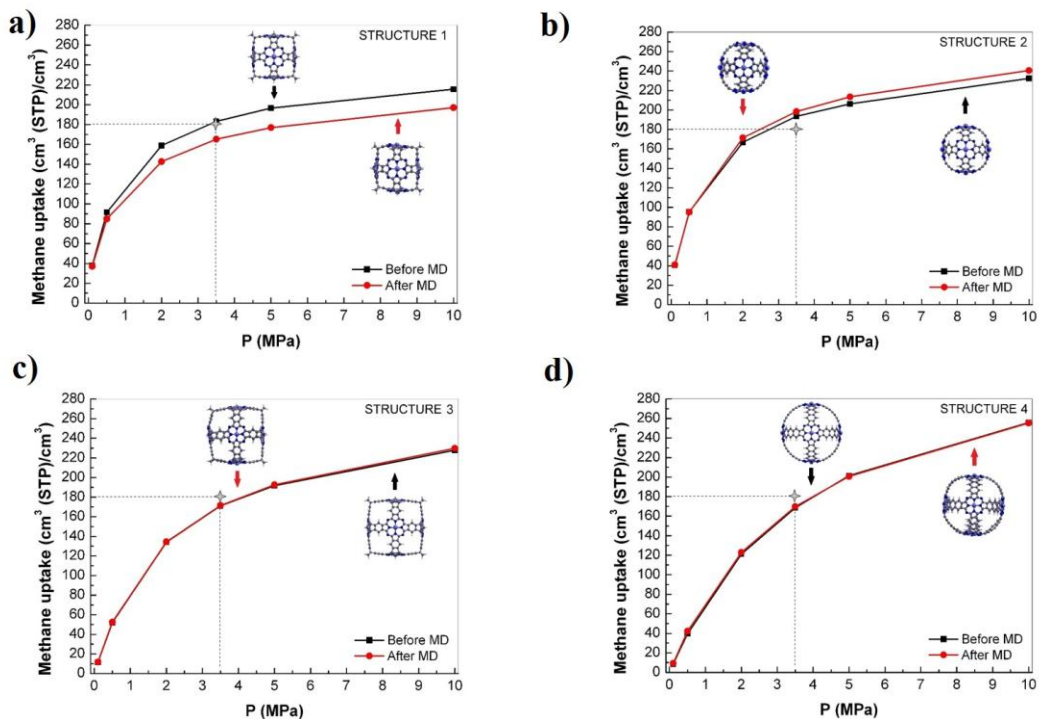


Figure S22. Adsorption isotherm of CH₄ in: (a) 1; (b) 2; (c) 3 and (d) 4 nanocages at T=298 K. Four-point star indicates the DOE target.

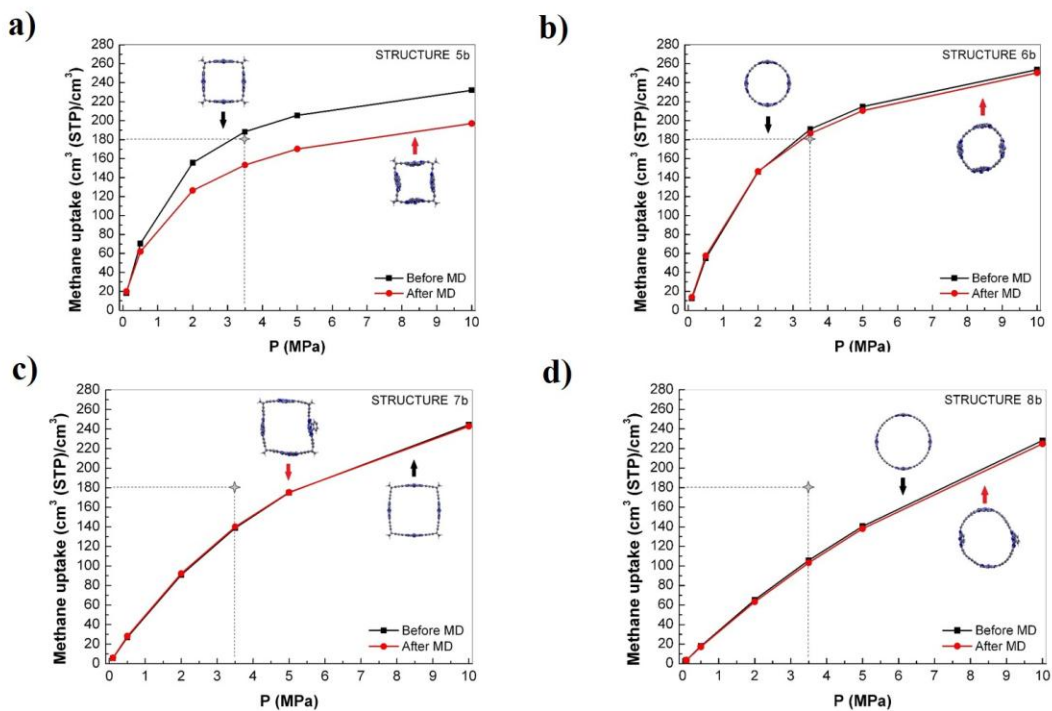


Figure S23. Adsorption isotherm of CH₄ for: (a) 5; (b) 6; (c) 7 and (d) 8 nanobarrels at T=298 K. Four-point star indicates the DOE target.

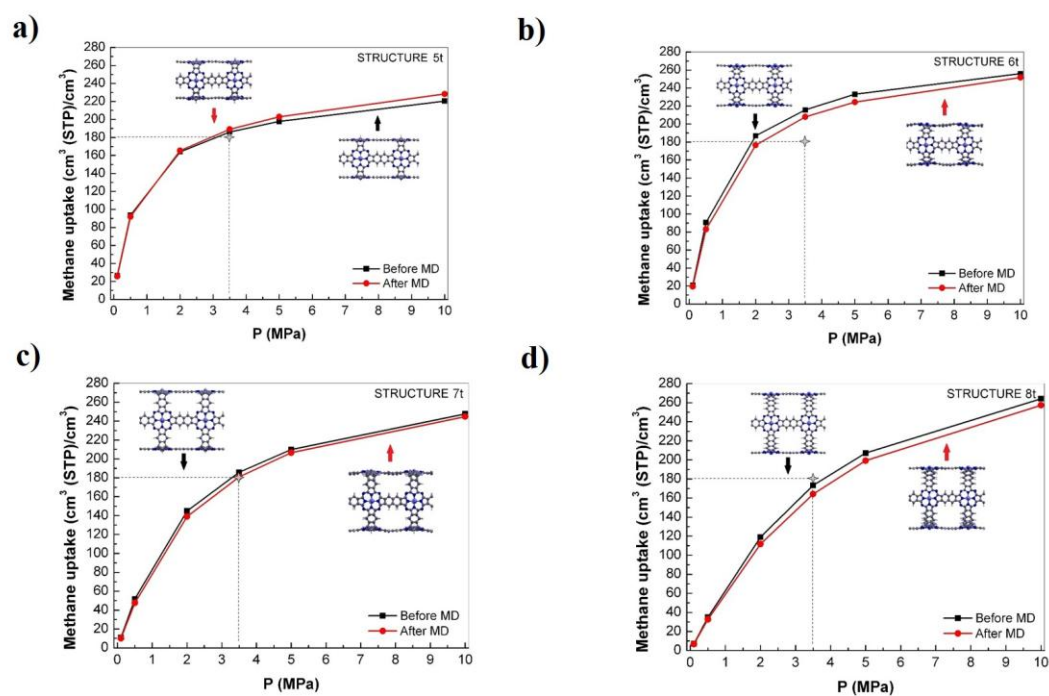


Figure S24. Adsorption isotherm of CH₄ for: (a) 5; (b) 6; (c) 7 and (d) 8 nanotubes at T=298 K. Four-point star indicates the DOE target.

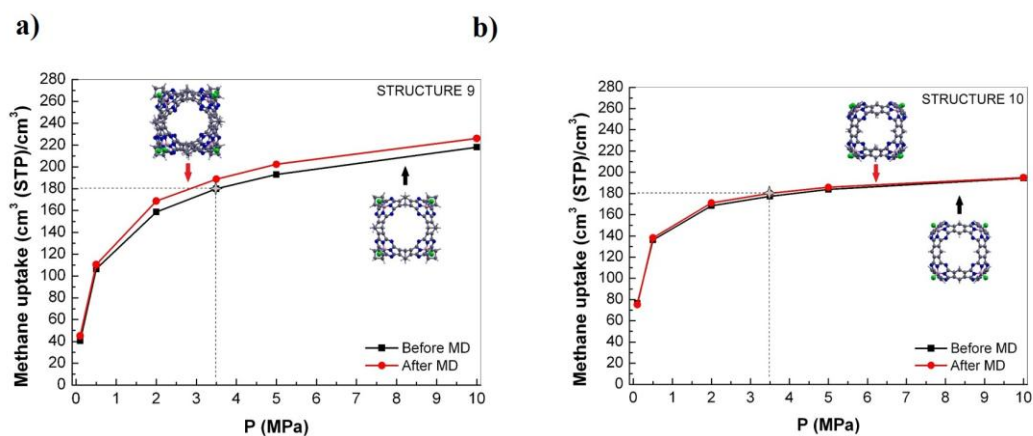


Figure S25. Adsorption isotherm of CH₄ for: (a) 9 and (b) 10 nanocages at T=298 K. Four-point star indicates the DOE target.

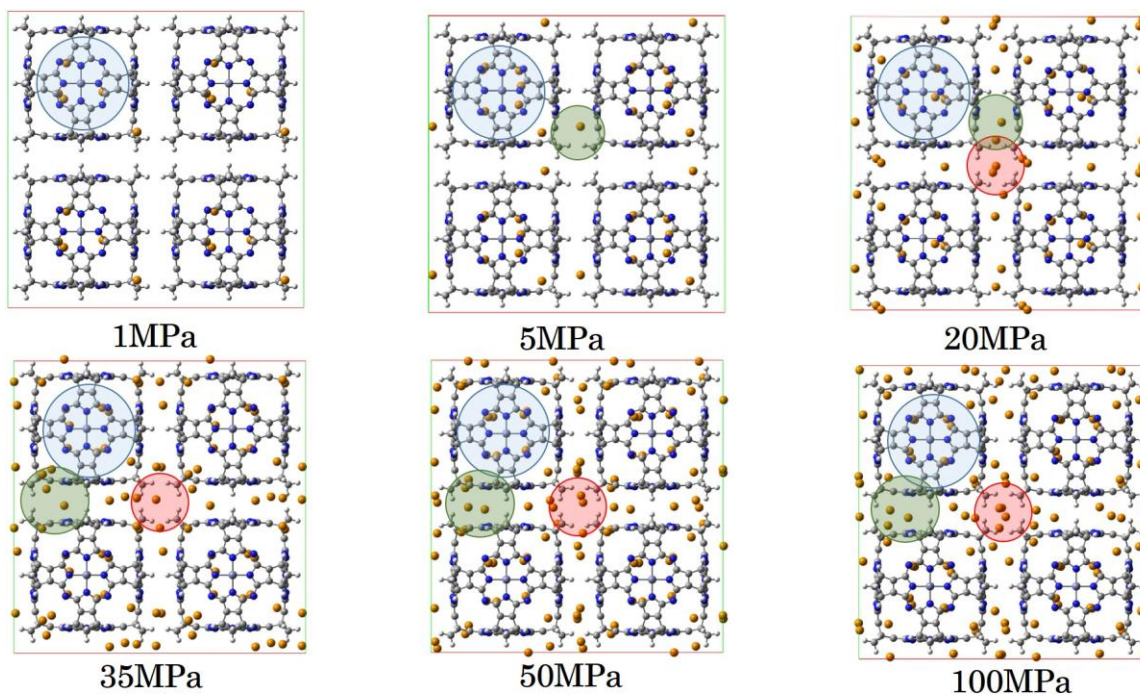


Figure S26. Distribution of the adsorbed methane in nanostructure **1** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

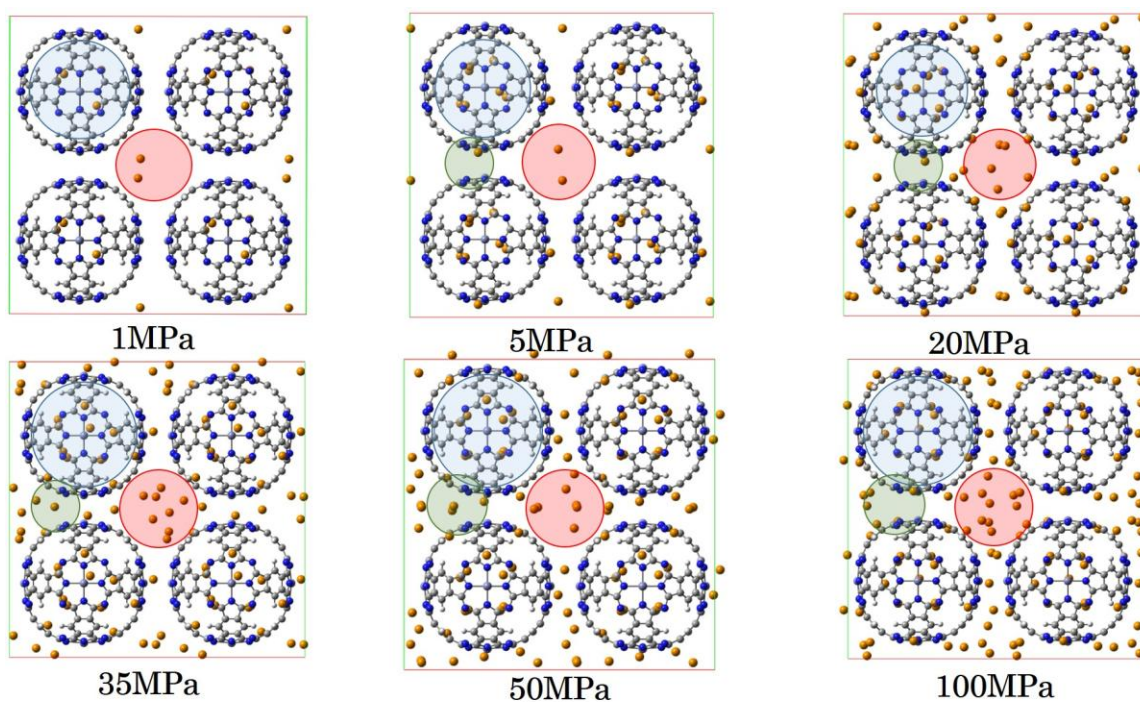


Figure S27. Distribution of the adsorbed methane in nanostructure **2** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

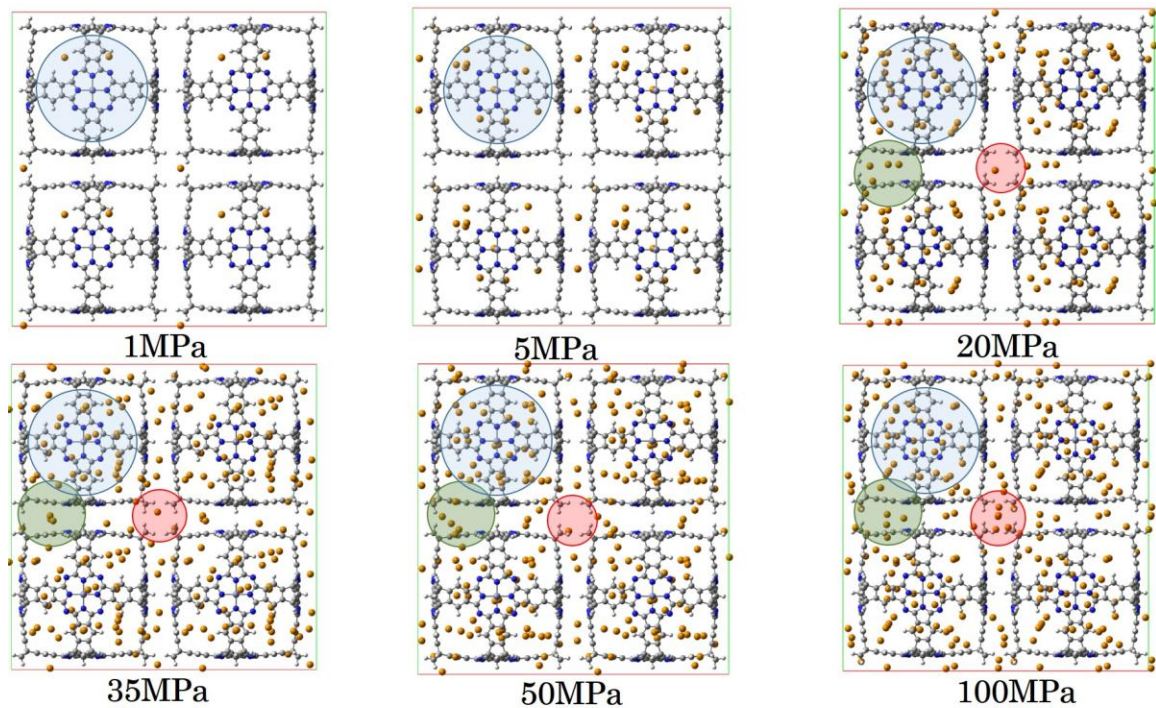


Figure S28. Distribution of the adsorbed methane in nanostructure **3** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

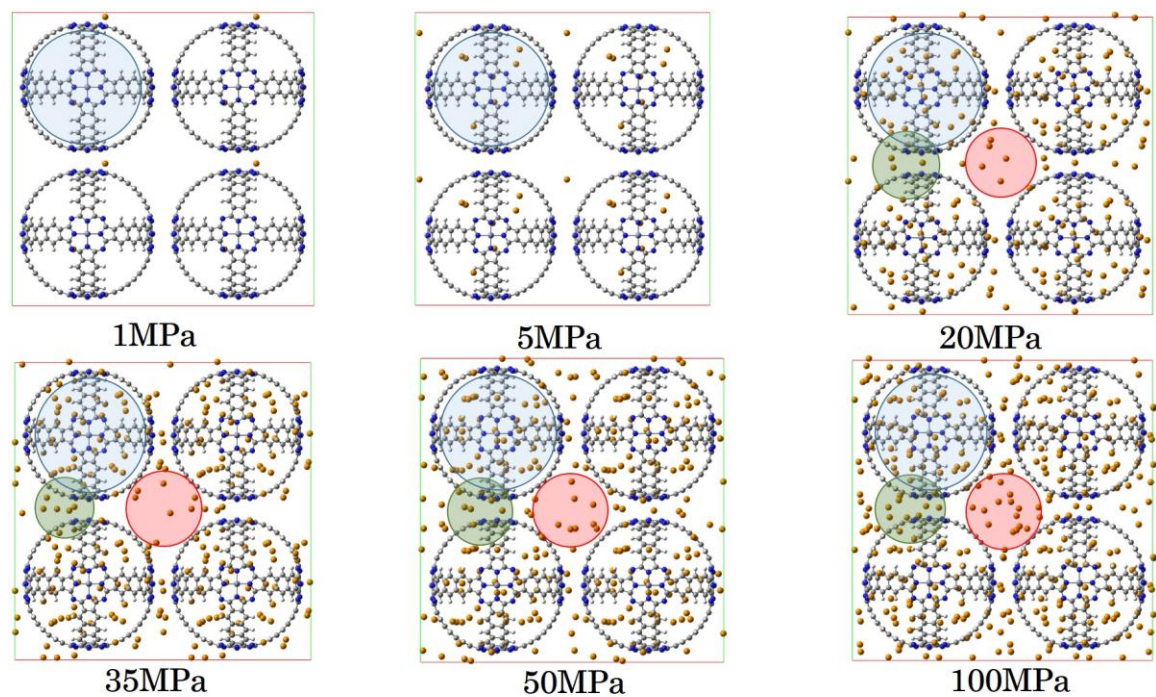


Figure S29. Distribution of the adsorbed methane in nanostructure **4** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

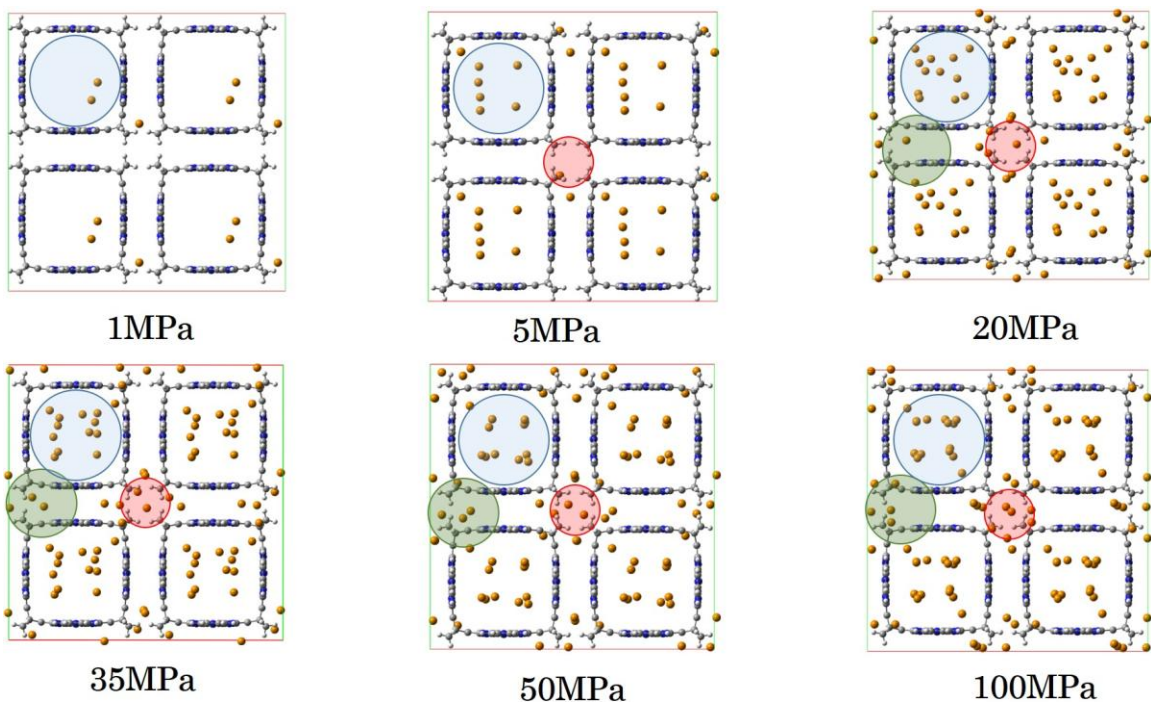


Figure S30. Distribution of the adsorbed methane in nanostructure **5** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

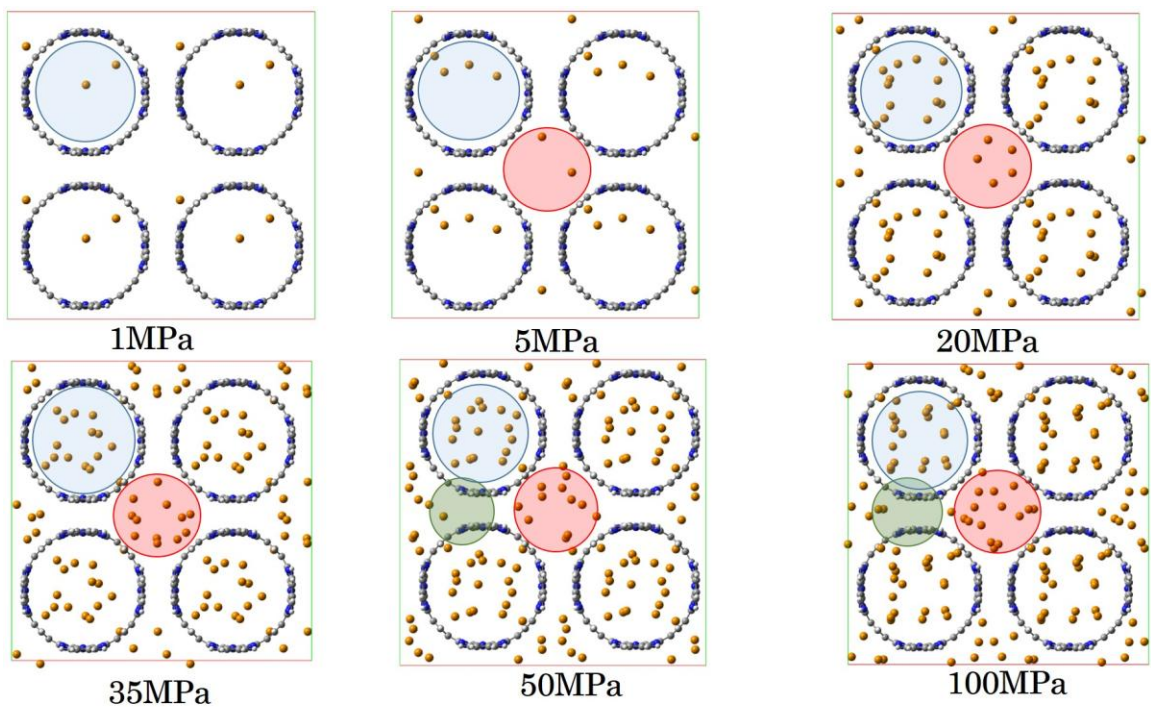


Figure S31. Distribution of the adsorbed methane in nanostructure **6** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

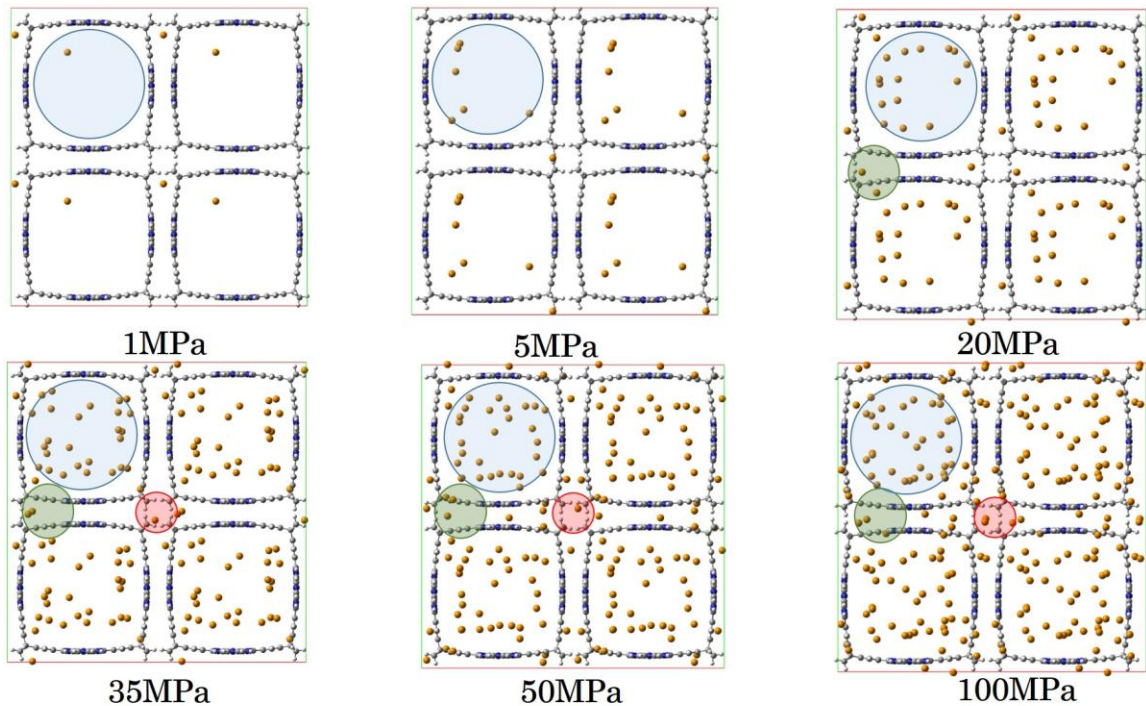


Figure S32. Distribution of the adsorbed methane in nanostructure **7** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

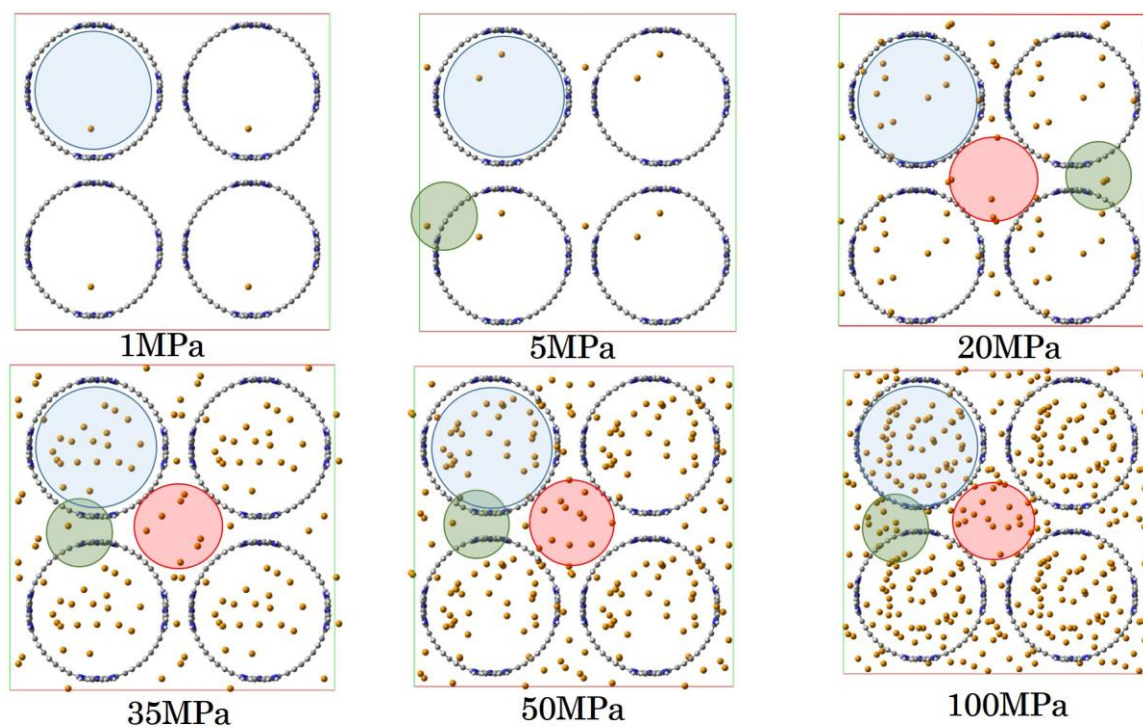


Figure S33. Distribution of the adsorbed methane in nanostructure **8** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

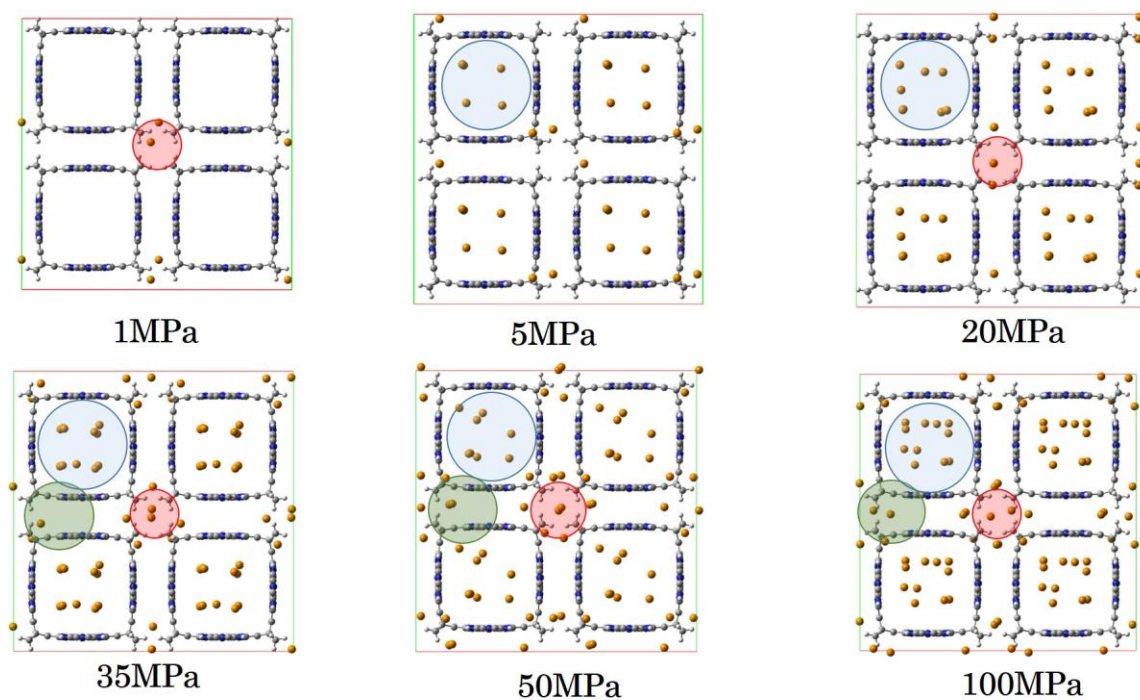


Figure S34. Distribution of the adsorbed methane in nanostructure **5t** in nanotube configuration at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

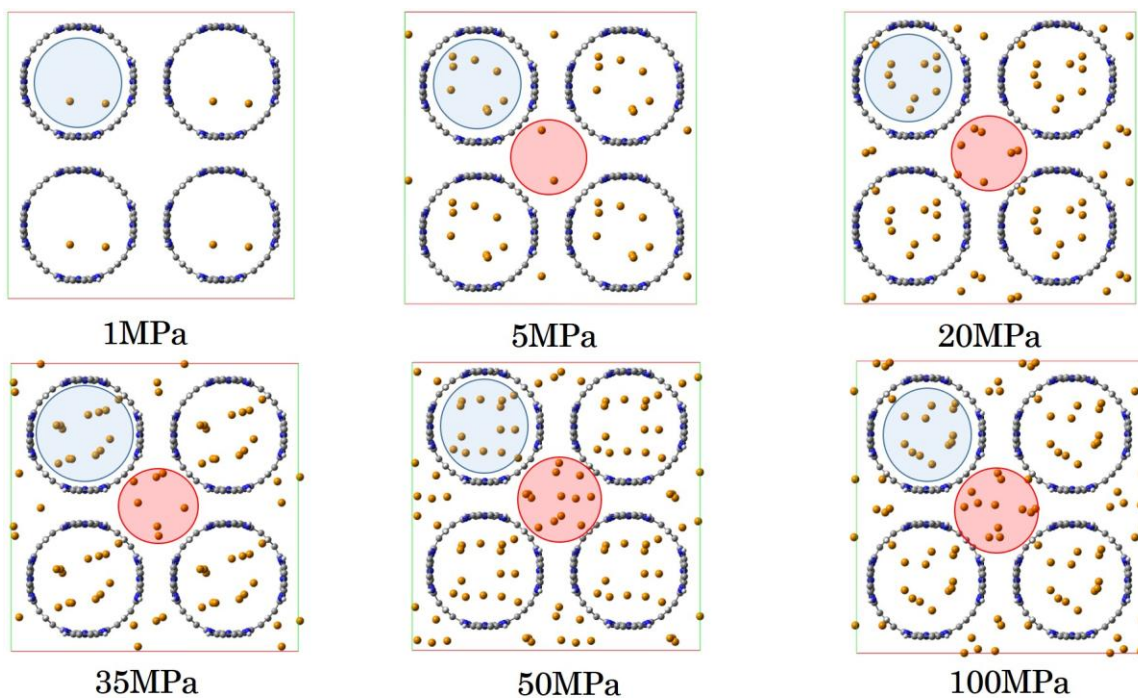


Figure S35. Distribution of the adsorbed methane in nanostructure **6t** in nanotube configuration at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

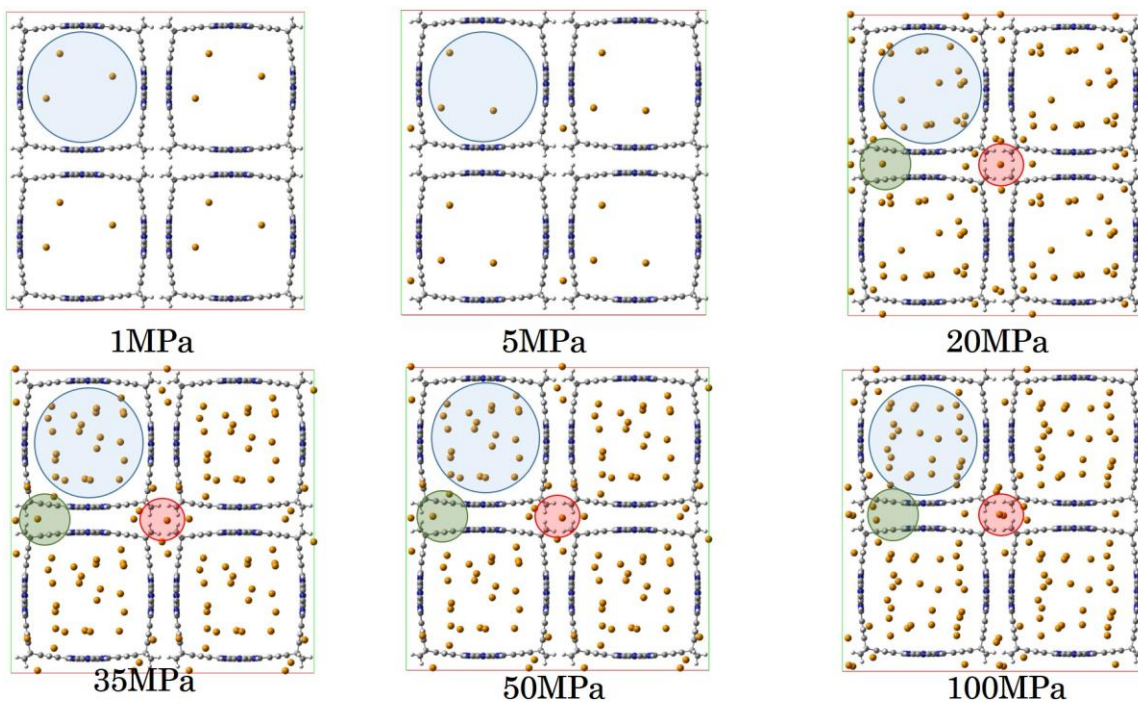


Figure S36. Distribution of the adsorbed methane in nanostructure **7t** in nanotube configuration at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

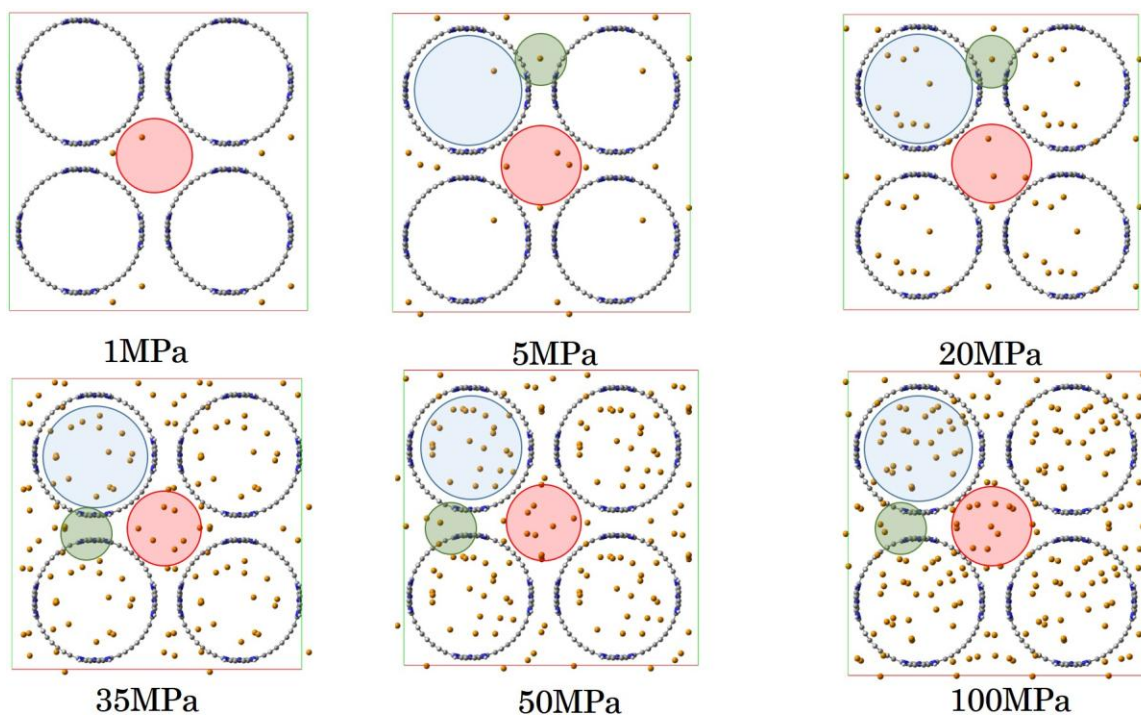


Figure S37. Distribution of the adsorbed methane in nanostructure **8t** in nanotube configuration at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

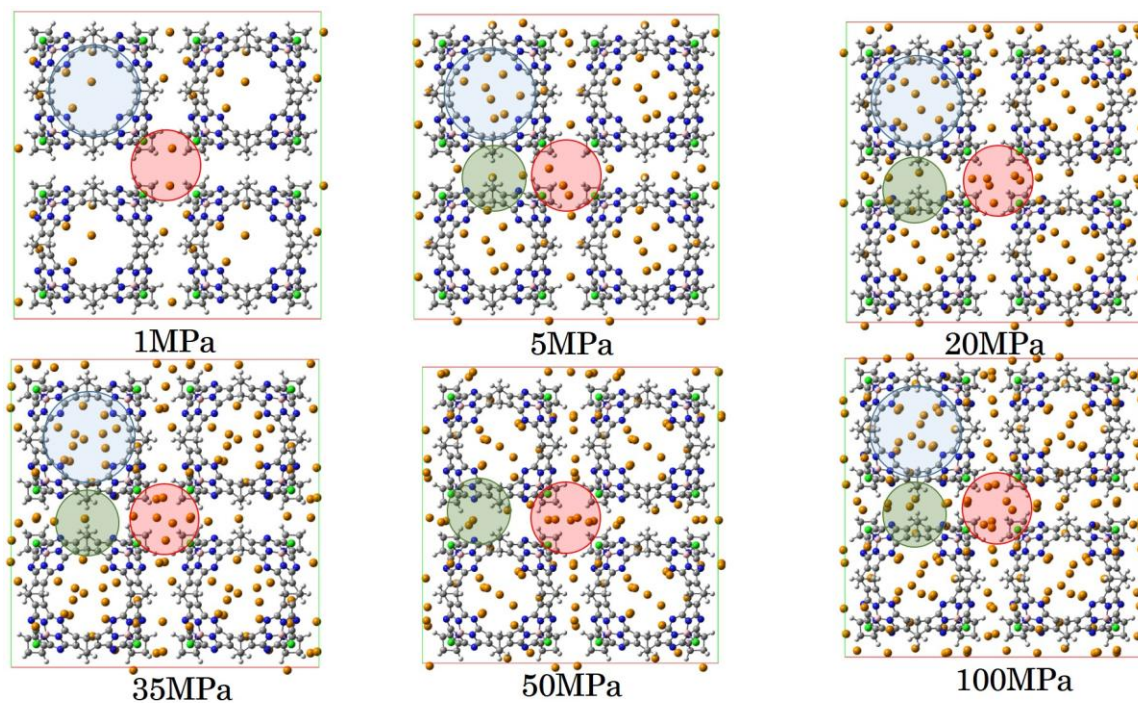


Figure S38. Distribution of the adsorbed methane in nanostructure **9** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

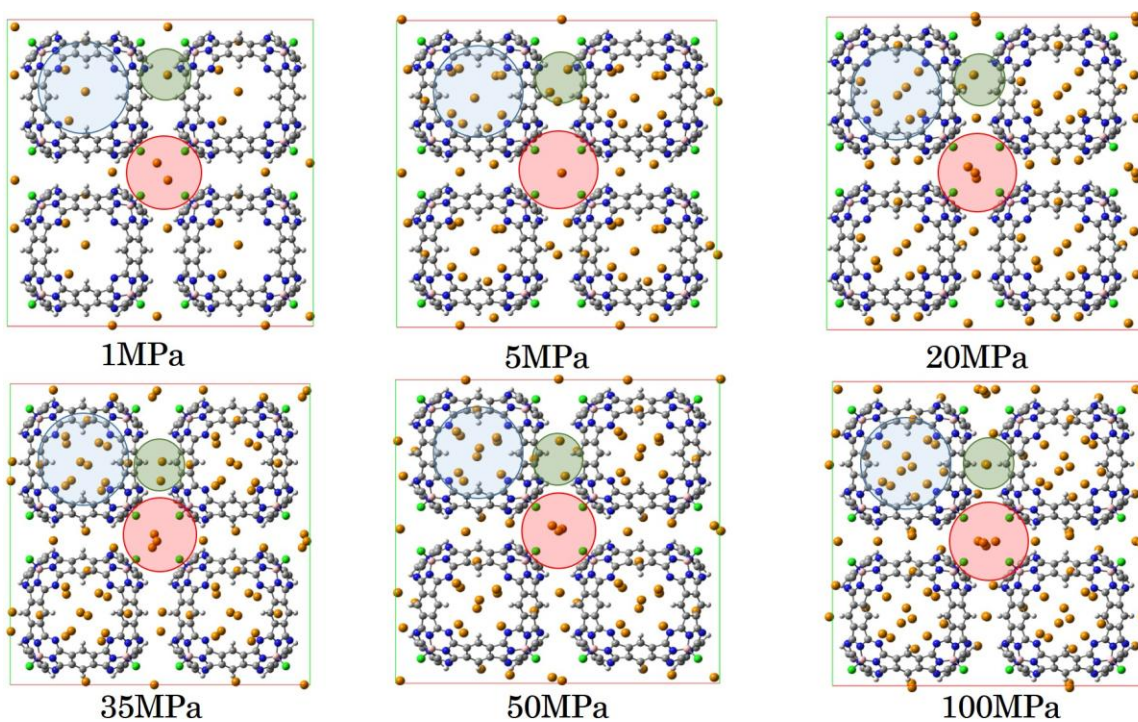
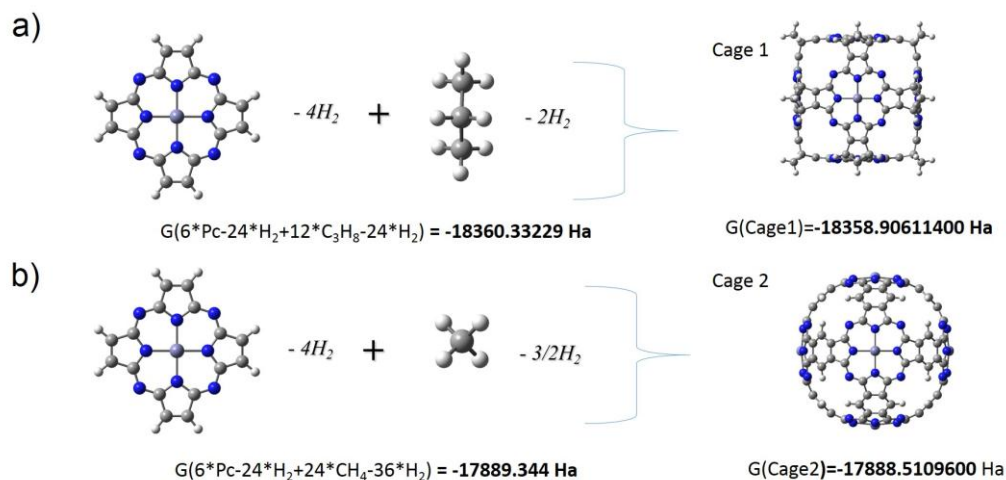


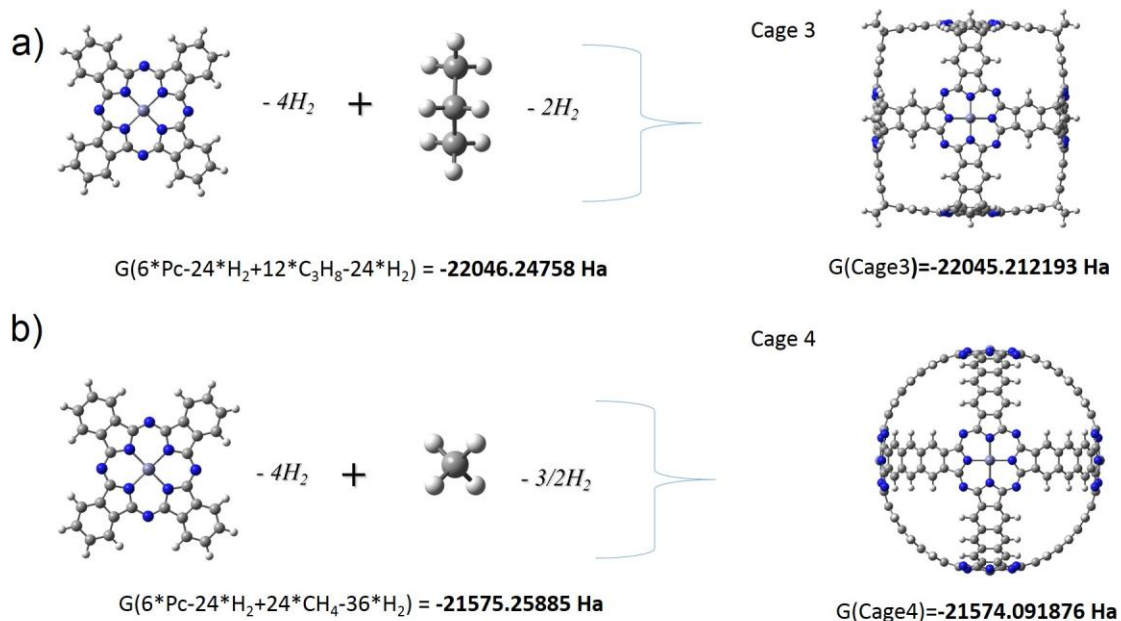
Figure S39. Distribution of the adsorbed methane in nanostructure **10** at different pressures. Blue, red and green cycles show the space in unit cell where the adsorption is occurred.

SCHEME



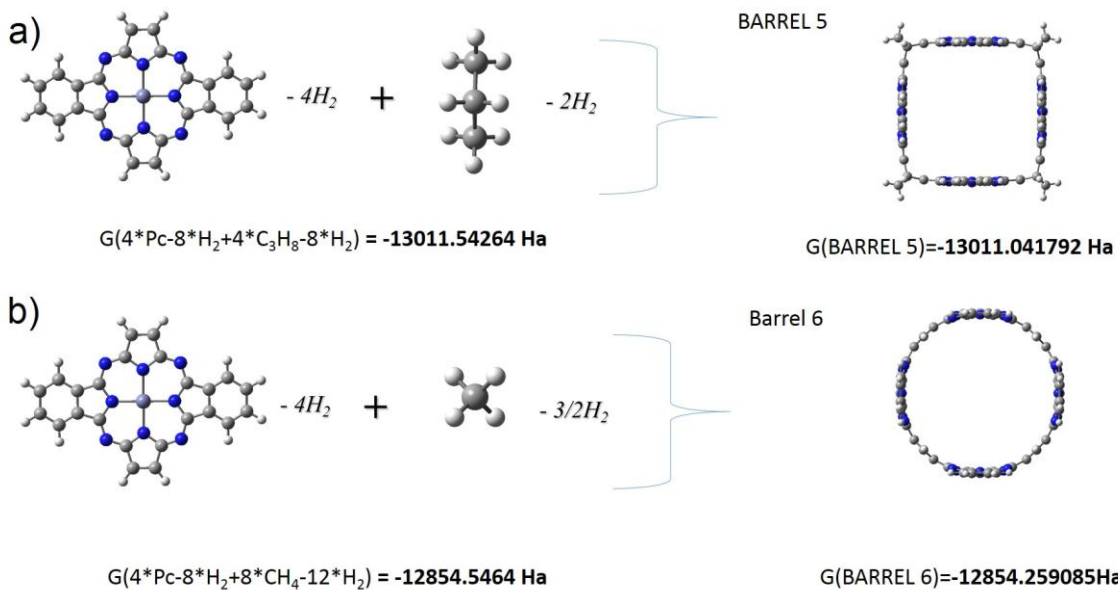
Scheme S1. Proposed reaction via monomers: (a) nanocage 1 and (b) nanocage 2.

SCHEME



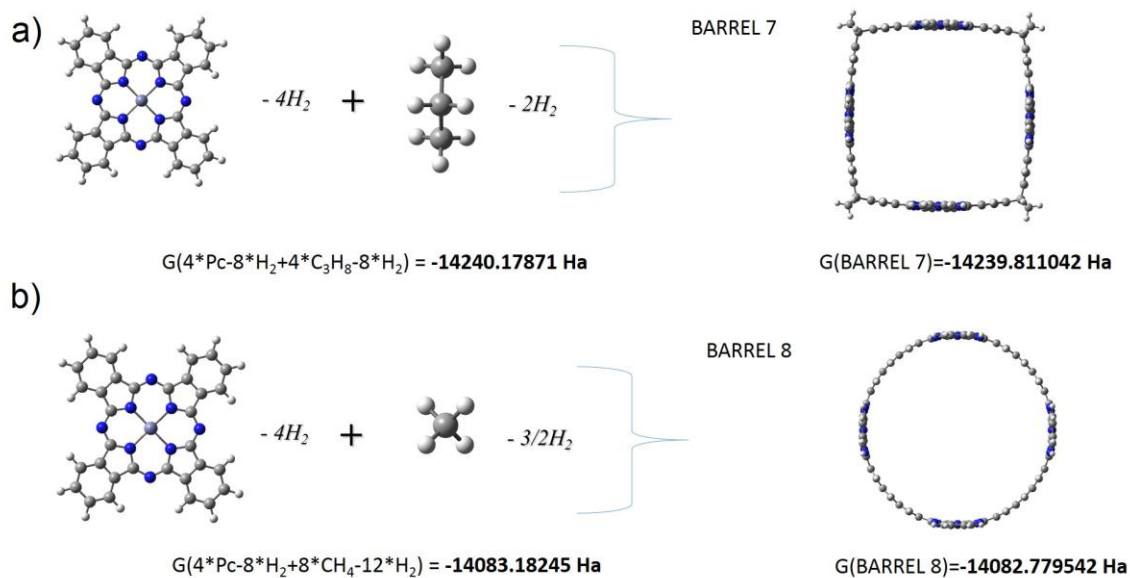
Scheme S2. Proposed reaction via monomers: (a) nanocage 3 and (b) nanocage 4.

SCHEME

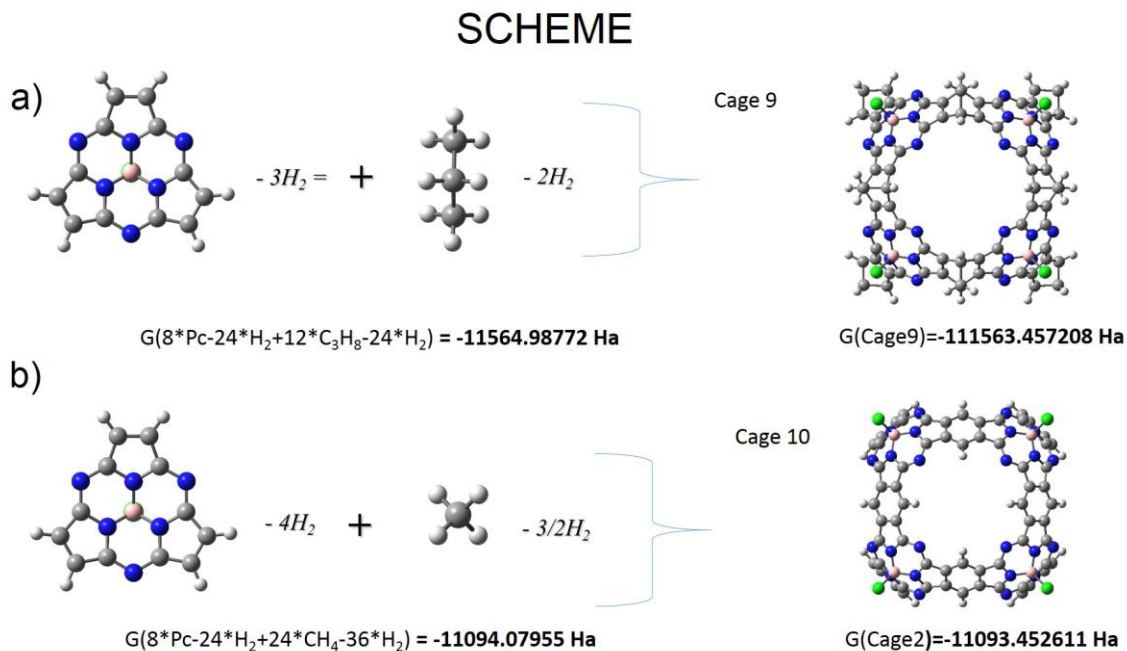


Scheme S3. Proposed reaction via monomers: (a) nanobarrel 5 and (b) nanobarrel 6.

SCHEME



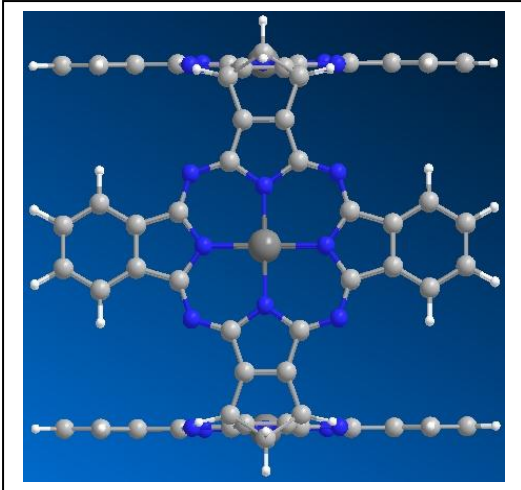
Scheme S4. Proposed reaction via monomers: (a) nanobarrel 7 and (b) nanobarrel 8.



Scheme S5. Proposed reaction via monomers: (a) nanocage 9 and (b) nanocage 10.

Supporting information Table 1: TDDFT predicted energies and expansion coefficients for nanostructures 1 – 10

PcTube01_LC-wPBE_TDDFT



Excited State 1: Singlet-A2G 1.6652 eV 744.58 nm f=0.0000 $\langle S^2 \rangle = 0.000$

Excited State 2: Singlet-EU 1.9053 eV 650.72 nm f=0.6537
 $\langle S^2 \rangle = 0.000$

517 -> 522	-0.15215
517 -> 523	-0.27784
518 -> 521	-0.32492
518 -> 524	-0.26277
519 -> 521	0.17793
519 -> 524	-0.14390
520 -> 522	0.16832
520 -> 523	-0.30738

Excited State 3: Singlet-EU 1.9053 eV 650.72 nm f=0.6537
 $\langle S^2 \rangle = 0.000$

517 -> 522	-0.27784
517 -> 523	0.15215
518 -> 521	0.17793
518 -> 524	0.14390
519 -> 521	0.32492
519 -> 524	-0.26277
520 -> 522	0.30738
520 -> 523	0.16832

Excited State 4: Singlet-B2G 2.0241 eV 612.53 nm f=0.0000 $\langle S^2 \rangle = 0.000$

Excited State 5: Singlet-B2U 2.2860 eV 542.36 nm f=0.0000 $\langle S^2 \rangle = 0.000$

Excited State 6: Singlet-EG 2.3115 eV 536.38 nm f=0.0000 $\langle S^2 \rangle = 0.000$

Excited State 7: Singlet-EG 2.3115 eV 536.38 nm f=0.0000 $\langle S^2 \rangle = 0.000$

Excited State 8: Singlet-A2U 2.3595 eV 525.47 nm f=0.8325
 $\langle S^2 \rangle = 0.000$

509 -> 524	0.10191
510 -> 522	0.10463
511 -> 523	0.10463
513 -> 521	-0.17111
514 -> 522	-0.12939

515 -> 523 -0.12939
 516 -> 524 0.12836
 517 -> 525 0.30692
 518 -> 527 0.30774
 519 -> 526 0.30774
 520 -> 528 0.30921
 Excited State 9: Singlet-EG 3.0984 eV 400.16 nm f=0.0000 <S**2>=0.000
 Excited State 10: Singlet-EG 3.0984 eV 400.16 nm f=0.0000 <S**2>=0.000
 Excited State 11: Singlet-B2U 3.0986 eV 400.13 nm f=0.0000 <S**2>=0.000
Excited State 12: Singlet-A2U 3.0996 eV 400.00 nm f=0.0216
<S2>=0.000**
 505 -> 524 0.26726
 506 -> 523 0.27256
 507 -> 522 -0.27256
 508 -> 521 0.31665
 509 -> 524 0.17877
 510 -> 522 0.18970
 511 -> 523 0.18970
 513 -> 521 -0.15080
 Excited State 13: Singlet-A1U 3.2411 eV 382.54 nm f=0.0000 <S**2>=0.000
 Excited State 14: Singlet-EG 3.2792 eV 378.09 nm f=0.0000 <S**2>=0.000
 Excited State 15: Singlet-EG 3.2792 eV 378.09 nm f=0.0000 <S**2>=0.000
 Excited State 16: Singlet-B2U 3.3410 eV 371.10 nm f=0.0000 <S**2>=0.000
 Excited State 17: Singlet-A2G 3.4309 eV 361.38 nm f=0.0000 <S**2>=0.000
 Excited State 18: Singlet-EU 3.4366 eV 360.77 nm f=0.0002 <S**2>=0.000
 Excited State 19: Singlet-EU 3.4366 eV 360.77 nm f=0.0002 <S**2>=0.000
 Excited State 20: Singlet-B1U 3.4495 eV 359.43 nm f=0.0000 <S**2>=0.000
 Excited State 21: Singlet-?Sym 3.4547 eV 358.88 nm f=0.0000 <S**2>=0.000
 Excited State 22: Singlet-?Sym 3.4578 eV 358.57 nm f=0.0000 <S**2>=0.000
 Excited State 23: Singlet-B2G 3.4627 eV 358.05 nm f=0.0000 <S**2>=0.000
Excited State 24: Singlet-EU 3.4660 eV 357.72 nm f=0.0220
<S2>=0.000**
 517 -> 522 0.33501
 517 -> 523 -0.11580
 518 -> 521 0.12836
 518 -> 524 -0.12147
 519 -> 521 0.37136
 519 -> 524 0.35143
 520 -> 522 0.24306
Excited State 25: Singlet-EU 3.4660 eV 357.72 nm f=0.0220
<S2>=0.000**
 517 -> 522 -0.11580
 517 -> 523 -0.33501
 518 -> 521 0.37136
 518 -> 524 -0.35143
 519 -> 521 -0.12836

519 -> 524 -0.12147
 520 -> 523 0.24306
 Excited State 26: Singlet-EG 3.5209 eV 352.13 nm f=0.0000 <S**2>=0.000
 Excited State 27: Singlet-EG 3.5209 eV 352.13 nm f=0.0000 <S**2>=0.000
Excited State 28: Singlet-A2U 3.5685 eV 347.44 nm f=0.0442
<S2>=0.000**
 481 -> 521 0.19483
 486 -> 523 0.14137
 487 -> 522 0.14137
 493 -> 524 0.10413
 505 -> 524 -0.13883
 506 -> 523 -0.16941
 507 -> 522 0.16941
 508 -> 521 -0.14838
 509 -> 524 0.25346
 510 -> 522 0.18748
 511 -> 523 0.18748
 512 -> 532 0.10248
 514 -> 522 0.16204
 515 -> 523 0.16204
 516 -> 524 -0.25255
 Excited State 29: Singlet-A2G 3.7684 eV 329.01 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-EU 3.7699 eV 328.88 nm f=0.0044
<S2>=0.000**
 489 -> 522 0.16271
 489 -> 523 0.18985
 490 -> 521 0.17389
 490 -> 524 -0.15308
 491 -> 521 0.20290
 491 -> 524 0.17861
 492 -> 522 -0.16303
 492 -> 523 0.19022
 505 -> 526 0.11739
 505 -> 527 0.13697
 506 -> 525 0.13371
 506 -> 528 0.12515
 507 -> 525 -0.11460
 507 -> 528 0.10726
 508 -> 526 -0.12009
 508 -> 527 0.14012
 511 -> 525 0.10131
Excited State 31: Singlet-EU 3.7699 eV 328.88 nm f=0.0044
<S2>=0.000**
 489 -> 522 -0.18985
 489 -> 523 0.16271
 490 -> 521 -0.20290

490 -> 524	0.17861				
491 -> 521	0.17389				
491 -> 524	0.15308				
492 -> 522	0.19022				
492 -> 523	0.16303				
505 -> 526	-0.13697				
505 -> 527	0.11739				
506 -> 525	0.11459				
506 -> 528	0.10726				
507 -> 525	0.13371				
507 -> 528	-0.12515				
508 -> 526	0.14012				
508 -> 527	0.12009				
510 -> 525	-0.10131				
Excited State 32:	Singlet-B2G	3.7706 eV	328.82 nm	f=0.0000	<S**2>=0.000
Excited State 33:	Singlet-A2G	3.8134 eV	325.13 nm	f=0.0000	<S**2>=0.000
Excited State 34:	Singlet-EU	3.8168 eV	324.84 nm	f=0.0084	<S**2>=0.000
489 -> 522	0.20648				
490 -> 521	0.22044				
490 -> 524	-0.19438				
492 -> 522	-0.20674				
505 -> 526	-0.19958				
507 -> 525	0.19637				
507 -> 528	-0.18397				
508 -> 526	0.20680				
509 -> 526	-0.13904				
510 -> 525	-0.14337				
510 -> 528	0.13327				
513 -> 526	-0.10830				
Excited State 35:	Singlet-EU	3.8168 eV	324.84 nm	f=0.0084	<S**2>=0.000
489 -> 523	0.20648				
491 -> 521	0.22044				
491 -> 524	0.19438				
492 -> 523	0.20674				
505 -> 527	-0.19958				
506 -> 525	-0.19638				
506 -> 528	-0.18397				
508 -> 527	-0.20680				
509 -> 527	-0.13904				
511 -> 525	-0.14337				
511 -> 528	-0.13327				
513 -> 527	0.10830				
Excited State 36:	Singlet-B2G	3.8189 eV	324.66 nm	f=0.0000	<S**2>=0.000
Excited State 37:	Singlet-B2U	3.9046 eV	317.53 nm	f=0.0000	<S**2>=0.000

Excited State 38: Singlet-EG 3.9883 eV 310.87 nm f=0.0000 <S**2>=0.000
 Excited State 39: Singlet-EG 3.9883 eV 310.87 nm f=0.0000 <S**2>=0.000
 Excited State 40: Singlet-B2G 4.0913 eV 303.05 nm f=0.0000 <S**2>=0.000
Excited State 41: Singlet-EU 4.1120 eV 301.52 nm f=0.0012
<S2>=0.000**
 517 -> 522 -0.36659
 517 -> 523 0.13520
 518 -> 524 -0.14900
 519 -> 521 -0.24459
 519 -> 524 0.40403
 520 -> 522 0.28408
 520 -> 523 0.10477
Excited State 42: Singlet-EU 4.1120 eV 301.52 nm f=0.0012
<S2>=0.000**
 517 -> 522 -0.13520
 517 -> 523 -0.36659
 518 -> 521 0.24459
 518 -> 524 0.40403
 519 -> 524 0.14900
 520 -> 522 0.10477
 520 -> 523 -0.28408
 Excited State 43: Singlet-?Sym 4.1183 eV 301.06 nm f=0.0000 <S**2>=0.000
 Excited State 44: Singlet-A2G 4.1498 eV 298.77 nm f=0.0000 <S**2>=0.000
Excited State 45: Singlet-A2U 4.1569 eV 298.26 nm f=4.6245
<S2>=0.000**
 510 -> 522 0.10568
 511 -> 523 0.10568
 513 -> 521 -0.27201
 514 -> 522 -0.26215
 515 -> 523 -0.26215
 516 -> 524 0.27185
 517 -> 525 -0.26488
 518 -> 527 -0.16910
 519 -> 526 -0.16910
 Excited State 46: Singlet-B2U 4.1727 eV 297.13 nm f=0.0000 <S**2>=0.000
 Excited State 47: Singlet-EG 4.1751 eV 296.96 nm f=0.0000 <S**2>=0.000
 Excited State 48: Singlet-EG 4.1751 eV 296.96 nm f=0.0000 <S**2>=0.000
Excited State 49: Singlet-A2U 4.1856 eV 296.21 nm f=0.1716
<S2>=0.000**
 517 -> 525 -0.43186
 520 -> 528 0.50959
 Excited State 50: Singlet-?Sym 4.1892 eV 295.96 nm f=0.0000 <S**2>=0.000
 Excited State 51: Singlet-?Sym 4.1911 eV 295.83 nm f=0.0000 <S**2>=0.000
 Excited State 52: Singlet-EG 4.1941 eV 295.62 nm f=0.0000 <S**2>=0.000
 Excited State 53: Singlet-EG 4.1941 eV 295.62 nm f=0.0000 <S**2>=0.000
 Excited State 54: Singlet-B1G 4.2345 eV 292.80 nm f=0.0000 <S**2>=0.000

Excited State 55: Singlet-EU 4.2389 eV 292.49 nm f=0.0035
<S2>=0.000**

473 -> 522 -0.18640
473 -> 523 -0.23833
477 -> 521 0.20164
477 -> 524 -0.17529
478 -> 521 -0.25782
478 -> 524 -0.22413
480 -> 522 0.19029
480 -> 523 -0.24330

Excited State 56: Singlet-EU 4.2389 eV 292.49 nm f=0.0035
<S2>=0.000**

473 -> 522 -0.23833
473 -> 523 0.18640
477 -> 521 0.25782
477 -> 524 -0.22413
478 -> 521 0.20164
478 -> 524 0.17529
480 -> 522 0.24330
480 -> 523 0.19029

Excited State 57: Singlet-A1G 4.2439 eV 292.15 nm f=0.0000 <S**2>=0.000

Excited State 58: Singlet-B1U 4.2674 eV 290.54 nm f=0.0000 <S**2>=0.000

Excited State 59: Singlet-EG 4.2715 eV 290.26 nm f=0.0000 <S**2>=0.000

Excited State 60: Singlet-EG 4.2715 eV 290.26 nm f=0.0000 <S**2>=0.000

Excited State 61: Singlet-A1U 4.2754 eV 289.99 nm f=0.0000 <S**2>=0.000

Excited State 62: Singlet-B2U 4.2929 eV 288.81 nm f=0.0000 <S**2>=0.000

Excited State 63: Singlet-EG 4.2957 eV 288.63 nm f=0.0000 <S**2>=0.000

Excited State 64: Singlet-EG 4.2957 eV 288.63 nm f=0.0000 <S**2>=0.000

Excited State 65: Singlet-A2U 4.2985 eV 288.44 nm f=0.0478
<S2>=0.000**

489 -> 525 0.31653
490 -> 526 -0.30807
491 -> 527 0.30807
492 -> 528 0.30037
517 -> 525 0.11431
520 -> 528 -0.14667

Excited State 66: Singlet-EU 4.3070 eV 287.87 nm f=1.3079
<S2>=0.000**

493 -> 526 0.17058
494 -> 525 0.12369
494 -> 528 -0.16983
497 -> 526 -0.20615
498 -> 525 0.14825
513 -> 526 0.17780
514 -> 525 -0.26103
514 -> 528 0.21181

516 -> 526	0.28661				
517 -> 522	0.10951				
519 -> 524	0.11225				
Excited State 67:		Singlet-EU	4.3070 eV	287.87 nm	f=1.3079
<S**2>=0.000					
493 -> 527	0.17058				
495 -> 525	0.12369				
495 -> 528	0.16983				
497 -> 527	0.20615				
499 -> 525	-0.14825				
513 -> 527	-0.17780				
515 -> 525	-0.26103				
515 -> 528	-0.21181				
516 -> 527	0.28660				
517 -> 523	0.10951				
518 -> 524	0.11225				
Excited State 68:		Singlet-B2G	4.4184 eV	280.61 nm	f=0.0000 <S**2>=0.000
Excited State 69:		Singlet-B1G	4.4632 eV	277.79 nm	f=0.0000 <S**2>=0.000
Excited State 70:		Singlet-A1U	4.4940 eV	275.89 nm	f=0.0000 <S**2>=0.000
Excited State 71:		Singlet-EG	4.4943 eV	275.87 nm	f=0.0000 <S**2>=0.000
Excited State 72:		Singlet-EG	4.4943 eV	275.87 nm	f=0.0000 <S**2>=0.000
Excited State 73:		Singlet-B1U	4.4944 eV	275.86 nm	f=0.0000 <S**2>=0.000
Excited State 74:		Singlet-EU	4.5007 eV	275.48 nm	f=0.0004
<S**2>=0.000					
498 -> 528	0.12141				
499 -> 528	0.10687				
500 -> 526	-0.10062				
500 -> 527	0.11432				
501 -> 522	-0.10894				
501 -> 523	-0.12377				
502 -> 521	-0.13905				
502 -> 524	-0.11893				
503 -> 521	-0.12239				
503 -> 524	0.10468				
504 -> 522	0.11659				
504 -> 523	-0.13246				
512 -> 527	0.11259				
517 -> 530	-0.12682				
517 -> 531	0.14408				
518 -> 529	-0.16647				
518 -> 532	0.13854				
519 -> 529	0.14653				
519 -> 532	0.12194				
520 -> 530	0.13942				
520 -> 531	0.15839				

Excited State 75: Singlet-EU 4.5007 eV 275.48 nm f=0.0004
<S2>=0.000**

498 -> 528 -0.10687
499 -> 528 0.12141
500 -> 526 -0.11432
500 -> 527 -0.10062
501 -> 522 -0.12377
501 -> 523 0.10894
502 -> 521 0.12239
502 -> 524 0.10468
503 -> 521 -0.13905
503 -> 524 0.11893
504 -> 522 0.13245
504 -> 523 0.11659
512 -> 526 0.11259
517 -> 530 -0.14408
517 -> 531 -0.12682
518 -> 529 0.14653
518 -> 532 -0.12194
519 -> 529 0.16647
519 -> 532 0.13854
520 -> 530 0.15839
520 -> 531 -0.13942

Excited State 76: Singlet-A1G 4.5215 eV 274.21 nm f=0.0000 <S**2>=0.000

Excited State 77: Singlet-A2G 4.6248 eV 268.09 nm f=0.0000 <S**2>=0.000

Excited State 78: Singlet-EU 4.6715 eV 265.41 nm f=0.8087
<S2>=0.000**

493 -> 526 -0.10323
494 -> 525 -0.11422
497 -> 526 0.16967
498 -> 525 -0.11399
505 -> 526 -0.16289
507 -> 525 0.18185
507 -> 528 -0.18133
508 -> 526 0.16616
509 -> 526 0.23203
510 -> 525 0.14351
510 -> 528 -0.22715
512 -> 527 -0.10750
513 -> 526 0.19595
514 -> 525 -0.16554

Excited State 79: Singlet-EU 4.6715 eV 265.41 nm f=0.8087
<S2>=0.000**

493 -> 527 -0.10323
495 -> 525 -0.11422
497 -> 527 -0.16967

499 -> 525	0.11399				
505 -> 527	-0.16289				
506 -> 525	-0.18185				
506 -> 528	-0.18133				
508 -> 527	-0.16616				
509 -> 527	0.23203				
511 -> 525	0.14351				
511 -> 528	0.22715				
512 -> 526	-0.10750				
513 -> 527	-0.19595				
515 -> 525	-0.16553				
Excited State 80:	Singlet-A2U	4.6940 eV	264.13 nm	f=0.0000	<S**2>=0.000
Excited State 81:	Singlet-EG	4.7047 eV	263.53 nm	f=0.0000	<S**2>=0.000
Excited State 82:	Singlet-EG	4.7047 eV	263.53 nm	f=0.0000	<S**2>=0.000
Excited State 83:	Singlet-B2U	4.7154 eV	262.93 nm	f=0.0000	<S**2>=0.000
Excited State 84:	Singlet-B2G	4.7265 eV	262.31 nm	f=0.0000	<S**2>=0.000
Excited State 85:	Singlet-B1G	4.7523 eV	260.89 nm	f=0.0000	<S**2>=0.000
Excited State 86:	Singlet-B1U	4.7573 eV	260.62 nm	f=0.0000	<S**2>=0.000
Excited State 87:	Singlet-EG	4.7736 eV	259.73 nm	f=0.0000	<S**2>=0.000
Excited State 88:	Singlet-EG	4.7736 eV	259.73 nm	f=0.0000	<S**2>=0.000
Excited State 89:	Singlet-A1U	4.7923 eV	258.72 nm	f=0.0000	<S**2>=0.000
Excited State 90:	Singlet-EU	4.7964 eV	258.50 nm	f=0.0024	<S**2>=0.000
474 -> 526	-0.14096				
474 -> 527	0.14109				
475 -> 525	0.15732				
475 -> 528	-0.14095				
476 -> 525	0.15747				
476 -> 528	0.14109				
479 -> 526	0.16602				
479 -> 527	0.16617				
486 -> 528	0.10162				
487 -> 528	-0.10172				
488 -> 526	-0.11760				
488 -> 527	0.11772				
510 -> 525	0.11005				
511 -> 525	0.10994				
512 -> 526	0.14523				
512 -> 527	0.14538				
Excited State 91:	Singlet-EU	4.7964 eV	258.50 nm	f=0.0024	<S**2>=0.000
474 -> 526	0.14110				
474 -> 527	0.14096				
475 -> 525	-0.15747				
475 -> 528	0.14109				
476 -> 525	0.15732				

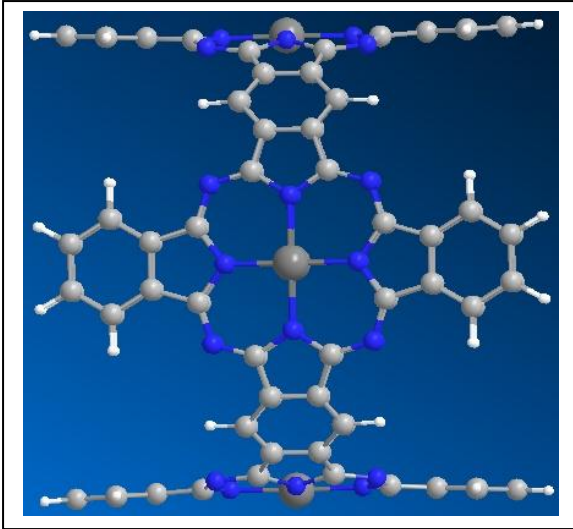
476 -> 528 0.14096
 479 -> 526 -0.16618
 479 -> 527 0.16601
 486 -> 528 -0.10172
 487 -> 528 -0.10162
 488 -> 526 0.11772
 488 -> 527 0.11760
 510 -> 525 0.10994
 511 -> 525 -0.11005
 512 -> 526 -0.14537
 512 -> 527 0.14523
 Excited State 92: Singlet-A1G 4.8005 eV 258.28 nm f=0.0000 <S**2>=0.000
 Excited State 93: Singlet-B1G 4.8052 eV 258.02 nm f=0.0000 <S**2>=0.000
 Excited State 94: Singlet-EG 4.8075 eV 257.90 nm f=0.0000 <S**2>=0.000
 Excited State 95: Singlet-EG 4.8075 eV 257.90 nm f=0.0000 <S**2>=0.000
 Excited State 96: Singlet-B1U 4.8081 eV 257.87 nm f=0.0000 <S**2>=0.000
 Excited State 97: Singlet-A1U 4.8141 eV 257.54 nm f=0.0000 <S**2>=0.000
 Excited State 98: Singlet-B2U 4.8166 eV 257.41 nm f=0.0000 <S**2>=0.000
 Excited State 99: Singlet-EG 4.8194 eV 257.26 nm f=0.0000 <S**2>=0.000
 Excited State 100: Singlet-EG 4.8194 eV 257.26 nm f=0.0000 <S**2>=0.000
 Excited State 101: Singlet-EU 4.8233 eV 257.05 nm f=0.0002 <S**2>=0.000
 Excited State 102: Singlet-EU 4.8233 eV 257.05 nm f=0.0002 <S**2>=0.000
Excited State 103: Singlet-A2U 4.8237 eV 257.03 nm f=0.4155
<S2>=0.000**
 481 -> 521 -0.12757
 493 -> 524 0.22793
 494 -> 522 0.20967
 495 -> 523 0.20967
 497 -> 521 0.31746
 498 -> 522 0.18765
 499 -> 523 -0.18765
 508 -> 521 0.12799
 516 -> 524 -0.17237
 Excited State 104: Singlet-B1G 4.8602 eV 255.10 nm f=0.0000 <S**2>=0.000
 Excited State 105: Singlet-A1G 4.8607 eV 255.08 nm f=0.0000 <S**2>=0.000
 Excited State 106: Singlet-EU 4.8868 eV 253.71 nm f=0.0215 <S**2>=0.000
 Excited State 107: Singlet-EU 4.8868 eV 253.71 nm f=0.0215 <S**2>=0.000
 Excited State 108: Singlet-A2G 4.8983 eV 253.12 nm f=0.0000 <S**2>=0.000
Excited State 109: Singlet-A2U 4.9266 eV 251.66 nm f=0.8048
<S2>=0.000**
 481 -> 521 0.31739
 486 -> 523 0.24129
 487 -> 522 0.24129
 493 -> 524 0.12680
 505 -> 524 0.16249
 510 -> 522 -0.12257

511 -> 523 -0.12257
 513 -> 521 0.24115
 516 -> 524 0.11600
 Excited State 110: Singlet-EG 4.9675 eV 249.59 nm f=0.0000 <S**2>=0.000
 Excited State 111: Singlet-EG 4.9675 eV 249.59 nm f=0.0000 <S**2>=0.000
 Excited State 112: Singlet-A1G 4.9830 eV 248.82 nm f=0.0000 <S**2>=0.000
Excited State 113: Singlet-EU 4.9967 eV 248.13 nm f=0.3488
<S2>=0.000**
 481 -> 526 0.12715
 487 -> 525 -0.14991
 493 -> 526 -0.18437
 494 -> 528 0.16988
 497 -> 526 0.10011
 502 -> 521 -0.10470
 504 -> 523 -0.10206
 509 -> 526 -0.11133
 510 -> 528 0.12887
 512 -> 527 0.12360
 514 -> 528 0.23274
 516 -> 526 0.26276
 518 -> 529 0.11268
 520 -> 531 -0.11272
Excited State 114: Singlet-EU 4.9967 eV 248.13 nm f=0.3488
<S2>=0.000**
 481 -> 527 -0.12715
 486 -> 525 -0.14991
 493 -> 527 -0.18437
 495 -> 528 -0.16988
 497 -> 527 -0.10011
 503 -> 521 -0.10470
 504 -> 522 0.10207
 509 -> 527 -0.11133
 511 -> 528 -0.12888
 512 -> 526 0.12359
 515 -> 528 -0.23274
 516 -> 527 0.26276
 519 -> 529 -0.11268
 520 -> 530 -0.11273
 Excited State 115: Singlet-B2G 5.0229 eV 246.84 nm f=0.0000 <S**2>=0.000
 Excited State 116: Singlet-B2U 5.0238 eV 246.79 nm f=0.0000 <S**2>=0.000
 Excited State 117: Singlet-B1U 5.0405 eV 245.98 nm f=0.0000 <S**2>=0.000
 Excited State 118: Singlet-EG 5.0663 eV 244.72 nm f=0.0000 <S**2>=0.000
 Excited State 119: Singlet-EG 5.0663 eV 244.72 nm f=0.0000 <S**2>=0.000
 Excited State 120: Singlet-A1U 5.0760 eV 244.25 nm f=0.0000 <S**2>=0.000
Excited State 121: Singlet-A2U 5.1337 eV 241.51 nm f=0.0567
<S2>=0.000**

469 -> 524 0.28997
 470 -> 522 -0.31132
 471 -> 523 0.31132
 472 -> 521 0.33617
 Excited State 122: Singlet-EG 5.1397 eV 241.23 nm f=0.0000 <S**2>=0.000
 Excited State 123: Singlet-EG 5.1397 eV 241.23 nm f=0.0000 <S**2>=0.000
 Excited State 124: Singlet-B2U 5.1456 eV 240.95 nm f=0.0000 <S**2>=0.000
 Excited State 125: Singlet-B1G 5.1464 eV 240.92 nm f=0.0000 <S**2>=0.000
Excited State 126: Singlet-EU 5.1578 eV 240.38 nm f=0.0010
<S2>=0.000**
 484 -> 529 0.10465
 494 -> 525 -0.15710
 494 -> 528 -0.12823
 496 -> 527 0.23709
 498 -> 525 0.18690
 498 -> 528 0.18509
 500 -> 527 0.21833
 517 -> 531 -0.13862
 518 -> 529 0.18177
 518 -> 532 -0.12390
 520 -> 531 -0.16281
Excited State 127: Singlet-EU 5.1578 eV 240.38 nm f=0.0010
<S2>=0.000**
 485 -> 529 -0.10465
 495 -> 525 -0.15710
 495 -> 528 0.12823
 496 -> 526 0.23708
 499 -> 525 -0.18690
 499 -> 528 0.18509
 500 -> 526 -0.21833
 517 -> 530 0.13862
 519 -> 529 -0.18177
 519 -> 532 -0.12390
 520 -> 530 -0.16281
 Excited State 128: Singlet-A1G 5.1723 eV 239.71 nm f=0.0000 <S**2>=0.000
 Excited State 129: Singlet-B2U 5.3064 eV 233.65 nm f=0.0000 <S**2>=0.000
 Excited State 130: Singlet-EG 5.3104 eV 233.47 nm f=0.0000 <S**2>=0.000
 Excited State 131: Singlet-EG 5.3104 eV 233.47 nm f=0.0000 <S**2>=0.000
Excited State 132: Singlet-A2U 5.3154 eV 233.25 nm f=0.1365
<S2>=0.000**
 482 -> 528 0.24131
 483 -> 525 0.25637
 484 -> 527 0.24854
 485 -> 526 0.24854
 494 -> 522 -0.11666
 495 -> 523 -0.11666

496 -> 532 -0.11245
 497 -> 521 -0.15354
 500 -> 529 0.11191
 Excited State 133: Singlet-B2U 5.4359 eV 228.08 nm f=0.0000 <S**2>=0.000
 Excited State 134: Singlet-EG 5.4360 eV 228.08 nm f=0.0000 <S**2>=0.000
 Excited State 135: Singlet-EG 5.4360 eV 228.08 nm f=0.0000 <S**2>=0.000
 Excited State 136: Singlet-?Sym 5.4402 eV 227.90 nm f=0.0000 <S**2>=0.000
Excited State 137: Singlet-EU 5.4481 eV 227.57 nm f=0.0005
<S2>=0.000**
 469 -> 526 -0.25050
 469 -> 527 0.14526
 470 -> 525 0.25593
 470 -> 528 -0.24269
 471 -> 525 0.14838
 471 -> 528 0.14072
 472 -> 526 0.24761
 472 -> 527 0.14357
 473 -> 530 -0.10439
 477 -> 529 0.11714
 480 -> 530 0.10478
 Excited State 138: Singlet-?Sym 5.4520 eV 227.41 nm f=0.0000 <S**2>=0.000
 Excited State 139: Singlet-EG 5.4673 eV 226.78 nm f=0.0000 <S**2>=0.000
 Excited State 140: Singlet-EG 5.4673 eV 226.78 nm f=0.0000 <S**2>=0.000

PcTube02_LC-wPBE_TDDFT



Excited State 1: Singlet-A2G 0.9686 eV 1280.06 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 2: Singlet-EU 1.7396 eV 712.70 nm f=1.1704 $\langle S^{*2} \rangle = 0.000$

501 -> 508 -0.20094
 503 -> 505 0.45554
 503 -> 512 -0.18147
 504 -> 508 0.41029

Excited State 3: Singlet-EU 1.7396 eV 712.70 nm f=1.1704 $\langle S^{*2} \rangle = 0.000$

501 -> 507 0.20094
 502 -> 505 0.45554
 502 -> 512 0.18147
 504 -> 507 0.41029

Excited State 4: Singlet-A2U 1.8574 eV 667.52 nm f=1.1779
 $\langle S^{*2} \rangle = 0.000$

498 -> 507 0.10288
 499 -> 508 0.10288
 500 -> 505 0.13296
 501 -> 511 0.20031
 502 -> 509 0.28830
 503 -> 510 0.28831
 504 -> 506 0.49695

Excited State 5: Singlet-EG 1.8708 eV 662.75 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 6: Singlet-EG 1.8708 eV 662.75 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 7: Singlet-B2U 1.9130 eV 648.10 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 8: Singlet-B2G 2.1400 eV 579.37 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 9: Singlet-EU 2.7874 eV 444.80 nm f=0.0207 $\langle S^{*2} \rangle = 0.000$

501 -> 507 -0.12489
 502 -> 505 -0.41856
 502 -> 512 0.10115
 503 -> 505 0.14582
 504 -> 507 0.47907
 504 -> 508 -0.16690

Excited State 10: Singlet-EU 2.7874 eV 444.80 nm f=0.0207

<S2>=0.000**

501 -> 508 0.12489
502 -> 505 -0.14582
503 -> 505 -0.41856
503 -> 512 -0.10115
504 -> 507 0.16690
504 -> 508 0.47907

Excited State 11: Singlet-A2G 2.9666 eV 417.93 nm f=0.0000 <S**2>=0.000

Excited State 12: Singlet-?Sym 3.1517 eV 393.39 nm f=0.0000 <S**2>=0.000

Excited State 13: Singlet-B2G 3.2680 eV 379.39 nm f=0.0000 <S**2>=0.000

Excited State 14: Singlet-?Sym 3.2693 eV 379.23 nm f=0.0000 <S**2>=0.000

Excited State 15: Singlet-EG 3.3076 eV 374.85 nm f=0.0000 <S**2>=0.000

Excited State 16: Singlet-EG 3.3076 eV 374.85 nm f=0.0000 <S**2>=0.000

Excited State 17: Singlet-A2U 3.3099 eV 374.59 nm f=0.0425

<S2>=0.000**

501 -> 511 -0.27695
502 -> 509 -0.26452
503 -> 510 -0.26452
504 -> 506 0.49306

Excited State 18: Singlet-B2U 3.3894 eV 365.80 nm f=0.0000 <S**2>=0.000

Excited State 19: Singlet-EU 3.4581 eV 358.53 nm f=0.5800

<S2>=0.000**

497 -> 510 -0.11433
499 -> 506 0.11898
499 -> 511 -0.11340
500 -> 510 0.11835
501 -> 507 0.12262
501 -> 508 0.39113
502 -> 512 0.10159
503 -> 505 0.24169
503 -> 512 0.32404
504 -> 508 0.15141
504 -> 517 0.11955

Excited State 20: Singlet-EU 3.4581 eV 358.53 nm f=0.5799

<S2>=0.000**

497 -> 509 0.11433
498 -> 506 0.11898
498 -> 511 0.11340
500 -> 509 0.11835
501 -> 507 -0.39113
501 -> 508 0.12262
502 -> 505 0.24169
502 -> 512 -0.32404
503 -> 512 0.10159
504 -> 507 0.15141

504 -> 518 -0.11956
 Excited State 21: Singlet-?Sym 3.4725 eV 357.05 nm f=0.0000 <S**2>=0.000
 Excited State 22: Singlet-?Sym 3.5027 eV 353.96 nm f=0.0000 <S**2>=0.000
 Excited State 23: Singlet-EG 3.5287 eV 351.36 nm f=0.0000 <S**2>=0.000
 Excited State 24: Singlet-EG 3.5287 eV 351.36 nm f=0.0000 <S**2>=0.000
Excited State 25: Singlet-A2U 3.6560 eV 339.12 nm f=0.3685
<S2>=0.000**
 472 -> 512 0.19009
 475 -> 507 -0.12865
 476 -> 508 -0.12865
 481 -> 508 -0.13647
 482 -> 507 0.13648
 486 -> 507 -0.15590
 487 -> 508 -0.15591
 488 -> 505 0.31029
 494 -> 508 -0.10546
 495 -> 507 0.10546
 496 -> 505 -0.21859
 497 -> 512 -0.13860
 498 -> 507 -0.16441
 499 -> 508 -0.16441
 500 -> 505 -0.22984
 Excited State 26: Singlet-EG 3.6733 eV 337.53 nm f=0.0000 <S**2>=0.000
 Excited State 27: Singlet-EG 3.6733 eV 337.53 nm f=0.0000 <S**2>=0.000
 Excited State 28: Singlet-B2U 3.6873 eV 336.24 nm f=0.0000 <S**2>=0.000
 Excited State 29: Singlet-A2G 3.7622 eV 329.55 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-EU 3.8158 eV 324.93 nm f=0.0560
<S2>=0.000**
 472 -> 509 0.14210
 472 -> 510 -0.19547
 476 -> 506 -0.12756
 476 -> 511 0.10692
 481 -> 506 -0.12039
 481 -> 511 0.10268
 486 -> 506 -0.10345
 487 -> 506 -0.14231
 487 -> 511 0.12898
 488 -> 509 0.14237
 488 -> 510 0.19585
 497 -> 509 -0.10842
 497 -> 510 0.14914
 498 -> 506 -0.12082
 499 -> 506 -0.16620
 499 -> 511 0.13671
 500 -> 509 -0.11137
 500 -> 510 -0.15320

501 -> 508 0.11619
Excited State 31: Singlet-EU 3.8158 eV 324.93 nm f=0.0560
<S2>=0.000**
 472 -> 509 -0.19547
 472 -> 510 -0.14210
 475 -> 506 0.12756
 475 -> 511 0.10692
 482 -> 506 -0.12039
 482 -> 511 -0.10269
 486 -> 506 0.14231
 486 -> 511 0.12897
 487 -> 506 -0.10345
 488 -> 509 -0.19585
 488 -> 510 0.14237
 497 -> 509 0.14914
 497 -> 510 0.10842
 498 -> 506 0.16620
 498 -> 511 0.13671
 499 -> 506 -0.12082
 500 -> 509 0.15320
 500 -> 510 -0.11137
 501 -> 507 0.11619
 Excited State 32: Singlet-B2G 3.8179 eV 324.74 nm f=0.0000 <S**2>=0.000
 Excited State 33: Singlet-B2G 3.9607 eV 313.04 nm f=0.0000 <S**2>=0.000
 Excited State 34: Singlet-B1U 3.9749 eV 311.92 nm f=0.0000 <S**2>=0.000
 Excited State 35: Singlet-EG 4.0202 eV 308.40 nm f=0.0000 <S**2>=0.000
 Excited State 36: Singlet-EG 4.0202 eV 308.40 nm f=0.0000 <S**2>=0.000
Excited State 37: Singlet-A2U 4.0639 eV 305.09 nm f=0.0157
<S2>=0.000**
 473 -> 505 -0.27493
 475 -> 507 -0.15130
 476 -> 508 -0.15130
 488 -> 505 0.11734
 493 -> 513 0.12476
 494 -> 508 0.23105
 495 -> 507 -0.23106
 496 -> 505 0.39268
 500 -> 505 -0.10932
 504 -> 519 -0.10291
 Excited State 38: Singlet-A2G 4.1623 eV 297.87 nm f=0.0000 <S**2>=0.000
 Excited State 39: Singlet-A2G 4.1927 eV 295.71 nm f=0.0000 <S**2>=0.000
 Excited State 40: Singlet-B2U 4.1939 eV 295.63 nm f=0.0000 <S**2>=0.000
Excited State 41: Singlet-EU 4.1968 eV 295.43 nm f=0.0125
<S2>=0.000**
 468 -> 508 -0.14014
 469 -> 508 0.24821

471 -> 505 0.37097
471 -> 512 -0.20061
474 -> 508 0.25653
477 -> 508 -0.14272
479 -> 505 -0.13391

Excited State 42: Singlet-EU 4.1968 eV 295.43 nm f=0.0125

<S2>=0.000**

468 -> 507 0.14014
469 -> 507 0.24821
470 -> 505 -0.37096
470 -> 512 -0.20061
474 -> 507 -0.25653
477 -> 507 -0.14271
478 -> 505 -0.13391

Excited State 43: Singlet-B2G 4.1984 eV 295.31 nm f=0.0000 <S**2>=0.000

Excited State 44: Singlet-B1G 4.2091 eV 294.56 nm f=0.0000 <S**2>=0.000

Excited State 45: Singlet-EG 4.2216 eV 293.69 nm f=0.0000 <S**2>=0.000

Excited State 46: Singlet-EG 4.2216 eV 293.69 nm f=0.0000 <S**2>=0.000

Excited State 47: Singlet-B2U 4.2554 eV 291.36 nm f=0.0000 <S**2>=0.000

Excited State 48: Singlet-A2U 4.2747 eV 290.04 nm f=0.6172

<S2>=0.000**

468 -> 511 0.12982
469 -> 506 0.24134
470 -> 509 -0.23218
471 -> 510 0.23217
472 -> 512 -0.10339
473 -> 505 0.11441
474 -> 511 -0.20414
475 -> 507 0.10140
476 -> 508 0.10139
477 -> 506 -0.10306
488 -> 505 -0.13263
498 -> 507 -0.12701
499 -> 508 -0.12700
500 -> 505 -0.22512
501 -> 511 0.11123

Excited State 49: Singlet-EG 4.3004 eV 288.31 nm f=0.0000 <S**2>=0.000

Excited State 50: Singlet-EG 4.3004 eV 288.31 nm f=0.0000 <S**2>=0.000

Excited State 51: Singlet-EU 4.3119 eV 287.54 nm f=0.0003

<S2>=0.000**

501 -> 507 -0.11043
501 -> 508 0.26813
501 -> 517 0.13989
502 -> 512 0.17762
502 -> 513 0.20373
503 -> 512 -0.43123

504 -> 508 -0.17348
 504 -> 517 0.11264
Excited State 52: Singlet-EU 4.3119 eV 287.54 nm f=0.0003
<S2>=0.000**
 501 -> 507 -0.26813
 501 -> 508 -0.11044
 501 -> 518 0.13989
 502 -> 512 0.43123
 503 -> 512 0.17762
 503 -> 513 0.20373
 504 -> 507 -0.17348
 504 -> 518 -0.11263
Excited State 53: Singlet-B2U 4.3334 eV 286.11 nm f=0.0000 <S2>=0.000**
Excited State 54: Singlet-EU 4.3395 eV 285.71 nm f=0.6092
<S2>=0.000**
 472 -> 510 -0.15431
 473 -> 510 -0.18319
 476 -> 506 -0.18767
 476 -> 511 0.19441
 485 -> 510 0.21521
 487 -> 506 0.11567
 487 -> 511 -0.10632
 494 -> 506 -0.18515
 494 -> 511 0.11985
 496 -> 510 -0.19858
 499 -> 506 0.13097
 500 -> 510 0.14183
 501 -> 508 -0.15986
Excited State 55: Singlet-EU 4.3395 eV 285.71 nm f=0.6092
<S2>=0.000**
 472 -> 509 -0.15431
 473 -> 509 0.18319
 475 -> 506 0.18768
 475 -> 511 0.19440
 485 -> 509 0.21521
 486 -> 506 -0.11567
 486 -> 511 -0.10632
 495 -> 506 -0.18516
 495 -> 511 -0.11986
 496 -> 509 0.19858
 498 -> 506 -0.13097
 500 -> 509 -0.14183
 501 -> 507 -0.15986
Excited State 56: Singlet-EG 4.3434 eV 285.45 nm f=0.0000 <S2>=0.000**
Excited State 57: Singlet-EG 4.3434 eV 285.45 nm f=0.0000 <S2>=0.000**
Excited State 58: Singlet-B1U 4.3439 eV 285.42 nm f=0.0000 <S2>=0.000**

Excited State 59: Singlet-A1U 4.3512 eV 284.94 nm f=0.0000 <S**2>=0.000

Excited State 60: Singlet-A2U 4.3519 eV 284.89 nm f=1.9492

<S2>=0.000**

469 -> 506 0.13148
470 -> 509 -0.14304
471 -> 510 0.14304
473 -> 505 -0.10329
474 -> 511 -0.14807
477 -> 506 -0.10573
496 -> 505 -0.12350
498 -> 507 0.15644
499 -> 508 0.15643
500 -> 505 0.30151
501 -> 511 0.19208
502 -> 509 -0.24266
503 -> 510 -0.24266

Excited State 61: Singlet-EG 4.3667 eV 283.93 nm f=0.0000 <S**2>=0.000

Excited State 62: Singlet-EG 4.3667 eV 283.93 nm f=0.0000 <S**2>=0.000

Excited State 63: Singlet-B2G 4.3863 eV 282.66 nm f=0.0000 <S**2>=0.000

Excited State 64: Singlet-EU 4.3950 eV 282.11 nm f=0.0102

<S2>=0.000**

461 -> 507 -0.10828
464 -> 507 -0.13071
467 -> 505 -0.16183
492 -> 507 0.11925
501 -> 508 0.31247
502 -> 513 -0.18315
502 -> 523 -0.13825
503 -> 505 0.10763
503 -> 512 -0.16729
504 -> 517 -0.27661

Excited State 65: Singlet-EU 4.3950 eV 282.11 nm f=0.0102

<S2>=0.000**

461 -> 508 0.10828
464 -> 508 -0.13070
466 -> 505 0.16183
492 -> 508 -0.11925
501 -> 507 0.31247
502 -> 505 -0.10763
502 -> 512 -0.16729
503 -> 513 0.18315
503 -> 523 -0.13825
504 -> 518 -0.27661

Excited State 66: Singlet-B1U 4.4011 eV 281.71 nm f=0.0000 <S**2>=0.000

Excited State 67: Singlet-A1G 4.4409 eV 279.18 nm f=0.0000 <S**2>=0.000

Excited State 68: Singlet-A2U 4.4477 eV 278.76 nm f=1.0483

<S2>=0.000**

474 -> 511	0.12831
477 -> 506	0.13431
478 -> 509	0.11450
479 -> 510	0.11450
501 -> 511	0.50861
502 -> 509	-0.16198
503 -> 510	-0.16198
504 -> 519	-0.13586

Excited State 69: Singlet-A2G 4.4563 eV 278.22 nm f=0.0000 <S**2>=0.000

Excited State 70: Singlet-EG 4.5176 eV 274.45 nm f=0.0000 <S**2>=0.000

Excited State 71: Singlet-EG 4.5176 eV 274.45 nm f=0.0000 <S**2>=0.000

Excited State 72: Singlet-A1U 4.5346 eV 273.42 nm f=0.0000 <S**2>=0.000

Excited State 73: Singlet-B1G 4.5776 eV 270.85 nm f=0.0000 <S**2>=0.000

Excited State 74: Singlet-EU 4.6085 eV 269.03 nm f=0.6217

<S2>=0.000**

458 -> 505	0.13660
461 -> 508	0.17419
464 -> 508	-0.17646
466 -> 505	0.22335
466 -> 512	-0.10849
482 -> 506	-0.11646
485 -> 509	-0.10715
486 -> 511	0.13986
488 -> 509	-0.12840
497 -> 509	-0.12968
498 -> 506	-0.12652
498 -> 511	-0.10038
500 -> 509	-0.10036
501 -> 507	-0.10837
504 -> 518	0.14005

Excited State 75: Singlet-EU 4.6085 eV 269.03 nm f=0.6217

<S2>=0.000**

459 -> 505	0.13661
461 -> 507	0.17419
464 -> 507	0.17646
467 -> 505	0.22336
467 -> 512	0.10849
481 -> 506	0.11646
485 -> 510	0.10715
487 -> 511	-0.13986
488 -> 510	-0.12840
497 -> 510	0.12968
499 -> 506	-0.12652
499 -> 511	0.10038

500 -> 510 -0.10037
 501 -> 508 0.10837
 504 -> 517 -0.14005
 Excited State 76: Singlet-A1U 4.6130 eV 268.77 nm f=0.0000 <S**2>=0.000
 Excited State 77: Singlet-EG 4.6162 eV 268.59 nm f=0.0000 <S**2>=0.000
 Excited State 78: Singlet-EG 4.6162 eV 268.59 nm f=0.0000 <S**2>=0.000
 Excited State 79: Singlet-B1G 4.6272 eV 267.94 nm f=0.0000 <S**2>=0.000
 Excited State 80: Singlet-B1U 4.6329 eV 267.62 nm f=0.0000 <S**2>=0.000
Excited State 81: Singlet-EU 4.6528 eV 266.47 nm f=0.5931
<S2>=0.000**
 461 -> 507 -0.10419
 464 -> 507 -0.11423
 467 -> 505 -0.13178
 481 -> 511 -0.11389
 485 -> 510 0.11181
 487 -> 506 0.16453
 488 -> 510 -0.15246
 489 -> 507 0.10253
 494 -> 511 0.10381
 497 -> 510 0.14389
 499 -> 506 -0.16610
 499 -> 511 0.10588
 500 -> 510 -0.12901
 503 -> 512 0.12999
 504 -> 517 0.10006
Excited State 82: Singlet-EU 4.6528 eV 266.47 nm f=0.5932
<S2>=0.000**
 461 -> 508 -0.10419
 464 -> 508 0.11423
 466 -> 505 -0.13178
 482 -> 511 -0.11389
 485 -> 509 -0.11181
 486 -> 506 0.16452
 488 -> 509 -0.15246
 489 -> 508 -0.10253
 495 -> 511 0.10381
 497 -> 509 -0.14390
 498 -> 506 -0.16610
 498 -> 511 -0.10589
 500 -> 509 -0.12901
 502 -> 512 -0.12999
 504 -> 518 -0.10006
 Excited State 83: Singlet-A1G 4.6648 eV 265.79 nm f=0.0000 <S**2>=0.000
 Excited State 84: Singlet-A2G 4.6669 eV 265.67 nm f=0.0000 <S**2>=0.000
 Excited State 85: Singlet-EG 4.6939 eV 264.14 nm f=0.0000 <S**2>=0.000
 Excited State 86: Singlet-EG 4.6939 eV 264.14 nm f=0.0000 <S**2>=0.000

Excited State 87: Singlet-B2G 4.7032 eV 263.62 nm f=0.0000 <S**2>=0.000

Excited State 88: Singlet-EU 4.7177 eV 262.80 nm f=0.0863

<S2>=0.000**

460 -> 510 -0.17558

462 -> 506 0.10673

463 -> 506 0.19565

463 -> 511 -0.17052

465 -> 509 0.10468

465 -> 510 0.19190

478 -> 505 0.18023

484 -> 508 0.11266

Excited State 89: Singlet-EU 4.7177 eV 262.80 nm f=0.0863

<S2>=0.000**

460 -> 509 0.17558

462 -> 506 0.19565

462 -> 511 0.17052

463 -> 506 -0.10672

465 -> 509 0.19190

465 -> 510 -0.10468

479 -> 505 0.18023

484 -> 507 0.11266

Excited State 90: Singlet-?Sym 4.7289 eV 262.19 nm f=0.0000 <S**2>=0.000

Excited State 91: Singlet-B1U 4.7290 eV 262.18 nm f=0.0000 <S**2>=0.000

Excited State 92: Singlet-EG 4.7469 eV 261.19 nm f=0.0000 <S**2>=0.000

Excited State 93: Singlet-EG 4.7469 eV 261.19 nm f=0.0000 <S**2>=0.000

Excited State 94: Singlet-A1U 4.7543 eV 260.79 nm f=0.0000 <S**2>=0.000

Excited State 95: Singlet-A1G 4.7780 eV 259.49 nm f=0.0000 <S**2>=0.000

Excited State 96: Singlet-B1G 4.7889 eV 258.90 nm f=0.0000 <S**2>=0.000

Excited State 97: Singlet-A2U 4.8005 eV 258.27 nm f=0.0170

<S2>=0.000**

496 -> 505 0.10369

500 -> 505 -0.10371

501 -> 511 0.21554

502 -> 515 0.23196

502 -> 522 0.10011

503 -> 516 -0.23196

503 -> 521 -0.10012

504 -> 519 0.52033

Excited State 98: Singlet-A1U 4.8051 eV 258.03 nm f=0.0000 <S**2>=0.000

Excited State 99: Singlet-EU 4.8100 eV 257.76 nm f=0.0678

<S2>=0.000**

458 -> 505 -0.12306

460 -> 509 -0.11011

460 -> 510 -0.15063

461 -> 508 -0.10346

462 -> 506 -0.11406

462 -> 511 -0.10443
463 -> 506 0.15604
463 -> 511 -0.14286
465 -> 509 -0.11109
465 -> 510 0.15197
475 -> 506 -0.11887
478 -> 505 -0.11923
480 -> 510 0.10395
495 -> 506 -0.10100

Excited State 100: Singlet-EU 4.8100 eV 257.76 nm f=0.0678

<S2>=0.000**

459 -> 505 -0.12307
460 -> 509 0.15063
460 -> 510 -0.11011
461 -> 507 -0.10346
462 -> 506 0.15604
462 -> 511 0.14286
463 -> 506 0.11406
463 -> 511 -0.10443
465 -> 509 0.15197
465 -> 510 0.11109
476 -> 506 -0.11887
479 -> 505 -0.11922
480 -> 509 0.10394
494 -> 506 0.10100

Excited State 101: Singlet-B1G 4.8312 eV 256.63 nm f=0.0000 <S2>=0.000**

Excited State 102: Singlet-EG 4.9058 eV 252.73 nm f=0.0000 <S2>=0.000**

Excited State 103: Singlet-EG 4.9058 eV 252.73 nm f=0.0000 <S2>=0.000**

Excited State 104: Singlet-EU 4.9065 eV 252.69 nm f=0.0090

<S2>=0.000**

480 -> 509 0.11248
481 -> 506 0.13080
483 -> 509 0.13345
489 -> 507 -0.15811
490 -> 505 0.27923
490 -> 512 0.12219
492 -> 507 0.16793
502 -> 513 0.18703
504 -> 517 0.27193

Excited State 105: Singlet-EU 4.9065 eV 252.69 nm f=0.0090

<S2>=0.000**

480 -> 510 -0.11248
482 -> 506 0.13080
483 -> 510 0.13345
489 -> 508 -0.15812
491 -> 505 0.27924

491 -> 512 -0.12219

492 -> 508 -0.16793

503 -> 513 -0.18703

504 -> 518 0.27193

Excited State 106: Singlet-B2U 4.9231 eV 251.84 nm f=0.0000 <S**2>=0.000

Excited State 107: Singlet-A2U 4.9718 eV 249.38 nm f=0.5664

<S2>=0.000**

468 -> 511 0.13223

473 -> 505 0.23500

475 -> 507 0.12616

476 -> 508 0.12616

477 -> 506 0.11319

478 -> 509 0.10049

479 -> 510 0.10050

485 -> 512 0.16521

486 -> 507 -0.14495

487 -> 508 -0.14495

488 -> 505 0.21926

489 -> 520 -0.10200

496 -> 505 0.12556

500 -> 505 0.13575

Excited State 108: Singlet-A2G 4.9814 eV 248.89 nm f=0.0000 <S**2>=0.000

Excited State 109: Singlet-EG 5.0092 eV 247.51 nm f=0.0000 <S**2>=0.000

Excited State 110: Singlet-EG 5.0092 eV 247.51 nm f=0.0000 <S**2>=0.000

Excited State 111: Singlet-A1G 5.0632 eV 244.87 nm f=0.0000 <S**2>=0.000

Excited State 112: Singlet-B1G 5.0748 eV 244.31 nm f=0.0000 <S**2>=0.000

Excited State 113: Singlet-B1U 5.0791 eV 244.10 nm f=0.0000 <S**2>=0.000

Excited State 114: Singlet-EU 5.1022 eV 243.00 nm f=0.1124

<S2>=0.000**

483 -> 509 -0.13239

483 -> 510 -0.12100

489 -> 507 -0.12043

489 -> 508 -0.11007

490 -> 505 0.24432

491 -> 505 0.22332

492 -> 507 0.13792

492 -> 508 -0.12606

493 -> 509 0.17697

493 -> 510 -0.16174

494 -> 506 0.17461

495 -> 506 0.15960

Excited State 115: Singlet-EU 5.1022 eV 243.00 nm f=0.1124

<S2>=0.000**

483 -> 509 0.12100

483 -> 510 -0.13239

489 -> 507 0.11007

489 -> 508 -0.12043
 490 -> 505 -0.22332
 491 -> 505 0.24433
 492 -> 507 -0.12605
 492 -> 508 -0.13792
 493 -> 509 -0.16175
 493 -> 510 -0.17696
 494 -> 506 -0.15959
 495 -> 506 0.17461
Excited State 116: Singlet-A1G 5.1126 eV 242.51 nm f=0.0000 <S**2>=0.000
Excited State 117: Singlet-?Sym 5.1179 eV 242.25 nm f=0.0000 <S**2>=0.000
Excited State 118: Singlet-B1G 5.1231 eV 242.01 nm f=0.0000 <S**2>=0.000
Excited State 119: Singlet-EU 5.1525 eV 240.63 nm f=0.3709
 <S**2>=0.000
 471 -> 505 0.13146
 473 -> 510 -0.12539
 476 -> 506 -0.14459
 478 -> 505 0.13036
 479 -> 505 0.28837
 480 -> 509 0.13864
 481 -> 506 0.11857
 483 -> 509 0.10372
 484 -> 507 0.17074
 489 -> 507 0.10584
 490 -> 505 -0.10504
 494 -> 506 0.17058
 496 -> 510 0.13517
Excited State 120: Singlet-EU 5.1525 eV 240.63 nm f=0.3709
 <S**2>=0.000
 470 -> 505 -0.13145
 473 -> 509 -0.12539
 475 -> 506 -0.14460
 478 -> 505 0.28838
 479 -> 505 -0.13037
 480 -> 510 0.13864
 482 -> 506 -0.11858
 483 -> 510 -0.10372
 484 -> 508 0.17075
 489 -> 508 -0.10585
 491 -> 505 0.10504
 495 -> 506 -0.17058
 496 -> 509 0.13518
Excited State 121: Singlet-EG 5.1687 eV 239.88 nm f=0.0000 <S**2>=0.000
Excited State 122: Singlet-EG 5.1687 eV 239.88 nm f=0.0000 <S**2>=0.000
Excited State 123: Singlet-A2G 5.1906 eV 238.86 nm f=0.0000 <S**2>=0.000
Excited State 124: Singlet-A1U 5.1998 eV 238.44 nm f=0.0000 <S**2>=0.000

Excited State 125: Singlet-B1U 5.2292 eV 237.10 nm f=0.0000 <S**2>=0.000
Excited State 126: Singlet-EG 5.2354 eV 236.82 nm f=0.0000 <S**2>=0.000
Excited State 127: Singlet-EG 5.2354 eV 236.82 nm f=0.0000 <S**2>=0.000
Excited State 128: Singlet-A1U 5.2516 eV 236.09 nm f=0.0000 <S**2>=0.000

**Excited State 129: Singlet-A2U 5.2765 eV 234.98 nm f=0.6750
<S**2>=0.000**

468 -> 511 -0.17233
469 -> 506 -0.13902
473 -> 505 0.25077
477 -> 506 -0.21101
478 -> 509 -0.18817
479 -> 510 -0.18821
485 -> 512 0.10654
486 -> 507 -0.15771
487 -> 508 -0.15773
488 -> 505 0.19125
496 -> 505 0.13927

Excited State 130: Singlet-EG 5.2793 eV 234.85 nm f=0.0000 <S**2>=0.000
Excited State 131: Singlet-EG 5.2793 eV 234.85 nm f=0.0000 <S**2>=0.000
Excited State 132: Singlet-A2G 5.2809 eV 234.78 nm f=0.0000 <S**2>=0.000
Excited State 133: Singlet-B2U 5.2836 eV 234.66 nm f=0.0000 <S**2>=0.000
Excited State 134: Singlet-A1G 5.3075 eV 233.60 nm f=0.0000 <S**2>=0.000

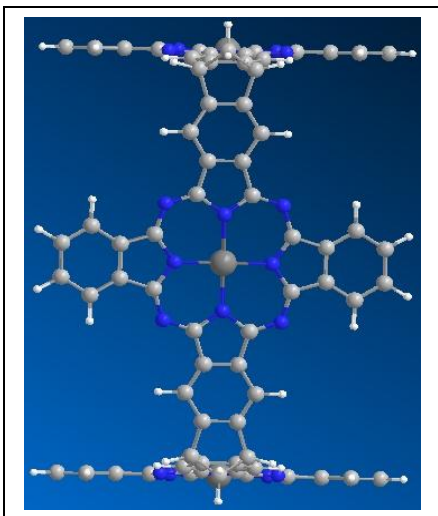
**Excited State 135: Singlet-EU 5.3081 eV 233.58 nm f=0.0214
<S**2>=0.000**

453 -> 509 0.13546
455 -> 506 0.14545
455 -> 511 0.12863
456 -> 509 0.13794
493 -> 510 0.11458
501 -> 518 0.11373
501 -> 527 0.13277
502 -> 525 0.22096
502 -> 528 0.18089
504 -> 518 0.11294
504 -> 526 -0.12358
504 -> 527 0.28945

**Excited State 136: Singlet-EU 5.3081 eV 233.58 nm f=0.0214
<S**2>=0.000**

453 -> 510 -0.13547
454 -> 506 -0.14546
454 -> 511 0.12863
456 -> 510 0.13794
493 -> 509 0.11475
501 -> 517 0.11369
501 -> 526 -0.13273
503 -> 525 0.22088

503 -> 528 -0.18083
504 -> 517 -0.11291
504 -> 526 0.28935
504 -> 527 0.12356
Excited State 137: Singlet-B2G 5.3312 eV 232.56 nm f=0.0000 <S**2>=0.000
Excited State 138: Singlet-A2U 5.3681 eV 230.97 nm f=0.2262
<S2>=0.000**
453 -> 512 0.21488
454 -> 508 -0.27319
455 -> 507 0.27313
456 -> 505 0.39305
465 -> 513 -0.11396
Excited State 139: Singlet-EU 5.3704 eV 230.86 nm f=0.0806
<S2>=0.000**
473 -> 509 -0.15233
475 -> 511 -0.16118
480 -> 510 -0.10545
493 -> 510 -0.28303
495 -> 511 -0.32600
496 -> 509 0.22816
498 -> 511 -0.13149
500 -> 509 -0.13795
504 -> 527 0.14541
Excited State 140: Singlet-EG 5.3968 eV 229.74 nm f=0.0000 <S**2>=0.000



Excited State 1: Singlet-A2G 1.8163 eV 682.64 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 2: Singlet-EU 1.9578 eV 633.30 nm f=1.1376 $\langle S^{*2} \rangle = 0.000$

616 -> 630 0.10517
621 -> 627 -0.32659
623 -> 625 0.34818
623 -> 632 0.32248
624 -> 627 0.34375

Excited State 3: Singlet-EU 1.9578 eV 633.30 nm f=1.1376 $\langle S^{*2} \rangle = 0.000$

616 -> 629 0.10517
621 -> 626 0.32659
622 -> 625 0.34818
622 -> 632 -0.32248
624 -> 626 0.34375

Excited State 4: Singlet-B2U 1.9881 eV 623.63 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 5: Singlet-EG 2.0048 eV 618.43 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 6: Singlet-EG 2.0048 eV 618.43 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 7: Singlet-B2G 2.0364 eV 608.84 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 8: Singlet-A2U 2.0402 eV 607.70 nm f=1.5331
 $\langle S^{*2} \rangle = 0.000$

616 -> 625 -0.11594
621 -> 628 -0.33053
622 -> 629 0.33350
623 -> 630 0.33350
624 -> 631 0.33665

Excited State 9: Singlet-B2U 3.6420 eV 340.43 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 10: Singlet-EG 3.6420 eV 340.43 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 11: Singlet-EG 3.6420 eV 340.43 nm f=0.0000 $\langle S^{*2} \rangle = 0.000$

Excited State 12: Singlet-A2U 3.6421 eV 340.42 nm f=0.0121
 $\langle S^{*2} \rangle = 0.000$

602 -> 625 0.23100
605 -> 626 0.23915
606 -> 627 0.23916

608 -> 632	0.33729				
610 -> 626	0.24558				
611 -> 627	-0.24559				
612 -> 625	-0.25891				
Excited State 13: Singlet-A2G 3.6963 eV 335.43 nm f=0.0000 <S**2>=0.000					
Excited State 14:	Singlet-EU	3.6972 eV	335.34 nm	f=0.0113	
<S**2>=0.000					
602 -> 630	0.21206				
605 -> 628	0.10282				
605 -> 631	-0.10122				
606 -> 628	0.22318				
606 -> 631	0.21971				
608 -> 629	0.14296				
608 -> 630	0.31030				
610 -> 628	0.10120				
611 -> 628	-0.21966				
611 -> 631	-0.21580				
612 -> 629	0.10360				
612 -> 630	-0.22487				
Excited State 15:	Singlet-EU	3.6972 eV	335.34 nm	f=0.0113	
<S**2>=0.000					
602 -> 629	-0.21206				
605 -> 628	0.22318				
605 -> 631	-0.21971				
606 -> 628	-0.10282				
606 -> 631	-0.10122				
608 -> 629	0.31030				
608 -> 630	-0.14296				
610 -> 628	0.21966				
610 -> 631	-0.21580				
611 -> 628	0.10120				
612 -> 629	0.22487				
612 -> 630	0.10360				
Excited State 16: Singlet-B2G 3.6976 eV 335.31 nm f=0.0000 <S**2>=0.000					
Excited State 17: Singlet-A2G 3.8878 eV 318.90 nm f=0.0000 <S**2>=0.000					
Excited State 18: Singlet-?Sym 3.8979 eV 318.08 nm f=0.0000 <S**2>=0.000					
Excited State 19:	Singlet-EU	3.8982 eV	318.06 nm	f=0.0427	
<S**2>=0.000					
621 -> 626	-0.43785				
621 -> 627	0.11312				
624 -> 626	0.50113				
624 -> 627	0.12947				
Excited State 20:	Singlet-EU	3.8982 eV	318.06 nm	f=0.0427	
<S**2>=0.000					
621 -> 626	0.11312				
621 -> 627	0.43785				

624 -> 626	-0.12947				
624 -> 627	0.50113				
Excited State	21:	Singlet-EU	3.9039 eV	317.59 nm	f=0.0584
<S**2>=0.000					
622 -> 625	0.41549				
622 -> 632	0.35531				
623 -> 625	-0.32068				
623 -> 632	0.27424				
Excited State	22:	Singlet-EU	3.9039 eV	317.59 nm	f=0.0584
<S**2>=0.000					
622 -> 625	0.32068				
622 -> 632	0.27424				
623 -> 625	0.41549				
623 -> 632	-0.35531				
Excited State 23:	Singlet-?Sym	3.9048 eV	317.52 nm	f=0.0000	<S**2>=0.000
Excited State 24:	Singlet-B2G	3.9114 eV	316.98 nm	f=0.0000	<S**2>=0.000
Excited State 25:	Singlet-A1U	3.9719 eV	312.15 nm	f=0.0000	<S**2>=0.000
Excited State 26:	Singlet-EG	3.9918 eV	310.59 nm	f=0.0000	<S**2>=0.000
Excited State 27:	Singlet-EG	3.9918 eV	310.59 nm	f=0.0000	<S**2>=0.000
Excited State 28:	Singlet-B2U	4.0101 eV	309.18 nm	f=0.0000	<S**2>=0.000
Excited State 29:	Singlet-EG	4.0163 eV	308.71 nm	f=0.0000	<S**2>=0.000
Excited State 30:	Singlet-EG	4.0163 eV	308.71 nm	f=0.0000	<S**2>=0.000
Excited State 31:	Singlet-?Sym	4.0177 eV	308.60 nm	f=0.0000	<S**2>=0.000
Excited State	32:	Singlet-A2U	4.0192 eV	308.48 nm	f=0.0001
<S**2>=0.000					
621 -> 628	0.48345				
624 -> 631	0.51188				
Excited State 33:	Singlet-?Sym	4.0207 eV	308.37 nm	f=0.0000	<S**2>=0.000
Excited State 34:	Singlet-EG	4.0221 eV	308.25 nm	f=0.0000	<S**2>=0.000
Excited State 35:	Singlet-EG	4.0221 eV	308.25 nm	f=0.0000	<S**2>=0.000
Excited State 36:	Singlet-B2U	4.0447 eV	306.53 nm	f=0.0000	<S**2>=0.000
Excited State 37:	Singlet-B1U	4.0568 eV	305.62 nm	f=0.0000	<S**2>=0.000
Excited State 38:	Singlet-A2G	4.0865 eV	303.40 nm	f=0.0000	<S**2>=0.000
Excited State 39:	Singlet-EG	4.0990 eV	302.48 nm	f=0.0000	<S**2>=0.000
Excited State 40:	Singlet-EG	4.0990 eV	302.48 nm	f=0.0000	<S**2>=0.000
Excited State	41:	Singlet-A2U	4.1199 eV	300.94 nm	f=0.2496
<S**2>=0.000					
588 -> 625	0.16158				
590 -> 627	0.11761				
591 -> 626	0.11761				
602 -> 625	-0.15406				
605 -> 626	-0.12416				
606 -> 627	-0.12416				
610 -> 626	0.13486				
611 -> 627	-0.13486				
612 -> 625	-0.17932				

613 -> 632	0.26600				
614 -> 626	-0.17769				
615 -> 627	-0.17769				
617 -> 636	-0.10004				
618 -> 627	0.16753				
619 -> 626	0.16753				
620 -> 632	0.22913				
Excited State 42:		Singlet-EU	4.1914 eV	295.81 nm	f=0.5324
<S**2>=0.000					
581 -> 626	-0.20218				
581 -> 627	-0.16972				
582 -> 625	-0.21867				
582 -> 632	0.20680				
583 -> 625	-0.18356				
583 -> 632	-0.17359				
584 -> 626	0.22110				
584 -> 627	-0.18560				
Excited State 43:		Singlet-EU	4.1914 eV	295.81 nm	f=0.5324
<S**2>=0.000					
581 -> 626	-0.16972				
581 -> 627	0.20218				
582 -> 625	-0.18356				
582 -> 632	0.17359				
583 -> 625	0.21867				
583 -> 632	0.20680				
584 -> 626	0.18560				
584 -> 627	0.22110				
Excited State 44:		Singlet-B2G	4.1946 eV	295.58 nm	f=0.0000 <S**2>=0.000
Excited State 45:		Singlet-A2G	4.1947 eV	295.57 nm	f=0.0000 <S**2>=0.000
Excited State 46:		Singlet-EU	4.2070 eV	294.71 nm	f=1.8630
<S**2>=0.000					
581 -> 626	-0.12190				
581 -> 627	-0.10090				
582 -> 625	-0.12188				
582 -> 632	0.12622				
583 -> 625	-0.10088				
583 -> 632	-0.10448				
584 -> 626	0.12312				
584 -> 627	-0.10191				
591 -> 628	0.11078				
594 -> 629	0.12850				
594 -> 630	0.10636				
614 -> 628	-0.10293				
614 -> 631	0.10176				
616 -> 629	0.15557				
616 -> 630	-0.12877				

618 -> 628	-0.10800				
619 -> 628	-0.13047				
619 -> 631	0.11918				
620 -> 629	-0.15312				
620 -> 630	-0.12674				
621 -> 626	-0.10936				
Excited State 47:	Singlet-EU	4.2070 eV	294.71 nm	f=1.8630	
<S**2>=0.000					
581 -> 626	-0.10090				
581 -> 627	0.12190				
582 -> 625	-0.10088				
582 -> 632	0.10448				
583 -> 625	0.12188				
583 -> 632	0.12622				
584 -> 626	0.10191				
584 -> 627	0.12312				
590 -> 628	-0.11078				
594 -> 629	0.10636				
594 -> 630	-0.12850				
615 -> 628	0.10293				
615 -> 631	0.10176				
616 -> 629	0.12877				
616 -> 630	0.15557				
618 -> 628	0.13047				
618 -> 631	0.11918				
619 -> 628	-0.10800				
620 -> 629	-0.12674				
620 -> 630	0.15312				
621 -> 627	0.10936				
Excited State 48:	Singlet-B2U	4.2267 eV	293.34 nm	f=0.0000	<S**2>=0.000
Excited State 49:	Singlet-EG	4.2277 eV	293.27 nm	f=0.0000	<S**2>=0.000
Excited State 50:	Singlet-EG	4.2277 eV	293.27 nm	f=0.0000	<S**2>=0.000
Excited State 51:	Singlet-A2U	4.2283 eV	293.23 nm	f=0.0003	
<S**2>=0.000					
581 -> 628	0.30853				
582 -> 629	-0.31959				
583 -> 630	0.31959				
584 -> 631	0.32661				
585 -> 628	-0.12570				
Excited State 52:	Singlet-B2U	4.2856 eV	289.31 nm	f=0.0000	<S**2>=0.000
Excited State 53:	Singlet-B2G	4.2974 eV	288.51 nm	f=0.0000	<S**2>=0.000
Excited State 54:	Singlet-B1G	4.3104 eV	287.64 nm	f=0.0000	<S**2>=0.000
Excited State 55:	Singlet-EG	4.3173 eV	287.18 nm	f=0.0000	<S**2>=0.000
Excited State 56:	Singlet-EG	4.3173 eV	287.18 nm	f=0.0000	<S**2>=0.000
Excited State 57:	Singlet-B2G	4.3287 eV	286.42 nm	f=0.0000	<S**2>=0.000

Excited State 58: Singlet-EU 4.3360 eV 285.94 nm f=0.0006
<S2>=0.000**

621 -> 626 0.34209
621 -> 627 0.16898
622 -> 625 -0.25691
622 -> 632 0.36294
623 -> 625 0.12690
623 -> 632 0.17928
624 -> 626 0.28770
624 -> 627 -0.14211

Excited State 59: Singlet-EU 4.3360 eV 285.94 nm f=0.0006
<S2>=0.000**

621 -> 626 -0.16898
621 -> 627 0.34209
622 -> 625 0.12690
622 -> 632 -0.17928
623 -> 625 0.25691
623 -> 632 0.36294
624 -> 626 -0.14211
624 -> 627 -0.28770

Excited State 60: Singlet-A2G 4.3436 eV 285.44 nm f=0.0000 <S**2>=0.000

Excited State 61: Singlet-A1U 4.3544 eV 284.74 nm f=0.0000 <S**2>=0.000

Excited State 62: Singlet-EG 4.3547 eV 284.71 nm f=0.0000 <S**2>=0.000

Excited State 63: Singlet-EG 4.3547 eV 284.71 nm f=0.0000 <S**2>=0.000

Excited State 64: Singlet-B1U 4.3548 eV 284.71 nm f=0.0000 <S**2>=0.000

Excited State 65: Singlet-EU 4.3580 eV 284.49 nm f=0.0281
<S2>=0.000**

595 -> 628 0.10588
604 -> 625 0.10313
607 -> 626 -0.11469
618 -> 628 -0.10131
621 -> 635 -0.22607
622 -> 633 0.24552
622 -> 636 -0.22395
623 -> 633 -0.10367
624 -> 634 -0.10210
624 -> 635 -0.24180

Excited State 66: Singlet-EU 4.3580 eV 284.49 nm f=0.0281
<S2>=0.000**

596 -> 628 -0.10588
603 -> 625 -0.10313
607 -> 627 -0.11469
619 -> 628 0.10131
621 -> 634 -0.22607
622 -> 633 0.10367
623 -> 633 0.24552

623 -> 636	0.22395					
624 -> 634	0.24180					
624 -> 635	-0.10210					
Excited State	67:	Singlet-A2U	4.3735 eV	283.49 nm	f=4.1933	
<S**2>=0.000						
613 -> 632	-0.15576					
614 -> 626	0.21095					
615 -> 627	0.21095					
616 -> 625	0.30732					
618 -> 627	0.23191					
619 -> 626	0.23191					
620 -> 632	0.27711					
621 -> 628	-0.10967					
622 -> 629	0.12498					
623 -> 630	0.12498					
624 -> 631	0.10550					
Excited State	68:	Singlet-A2U	4.3803 eV	283.05 nm	f=0.0026	
<S**2>=0.000						
621 -> 628	0.37909					
622 -> 629	0.35022					
623 -> 630	0.35022					
624 -> 631	-0.33271					
Excited State 69:	Singlet-EG	4.3830 eV	282.88 nm	f=0.0000	<S**2>=0.000	
Excited State 70:	Singlet-EG	4.3830 eV	282.88 nm	f=0.0000	<S**2>=0.000	
Excited State 71:	Singlet-A1G	4.3848 eV	282.76 nm	f=0.0000	<S**2>=0.000	
Excited State 72:	Singlet-B2U	4.3856 eV	282.70 nm	f=0.0000	<S**2>=0.000	
Excited State 73:	Singlet-A2G	4.5043 eV	275.26 nm	f=0.0000	<S**2>=0.000	
Excited State	74:	Singlet-EU	4.5352 eV	273.38 nm	f=0.9745	
<S**2>=0.000						
594 -> 629	-0.11914					
594 -> 630	-0.11515					
602 -> 629	0.13556					
602 -> 630	-0.13102					
605 -> 628	-0.11696					
606 -> 628	-0.11304					
612 -> 629	0.10065					
613 -> 629	0.19037					
613 -> 630	0.18399					
614 -> 628	-0.14735					
614 -> 631	0.17090					
615 -> 628	-0.14241					
615 -> 631	-0.16517					
616 -> 629	0.13467					
616 -> 630	-0.13016					
Excited State	75:	Singlet-EU	4.5352 eV	273.38 nm	f=0.9746	
<S**2>=0.000						

594 -> 629 0.11515
594 -> 630 -0.11914
602 -> 629 -0.13102
602 -> 630 -0.13556
605 -> 628 0.11304
606 -> 628 -0.11696
612 -> 630 -0.10065
613 -> 629 -0.18399
613 -> 630 0.19037
614 -> 628 0.14241
614 -> 631 -0.16517
615 -> 628 -0.14735
615 -> 631 -0.17090
616 -> 629 -0.13016
616 -> 630 -0.13467

Excited State 76: Singlet-B2G 4.5621 eV 271.77 nm f=0.0000 <S**2>=0.000

Excited State 77: Singlet-B1G 4.6057 eV 269.20 nm f=0.0000 <S**2>=0.000

Excited State 78: Singlet-EU 4.6068 eV 269.13 nm f=0.0128
<S2>=0.000**

569 -> 625 -0.12184
569 -> 632 -0.11567
570 -> 625 -0.13319
570 -> 632 0.12645
572 -> 626 -0.17359
572 -> 627 -0.15879
573 -> 629 0.14674
573 -> 630 -0.13423
574 -> 628 0.14718
574 -> 631 -0.14761
575 -> 628 -0.13464
575 -> 631 -0.13503
576 -> 629 -0.14812
576 -> 630 -0.13549
577 -> 626 0.17395
577 -> 627 -0.15913
578 -> 625 -0.10812
578 -> 632 -0.10372
579 -> 625 -0.11819
579 -> 632 0.11338

Excited State 79: Singlet-EU 4.6068 eV 269.13 nm f=0.0128
<S2>=0.000**

569 -> 625 0.13319
569 -> 632 0.12645
570 -> 625 -0.12184
570 -> 632 0.11567
572 -> 626 -0.15879

572 -> 627 0.17359
 573 -> 629 0.13423
 573 -> 630 0.14674
 574 -> 628 0.13464
 574 -> 631 -0.13503
 575 -> 628 0.14719
 575 -> 631 0.14761
 576 -> 629 -0.13549
 576 -> 630 0.14812
 577 -> 626 0.15913
 577 -> 627 0.17395
 578 -> 625 0.11819
 578 -> 632 0.11338
 579 -> 625 -0.10812
 579 -> 632 0.10372
Excited State 80: Singlet-A1G 4.6083 eV 269.04 nm f=0.0000 <S**2>=0.000
Excited State 81: Singlet-B1U 4.6733 eV 265.30 nm f=0.0000 <S**2>=0.000
Excited State 82: Singlet-EG 4.6733 eV 265.30 nm f=0.0000 <S**2>=0.000
Excited State 83: Singlet-EG 4.6733 eV 265.30 nm f=0.0000 <S**2>=0.000
Excited State 84: Singlet-A1U 4.6733 eV 265.30 nm f=0.0000 <S**2>=0.000
Excited State 85: Singlet-B1G 4.7081 eV 263.34 nm f=0.0000 <S**2>=0.000
Excited State 86: Singlet-EU 4.7306 eV 262.09 nm f=0.1519
 <S**2>=0.000
 591 -> 631 0.11573
 614 -> 628 0.11349
 617 -> 629 0.15253
 617 -> 630 0.19613
 618 -> 628 -0.14913
 619 -> 628 -0.19176
Excited State 87: Singlet-EU 4.7306 eV 262.09 nm f=0.1519
 <S**2>=0.000
 590 -> 631 -0.11573
 615 -> 628 0.11349
 617 -> 629 0.19613
 617 -> 630 -0.15253
 618 -> 628 -0.19176
 619 -> 628 0.14913
Excited State 88: Singlet-A1U 4.7465 eV 261.21 nm f=0.0000 <S**2>=0.000
Excited State 89: Singlet-EG 4.7466 eV 261.21 nm f=0.0000 <S**2>=0.000
Excited State 90: Singlet-EG 4.7466 eV 261.21 nm f=0.0000 <S**2>=0.000
Excited State 91: Singlet-B1U 4.7467 eV 261.20 nm f=0.0000 <S**2>=0.000
Excited State 92: Singlet-A2G 4.7595 eV 260.50 nm f=0.0000 <S**2>=0.000
Excited State 93: Singlet-A1G 4.7886 eV 258.92 nm f=0.0000 <S**2>=0.000
Excited State 94: Singlet-EU 4.7936 eV 258.65 nm f=0.0141
 <S**2>=0.000
 569 -> 625 -0.12360

569 -> 632	-0.13030				
572 -> 626	-0.13005				
572 -> 627	-0.16988				
573 -> 629	-0.15103				
573 -> 630	0.19729				
574 -> 628	-0.15204				
574 -> 631	0.15026				
575 -> 628	0.19861				
575 -> 631	0.19628				
576 -> 629	0.15135				
576 -> 630	0.19771				
577 -> 626	0.13215				
577 -> 627	-0.17263				
578 -> 625	-0.12150				
578 -> 632	-0.10936				
Excited State 95:		Singlet-EU	4.7936 eV	258.65 nm	f=0.0141
<S**2>=0.000					
570 -> 625	0.12360				
570 -> 632	-0.13030				
572 -> 626	0.16988				
572 -> 627	-0.13005				
573 -> 629	0.19729				
573 -> 630	0.15103				
574 -> 628	0.19861				
574 -> 631	-0.19628				
575 -> 628	0.15204				
575 -> 631	0.15026				
576 -> 629	-0.19771				
576 -> 630	0.15135				
577 -> 626	-0.17263				
577 -> 627	-0.13215				
579 -> 625	0.12150				
579 -> 632	-0.10936				
Excited State 96:		Singlet-B1G	4.7940 eV	258.62 nm	f=0.0000 <S**2>=0.000
Excited State 97:		Singlet-A1G	4.8067 eV	257.94 nm	f=0.0000 <S**2>=0.000
Excited State 98:		Singlet-EU	4.8421 eV	256.05 nm	f=0.3613
<S**2>=0.000					
588 -> 629	-0.12088				
588 -> 630	0.10649				
590 -> 628	0.12224				
591 -> 628	0.13877				
594 -> 629	0.10121				
596 -> 631	-0.10111				
598 -> 632	-0.10194				
618 -> 631	0.14070				
619 -> 631	-0.15972				

620 -> 629	0.16379				
620 -> 630	0.14429				
Excited State 99:	Singlet-EU	4.8421 eV	256.05 nm	f=0.3613	
<S**2>=0.000					
588 -> 629	0.10649				
588 -> 630	0.12088				
590 -> 628	0.13877				
591 -> 628	-0.12224				
594 -> 630	0.10121				
595 -> 631	0.10111				
599 -> 632	0.10194				
618 -> 631	0.15972				
619 -> 631	0.14070				
620 -> 629	-0.14429				
620 -> 630	0.16379				
Excited State 100:	Singlet-B2G	4.8805 eV	254.04 nm	f=0.0000	<S**2>=0.000
Excited State 101:	Singlet-B1G	4.8814 eV	253.99 nm	f=0.0000	<S**2>=0.000
Excited State 102:	Singlet-EU	4.9109 eV	252.46 nm	f=0.0047	
<S**2>=0.000					
593 -> 630	0.11037				
595 -> 628	0.10961				
596 -> 628	0.13424				
596 -> 631	0.11592				
597 -> 629	0.11078				
597 -> 630	0.13567				
598 -> 625	0.11365				
600 -> 627	-0.10374				
609 -> 629	0.11505				
609 -> 630	-0.14090				
617 -> 629	0.14000				
617 -> 630	0.17146				
618 -> 631	0.12093				
619 -> 631	-0.14811				
Excited State 103:	Singlet-EU	4.9109 eV	252.46 nm	f=0.0047	
<S**2>=0.000					
593 -> 629	-0.11037				
595 -> 628	0.13424				
595 -> 631	-0.11592				
596 -> 628	-0.10961				
597 -> 629	0.13567				
597 -> 630	-0.11078				
599 -> 625	0.11365				
600 -> 626	0.10374				
609 -> 629	0.14090				
609 -> 630	0.11505				
617 -> 629	0.17146				

617 -> 630 -0.14000
 618 -> 631 0.14811
 619 -> 631 0.12093
 Excited State 104: Singlet-A1U 4.9246 eV 251.77 nm f=0.0000 <S**2>=0.000
 Excited State 105: Singlet-EG 4.9313 eV 251.42 nm f=0.0000 <S**2>=0.000
 Excited State 106: Singlet-EG 4.9313 eV 251.42 nm f=0.0000 <S**2>=0.000
 Excited State 107: Singlet-A1G 4.9338 eV 251.30 nm f=0.0000 <S**2>=0.000
 Excited State 108: Singlet-B1U 4.9378 eV 251.09 nm f=0.0000 <S**2>=0.000
 Excited State 109: Singlet-B2U 4.9939 eV 248.27 nm f=0.0000 <S**2>=0.000
 Excited State 110: Singlet-EG 4.9969 eV 248.12 nm f=0.0000 <S**2>=0.000
 Excited State 111: Singlet-EG 4.9969 eV 248.12 nm f=0.0000 <S**2>=0.000
Excited State 112: Singlet-A2U 5.0017 eV 247.88 nm f=0.2953
<S2>=0.000**
 571 -> 628 0.10113
 580 -> 631 0.11653
 585 -> 628 0.16633
 586 -> 630 0.15467
 587 -> 629 0.15467
 588 -> 625 -0.13934
 590 -> 627 -0.14217
 591 -> 626 -0.14217
 592 -> 631 0.17049
 594 -> 632 -0.16525
 Excited State 113: Singlet-B1G 5.0414 eV 245.93 nm f=0.0000 <S**2>=0.000
Excited State 114: Singlet-EU 5.0489 eV 245.57 nm f=0.0117
<S2>=0.000**
 589 -> 626 0.10441
 601 -> 626 -0.14965
 601 -> 627 -0.12733
 603 -> 625 -0.16449
 603 -> 632 -0.14110
 604 -> 625 -0.19333
 604 -> 632 0.16584
 607 -> 626 0.20241
 607 -> 627 -0.17221
 617 -> 629 0.12557
 617 -> 630 0.10684
 622 -> 633 0.10621
Excited State 115: Singlet-EU 5.0489 eV 245.57 nm f=0.0117
<S2>=0.000**
 589 -> 627 -0.10441
 601 -> 626 -0.12733
 601 -> 627 0.14965
 603 -> 625 0.19333
 603 -> 632 0.16584
 604 -> 625 -0.16449

604 -> 632 0.14110
 607 -> 626 0.17221
 607 -> 627 0.20241
 617 -> 629 0.10684
 617 -> 630 -0.12557
 623 -> 633 0.10621
 Excited State 116: Singlet-A1G 5.0618 eV 244.94 nm f=0.0000 <S**2>=0.000
 Excited State 117: Singlet-A2G 5.1084 eV 242.71 nm f=0.0000 <S**2>=0.000
Excited State 118: Singlet-EU 5.1403 eV 241.20 nm f=0.2360
<S2>=0.000**
 585 -> 626 -0.13830
 585 -> 627 -0.12113
 586 -> 625 -0.12734
 586 -> 632 -0.10397
 587 -> 625 0.14538
 587 -> 632 -0.11870
 592 -> 626 0.17074
 592 -> 627 -0.14954
 613 -> 629 -0.11586
 613 -> 630 -0.10148
 619 -> 631 0.10784
 620 -> 629 -0.11844
 620 -> 630 -0.10374
Excited State 119: Singlet-EU 5.1403 eV 241.20 nm f=0.2360
<S2>=0.000**
 585 -> 626 -0.12113
 585 -> 627 0.13830
 586 -> 625 0.14538
 586 -> 632 0.11870
 587 -> 625 0.12734
 587 -> 632 -0.10397
 592 -> 626 0.14954
 592 -> 627 0.17074
 613 -> 629 -0.10148
 613 -> 630 0.11586
 618 -> 631 0.10784
 620 -> 629 -0.10374
 620 -> 630 0.11844
 Excited State 120: Singlet-A1U 5.1574 eV 240.40 nm f=0.0000 <S**2>=0.000
 Excited State 121: Singlet-B2G 5.1682 eV 239.90 nm f=0.0000 <S**2>=0.000
 Excited State 122: Singlet-EG 5.1715 eV 239.75 nm f=0.0000 <S**2>=0.000
 Excited State 123: Singlet-EG 5.1715 eV 239.75 nm f=0.0000 <S**2>=0.000
 Excited State 124: Singlet-B1U 5.1862 eV 239.07 nm f=0.0000 <S**2>=0.000
 Excited State 125: Singlet-B1G 5.2211 eV 237.47 nm f=0.0000 <S**2>=0.000
Excited State 126: Singlet-EU 5.2386 eV 236.67 nm f=0.0010
<S2>=0.000**

589 -> 627 -0.14054
593 -> 630 0.16670
596 -> 628 0.15713
596 -> 631 0.16467
597 -> 630 0.17063
598 -> 625 -0.18716
598 -> 632 -0.20301
600 -> 627 0.24470
601 -> 627 -0.21903
603 -> 625 -0.17567
603 -> 632 -0.15326

Excited State 127: Singlet-EU 5.2386 eV 236.67 nm f=0.0010

<S2>=0.000**

589 -> 626 0.14054
593 -> 629 0.16670
595 -> 628 -0.15713
595 -> 631 0.16467
597 -> 629 -0.17063
599 -> 625 0.18716
599 -> 632 -0.20301
600 -> 626 0.24470
601 -> 626 0.21903
604 -> 625 0.17567
604 -> 632 -0.15326

Excited State 128: Singlet-A1G 5.2523 eV 236.06 nm f=0.0000 <S**2>=0.000

Excited State 129: Singlet-B2U 5.3212 eV 233.00 nm f=0.0000 <S**2>=0.000

Excited State 130: Singlet-EG 5.3290 eV 232.66 nm f=0.0000 <S**2>=0.000

Excited State 131: Singlet-EG 5.3290 eV 232.66 nm f=0.0000 <S**2>=0.000

Excited State 132: Singlet-A2U 5.3405 eV 232.16 nm f=1.2179

<S2>=0.000**

585 -> 628 0.16723
586 -> 630 0.15548
587 -> 629 0.15548
588 -> 625 0.21324
590 -> 627 0.21389
591 -> 626 0.21389
592 -> 631 0.17509
594 -> 632 0.25318
602 -> 625 0.15685
605 -> 626 0.10923
606 -> 627 0.10923

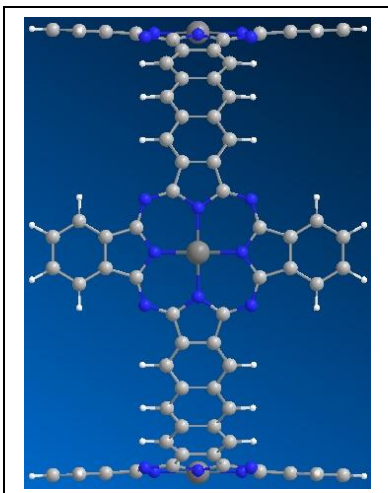
Excited State 133: Singlet-B2U 5.4209 eV 228.71 nm f=0.0000 <S**2>=0.000

Excited State 134: Singlet-A2U 5.4209 eV 228.71 nm f=0.0231

<S2>=0.000**

565 -> 625 0.30800
566 -> 627 0.30280

567 -> 626 0.30283
568 -> 632 0.29836
574 -> 635 0.10124
575 -> 634 0.10123
576 -> 636 0.10453
Excited State 135: Singlet-EG 5.4210 eV 228.71 nm f=0.0000 <S**2>=0.000
Excited State 136: Singlet-EG 5.4210 eV 228.71 nm f=0.0000 <S**2>=0.000
Excited State 137: Singlet-A2G 5.4338 eV 228.17 nm f=0.0000 <S**2>=0.000
Excited State 138: Singlet-EU 5.4342 eV 228.16 nm f=0.0001
<S2>=0.000**
565 -> 630 0.27772
566 -> 628 0.27929
566 -> 631 0.27649
568 -> 630 0.27838
Excited State 139: Singlet-EU 5.4342 eV 228.16 nm f=0.0001
<S2>=0.000**
565 -> 629 -0.27772
567 -> 628 0.27929
567 -> 631 -0.27649
568 -> 629 0.27838
Excited State 140: Singlet-B2U 5.4743 eV 226.48 nm f=0.0000 <S**2>=0.000



Excited State 1: Singlet-A2G 1.5396 eV 805.31 nm f=0.0000 <S**2>=0.000
 Excited State 2: Singlet-EG 1.6647 eV 744.79 nm f=0.0000 <S**2>=0.000
 Excited State 3: Singlet-EG 1.6647 eV 744.79 nm f=0.0000 <S**2>=0.000
 Excited State 4: Singlet-B2U 1.6701 eV 742.39 nm f=0.0000 <S**2>=0.000

Excited State 5: Singlet-A2U 1.6760 eV 739.78 nm f=1.5790

<S2>=0.000**

605 -> 613 0.27441

606 -> 611 0.33057

607 -> 612 0.33057

608 -> 609 0.41284

Excited State 6: Singlet-EU 1.8557 eV 668.13 nm f=1.8313 <S2>=0.000**

605 -> 614 -0.13388

605 -> 615 -0.24143

606 -> 610 -0.19191

606 -> 616 -0.13072

607 -> 610 0.34607

607 -> 616 -0.23573

608 -> 614 -0.18876

608 -> 615 0.34039

Excited State 7: Singlet-EU 1.8557 eV 668.13 nm f=1.8313 <S2>=0.000**

605 -> 614 0.24143

605 -> 615 -0.13388

606 -> 610 0.34607

606 -> 616 0.23573

607 -> 610 0.19191

607 -> 616 -0.13072

608 -> 614 0.34039

608 -> 615 0.18876

Excited State 8: Singlet-B2G 2.0522 eV 604.14 nm f=0.0000 <S**2>=0.000

Excited State 9: Singlet-B1U 3.0176 eV 410.87 nm f=0.0000 <S**2>=0.000

Excited State 10: Singlet-EG 3.0861 eV 401.75 nm f=0.0000 <S**2>=0.000

Excited State 11: Singlet-EG 3.0861 eV 401.75 nm f=0.0000 <S**2>=0.000

Excited State 12: Singlet-A2U 3.1555 eV 392.91 nm f=0.0474

<S2>=0.000**

601 -> 609 -0.11913
602 -> 611 -0.11133
603 -> 612 0.11133
604 -> 617 0.14326
605 -> 613 -0.26291
606 -> 618 -0.21523
607 -> 619 0.21523
608 -> 609 0.38121
608 -> 620 -0.28865

Excited State 13: Singlet-?Sym 3.2788 eV 378.14 nm f=0.0000 <S**2>=0.000

Excited State 14: Singlet-EG 3.2902 eV 376.82 nm f=0.0000 <S**2>=0.000

Excited State 15: Singlet-EG 3.2902 eV 376.82 nm f=0.0000 <S**2>=0.000

Excited State 16: Singlet-?Sym 3.3306 eV 372.25 nm f=0.0000 <S**2>=0.000

Excited State 17: Singlet-B2U 3.3597 eV 369.04 nm f=0.0000 <S**2>=0.000

Excited State 18: Singlet-A2G 3.3910 eV 365.63 nm f=0.0000 <S**2>=0.000

Excited State 19: Singlet-EU 3.4265 eV 361.84 nm f=0.9049

<S2>=0.000**

601 -> 614 0.11018
602 -> 610 0.18959
603 -> 610 0.15389
604 -> 614 -0.11228
604 -> 615 0.13832
605 -> 614 0.21387
605 -> 615 0.17361
606 -> 610 -0.14802
606 -> 616 0.18921
607 -> 610 0.12015
607 -> 616 0.15358
607 -> 621 0.11243
608 -> 614 -0.18727
608 -> 615 0.15201
608 -> 622 0.11362

Excited State 20: Singlet-EU 3.4265 eV 361.84 nm f=0.9049

<S2>=0.000**

601 -> 615 -0.11018
602 -> 610 -0.15389
603 -> 610 0.18959
604 -> 614 -0.13832
604 -> 615 -0.11228
605 -> 614 -0.17361
605 -> 615 0.21387
606 -> 610 0.12015
606 -> 616 -0.15358
606 -> 621 -0.11243

607 -> 610	0.14802
607 -> 616	0.18921
608 -> 614	0.15201
608 -> 615	0.18727
608 -> 623	0.11362
Excited State 21: Singlet-EU	3.4761 eV 356.68 nm f=0.0053
<S**2>=0.000	
604 -> 614	-0.12279
605 -> 615	-0.14463
607 -> 610	0.44099
607 -> 616	0.20313
608 -> 615	-0.43651
Excited State 22: Singlet-EU	3.4761 eV 356.68 nm f=0.0053
<S**2>=0.000	
604 -> 615	-0.12279
605 -> 614	0.14463
606 -> 610	0.44099
606 -> 616	-0.20313
608 -> 614	-0.43651
Excited State 23: Singlet-?Sym	3.5359 eV 350.65 nm f=0.0000 <S**2>=0.000
Excited State 24: Singlet-A2U	3.5579 eV 348.47 nm f=0.0105
<S**2>=0.000	
604 -> 617	-0.13766
605 -> 613	-0.10782
606 -> 611	-0.21935
606 -> 618	0.19326
607 -> 612	-0.21935
607 -> 619	-0.19326
608 -> 609	0.42043
608 -> 620	0.29069
Excited State 25: Singlet-?Sym	3.5695 eV 347.35 nm f=0.0000 <S**2>=0.000
Excited State 26: Singlet-EG	3.6016 eV 344.25 nm f=0.0000 <S**2>=0.000
Excited State 27: Singlet-EG	3.6016 eV 344.25 nm f=0.0000 <S**2>=0.000
Excited State 28: Singlet-B2G	3.6562 eV 339.11 nm f=0.0000 <S**2>=0.000
Excited State 29: Singlet-A2G	3.6638 eV 338.40 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-EU	3.6748 eV 337.39 nm f=0.0782
<S**2>=0.000	
577 -> 611	0.15255
578 -> 609	0.18737
578 -> 613	0.17613
580 -> 611	0.22583
585 -> 611	0.23914
587 -> 609	0.20854
587 -> 613	0.20304
588 -> 611	-0.17174
593 -> 611	-0.10242

595 -> 613 -0.10570
597 -> 611 0.15007
598 -> 609 0.13056
598 -> 613 0.10436
600 -> 611 0.11631

Excited State 31: Singlet-EU 3.6748 eV 337.39 nm f=0.0782

<S2>=0.000**

577 -> 612 0.15255
579 -> 609 0.18737
579 -> 613 -0.17613
580 -> 612 -0.22583
585 -> 612 0.23914
586 -> 609 -0.20854
586 -> 613 0.20304
588 -> 612 0.17174
593 -> 612 -0.10242
594 -> 613 0.10570
597 -> 612 -0.15007
599 -> 609 0.13056
599 -> 613 -0.10436
600 -> 612 0.11631

Excited State 32: Singlet-B2G 3.6802 eV 336.90 nm f=0.0000 <S**2>=0.000

Excited State 33: Singlet-A1U 3.7188 eV 333.40 nm f=0.0000 <S**2>=0.000

Excited State 34: Singlet-EG 3.8101 eV 325.41 nm f=0.0000 <S**2>=0.000

Excited State 35: Singlet-EG 3.8101 eV 325.41 nm f=0.0000 <S**2>=0.000

Excited State 36: Singlet-B2U 3.8874 eV 318.94 nm f=0.0000 <S**2>=0.000

Excited State 37: Singlet-B2U 3.9307 eV 315.42 nm f=0.0000 <S**2>=0.000

Excited State 38: Singlet-A2G 3.9389 eV 314.77 nm f=0.0000 <S**2>=0.000

Excited State 39: Singlet-EG 3.9603 eV 313.06 nm f=0.0000 <S**2>=0.000

Excited State 40: Singlet-EG 3.9603 eV 313.06 nm f=0.0000 <S**2>=0.000

Excited State 41: Singlet-A2G 3.9668 eV 312.55 nm f=0.0000 <S**2>=0.000

Excited State 42: Singlet-A2U 4.0040 eV 309.65 nm f=0.2438

<S2>=0.000**

577 -> 610 0.15599
578 -> 614 0.17566
579 -> 615 0.17566
580 -> 616 0.21032
585 -> 610 0.26072
586 -> 615 -0.20390
587 -> 614 0.20390
588 -> 616 -0.15821
593 -> 610 -0.15622
594 -> 615 -0.13056
595 -> 614 -0.13056
597 -> 616 0.16434
598 -> 614 0.12360

599 -> 615 0.12360
 600 -> 610 0.12693
 Excited State 43: Singlet-EG 4.0059 eV 309.51 nm f=0.0000 <S**2>=0.000
 Excited State 44: Singlet-EG 4.0059 eV 309.51 nm f=0.0000 <S**2>=0.000
 Excited State 45: Singlet-B2U 4.0115 eV 309.07 nm f=0.0000 <S**2>=0.000
Excited State 46: Singlet-A2U 4.0205 eV 308.38 nm f=0.0119
<S2>=0.000**
 601 -> 609 0.13098
 602 -> 611 0.11622
 603 -> 612 -0.11622
 605 -> 613 0.46968
 606 -> 611 -0.26195
 607 -> 612 -0.26195
 608 -> 620 -0.19777
 Excited State 47: Singlet-B1U 4.0754 eV 304.23 nm f=0.0000 <S**2>=0.000
Excited State 48: Singlet-EU 4.0821 eV 303.72 nm f=1.9839
<S2>=0.000**
 577 -> 612 -0.12840
 579 -> 609 -0.12778
 579 -> 613 0.15171
 580 -> 612 0.14950
 593 -> 619 0.11300
 594 -> 620 -0.11138
 595 -> 617 -0.13687
 596 -> 611 0.11621
 596 -> 618 -0.16885
 597 -> 612 -0.10053
 598 -> 617 -0.13170
 599 -> 609 0.21438
 600 -> 612 0.19679
 600 -> 619 0.11317
 603 -> 610 -0.11221
 604 -> 614 0.13088
 605 -> 615 0.10901
 607 -> 610 0.20764
 608 -> 615 0.10586
Excited State 49: Singlet-EU 4.0821 eV 303.72 nm f=1.9839
<S2>=0.000**
 577 -> 611 -0.12840
 578 -> 609 -0.12778
 578 -> 613 -0.15171
 580 -> 611 -0.14950
 593 -> 618 -0.11300
 594 -> 617 -0.13687
 595 -> 620 -0.11138
 596 -> 612 0.11621

596 -> 619 0.16886
 597 -> 611 0.10053
 598 -> 609 0.21438
 599 -> 617 -0.13170
 600 -> 611 0.19679
 600 -> 618 -0.11317
 602 -> 610 0.11221
 604 -> 615 0.13088
 605 -> 614 -0.10901
 606 -> 610 0.20764
 608 -> 614 0.10586
Excited State 50: Singlet-?Sym 4.1061 eV 301.95 nm f=0.0000 <S**2>=0.000
Excited State 51: Singlet-EG 4.1261 eV 300.48 nm f=0.0000 <S**2>=0.000
Excited State 52: Singlet-EG 4.1261 eV 300.48 nm f=0.0000 <S**2>=0.000
Excited State 53: Singlet-?Sym 4.1609 eV 297.98 nm f=0.0000 <S**2>=0.000
Excited State 54: Singlet-A2U 4.1809 eV 296.55 nm f=0.0754
 <S**2>=0.000
 568 -> 609 -0.11007
 569 -> 613 0.21251
 570 -> 612 0.19799
 571 -> 611 0.19800
 573 -> 609 0.28596
 574 -> 611 0.22164
 575 -> 612 -0.22164
 576 -> 613 0.20868
 605 -> 613 -0.19451
Excited State 55: Singlet-B2U 4.1838 eV 296.35 nm f=0.0000 <S**2>=0.000
Excited State 56: Singlet-EU 4.1840 eV 296.33 nm f=0.8733
 <S**2>=0.000
 577 -> 612 0.11414
 579 -> 609 0.11158
 579 -> 613 -0.11289
 580 -> 612 -0.10898
 603 -> 610 -0.14133
 605 -> 615 0.12448
 606 -> 616 -0.22052
 606 -> 621 0.12251
 607 -> 616 0.33987
 608 -> 614 0.11980
 608 -> 615 0.18464
 608 -> 623 -0.10469
Excited State 57: Singlet-EU 4.1840 eV 296.33 nm f=0.8733
 <S**2>=0.000
 577 -> 611 -0.11414
 578 -> 609 -0.11158
 578 -> 613 -0.11289

580 -> 611 -0.10898
 602 -> 610 -0.14133
 605 -> 614 0.12448
 606 -> 616 0.33987
 607 -> 616 0.22052
 607 -> 621 -0.12251
 608 -> 614 -0.18464
 608 -> 615 0.11980
 608 -> 622 -0.10469
 Excited State 58: Singlet-EG 4.1883 eV 296.03 nm f=0.0000 <S**2>=0.000
 Excited State 59: Singlet-EG 4.1883 eV 296.03 nm f=0.0000 <S**2>=0.000
 Excited State 60: Singlet-A1U 4.2177 eV 293.96 nm f=0.0000 <S**2>=0.000
 Excited State 61: Singlet-B2G 4.2496 eV 291.75 nm f=0.0000 <S**2>=0.000
 Excited State 62: Singlet-B1G 4.2514 eV 291.63 nm f=0.0000 <S**2>=0.000
Excited State 63: Singlet-EU 4.2595 eV 291.08 nm f=0.1694
<S2>=0.000**
 604 -> 615 -0.13178
 605 -> 614 0.38017
 605 -> 615 0.25975
 606 -> 610 -0.18696
 606 -> 616 -0.25448
 607 -> 610 0.12774
 607 -> 616 -0.17387
 608 -> 614 0.13822
Excited State 64: Singlet-EU 4.2595 eV 291.08 nm f=0.1694
<S2>=0.000**
 604 -> 614 0.13178
 605 -> 614 -0.25975
 605 -> 615 0.38017
 606 -> 610 0.12774
 606 -> 616 0.17387
 607 -> 610 0.18696
 607 -> 616 -0.25448
 608 -> 615 -0.13822
 Excited State 65: Singlet-B1U 4.2834 eV 289.45 nm f=0.0000 <S**2>=0.000
 Excited State 66: Singlet-EG 4.2946 eV 288.70 nm f=0.0000 <S**2>=0.000
 Excited State 67: Singlet-EG 4.2946 eV 288.70 nm f=0.0000 <S**2>=0.000
 Excited State 68: Singlet-A1G 4.2958 eV 288.62 nm f=0.0000 <S**2>=0.000
Excited State 69: Singlet-EU 4.3057 eV 287.95 nm f=0.0489
<S2>=0.000**
 601 -> 614 -0.15227
 602 -> 610 -0.10343
 602 -> 616 -0.11763
 605 -> 622 -0.21285
 606 -> 616 0.12902
 607 -> 621 0.25994

607 -> 627 0.23138
 608 -> 622 0.27363
Excited State 70: Singlet-EU 4.3057 eV 287.95 nm f=0.0489
<S2>=0.000**
 601 -> 615 0.15227
 603 -> 610 -0.10343
 603 -> 616 0.11763
 605 -> 623 0.21285
 606 -> 621 -0.25994
 606 -> 627 0.23138
 607 -> 616 0.12902
 608 -> 623 0.27363
Excited State 71: Singlet-A2U 4.3120 eV 287.53 nm f=0.0513
<S2>=0.000**
 574 -> 611 -0.10515
 575 -> 612 0.10515
 576 -> 613 -0.11132
 601 -> 609 0.27482
 601 -> 620 -0.14359
 602 -> 611 0.21191
 602 -> 618 -0.16993
 603 -> 612 -0.21191
 603 -> 619 -0.16993
 604 -> 617 -0.21290
 605 -> 613 -0.18074
 608 -> 620 -0.20117
Excited State 72: Singlet-A2G 4.4022 eV 281.64 nm f=0.0000 <S2>=0.000**
Excited State 73: Singlet-B2G 4.4072 eV 281.32 nm f=0.0000 <S2>=0.000**
Excited State 74: Singlet-EU 4.4078 eV 281.29 nm f=0.1552
<S2>=0.000**
 568 -> 615 -0.10807
 569 -> 615 -0.19620
 570 -> 610 0.19151
 570 -> 616 -0.17052
 573 -> 614 -0.12872
 573 -> 615 0.25480
 574 -> 610 -0.11419
 575 -> 610 -0.22603
 575 -> 616 0.18714
 576 -> 615 -0.19420
Excited State 75: Singlet-EU 4.4078 eV 281.29 nm f=0.1553
<S2>=0.000**
 577 -> 611 0.12329
 578 -> 609 0.10464
 585 -> 611 -0.20655
 587 -> 609 -0.23073

587 -> 613 -0.22256
 588 -> 611 0.24622
 593 -> 611 -0.15288
 595 -> 609 -0.11244
 595 -> 613 -0.16016
 597 -> 611 0.15707
 598 -> 609 0.12795
 Excited State 76: Singlet-A2G 4.4205 eV 280.48 nm f=0.0000 <S**2>=0.000
Excited State 77: Singlet-EU 4.4398 eV 279.26 nm f=0.9508
<S2>=0.000**
 577 -> 612 -0.12329
 579 -> 609 -0.10464
 585 -> 612 0.20655
 586 -> 609 -0.23073
 586 -> 613 0.22256
 588 -> 612 0.24622
 593 -> 612 0.15288
 594 -> 609 0.11244
 594 -> 613 -0.16016
 597 -> 612 0.15707
 599 -> 609 -0.12795
Excited State 78: Singlet-EU 4.4398 eV 279.26 nm f=0.9508
<S2>=0.000**
 577 -> 612 -0.12329
 579 -> 609 -0.10464
 585 -> 612 0.20655
 586 -> 609 -0.23073
 586 -> 613 0.22256
 588 -> 612 0.24622
 593 -> 612 0.15288
 594 -> 609 0.11244
 594 -> 613 -0.16016
 597 -> 612 0.15707
 599 -> 609 -0.12795
 Excited State 79: Singlet-B2G 4.4629 eV 277.81 nm f=0.0000 <S**2>=0.000
 Excited State 80: Singlet-B2U 4.4713 eV 277.29 nm f=0.0000 <S**2>=0.000
 Excited State 81: Singlet-EG 4.4751 eV 277.06 nm f=0.0000 <S**2>=0.000
 Excited State 82: Singlet-EG 4.4751 eV 277.06 nm f=0.0000 <S**2>=0.000
 Excited State 83: Singlet-A1U 4.4874 eV 276.29 nm f=0.0000 <S**2>=0.000
Excited State 84: Singlet-A2U 4.4891 eV 276.19 nm f=2.6367
<S2>=0.000**
 577 -> 610 0.21245
 578 -> 614 0.18537
 579 -> 615 0.18537
 580 -> 616 0.16839
 593 -> 610 0.24275

594 -> 615 0.20162
 595 -> 614 0.20162
 597 -> 616 -0.22950
 598 -> 614 -0.15172
 599 -> 615 -0.15172
 600 -> 610 -0.14460
 605 -> 613 0.16694
Excited State 85: Singlet-B1G 4.5248 eV 274.01 nm f=0.0000 <S2>=0.000**
Excited State 86: Singlet-EG 4.5394 eV 273.13 nm f=0.0000 <S2>=0.000**
Excited State 87: Singlet-EG 4.5394 eV 273.13 nm f=0.0000 <S2>=0.000**
Excited State 88: Singlet-A2G 4.5647 eV 271.62 nm f=0.0000 <S2>=0.000**
Excited State 89: Singlet-B1U 4.5802 eV 270.69 nm f=0.0000 <S2>=0.000**
Excited State 90: Singlet-A1U 4.5965 eV 269.73 nm f=0.0000 <S2>=0.000**
Excited State 91: Singlet-EG 4.5972 eV 269.69 nm f=0.0000 <S2>=0.000**
Excited State 92: Singlet-EG 4.5972 eV 269.69 nm f=0.0000 <S2>=0.000**
Excited State 93: Singlet-B2U 4.5987 eV 269.61 nm f=0.0000 <S2>=0.000**
Excited State 94: Singlet-EU 4.6212 eV 268.30 nm f=0.1928
<S2>=0.000**
 572 -> 614 -0.12320
 593 -> 612 -0.11569
 594 -> 609 -0.13488
 603 -> 610 -0.22422
 603 -> 616 -0.18558
 604 -> 614 0.31763
 605 -> 615 -0.18138
 607 -> 616 0.11921
 608 -> 623 0.11559
Excited State 95: Singlet-EU 4.6212 eV 268.30 nm f=0.1928
<S2>=0.000**
 572 -> 615 0.12320
 593 -> 611 -0.11569
 595 -> 609 -0.13488
 602 -> 610 0.22422
 602 -> 616 -0.18558
 604 -> 615 0.31763
 605 -> 614 0.18138
 606 -> 616 -0.11921
 608 -> 622 -0.11559
Excited State 96: Singlet-B1U 4.6483 eV 266.73 nm f=0.0000 <S2>=0.000**
Excited State 97: Singlet-A1G 4.6601 eV 266.05 nm f=0.0000 <S2>=0.000**
Excited State 98: Singlet-B1G 4.6636 eV 265.85 nm f=0.0000 <S2>=0.000**
Excited State 99: Singlet-EU 4.6714 eV 265.41 nm f=0.0083
<S2>=0.000**
 561 -> 611 0.30167
 563 -> 609 0.30736
 563 -> 613 0.29941

564 -> 611 0.30290
 608 -> 623 -0.10283
Excited State 100: Singlet-EU 4.6714 eV 265.41 nm f=0.0083
<S2>=0.000**
 561 -> 612 -0.30167
 562 -> 609 0.30736
 562 -> 613 -0.29941
 564 -> 612 0.30290
 608 -> 622 0.10283
 Excited State 101: Singlet-EG 4.7052 eV 263.50 nm f=0.0000 <S**2>=0.000
 Excited State 102: Singlet-EG 4.7052 eV 263.50 nm f=0.0000 <S**2>=0.000
 Excited State 103: Singlet-A1G 4.7341 eV 261.90 nm f=0.0000 <S**2>=0.000
 Excited State 104: Singlet-B1U 4.7657 eV 260.16 nm f=0.0000 <S**2>=0.000
 Excited State 105: Singlet-EG 4.7801 eV 259.38 nm f=0.0000 <S**2>=0.000
 Excited State 106: Singlet-EG 4.7801 eV 259.38 nm f=0.0000 <S**2>=0.000
 Excited State 107: Singlet-A1U 4.7890 eV 258.89 nm f=0.0000 <S**2>=0.000
Excited State 108: Singlet-A2U 4.7921 eV 258.73 nm f=0.0003
<S2>=0.000**
 593 -> 610 0.22603
 594 -> 615 0.15084
 595 -> 614 0.15084
 596 -> 621 -0.10768
 598 -> 614 0.18176
 599 -> 615 0.18176
 600 -> 610 0.29159
 601 -> 609 0.20237
 602 -> 611 0.15242
 603 -> 612 -0.15242
 605 -> 613 -0.14193
 Excited State 109: Singlet-B1G 4.8079 eV 257.87 nm f=0.0000 <S**2>=0.000
Excited State 110: Singlet-EU 4.8092 eV 257.81 nm f=0.0014
<S2>=0.000**
 593 -> 610 0.22603
 594 -> 615 0.15084
 595 -> 614 0.15084
 596 -> 621 -0.10768
 598 -> 614 0.18176
 599 -> 615 0.18176
 600 -> 610 0.29159
 601 -> 609 0.20237
 602 -> 611 0.15242
 603 -> 612 -0.15242
 605 -> 613 -0.14193
Excited State 111: Singlet-EU 4.8092 eV 257.81 nm f=0.0014
<S2>=0.000**
 558 -> 610 0.11563

558 -> 616 -0.10744
 560 -> 615 -0.18716
 565 -> 615 0.19169
 567 -> 610 0.17386
 567 -> 616 -0.14178
 581 -> 612 0.18089
 583 -> 609 0.17819
 583 -> 613 -0.17751
 584 -> 612 -0.18489
Excited State 112: Singlet-A1G 4.8205 eV 257.20 nm f=0.0000 <S**2>=0.000
Excited State 113: Singlet-A2U 4.8578 eV 255.23 nm f=0.7063 <S**2>=0.000
Excited State 114: Singlet-A1U 4.8690 eV 254.64 nm f=0.0000 <S**2>=0.000
Excited State 115: Singlet-B1G 4.8894 eV 253.58 nm f=0.0000 <S**2>=0.000
Excited State 116: Singlet-A2G 4.8953 eV 253.27 nm f=0.0000 <S**2>=0.000
Excited State 117: Singlet-EG 4.8980 eV 253.13 nm f=0.0000 <S**2>=0.000
Excited State 118: Singlet-EG 4.8980 eV 253.13 nm f=0.0000 <S**2>=0.000
Excited State 119: Singlet-EU 4.8994 eV 253.06 nm f=0.1691
<S2>=0.000**
 559 -> 610 0.14821
 559 -> 616 0.10374
 560 -> 614 0.19818
 560 -> 615 0.10081
 565 -> 614 0.19722
 565 -> 615 -0.10032
 566 -> 610 0.16189
 566 -> 616 0.15153
 581 -> 611 -0.15508
 582 -> 609 -0.15281
 582 -> 613 -0.15136
 584 -> 611 -0.15796
 608 -> 623 -0.10752
Excited State 120: Singlet-EU 4.8994 eV 253.06 nm f=0.1691
<S2>=0.000**
 558 -> 610 -0.14821
 558 -> 616 0.10375
 560 -> 614 -0.10081
 560 -> 615 0.19818
 565 -> 614 -0.10032
 565 -> 615 -0.19722
 567 -> 610 -0.16189
 567 -> 616 0.15153
 581 -> 612 0.15508
 583 -> 609 0.15281
 583 -> 613 -0.15136
 584 -> 612 -0.15797
 608 -> 622 -0.10752

Excited State 121: Singlet-B1U 4.9026 eV 252.90 nm f=0.0000 <S**2>=0.000
Excited State 122: Singlet-EG 4.9097 eV 252.53 nm f=0.0000 <S**2>=0.000
Excited State 123: Singlet-EG 4.9097 eV 252.53 nm f=0.0000 <S**2>=0.000
Excited State 124: Singlet-B1U 4.9183 eV 252.09 nm f=0.0000 <S**2>=0.000
Excited State 125: Singlet-A1G 4.9209 eV 251.95 nm f=0.0000 <S**2>=0.000

Excited State 126: Singlet-EU 4.9247 eV 251.76 nm f=0.1781
<S2>=0.000**

593 -> 612 -0.11506
594 -> 609 -0.16649
595 -> 609 0.10935
596 -> 611 -0.11942
597 -> 612 -0.11357
599 -> 613 -0.11300
601 -> 614 -0.16577
601 -> 615 0.25239
602 -> 610 -0.12004
602 -> 616 -0.14160
603 -> 610 -0.18277
603 -> 616 0.21560
604 -> 614 -0.10108

Excited State 127: Singlet-EU 4.9247 eV 251.76 nm f=0.1781
<S2>=0.000**

593 -> 611 -0.11506
594 -> 609 -0.10935
595 -> 609 -0.16649
596 -> 612 -0.11942
597 -> 611 0.11357
598 -> 613 0.11300
601 -> 614 0.25239
601 -> 615 0.16577
602 -> 610 0.18277
602 -> 616 0.21560
603 -> 610 -0.12004
603 -> 616 0.14160
604 -> 615 -0.10108

Excited State 128: Singlet-B2G 4.9264 eV 251.67 nm f=0.0000 <S**2>=0.000
Excited State 129: Singlet-A1U 4.9407 eV 250.95 nm f=0.0000 <S**2>=0.000
Excited State 130: Singlet-EG 4.9747 eV 249.23 nm f=0.0000 <S**2>=0.000
Excited State 131: Singlet-EG 4.9747 eV 249.23 nm f=0.0000 <S**2>=0.000
Excited State 132: Singlet-B2U 4.9898 eV 248.48 nm f=0.0000 <S**2>=0.000
Excited State 133: Singlet-EG 5.0587 eV 245.09 nm f=0.0000 <S**2>=0.000
Excited State 134: Singlet-EG 5.0587 eV 245.09 nm f=0.0000 <S**2>=0.000
Excited State 135: Singlet-?Sym 5.0614 eV 244.96 nm f=0.0000 <S**2>=0.000
Excited State 136: Singlet-B2U 5.0967 eV 243.26 nm f=0.0000 <S**2>=0.000
Excited State 137: Singlet-A2G 5.1202 eV 242.15 nm f=0.0000 <S**2>=0.000

Excited State 138: Singlet-A2U 5.1451 eV 240.97 nm f=0.0676

<S2>=0.000**

606 -> 618 -0.35320

607 -> 619 0.35320

608 -> 620 0.45495

Excited State 139: Singlet-EU 5.1677 eV 239.92 nm f=0.0665

<S2>=0.000**

605 -> 623 0.13078

605 -> 634 -0.11606

605 -> 635 -0.19770

606 -> 629 -0.16255

606 -> 636 -0.13330

607 -> 629 0.27689

607 -> 636 -0.22707

608 -> 623 -0.10882

608 -> 634 -0.16649

608 -> 635 0.28359

Excited State 140: Singlet-EU 5.1677 eV 239.92 nm f=0.0665

<S2>=0.000**

605 -> 622 0.13078

605 -> 634 0.19770

605 -> 635 -0.11606

606 -> 629 0.27689

606 -> 636 0.22707

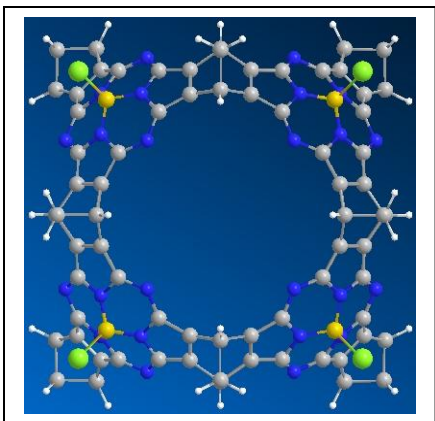
607 -> 629 0.16255

607 -> 636 -0.13330

608 -> 622 0.10882

608 -> 634 0.28360

608 -> 635 0.16648



Excited State 1: Singlet-EU 2.8230 eV 439.20 nm f=0.0000 <S**2>=0.000
 Excited State 2: Singlet-EU 2.8230 eV 439.20 nm f=0.0000 <S**2>=0.000
 Excited State 3: Singlet-T1G 2.8273 eV 438.53 nm f=0.0000 <S**2>=0.000
 Excited State 4: Singlet-T1G 2.8273 eV 438.53 nm f=0.0000 <S**2>=0.000
 Excited State 5: Singlet-T1G 2.8273 eV 438.53 nm f=0.0000 <S**2>=0.000

Excited State 6: Singlet-T1U 2.9714 eV 417.26 nm f=0.9137

<S2>=0.000**

669 -> 687 -0.20106
 670 -> 683 -0.10557
 670 -> 689 -0.17193
 671 -> 677 -0.20621
 672 -> 682 0.10557
 672 -> 690 0.17193
 673 -> 680 0.19698
 673 -> 686 0.10660
 674 -> 681 0.19698
 674 -> 685 0.10660
 675 -> 691 0.11085
 675 -> 692 0.16864
 676 -> 684 0.22435

Excited State 7: Singlet-T1U 2.9714 eV 417.26 nm f=0.9137

<S2>=0.000**

669 -> 685 0.15157
 669 -> 686 0.15178
 670 -> 677 0.13303
 670 -> 678 -0.10270
 670 -> 688 0.12978
 671 -> 689 0.12961
 671 -> 690 -0.12979
 672 -> 678 0.16678
 672 -> 688 -0.12961
 673 -> 679 0.14870
 673 -> 692 -0.13594

674 -> 679 -0.14850
674 -> 691 -0.15209
675 -> 680 -0.14850
675 -> 681 -0.14870
676 -> 682 0.16913
676 -> 683 -0.16936

Excited State 8: Singlet-T1U 2.9714 eV 417.26 nm f=0.9137

<S2>=0.000**

669 -> 685 0.14387
669 -> 686 -0.14059
670 -> 677 0.12626
670 -> 688 -0.12022
671 -> 689 0.12302
671 -> 690 0.12022
672 -> 678 -0.15449
672 -> 688 -0.12302
673 -> 679 -0.13774
673 -> 692 -0.12903
674 -> 679 -0.14095
674 -> 691 0.14088
675 -> 680 -0.14095
675 -> 681 0.13774
676 -> 682 0.16053
676 -> 683 0.15688

Excited State 9: Singlet-T2G 3.0003 eV 413.23 nm f=0.0000 <S**2>=0.000
Excited State 10: Singlet-T2G 3.0003 eV 413.23 nm f=0.0000 <S**2>=0.000
Excited State 11: Singlet-?Sym 3.0003 eV 413.23 nm f=0.0000 <S**2>=0.000
Excited State 12: Singlet-?Sym 3.0340 eV 408.65 nm f=0.0000 <S**2>=0.000
Excited State 13: Singlet-T2U 3.0340 eV 408.65 nm f=0.0000 <S**2>=0.000
Excited State 14: Singlet-T2U 3.0340 eV 408.65 nm f=0.0000 <S**2>=0.000
Excited State 15: Singlet-?Sym 3.0433 eV 407.41 nm f=0.0000 <S**2>=0.000
Excited State 16: Singlet-?Sym 3.0433 eV 407.41 nm f=0.0000 <S**2>=0.000
Excited State 17: Singlet-?Sym 3.5297 eV 351.26 nm f=0.0000 <S**2>=0.000
Excited State 18: Singlet-?Sym 3.5689 eV 347.40 nm f=0.0000 <S**2>=0.000
Excited State 19: Singlet-?Sym 3.5689 eV 347.40 nm f=0.0000 <S**2>=0.000
Excited State 20: Singlet-?Sym 3.5689 eV 347.40 nm f=0.0000 <S**2>=0.000
Excited State 21: Singlet-?Sym 3.6202 eV 342.48 nm f=0.0000 <S**2>=0.000
Excited State 22: Singlet-?Sym 3.6202 eV 342.48 nm f=0.0000 <S**2>=0.000
Excited State 23: Singlet-?Sym 3.6202 eV 342.48 nm f=0.0000 <S**2>=0.000
Excited State 24: Singlet-?Sym 3.7254 eV 332.81 nm f=0.0000 <S**2>=0.000
Excited State 25: Singlet-?Sym 3.7664 eV 329.19 nm f=0.0000 <S**2>=0.000
Excited State 26: Singlet-?Sym 3.7664 eV 329.19 nm f=0.0000 <S**2>=0.000
Excited State 27: Singlet-?Sym 3.7672 eV 329.12 nm f=0.0000 <S**2>=0.000
Excited State 28: Singlet-?Sym 3.7672 eV 329.12 nm f=0.0000 <S**2>=0.000
Excited State 29: Singlet-?Sym 3.7672 eV 329.12 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-?Sym 3.8714 eV 320.26 nm f=0.0000 <S**2>=0.000

Excited State 31: Singlet-?Sym 3.8714 eV 320.26 nm f=0.0000 <S**2>=0.000
Excited State 32: Singlet-?Sym 3.8714 eV 320.26 nm f=0.0000 <S**2>=0.000
Excited State 33: Singlet-?Sym 3.9142 eV 316.75 nm f=0.0000 <S**2>=0.000
Excited State 34: Singlet-?Sym 3.9142 eV 316.75 nm f=0.0000 <S**2>=0.000
Excited State 35: Singlet-?Sym 3.9142 eV 316.75 nm f=0.0000 <S**2>=0.000

Excited State 36: Singlet-?Sym 3.9537 eV 313.59 nm f=0.0205

<S2>=0.000**

637 -> 679 0.10412
640 -> 678 0.11350
644 -> 688 -0.10811
646 -> 682 0.10115
647 -> 683 -0.10115
652 -> 691 0.10465
661 -> 690 -0.12941
662 -> 689 0.12941
664 -> 692 0.12587
665 -> 686 -0.15934
666 -> 685 -0.15934
667 -> 684 0.16070
668 -> 688 0.15483

Excited State 37: Singlet-?Sym 3.9537 eV 313.59 nm f=0.0205

<S2>=0.000**

637 -> 681 0.11168
638 -> 678 -0.10417
644 -> 690 -0.11596
645 -> 683 0.10850
646 -> 684 0.10850
650 -> 691 -0.12003
660 -> 691 0.11300
661 -> 688 -0.13881
663 -> 689 0.13881
664 -> 686 -0.17091
665 -> 692 -0.14435
666 -> 687 0.17091
667 -> 690 0.14919
668 -> 682 -0.15484

Excited State 38: Singlet-?Sym 3.9537 eV 313.59 nm f=0.0205

<S2>=0.000**

637 -> 680 -0.10322
639 -> 677 0.12055
644 -> 689 -0.10718
645 -> 682 -0.10028
646 -> 678 -0.10164
647 -> 684 0.10028
648 -> 680 0.10372
651 -> 692 0.12395

659 -> 692 -0.11669
 662 -> 688 0.12829
 663 -> 690 0.12829
 664 -> 685 -0.15796
 665 -> 687 0.15796
 666 -> 691 -0.14907
 667 -> 689 -0.12797
 668 -> 683 -0.13281
Excited State 39: Singlet-?Sym 3.9579 eV 313.26 nm f=0.0000 <S2>=0.000**
Excited State 40: Singlet-?Sym 3.9579 eV 313.26 nm f=0.0000 <S2>=0.000**
Excited State 41: Singlet-?Sym 4.1601 eV 298.03 nm f=0.0000 <S2>=0.000**
Excited State 42: Singlet-?Sym 4.1632 eV 297.81 nm f=0.0000 <S2>=0.000**
Excited State 43: Singlet-?Sym 4.1632 eV 297.81 nm f=0.0000 <S2>=0.000**
Excited State 44: Singlet-?Sym 4.1632 eV 297.81 nm f=0.0000 <S2>=0.000**
Excited State 45: Singlet-?Sym 4.1673 eV 297.52 nm f=0.0103
<S2>=0.000**
 610 -> 678 0.11965
 611 -> 682 0.11046
 612 -> 683 -0.11046
 613 -> 681 -0.11583
 614 -> 692 -0.10456
 615 -> 680 -0.11583
 621 -> 679 0.15753
 622 -> 687 -0.15376
 623 -> 677 0.16171
 624 -> 690 0.13800
 625 -> 689 -0.13800
 629 -> 685 -0.13659
 630 -> 686 0.13659
 631 -> 691 0.12656
 635 -> 684 0.12412
 636 -> 688 -0.11478
Excited State 46: Singlet-?Sym 4.1673 eV 297.52 nm f=0.0103
<S2>=0.000**
 610 -> 682 -0.10502
 611 -> 677 0.12188
 612 -> 684 0.10502
 613 -> 691 0.11877
 614 -> 681 0.11013
 615 -> 679 0.11013
 619 -> 683 0.11105
 620 -> 689 0.10297
 621 -> 680 -0.11942
 621 -> 686 0.10151
 622 -> 680 0.10400
 622 -> 686 0.11656

623 -> 690 0.13121
624 -> 678 0.16472
625 -> 688 -0.13121
629 -> 692 0.14375
630 -> 687 -0.12986
631 -> 685 0.12986

**Excited State 47: Singlet-?Sym 4.1673 eV 297.52 nm f=0.0103
<S**2>=0.000**

610 -> 683 -0.10405
611 -> 684 0.10405
613 -> 679 -0.10911
614 -> 680 0.10911
615 -> 692 0.10532
620 -> 682 -0.10359
621 -> 685 -0.15029
622 -> 681 0.15398
623 -> 689 -0.13000
624 -> 688 0.13000
625 -> 677 0.13035
625 -> 678 -0.10063
629 -> 687 0.12866
630 -> 691 -0.12747
631 -> 686 -0.12866
636 -> 682 0.10600

Excited State 48: Singlet-?Sym 4.1734 eV 297.08 nm f=0.0000 <S**2>=0.000

Excited State 49: Singlet-?Sym 4.4115 eV 281.05 nm f=0.0000 <S**2>=0.000

Excited State 50: Singlet-?Sym 4.4115 eV 281.05 nm f=0.0000 <S**2>=0.000

Excited State 51: Singlet-?Sym 4.4121 eV 281.01 nm f=0.0000 <S**2>=0.000

Excited State 52: Singlet-?Sym 4.4121 eV 281.01 nm f=0.0000 <S**2>=0.000

Excited State 53: Singlet-?Sym 4.4121 eV 281.01 nm f=0.0000 <S**2>=0.000

**Excited State 54: Singlet-?Sym 4.4153 eV 280.80 nm f=0.0230
<S**2>=0.000**

621 -> 679 -0.12448
622 -> 687 -0.11515
623 -> 677 0.12102
624 -> 682 0.12972
625 -> 683 -0.12972
629 -> 681 -0.12158
630 -> 680 0.12158
631 -> 691 -0.10919

**Excited State 55: Singlet-?Sym 4.4153 eV 280.80 nm f=0.0230
<S**2>=0.000**

**Excited State 56: Singlet-?Sym 4.4153 eV 280.80 nm f=0.0230
<S**2>=0.000**

623 -> 682 0.11674
624 -> 678 -0.11668

625 -> 684 0.11674
 629 -> 692 0.11740
 630 -> 679 -0.10941
 631 -> 681 0.10941

Excited State 57: Singlet-?Sym 4.4195 eV 280.54 nm
f=0.0000 <S2>=0.000**

Excited State 58: Singlet-?Sym 4.4195 eV 280.54 nm f=0.0000 <S**2>=0.000
 Excited State 59: Singlet-?Sym 4.4235 eV 280.28 nm f=0.0000 <S**2>=0.000
 Excited State 60: Singlet-?Sym 4.4235 eV 280.28 nm f=0.0000 <S**2>=0.000
 Excited State 61: Singlet-?Sym 4.4235 eV 280.28 nm f=0.0000 <S**2>=0.000
 Excited State 62: Singlet-?Sym 4.4244 eV 280.23 nm f=0.0000 <S**2>=0.000
 Excited State 63: Singlet-?Sym 4.4244 eV 280.23 nm f=0.0000 <S**2>=0.000
 Excited State 64: Singlet-?Sym 4.4244 eV 280.23 nm f=0.0000 <S**2>=0.000
 Excited State 65: Singlet-EU 4.4518 eV 278.51 nm f=0.0000 <S**2>=0.000
 Excited State 66: Singlet-EU 4.4518 eV 278.51 nm f=0.0000 <S**2>=0.000
 Excited State 67: Singlet-T1G 4.4875 eV 276.29 nm f=0.0000 <S**2>=0.000
 Excited State 68: Singlet-T1G 4.4875 eV 276.29 nm f=0.0000 <S**2>=0.000
 Excited State 69: Singlet-T1G 4.4875 eV 276.29 nm f=0.0000 <S**2>=0.000
 Excited State 70: Singlet-T2G 4.6298 eV 267.79 nm f=0.0000 <S**2>=0.000
 Excited State 71: Singlet-T2G 4.6298 eV 267.79 nm f=0.0000 <S**2>=0.000
 Excited State 72: Singlet-?Sym 4.6298 eV 267.79 nm f=0.0000 <S**2>=0.000
 Excited State 73: Singlet-T2U 4.6675 eV 265.63 nm f=0.0000 <S**2>=0.000
 Excited State 74: Singlet-T2U 4.6675 eV 265.63 nm f=0.0000 <S**2>=0.000
 Excited State 75: Singlet-T2U 4.6675 eV 265.63 nm f=0.0000 <S**2>=0.000

Excited State 76: Singlet-T1U 4.6692 eV 265.54 nm f=1.9884
<S2>=0.000**

644 -> 688 -0.10637
 653 -> 683 0.10596
 654 -> 682 -0.10596
 655 -> 678 0.11213
 656 -> 679 0.13843
 656 -> 681 0.12144
 657 -> 688 0.10750

Excited State 77: Singlet-T1U 4.6692 eV 265.54 nm f=1.9884
<S2>=0.000**

654 -> 677 0.10982
 656 -> 679 0.10415
 656 -> 680 0.12654

Excited State 78: Singlet-T1U 4.6692 eV 265.54 nm f=1.9884
<S2>=0.000**

644 -> 689 0.10280
 653 -> 684 -0.10240
 654 -> 677 0.11610
 655 -> 682 0.10240
 656 -> 680 0.13378
 656 -> 681 0.11006
 657 -> 689 -0.10389

Excited State 79: Singlet-?Sym 4.7091 eV 263.28 nm f=0.0000 <S**2>=0.000
Excited State 80: Singlet-?Sym 4.7091 eV 263.28 nm f=0.0000 <S**2>=0.000
Excited State 81: Singlet-?Sym 4.7572 eV 260.63 nm f=0.0000 <S**2>=0.000
Excited State 82: Singlet-?Sym 4.7626 eV 260.33 nm f=0.0000 <S**2>=0.000
Excited State 83: Singlet-?Sym 4.7626 eV 260.33 nm f=0.0000 <S**2>=0.000
Excited State 84: Singlet-?Sym 4.7626 eV 260.33 nm f=0.0000 <S**2>=0.000

Excited State 85: Singlet-?Sym 4.7693 eV 259.96 nm f=0.0439

<S2>=0.000**

645 -> 677 0.10490
646 -> 690 -0.10211
647 -> 689 0.10211
649 -> 679 0.12690
650 -> 686 -0.11506
651 -> 685 0.11506
655 -> 678 -0.12405
661 -> 682 0.12631
662 -> 683 -0.12631
663 -> 678 0.15270
664 -> 692 -0.13669
665 -> 680 0.17704
665 -> 686 -0.11600
666 -> 681 0.17704
666 -> 685 -0.11600
667 -> 684 -0.17511
668 -> 688 0.20427

Excited State 86: Singlet-?Sym 4.7693 eV 259.96 nm f=0.0439

<S2>=0.000**

648 -> 680 0.10150
661 -> 677 -0.11626
664 -> 680 -0.12781
664 -> 681 -0.12581
665 -> 679 0.12582
665 -> 692 0.10551
666 -> 679 -0.12781
666 -> 691 0.11605
667 -> 689 -0.12102
667 -> 690 0.13247
668 -> 682 0.11356
668 -> 683 0.10375

Excited State 87: Singlet-?Sym 4.7693 eV 259.96 nm f=0.0439

<S2>=0.000**

648 -> 680 -0.10434
661 -> 677 0.11952
664 -> 680 -0.12267
664 -> 681 0.12934
665 -> 679 -0.12934

665 -> 692 0.10127
 666 -> 679 -0.12267
 666 -> 691 -0.11930
 667 -> 689 0.12441
 667 -> 690 0.12714
 668 -> 682 0.10900
 668 -> 683 -0.10666
Excited State 88: Singlet-?Sym 4.7790 eV 259.44 nm f=0.0000 <S**2>=0.000
Excited State 89: Singlet-?Sym 4.8713 eV 254.52 nm f=0.0000 <S**2>=0.000
Excited State 90: Singlet-EU 4.8713 eV 254.52 nm f=0.0000 <S**2>=0.000
Excited State 91: Singlet-T1G 4.8775 eV 254.19 nm f=0.0000 <S**2>=0.000
Excited State 92: Singlet-T1G 4.8775 eV 254.19 nm f=0.0000 <S**2>=0.000
Excited State 93: Singlet-T1G 4.8775 eV 254.19 nm f=0.0000 <S**2>=0.000
Excited State 94: Singlet-?Sym 4.9080 eV 252.62 nm f=0.0000 <S**2>=0.000
Excited State 95: Singlet-?Sym 4.9176 eV 252.13 nm f=0.0000 <S**2>=0.000
Excited State 96: Singlet-?Sym 4.9176 eV 252.13 nm f=0.0000 <S**2>=0.000
Excited State 97: Singlet-?Sym 4.9176 eV 252.13 nm f=0.0000 <S**2>=0.000
Excited State 98: Singlet-?Sym 4.9291 eV 251.53 nm f=0.0000 <S**2>=0.000
Excited State 99: Singlet-?Sym 4.9291 eV 251.53 nm f=0.0000 <S**2>=0.000
Excited State 100: Singlet-?Sym 4.9291 eV 251.53 nm f=0.0000 <S**2>=0.000
Excited State 101: Singlet-?Sym 4.9386 eV 251.05 nm f=0.0000 <S**2>=0.000
Excited State 102: Singlet-T1U 4.9868 eV 248.62 nm f=1.1005
 <S**2>=0.000
 637 -> 679 0.10220
 657 -> 688 -0.10962
 663 -> 678 -0.11977
 669 -> 687 0.16861
 670 -> 683 0.12873
 671 -> 677 -0.13600
 672 -> 682 -0.12873
 673 -> 680 0.13960
 673 -> 686 0.13242
 674 -> 681 0.13960
 674 -> 685 0.13242
 676 -> 684 0.23844
Excited State 103: Singlet-T1U 4.9868 eV 248.62 nm f=1.1004
 <S**2>=0.000
 661 -> 677 -0.11365
 669 -> 686 0.14933
 670 -> 684 0.11401
 671 -> 682 0.11401
 672 -> 678 -0.12905
 673 -> 679 -0.12363
 673 -> 687 0.11728
 675 -> 681 0.12363
 675 -> 685 -0.11728

676 -> 682 0.11089
 676 -> 683 0.21117
Excited State 104: Singlet-T1U 4.9868 eV 248.62 nm f=1.1005
<S2>=0.000**
 657 -> 690 -0.10438
 669 -> 685 -0.16055
 670 -> 677 0.11082
 671 -> 683 0.12258
 672 -> 684 -0.12258
 674 -> 679 -0.13293
 674 -> 687 -0.12610
 675 -> 680 -0.13293
 675 -> 686 0.12610
 676 -> 682 0.22704
 676 -> 683 -0.11659
 Excited State 105: Singlet-T2G 4.9896 eV 248.48 nm f=0.0000 <S**2>=0.000
 Excited State 106: Singlet-T2G 4.9896 eV 248.48 nm f=0.0000 <S**2>=0.000
 Excited State 107: Singlet-T2G 4.9896 eV 248.48 nm f=0.0000 <S**2>=0.000
 Excited State 108: Singlet-EU 4.9987 eV 248.03 nm f=0.0000 <S**2>=0.000
 Excited State 109: Singlet-EU 4.9987 eV 248.03 nm f=0.0000 <S**2>=0.000
 Excited State 110: Singlet-T2G 5.0002 eV 247.96 nm f=0.0000 <S**2>=0.000
 Excited State 111: Singlet-T2G 5.0002 eV 247.96 nm f=0.0000 <S**2>=0.000
 Excited State 112: Singlet-T2G 5.0002 eV 247.96 nm f=0.0000 <S**2>=0.000
 Excited State 113: Singlet-T1G 5.0040 eV 247.77 nm f=0.0000 <S**2>=0.000
 Excited State 114: Singlet-T1G 5.0040 eV 247.77 nm f=0.0000 <S**2>=0.000
 Excited State 115: Singlet-T1G 5.0040 eV 247.77 nm f=0.0000 <S**2>=0.000
 Excited State 116: Singlet-T2U 5.0045 eV 247.75 nm f=0.0000 <S**2>=0.000
 Excited State 117: Singlet-T2U 5.0045 eV 247.75 nm f=0.0000 <S**2>=0.000
 Excited State 118: Singlet-T2U 5.0045 eV 247.75 nm f=0.0000 <S**2>=0.000
Excited State 119: Singlet-?Sym 5.0053 eV 247.70 nm f=0.0486
<S2>=0.000**
 670 -> 683 0.17304
 670 -> 684 0.12866
 670 -> 689 -0.11335
 671 -> 677 0.15077
 671 -> 682 0.12866
 672 -> 678 0.12012
 672 -> 682 -0.17303
 672 -> 690 0.11335
 673 -> 679 0.10729
 673 -> 680 -0.14428
 673 -> 686 0.18514
 673 -> 687 0.13767
 674 -> 681 -0.14429
 674 -> 685 0.18514
 674 -> 691 0.10375

675 -> 681 -0.10729
675 -> 685 -0.13767
675 -> 692 0.11679
676 -> 683 0.10701
676 -> 684 0.14392

Excited State 120: Singlet-?Sym 5.0053 eV 247.70 nm f=0.0486

<S2>=0.000**

670 -> 684 0.18378
670 -> 688 -0.12039
671 -> 682 0.18378
671 -> 690 0.12039
672 -> 678 0.17157
673 -> 679 0.15324
673 -> 686 -0.10676
673 -> 687 0.19664
674 -> 685 -0.10676
674 -> 691 0.14819
675 -> 681 -0.15324
675 -> 685 -0.19664
676 -> 683 0.15285

Excited State 121: Singlet-?Sym 5.0053 eV 247.70 nm f=0.0486

<S2>=0.000**

670 -> 677 -0.14646
670 -> 678 0.11308
670 -> 683 -0.10838
671 -> 683 0.19643
671 -> 689 0.12868
672 -> 682 0.10838
672 -> 684 -0.19643
672 -> 688 -0.12868
673 -> 686 -0.11596
673 -> 692 -0.14176
674 -> 679 0.16379
674 -> 685 -0.11596
674 -> 687 -0.21017
675 -> 680 0.16379
675 -> 686 0.21017
676 -> 682 0.16337

Excited State 122: Singlet-EG 5.0090 eV 247.52 nm f=0.0000 <S**2>=0.000

Excited State 123: Singlet-EG 5.0090 eV 247.52 nm f=0.0000 <S**2>=0.000

Excited State 124: Singlet-?Sym 5.0099 eV 247.48 nm f=0.0000 <S**2>=0.000

Excited State 125: Singlet-?Sym 5.0102 eV 247.46 nm f=0.0000 <S**2>=0.000

Excited State 126: Singlet-?Sym 5.0179 eV 247.09 nm f=0.0000 <S**2>=0.000

Excited State 127: Singlet-?Sym 5.0179 eV 247.09 nm f=0.0000 <S**2>=0.000

Excited State 128: Singlet-?Sym 5.0179 eV 247.09 nm f=0.0000 <S**2>=0.000

Excited State 129: Singlet-T1U 5.0374 eV 246.13 nm f=1.4705

<S2>=0.000**

657 -> 688	-0.13387
659 -> 685	0.10133
660 -> 686	-0.10133
663 -> 678	-0.11006
669 -> 686	-0.11583
669 -> 687	-0.17439
670 -> 688	-0.10498
670 -> 689	-0.15805
671 -> 690	0.10498
672 -> 690	0.15805
674 -> 691	0.12596
675 -> 691	0.10434
675 -> 692	0.15874

Excited State 130: Singlet-T1U 5.0374 eV 246.13 nm f=1.4705

<S2>=0.000**

657 -> 690	-0.15306
658 -> 680	0.10093
658 -> 686	0.11586
659 -> 679	-0.10093
659 -> 687	0.11586
660 -> 691	0.11139
661 -> 684	-0.10980
662 -> 678	0.10768
663 -> 683	0.10980
669 -> 685	0.19938
671 -> 683	-0.10172
671 -> 689	0.18070
672 -> 684	0.10172
672 -> 688	-0.18070
673 -> 692	-0.19406
674 -> 679	0.10454
675 -> 680	0.10454

Excited State 131: Singlet-?Sym 5.0374 eV 246.13 nm f=1.4705

<S2>=0.000**

657 -> 689	0.12466
659 -> 692	0.10137
661 -> 677	-0.10981
669 -> 686	-0.16240
669 -> 687	0.12167
670 -> 688	-0.14718
670 -> 689	0.11027
671 -> 690	0.14718
672 -> 690	-0.11027
674 -> 691	0.17660

675 -> 692 -0.11075

Excited State 132: Singlet-T2U 5.0538 eV 245.33 nm f=0.0000 <S**2>=0.000

Excited State 133: Singlet-T2U 5.0538 eV 245.33 nm f=0.0000 <S**2>=0.000

Excited State 134: Singlet-T2U 5.0538 eV 245.33 nm f=0.0000 <S**2>=0.000

Excited State 135: Singlet-EG 5.1251 eV 241.91 nm f=0.0000 <S**2>=0.000

Excited State 136: Singlet-?Sym 5.1251 eV 241.91 nm f=0.0000 <S**2>=0.000

Excited State 137: Singlet-?Sym 5.1833 eV 239.20 nm f=0.1047

<S2>=0.000**

637 -> 679 -0.11525

640 -> 678 -0.12042

646 -> 682 -0.10452

647 -> 683 0.10453

650 -> 680 -0.10982

651 -> 681 0.10982

655 -> 678 0.14001

656 -> 679 0.12426

Excited State 138: Singlet-?Sym 5.1833 eV 239.20 nm f=0.1047

<S2>=0.000**

637 -> 680 0.12784

639 -> 677 -0.14311

645 -> 682 0.11595

646 -> 678 0.11799

647 -> 684 -0.11594

648 -> 680 -0.12205

649 -> 686 -0.10954

650 -> 679 0.12183

652 -> 681 0.12181

653 -> 684 0.10637

654 -> 677 -0.16639

655 -> 682 -0.10639

656 -> 680 -0.13784

659 -> 692 -0.11746

Excited State 139: Singlet-T1U 5.1833 eV 239.20 nm f=0.1047

<S2>=0.000**

637 -> 681 0.10817

651 -> 679 -0.10307

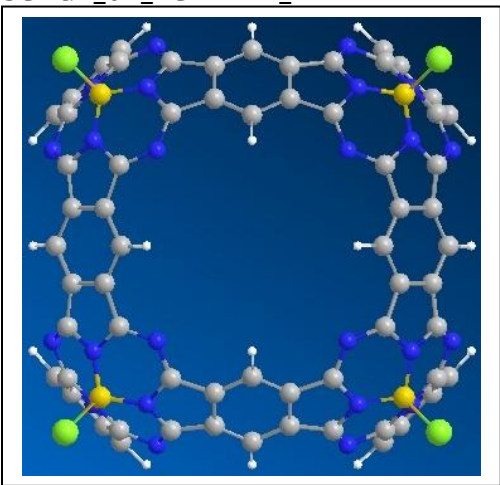
652 -> 680 0.10309

653 -> 678 0.11244

656 -> 681 -0.11663

Excited State 140: Singlet-?Sym 5.1887 eV 238.95 nm f=0.0000 <S**2>=0.000

SCAGE_02_LC-wPBE_TDDFT



Excited State 1: Singlet-T1G 1.7030 eV 728.04 nm f=0.0000 <S**2>=0.000
Excited State 2: Singlet-T1G 1.7030 eV 728.04 nm f=0.0000 <S**2>=0.000
Excited State 3: Singlet-T1G 1.7030 eV 728.04 nm f=0.0000 <S**2>=0.000
Excited State 4: Singlet-EU 1.7888 eV 693.12 nm f=0.0000 <S**2>=0.000
Excited State 5: Singlet-EU 1.7888 eV 693.12 nm f=0.0000 <S**2>=0.000

Excited State 6: Singlet-T1U 2.3196 eV 534.50 nm f=1.6959

<S2>=0.000**

624 -> 632 -0.16960
625 -> 637 0.10305
625 -> 638 -0.15275
626 -> 629 -0.27534
627 -> 631 0.27534
628 -> 635 0.43949

Excited State 7: Singlet-T1U 2.3196 eV 534.50 nm f=1.6959

<S2>=0.000**

623 -> 632 0.15983
623 -> 633 0.10233
625 -> 629 -0.27361
626 -> 637 0.18266
627 -> 630 0.27361
628 -> 634 0.43673

Excited State 8: Singlet-T1U 2.3196 eV 534.50 nm f=1.6959

<S2>=0.000**

622 -> 633 -0.18961
625 -> 631 -0.27366
626 -> 630 0.27366
627 -> 638 0.16461
628 -> 636 0.43681

Excited State 9: Singlet-EG 2.6933 eV 460.34 nm f=0.0000 <S**2>=0.000

Excited State 10: Singlet-?Sym 2.6933 eV 460.34 nm f=0.0000 <S**2>=0.000

Excited State 11: Singlet-?Sym 2.7223 eV 455.44 nm f=0.0000 <S**2>=0.000

Excited State 12: Singlet-?Sym 2.7223 eV 455.44 nm f=0.0000 <S**2>=0.000

Excited State 13: Singlet-?Sym 2.7223 eV 455.44 nm f=0.0000 <S**2>=0.000

Excited State 14: Singlet-T2U 2.8134 eV 440.70 nm f=0.0000 <S**2>=0.000

Excited State 15: Singlet-T2U 2.8134 eV 440.70 nm f=0.0000 <S**2>=0.000

Excited State 16: Singlet-T2U 2.8134 eV 440.70 nm f=0.0000 <S**2>=0.000

Excited State 17: Singlet-T1U 3.4019 eV 364.46 nm f=0.1091

<S2>=0.000**

624 -> 632 0.18777
626 -> 629 0.29678
627 -> 631 -0.29678
628 -> 635 0.48101

Excited State 18: Singlet-T1U 3.4019 eV 364.46 nm f=0.1091

<S2>=0.000**

623 -> 632 -0.17560
623 -> 633 -0.11243

625 -> 629 0.29267
627 -> 630 -0.29267
628 -> 634 0.47435

Excited State 19: Singlet-T1U 3.4019 eV 364.46 nm f=0.1091

<S2>=0.000**

622 -> 633 0.20827
625 -> 631 0.29264
626 -> 630 -0.29264
628 -> 636 0.47431

Excited State 20: Singlet-T1G 3.4301 eV 361.46 nm f=0.0000 <S**2>=0.000
Excited State 21: Singlet-T1G 3.4301 eV 361.46 nm f=0.0000 <S**2>=0.000
Excited State 22: Singlet-T1G 3.4301 eV 361.46 nm f=0.0000 <S**2>=0.000
Excited State 23: Singlet-EU 3.4505 eV 359.33 nm f=0.0000 <S**2>=0.000
Excited State 24: Singlet-EU 3.4505 eV 359.33 nm f=0.0000 <S**2>=0.000
Excited State 25: Singlet-?Sym 3.5496 eV 349.29 nm f=0.0000 <S**2>=0.000
Excited State 26: Singlet-?Sym 3.6906 eV 335.95 nm f=0.0000 <S**2>=0.000
Excited State 27: Singlet-?Sym 3.6906 eV 335.95 nm f=0.0000 <S**2>=0.000
Excited State 28: Singlet-?Sym 3.6906 eV 335.95 nm f=0.0000 <S**2>=0.000
Excited State 29: Singlet-?Sym 3.7014 eV 334.96 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-?Sym 3.7014 eV 334.96 nm f=0.0000 <S**2>=0.000
Excited State 31: Singlet-?Sym 3.7014 eV 334.96 nm f=0.0000 <S**2>=0.000
Excited State 32: Singlet-?Sym 3.7140 eV 333.83 nm f=0.0000 <S**2>=0.000
Excited State 33: Singlet-?Sym 3.7140 eV 333.83 nm f=0.0000 <S**2>=0.000
Excited State 34: Singlet-?Sym 3.7140 eV 333.83 nm f=0.0000 <S**2>=0.000
Excited State 35: Singlet-EG 3.8079 eV 325.60 nm f=0.0000 <S**2>=0.000
Excited State 36: Singlet-EG 3.8079 eV 325.60 nm f=0.0000 <S**2>=0.000
Excited State 37: Singlet-?Sym 3.8313 eV 323.61 nm f=0.0000 <S**2>=0.000

Excited State 38: Singlet-?Sym 4.0551 eV 305.75 nm f=0.4920

<S2>=0.000**

622 -> 633 0.15309
623 -> 635 0.19347
624 -> 634 0.19347
625 -> 647 -0.11344
626 -> 645 -0.11344
627 -> 637 0.15559
627 -> 638 0.31906
628 -> 636 -0.16539
628 -> 650 -0.23686

Excited State 39: Singlet-?Sym 4.0551 eV 305.75 nm f=0.4920

<S2>=0.000**

622 -> 634 -0.19050
623 -> 636 -0.19050
624 -> 632 -0.13400
625 -> 637 -0.19547
625 -> 638 0.28975
626 -> 646 -0.11170

627 -> 647 -0.11170
628 -> 635 0.16285
628 -> 651 0.23322

Excited State 40: Singlet-?Sym 4.0551 eV 305.75 nm f=0.4920

<S2>=0.000**

622 -> 635 0.19249
623 -> 632 -0.12841
624 -> 636 0.19249
625 -> 646 0.11287
626 -> 637 0.35232
627 -> 645 -0.11287
628 -> 634 -0.16455
628 -> 649 0.23566

Excited State 41: Singlet-?Sym 4.0687 eV 304.73 nm f=0.0000 <S**2>=0.000
Excited State 42: Singlet-?Sym 4.0687 eV 304.73 nm f=0.0000 <S**2>=0.000
Excited State 43: Singlet-?Sym 4.0687 eV 304.73 nm f=0.0000 <S**2>=0.000
Excited State 44: Singlet-?Sym 4.0842 eV 303.57 nm f=0.0000 <S**2>=0.000
Excited State 45: Singlet-T2G 4.1139 eV 301.38 nm f=0.0000 <S**2>=0.000
Excited State 46: Singlet-T2G 4.1139 eV 301.38 nm f=0.0000 <S**2>=0.000
Excited State 47: Singlet-T2G 4.1139 eV 301.38 nm f=0.0000 <S**2>=0.000
Excited State 48: Singlet-?Sym 4.1508 eV 298.70 nm f=0.0000 <S**2>=0.000
Excited State 49: Singlet-?Sym 4.1508 eV 298.70 nm f=0.0000 <S**2>=0.000
Excited State 50: Singlet-?Sym 4.1709 eV 297.26 nm f=0.0000 <S**2>=0.000
Excited State 51: Singlet-?Sym 4.1709 eV 297.26 nm f=0.0000 <S**2>=0.000
Excited State 52: Singlet-?Sym 4.1709 eV 297.26 nm f=0.0000 <S**2>=0.000
Excited State 53: Singlet-T2U 4.2730 eV 290.16 nm f=0.0000 <S**2>=0.000
Excited State 54: Singlet-T2U 4.2730 eV 290.16 nm f=0.0000 <S**2>=0.000
Excited State 55: Singlet-T2U 4.2730 eV 290.16 nm f=0.0000 <S**2>=0.000
Excited State 56: Singlet-?Sym 4.3008 eV 288.28 nm f=0.0000 <S**2>=0.000
Excited State 57: Singlet-T2G 4.3008 eV 288.28 nm f=0.0000 <S**2>=0.000
Excited State 58: Singlet-?Sym 4.3008 eV 288.28 nm f=0.0000 <S**2>=0.000
Excited State 59: Singlet-?Sym 4.3123 eV 287.52 nm f=0.0000 <S**2>=0.000

Excited State 60: Singlet-?Sym 4.3295 eV 286.37 nm f=0.0442

<S2>=0.000**

621 -> 639 -0.10836
622 -> 642 -0.12540
623 -> 643 -0.12540
624 -> 632 0.27987
624 -> 633 -0.14489
625 -> 637 -0.11439
625 -> 638 0.16957
626 -> 629 -0.23318
626 -> 640 0.20965
627 -> 631 0.23318
627 -> 641 -0.20965
628 -> 635 0.16402

628 -> 651 -0.11195

Excited State 61: Singlet-?Sym 4.3295 eV 286.37 nm f=0.0443
<S2>=0.000**

622 -> 633 0.24448
623 -> 632 0.16770
623 -> 633 0.10737
625 -> 629 0.14733
625 -> 631 -0.18108
625 -> 640 0.13247
625 -> 641 -0.16281
626 -> 630 0.18108
626 -> 637 0.12893
626 -> 639 -0.16281
627 -> 630 -0.14733
627 -> 638 -0.14278
627 -> 639 -0.13247
628 -> 634 -0.10364
628 -> 636 0.12738

Excited State 62: Singlet-?Sym 4.3295 eV 286.37 nm f=0.0443
<S2>=0.000**

622 -> 633 -0.19877
623 -> 632 0.20583
623 -> 633 0.13178
625 -> 629 0.18083
625 -> 631 0.14723
625 -> 640 0.16258
625 -> 641 0.13237
626 -> 630 -0.14723
626 -> 637 0.15824
626 -> 639 0.13237
627 -> 630 -0.18083
627 -> 638 0.11608
627 -> 639 -0.16258
628 -> 634 -0.12720
628 -> 636 -0.10356

Excited State 63: Singlet-?Sym 4.3737 eV 283.48 nm f=0.0000 <S**2>=0.000
Excited State 64: Singlet-?Sym 4.3901 eV 282.42 nm f=0.0000 <S**2>=0.000
Excited State 65: Singlet-?Sym 4.3901 eV 282.42 nm f=0.0000 <S**2>=0.000
Excited State 66: Singlet-?Sym 4.4402 eV 279.23 nm f=0.0000 <S**2>=0.000
Excited State 67: Singlet-?Sym 4.4402 eV 279.23 nm f=0.0000 <S**2>=0.000
Excited State 68: Singlet-?Sym 4.4402 eV 279.23 nm f=0.0000 <S**2>=0.000
Excited State 69: Singlet-?Sym 4.4629 eV 277.81 nm f=0.0000 <S**2>=0.000
Excited State 70: Singlet-?Sym 4.4629 eV 277.81 nm f=0.0000 <S**2>=0.000
Excited State 71: Singlet-?Sym 4.4629 eV 277.81 nm f=0.0000 <S**2>=0.000
Excited State 72: Singlet-?Sym 4.5413 eV 273.02 nm f=0.0000 <S**2>=0.000
Excited State 73: Singlet-?Sym 4.5413 eV 273.02 nm f=0.0000 <S**2>=0.000

Excited State 74: Singlet-?Sym 4.5413 eV 273.02 nm f=0.0000 <S**2>=0.000
Excited State 75: Singlet-?Sym 4.5502 eV 272.48 nm f=0.0000 <S**2>=0.000
Excited State 76: Singlet-?Sym 4.5502 eV 272.48 nm f=0.0000 <S**2>=0.000
Excited State 77: Singlet-?Sym 4.5700 eV 271.30 nm f=0.0000 <S**2>=0.000
Excited State 78: Singlet-?Sym 4.5700 eV 271.30 nm f=0.0000 <S**2>=0.000
Excited State 79: Singlet-?Sym 4.5788 eV 270.78 nm f=0.0000 <S**2>=0.000
Excited State 80: Singlet-?Sym 4.5788 eV 270.78 nm f=0.0000 <S**2>=0.000
Excited State 81: Singlet-?Sym 4.5788 eV 270.78 nm f=0.0000 <S**2>=0.000

Excited State 82: Singlet-?Sym 4.6052 eV 269.23 nm f=0.0909

<S2>=0.000**

596 -> 631 -0.15021
599 -> 633 0.14253
609 -> 635 -0.11853
610 -> 632 -0.14170
611 -> 636 0.11852
612 -> 631 0.11449
613 -> 631 -0.11526
614 -> 629 -0.15521
616 -> 630 -0.15521
619 -> 633 -0.12798
622 -> 635 -0.18961
624 -> 636 -0.18961
625 -> 640 0.10660
627 -> 639 -0.10660

Excited State 83: Singlet-?Sym 4.6052 eV 269.23 nm f=0.0909

<S2>=0.000**

596 -> 629 -0.15002
597 -> 632 0.16884
609 -> 633 0.16786
610 -> 635 -0.11837
611 -> 634 -0.11837
613 -> 629 0.15659
614 -> 631 -0.15501
615 -> 630 0.15501
617 -> 632 0.15161
622 -> 633 0.11785
623 -> 635 0.18937
624 -> 634 0.18937
625 -> 641 -0.10646
626 -> 639 -0.10646

Excited State 84: Singlet-?Sym 4.6052 eV 269.23 nm f=0.0909

<S2>=0.000**

596 -> 630 -0.15220
598 -> 633 -0.15229
600 -> 629 -0.10042
602 -> 631 0.10042

609 -> 634 0.12010
610 -> 636 -0.12010
611 -> 632 -0.15140
612 -> 630 -0.15915
615 -> 629 0.15727
616 -> 631 -0.15727
618 -> 633 0.13674
622 -> 634 0.19214
623 -> 636 0.19213
624 -> 632 0.10630
626 -> 640 0.10801
627 -> 641 -0.10801

Excited State 85: Singlet-?Sym 4.6642 eV 265.82 nm f=0.0371
<S2>=0.000**

622 -> 633 0.27959
623 -> 635 -0.19321
624 -> 634 -0.19321
625 -> 631 -0.14380
625 -> 641 0.16375
626 -> 630 0.14380
626 -> 639 0.16375
627 -> 638 0.12449

Excited State 86: Singlet-?Sym 4.6642 eV 265.82 nm f=0.0371
<S2>=0.000**

622 -> 634 -0.15441
622 -> 635 0.12646
623 -> 632 0.15427
623 -> 636 -0.15441
624 -> 632 0.19863
624 -> 633 -0.10283
624 -> 636 0.12646
625 -> 640 -0.10718
626 -> 629 -0.11492
626 -> 640 -0.13086
627 -> 631 0.11492
627 -> 639 0.10718
627 -> 641 0.13086

Excited State 87: Singlet-?Sym 4.6642 eV 265.82 nm f=0.0371
<S2>=0.000**

622 -> 634 -0.13612
622 -> 635 -0.14617
623 -> 632 -0.17832
623 -> 633 -0.11417
623 -> 636 -0.13612
624 -> 632 0.17511
624 -> 636 -0.14617

625 -> 629 -0.10879
 625 -> 640 0.12388
 626 -> 629 -0.10131
 626 -> 637 0.10453
 626 -> 640 -0.11536
 627 -> 630 0.10879
 627 -> 631 0.10131
 627 -> 639 -0.12388
 627 -> 641 0.11536
Excited State 88: Singlet-?Sym 4.6708 eV 265.45 nm f=0.0000 <S2>=0.000**
Excited State 89: Singlet-?Sym 4.6708 eV 265.45 nm f=0.0000 <S2>=0.000**
Excited State 90: Singlet-A2G 4.7008 eV 263.75 nm f=0.0000 <S2>=0.000**
Excited State 91: Singlet-T1G 4.7120 eV 263.12 nm f=0.0000 <S2>=0.000**
Excited State 92: Singlet-T1G 4.7120 eV 263.12 nm f=0.0000 <S2>=0.000**
Excited State 93: Singlet-T1G 4.7120 eV 263.12 nm f=0.0000 <S2>=0.000**
Excited State 94: Singlet-?Sym 4.7123 eV 263.11 nm f=0.0000 <S2>=0.000**
Excited State 95: Singlet-?Sym 4.7260 eV 262.35 nm f=0.0864
<S2>=0.000**
 576 -> 633 0.12052
 578 -> 631 -0.14999
 579 -> 629 0.14999
 585 -> 633 -0.11489
 591 -> 639 -0.10458
 592 -> 630 0.16370
 594 -> 632 0.14615
 622 -> 634 0.11780
 623 -> 636 0.11780
 624 -> 632 -0.12036
 625 -> 638 0.10455
Excited State 96: Singlet-?Sym 4.7260 eV 262.35 nm f=0.0864
<S2>=0.000**
 577 -> 629 -0.11337
 578 -> 630 0.11337
 591 -> 631 0.11691
 593 -> 633 0.10785
 595 -> 632 -0.10476
Excited State 97: Singlet-?Sym 4.7260 eV 262.35 nm f=0.0864
<S2>=0.000**
 575 -> 632 0.10260
 577 -> 631 0.11352
 579 -> 630 -0.11352
 591 -> 631 -0.10127
 593 -> 633 0.12443
 622 -> 633 -0.10247
Excited State 98: Singlet-?Sym 4.7371 eV 261.73 nm f=0.0000 <S2>=0.000**
Excited State 99: Singlet-?Sym 4.7371 eV 261.73 nm f=0.0000 <S2>=0.000**

Excited State 100: Singlet-?Sym 4.7371 eV 261.73 nm f=0.0000 <S**2>=0.000
Excited State 101: Singlet-?Sym 4.7718 eV 259.83 nm f=0.0000 <S**2>=0.000
Excited State 102: Singlet-?Sym 4.7718 eV 259.83 nm f=0.0000 <S**2>=0.000
Excited State 103: Singlet-T2U 4.7945 eV 258.59 nm f=0.0000 <S**2>=0.000
Excited State 104: Singlet-T2U 4.7945 eV 258.59 nm f=0.0000 <S**2>=0.000
Excited State 105: Singlet-T2U 4.7945 eV 258.59 nm f=0.0000 <S**2>=0.000
Excited State 106: Singlet-?Sym 4.7986 eV 258.37 nm f=0.0000 <S**2>=0.000
Excited State 107: Singlet-?Sym 4.7986 eV 258.37 nm f=0.0000 <S**2>=0.000
Excited State 108: Singlet-?Sym 4.7986 eV 258.37 nm f=0.0000 <S**2>=0.000
Excited State 109: Singlet-T1U 4.8178 eV 257.34 nm f=0.0189

<S2>=0.000**

566 -> 629 0.10202
567 -> 631 -0.10202
576 -> 633 -0.10698
578 -> 641 -0.10375
579 -> 640 0.10375
585 -> 633 0.12888
592 -> 630 -0.19401
593 -> 634 0.13036
594 -> 632 0.12479
595 -> 636 -0.13036
628 -> 651 0.24213

Excited State 110: Singlet-T1U 4.8178 eV 257.34 nm f=0.0189

<S2>=0.000**

583 -> 633 -0.11205
591 -> 631 -0.16805
593 -> 635 -0.11951
594 -> 636 -0.11951
595 -> 632 -0.10850
628 -> 649 0.22198

Excited State 111: Singlet-T1U 4.8178 eV 257.34 nm f=0.0189

<S2>=0.000**

575 -> 632 -0.11032
584 -> 632 0.13291
591 -> 629 0.14002
592 -> 629 0.11321
593 -> 633 0.12869
594 -> 634 0.11951
595 -> 635 -0.11951
628 -> 650 0.22198

Excited State 112: Singlet-T2G 4.8222 eV 257.11 nm f=0.0000 <S**2>=0.000
Excited State 113: Singlet-T2G 4.8222 eV 257.11 nm f=0.0000 <S**2>=0.000
Excited State 114: Singlet-T2G 4.8222 eV 257.11 nm f=0.0000 <S**2>=0.000
Excited State 115: Singlet-?Sym 4.8335 eV 256.51 nm f=0.0000 <S**2>=0.000
Excited State 116: Singlet-?Sym 4.8335 eV 256.51 nm f=0.0000 <S**2>=0.000
Excited State 117: Singlet-?Sym 4.8335 eV 256.51 nm f=0.0000 <S**2>=0.000

Excited State 118: Singlet-?Sym 4.8434 eV 255.98 nm f=0.0000 <S**2>=0.000
Excited State 119: Singlet-?Sym 4.8434 eV 255.98 nm f=0.0000 <S**2>=0.000
Excited State 120: Singlet-?Sym 4.8475 eV 255.77 nm f=0.0000 <S**2>=0.000
Excited State 121: Singlet-?Sym 4.8475 eV 255.77 nm f=0.0000 <S**2>=0.000
Excited State 122: Singlet-?Sym 4.8475 eV 255.77 nm f=0.0000 <S**2>=0.000

Excited State 123: Singlet-?Sym 4.8498 eV 255.65 nm f=1.3910

<S2>=0.000**

615 -> 629 -0.11379
616 -> 631 0.11379
617 -> 634 -0.14125
618 -> 633 -0.15818
619 -> 636 0.14125
620 -> 630 0.23080
624 -> 632 0.27173
624 -> 633 -0.14067
625 -> 638 0.10622
628 -> 651 0.23502

Excited State 124: Singlet-?Sym 4.8498 eV 255.65 nm f=1.3910

<S2>=0.000**

614 -> 629 0.11394
616 -> 630 0.11394
617 -> 635 -0.14144
618 -> 636 -0.14144
619 -> 633 0.15021
620 -> 631 0.23111
623 -> 632 0.25804
623 -> 633 0.16521
626 -> 637 0.12799
628 -> 649 0.23533

Excited State 125: Singlet-?Sym 4.8498 eV 255.65 nm f=1.3910

<S2>=0.000**

614 -> 631 0.11398
615 -> 630 -0.11398
617 -> 632 -0.17824
618 -> 634 -0.14149
619 -> 635 -0.14149
620 -> 629 0.23120
622 -> 633 0.30618
627 -> 638 -0.11536
628 -> 650 0.23542

Excited State 126: Singlet-?Sym 4.8546 eV 255.40 nm f=0.0000 <S**2>=0.000

Excited State 127: Singlet-?Sym 4.8546 eV 255.40 nm f=0.0000 <S**2>=0.000

Excited State 128: Singlet-T2G 4.8910 eV 253.50 nm f=0.0000 <S**2>=0.000

Excited State 129: Singlet-T2G 4.8910 eV 253.50 nm f=0.0000 <S**2>=0.000

Excited State 130: Singlet-T2G 4.8910 eV 253.50 nm f=0.0000 <S**2>=0.000

Excited State 131: Singlet-T1U 4.9177 eV 252.12 nm f=2.6855

<S2>=0.000**

612 -> 630 0.12949
614 -> 637 0.14610
617 -> 634 0.15366
619 -> 636 -0.15366
620 -> 630 -0.20534
628 -> 651 0.22693

Excited State 132: Singlet-T1U 4.9177 eV 252.12 nm f=2.6855

<S2>=0.000**

615 -> 638 -0.11715
616 -> 637 -0.11812
617 -> 635 -0.10239
618 -> 634 0.11458
618 -> 636 -0.10239
619 -> 635 0.11458
620 -> 629 -0.15312
620 -> 631 0.13683
628 -> 649 -0.15122
628 -> 650 0.16922

Excited State 133: Singlet-T1U 4.9177 eV 252.12 nm f=2.6855

<S2>=0.000**

615 -> 638 0.13113
616 -> 637 -0.10554
617 -> 635 0.11461
618 -> 634 0.10238
618 -> 636 0.11461
619 -> 635 0.10239
620 -> 629 -0.13682
620 -> 631 -0.15316
628 -> 649 0.16927
628 -> 650 0.15121

Excited State 134: Singlet-?Sym 4.9250 eV 251.75 nm f=0.0000 <S**2>=0.000

Excited State 135: Singlet-?Sym 4.9250 eV 251.75 nm f=0.0000 <S**2>=0.000

Excited State 136: Singlet-?Sym 4.9250 eV 251.75 nm f=0.0000 <S**2>=0.000

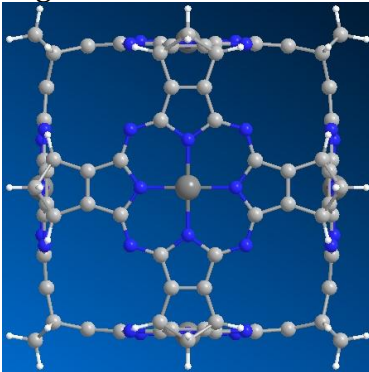
Excited State 137: Singlet-?Sym 4.9370 eV 251.13 nm f=0.0000 <S**2>=0.000

Excited State 138: Singlet-?Sym 4.9370 eV 251.13 nm f=0.0000 <S**2>=0.000

Excited State 139: Singlet-?Sym 4.9370 eV 251.13 nm f=0.0000 <S**2>=0.000

Excited State 140: Singlet-?Sym 4.9500 eV 250.47 nm f=0.0000 <S**2>=0.000

Cage01_LC-wPBE_TDDFT



Excited State 1: Singlet-T1G 2.0816 eV 595.62 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 2: Singlet-T1G 2.0816 eV 595.62 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 3: Singlet-T1G 2.0816 eV 595.62 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 4: Singlet-T2U 2.1717 eV 570.90 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 5: Singlet-T2U 2.1717 eV 570.90 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 6: Singlet-T2U 2.1717 eV 570.90 nm f=0.0000 $\langle S^2 \rangle = 0.000$
Excited State 7: Singlet-?Sym 2.2603 eV 548.52 nm f=0.5552
 $\langle S^2 \rangle = 0.000$
663 -> 681 -0.11272
672 -> 690 -0.11715
673 -> 683 0.24577
674 -> 684 -0.14384
674 -> 686 -0.13325
675 -> 679 0.19303
675 -> 688 0.16165
676 -> 679 0.11647
677 -> 680 -0.19303
677 -> 681 -0.11647

677 -> 689 -0.16165
678 -> 686 -0.20905
678 -> 687 -0.12613

Excited State 8: Singlet-?Sym 2.2603 eV 548.52 nm f=0.5552

<S2>=0.000**

663 -> 680 -0.12044
673 -> 683 0.11869
673 -> 687 -0.13810
674 -> 684 0.25472
676 -> 679 -0.20625
676 -> 688 0.17272
677 -> 681 0.20625
677 -> 690 0.17272
678 -> 686 -0.10096
678 -> 687 0.22337

Excited State 9: Singlet-T1U 2.2603 eV 548.52 nm f=0.5552

<S2>=0.000**

663 -> 679 -0.12387
671 -> 688 0.12737
673 -> 682 -0.18368
673 -> 683 0.13419
673 -> 685 -0.11159
674 -> 682 -0.20582
675 -> 679 0.10539
675 -> 681 -0.21212
675 -> 690 0.17764
676 -> 680 0.21212
676 -> 689 -0.17764
677 -> 680 -0.10539
678 -> 685 -0.22973
678 -> 686 -0.11413

Excited State 10: Singlet-?Sym 2.2907 eV 541.25 nm f=0.0000 <S**2>=0.000

Excited State 11: Singlet-?Sym 2.2907 eV 541.25 nm f=0.0000 <S**2>=0.000

Excited State 12: Singlet-?Sym 2.2907 eV 541.25 nm f=0.0000 <S**2>=0.000

Excited State 13: Singlet-?Sym 3.2096 eV 386.29 nm f=0.0000 <S**2>=0.000

Excited State 14: Singlet-?Sym 3.2096 eV 386.29 nm f=0.0000 <S**2>=0.000

Excited State 15: Singlet-?Sym 3.2096 eV 386.29 nm f=0.0000 <S**2>=0.000

Excited State 16: Singlet-?Sym 3.2100 eV 386.25 nm f=0.0001

<S2>=0.000**

651 -> 689 0.14405
651 -> 690 0.16785
655 -> 682 0.13485
655 -> 685 -0.12621
656 -> 682 0.15714
656 -> 685 0.14708
657 -> 683 0.13487

657 -> 684 0.15713
657 -> 686 0.12623
657 -> 687 0.14707
658 -> 680 0.18913
658 -> 690 0.12722
659 -> 680 0.10880
659 -> 681 0.25424
667 -> 690 -0.10026

**Excited State 17: Singlet-?Sym 3.2100 eV 386.25 nm f=0.0001
<S**2>=0.000**

651 -> 689 -0.15433
651 -> 690 0.15625
655 -> 682 -0.14448
655 -> 685 0.13523
656 -> 682 0.14628
656 -> 685 0.13692
657 -> 683 -0.14449
657 -> 684 0.14627
657 -> 686 -0.13524
657 -> 687 0.13690
658 -> 680 -0.20263
658 -> 690 0.11842
659 -> 680 -0.11657
659 -> 681 0.23667
659 -> 689 -0.10140

**Excited State 18: Singlet-?Sym 3.2100 eV 386.25 nm f=0.0001
<S**2>=0.000**

651 -> 688 -0.21111
655 -> 684 -0.19763
655 -> 687 0.18498
656 -> 683 0.19765
656 -> 686 -0.18499
658 -> 679 -0.27667
658 -> 680 0.11756
659 -> 679 0.16033
659 -> 688 0.13845
664 -> 684 0.11044
664 -> 687 -0.10340
665 -> 683 0.11045
665 -> 686 -0.10341
667 -> 688 0.12611

Excited State 19: Singlet-?Sym 3.2101 eV 386.23 nm f=0.0000 <S**2>=0.000
Excited State 20: Singlet-?Sym 3.2101 eV 386.23 nm f=0.0000 <S**2>=0.000
Excited State 21: Singlet-?Sym 3.2101 eV 386.23 nm f=0.0000 <S**2>=0.000
Excited State 22: Singlet-?Sym 3.2105 eV 386.18 nm f=0.0000 <S**2>=0.000
Excited State 23: Singlet-?Sym 3.2105 eV 386.18 nm f=0.0000 <S**2>=0.000

Excited State 24: Singlet-?Sym 3.2105 eV 386.18 nm f=0.0000 <S**2>=0.000
 Excited State 25: Singlet-?Sym 3.3681 eV 368.11 nm f=0.0000 <S**2>=0.000
 Excited State 26: Singlet-?Sym 3.4037 eV 364.27 nm f=0.0000 <S**2>=0.000
 Excited State 27: Singlet-?Sym 3.4037 eV 364.27 nm f=0.0000 <S**2>=0.000
 Excited State 28: Singlet-?Sym 3.4080 eV 363.80 nm f=0.0000 <S**2>=0.000
 Excited State 29: Singlet-?Sym 3.4080 eV 363.80 nm f=0.0000 <S**2>=0.000
 Excited State 30: Singlet-?Sym 3.4080 eV 363.80 nm f=0.0000 <S**2>=0.000
 Excited State 31: Singlet-?Sym 3.4401 eV 360.41 nm f=0.0000 <S**2>=0.000
 Excited State 32: Singlet-?Sym 3.4401 eV 360.41 nm f=0.0000 <S**2>=0.000
 Excited State 33: Singlet-?Sym 3.4401 eV 360.41 nm f=0.0000 <S**2>=0.000
 Excited State 34: Singlet-T2U 3.4644 eV 357.88 nm f=0.0000 <S**2>=0.000
 Excited State 35: Singlet-T2U 3.4644 eV 357.88 nm f=0.0000 <S**2>=0.000
 Excited State 36: Singlet-T2U 3.4644 eV 357.88 nm f=0.0000 <S**2>=0.000
 Excited State 37: Singlet-?Sym 3.6307 eV 341.49 nm f=0.0000 <S**2>=0.000
 Excited State 38: Singlet-?Sym 3.6307 eV 341.49 nm f=0.0000 <S**2>=0.000
 Excited State 39: Singlet-T1G 3.6352 eV 341.07 nm f=0.0000 <S**2>=0.000
 Excited State 40: Singlet-T1G 3.6352 eV 341.07 nm f=0.0000 <S**2>=0.000
 Excited State 41: Singlet-T1G 3.6352 eV 341.07 nm f=0.0000 <S**2>=0.000
 Excited State 42: Singlet-?Sym 3.6650 eV 338.30 nm f=0.0000 <S**2>=0.000
 Excited State 43: Singlet-T2G 3.6928 eV 335.74 nm f=0.0000 <S**2>=0.000
 Excited State 44: Singlet-T2G 3.6928 eV 335.74 nm f=0.0000 <S**2>=0.000
 Excited State 45: Singlet-T2G 3.6928 eV 335.74 nm f=0.0000 <S**2>=0.000

Excited State 46: Singlet-T1U 3.7090 eV 334.28 nm f=0.1376
<S2>=0.000**

632 -> 679 0.12156
 649 -> 688 0.16601
 649 -> 689 0.10398
 650 -> 689 -0.10970
 664 -> 684 -0.10725
 664 -> 687 0.10836
 665 -> 683 -0.10725
 665 -> 686 0.10836
 667 -> 688 -0.18378
 667 -> 689 0.16273

Excited State 47: Singlet-T1U 3.7090 eV 334.28 nm f=0.1376
<S2>=0.000**

632 -> 679 -0.10314
 633 -> 681 0.10869
 649 -> 688 -0.14085
 650 -> 690 -0.15723
 665 -> 682 0.10306
 665 -> 685 0.10412
 666 -> 684 0.10306
 666 -> 687 0.10412
 667 -> 688 0.15593
 667 -> 690 -0.17658

Excited State 48: Singlet-T1U 3.7090 eV 334.28 nm f=0.1376

<S2>=0.000**

633 -> 681 -0.10495
649 -> 689 0.10884
650 -> 689 -0.11483
650 -> 690 0.15183
664 -> 685 -0.10043
665 -> 685 -0.10053
666 -> 686 -0.10043
666 -> 687 -0.10054
667 -> 689 0.17034
667 -> 690 0.17050

Excited State 49: Singlet-?Sym 3.8336 eV 323.41 nm f=0.0000 <S**2>=0.000

Excited State 50: Singlet-?Sym 3.8336 eV 323.41 nm f=0.0000 <S**2>=0.000

Excited State 51: Singlet-T1G 3.8336 eV 323.41 nm f=0.0000 <S**2>=0.000

Excited State 52: Singlet-?Sym 3.8512 eV 321.94 nm f=0.0000 <S**2>=0.000

Excited State 53: Singlet-?Sym 3.8512 eV 321.94 nm f=0.0000 <S**2>=0.000

Excited State 54: Singlet-?Sym 3.8512 eV 321.94 nm f=0.0000 <S**2>=0.000

Excited State 55: Singlet-?Sym 3.8548 eV 321.64 nm f=0.0000 <S**2>=0.000

Excited State 56: Singlet-?Sym 3.8548 eV 321.64 nm f=0.0000 <S**2>=0.000

Excited State 57: Singlet-?Sym 3.8548 eV 321.64 nm f=0.0000 <S**2>=0.000

Excited State 58: Singlet-?Sym 3.8622 eV 321.02 nm f=0.0026

<S2>=0.000**

640 -> 682 -0.22809
640 -> 684 -0.13065
644 -> 681 0.20062
644 -> 690 -0.17700
645 -> 679 0.11492
645 -> 680 0.20062
645 -> 688 -0.10139
645 -> 689 -0.17700
646 -> 681 -0.11492
646 -> 690 -0.10139
647 -> 685 0.23307
648 -> 682 -0.14289
648 -> 685 0.13868
648 -> 687 0.15534

Excited State 59: Singlet-?Sym 3.8622 eV 321.02 nm f=0.0026

<S2>=0.000**

640 -> 682 0.13059
640 -> 683 0.14867
640 -> 684 -0.17842
644 -> 679 -0.13077
644 -> 681 -0.11486
644 -> 688 -0.11537
644 -> 690 0.10134

645 -> 679 0.15693
645 -> 680 -0.11486
645 -> 688 -0.13846
645 -> 689 0.10134
646 -> 680 0.13077
646 -> 681 -0.15693
646 -> 689 0.11538
646 -> 690 -0.13846
647 -> 684 -0.13005
647 -> 685 -0.13344
647 -> 686 0.15425
648 -> 687 0.21214

**Excited State 60: Singlet-?Sym 3.8622 eV 321.02 nm f=0.0026
<S**2>=0.000**

640 -> 683 0.21677
640 -> 684 0.14861
644 -> 679 -0.19067
644 -> 688 -0.16822
645 -> 679 -0.13071
645 -> 688 0.11533
646 -> 680 0.19066
646 -> 681 0.13072
646 -> 689 0.16822
646 -> 690 0.11533
647 -> 684 0.10833
647 -> 686 0.22490
648 -> 683 -0.13788
648 -> 686 -0.12593
648 -> 687 -0.17670

Excited State 61: Singlet-?Sym 3.8635 eV 320.91 nm f=0.0000 <S**2>=0.000
Excited State 62: Singlet-T2G 3.8635 eV 320.91 nm f=0.0000 <S**2>=0.000
Excited State 63: Singlet-T2G 3.8635 eV 320.91 nm f=0.0000 <S**2>=0.000
Excited State 64: Singlet-T2U 3.8819 eV 319.39 nm f=0.0000 <S**2>=0.000
Excited State 65: Singlet-T2U 3.8819 eV 319.39 nm f=0.0000 <S**2>=0.000
Excited State 66: Singlet-T2U 3.8819 eV 319.39 nm f=0.0000 <S**2>=0.000
Excited State 67: Singlet-?Sym 3.9661 eV 312.61 nm f=0.0000 <S**2>=0.000
Excited State 68: Singlet-?Sym 3.9783 eV 311.65 nm f=0.0000 <S**2>=0.000
Excited State 69: Singlet-?Sym 3.9783 eV 311.65 nm f=0.0000 <S**2>=0.000
Excited State 70: Singlet-T2U 3.9997 eV 309.98 nm f=0.0000 <S**2>=0.000
Excited State 71: Singlet-T2U 3.9997 eV 309.98 nm f=0.0000 <S**2>=0.000
Excited State 72: Singlet-T2U 3.9997 eV 309.98 nm f=0.0000 <S**2>=0.000
Excited State 73: Singlet-T1G 4.0131 eV 308.95 nm f=0.0000 <S**2>=0.000
Excited State 74: Singlet-T1G 4.0131 eV 308.95 nm f=0.0000 <S**2>=0.000
Excited State 75: Singlet-T1G 4.0131 eV 308.95 nm f=0.0000 <S**2>=0.000

**Excited State 76: Singlet-?Sym 4.0429 eV 306.67 nm f=0.0604
<S**2>=0.000**

675 -> 679 -0.25258
675 -> 681 -0.15897
675 -> 688 0.18799
675 -> 690 -0.11832
676 -> 680 0.15897
676 -> 689 0.11831
677 -> 680 0.25258
677 -> 689 -0.18799
678 -> 686 -0.10857

**Excited State 77: Singlet-?Sym 4.0429 eV 306.67 nm f=0.0604
<S**2>=0.000**

676 -> 679 0.29296
676 -> 688 0.21805
677 -> 681 -0.29296
677 -> 690 0.21805
678 -> 687 0.12592

**Excited State 78: Singlet-?Sym 4.0429 eV 306.67 nm f=0.0604
<S**2>=0.000**

675 -> 679 -0.16299
675 -> 681 0.24608
675 -> 688 0.12132
675 -> 690 0.18315
676 -> 680 -0.24608
676 -> 689 -0.18315
677 -> 680 0.16299
677 -> 689 -0.12131
678 -> 685 -0.10577

Excited State 79: Singlet-?Sym 4.0577 eV 305.55 nm f=0.0000 <S**2>=0.000

Excited State 80: Singlet-?Sym 4.0577 eV 305.55 nm f=0.0000 <S**2>=0.000

Excited State 81: Singlet-?Sym 4.0611 eV 305.29 nm f=0.0000 <S**2>=0.000

Excited State 82: Singlet-?Sym 4.0765 eV 304.14 nm f=0.0000 <S**2>=0.000

Excited State 83: Singlet-?Sym 4.0765 eV 304.14 nm f=0.0000 <S**2>=0.000

Excited State 84: Singlet-T2G 4.0765 eV 304.14 nm f=0.0000 <S**2>=0.000

Excited State 85: Singlet-?Sym 4.0832 eV 303.65 nm f=0.0000 <S**2>=0.000

Excited State 86: Singlet-?Sym 4.0888 eV 303.23 nm f=0.0000 <S**2>=0.000

Excited State 87: Singlet-?Sym 4.0888 eV 303.23 nm f=0.0000 <S**2>=0.000

Excited State 88: Singlet-T1U 4.1077 eV 301.83 nm f=0.0803

<S2>=0.000**

673 -> 685 -0.12767
674 -> 682 -0.10745
674 -> 685 0.11393
675 -> 681 -0.12271
676 -> 680 0.12271
678 -> 685 0.33872
678 -> 686 -0.17919
678 -> 687 -0.11202

Excited State 89: Singlet-T1U 4.1077 eV 301.83 nm f=0.0803

<S2>=0.000**

673 -> 683 0.14847
674 -> 686 -0.17641
675 -> 679 0.12922
677 -> 680 -0.12922
678 -> 685 0.17293
678 -> 686 0.35667

Excited State 90: Singlet-T1U 4.1077 eV 301.83 nm f=0.0803

<S2>=0.000**

625 -> 681 0.10206
626 -> 679 0.10206
647 -> 693 -0.10223
673 -> 687 0.18242
674 -> 684 -0.15352
676 -> 679 0.13775
677 -> 681 -0.13775
678 -> 685 0.12147
678 -> 687 0.38022

Excited State 91: Singlet-?Sym 4.1237 eV 300.66 nm f=0.0000 <S**2>=0.000

Excited State 92: Singlet-?Sym 4.1238 eV 300.66 nm f=0.0000 <S**2>=0.000

Excited State 93: Singlet-?Sym 4.1238 eV 300.66 nm f=0.0000 <S**2>=0.000

Excited State 94: Singlet-T1U 4.1318 eV 300.07 nm f=0.2495

<S2>=0.000**

673 -> 685 0.11683
673 -> 687 0.11137
674 -> 685 -0.10425
674 -> 686 -0.13640
675 -> 679 -0.11415
675 -> 681 -0.12829
676 -> 680 0.12828
677 -> 680 0.11414
678 -> 685 -0.25678
678 -> 686 0.22847
678 -> 687 0.19232

Excited State 95: Singlet-T1U 4.1318 eV 300.07 nm f=0.2495

<S2>=0.000**

673 -> 683 0.13785
674 -> 686 -0.19098
675 -> 679 -0.15983
675 -> 688 0.12102
677 -> 680 0.15983
677 -> 689 -0.12102
678 -> 685 0.16460
678 -> 686 0.31991
678 -> 687 -0.16027

Excited State 96: Singlet-T1U 4.1318 eV 300.07 nm f=0.2495

<S2>=0.000**

673 -> 685 -0.11337
673 -> 687 0.17607
674 -> 684 -0.12708
674 -> 685 0.10117
675 -> 681 0.12449
676 -> 679 -0.15191
676 -> 680 -0.12449
676 -> 688 -0.11502
677 -> 681 0.15191
677 -> 690 -0.11502
678 -> 685 0.24918
678 -> 687 0.30405

Excited State 97: Singlet-?Sym 4.1623 eV 297.88 nm f=0.0000 <S**2>=0.000
Excited State 98: Singlet-?Sym 4.1623 eV 297.88 nm f=0.0000 <S**2>=0.000
Excited State 99: Singlet-?Sym 4.1623 eV 297.88 nm f=0.0000 <S**2>=0.000
Excited State 100: Singlet-?Sym 4.1710 eV 297.26 nm f=0.0000 <S**2>=0.000
Excited State 101: Singlet-?Sym 4.1710 eV 297.26 nm f=0.0000 <S**2>=0.000
Excited State 102: Singlet-?Sym 4.1788 eV 296.70 nm f=0.0000 <S**2>=0.000
Excited State 103: Singlet-?Sym 4.1943 eV 295.60 nm f=0.0000 <S**2>=0.000
Excited State 104: Singlet-?Sym 4.1943 eV 295.60 nm f=0.0000 <S**2>=0.000
Excited State 105: Singlet-?Sym 4.1943 eV 295.60 nm f=0.0000 <S**2>=0.000
Excited State 106: Singlet-?Sym 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000
Excited State 107: Singlet-?Sym 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000
Excited State 108: Singlet-?Sym 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000
Excited State 109: Singlet-?Sym 4.2335 eV 292.87 nm f=0.0000 <S**2>=0.000
Excited State 110: Singlet-?Sym 4.2335 eV 292.87 nm f=0.0000 <S**2>=0.000
Excited State 111: Singlet-?Sym 4.2335 eV 292.87 nm f=0.0000 <S**2>=0.000
Excited State 112: Singlet-?Sym 4.2348 eV 292.77 nm f=0.0000 <S**2>=0.000
Excited State 113: Singlet-?Sym 4.2434 eV 292.18 nm f=0.0000 <S**2>=0.000
Excited State 114: Singlet-?Sym 4.2434 eV 292.18 nm f=0.0000 <S**2>=0.000
Excited State 115: Singlet-?Sym 4.2678 eV 290.51 nm f=0.0000 <S**2>=0.000
Excited State 116: Singlet-?Sym 4.2678 eV 290.51 nm f=0.0000 <S**2>=0.000
Excited State 117: Singlet-?Sym 4.2678 eV 290.51 nm f=0.0000 <S**2>=0.000

Excited State 118: Singlet-?Sym 4.2708 eV 290.31 nm f=0.1070

<S2>=0.000**

673 -> 682 -0.20439
673 -> 683 -0.17081
673 -> 685 0.24316
673 -> 687 0.30816
674 -> 682 -0.22903
674 -> 684 0.29027
674 -> 685 -0.21700
674 -> 686 -0.18134
674 -> 687 0.10164

Excited State 119: Singlet-?Sym 4.2708 eV 290.31 nm f=0.1071
<S2>=0.000**

673 -> 683 0.41340
673 -> 687 0.19553
674 -> 684 0.18417
674 -> 686 0.43888

Excited State 120: Singlet-?Sym 4.2708 eV 290.31 nm f=0.1070
<S2>=0.000**

673 -> 682 -0.23224
673 -> 685 0.27629
673 -> 687 -0.29749
674 -> 682 -0.26024
674 -> 684 -0.28022
674 -> 685 -0.24656
674 -> 686 0.10061

Excited State 121: Singlet-?Sym 4.2866 eV 289.24 nm f=0.0000 <S**2>=0.000

Excited State 122: Singlet-?Sym 4.3274 eV 286.51 nm f=0.0000 <S**2>=0.000

Excited State 123: Singlet-?Sym 4.3274 eV 286.51 nm f=0.0000 <S**2>=0.000

Excited State 124: Singlet-?Sym 4.3274 eV 286.51 nm f=0.0000 <S**2>=0.000

Excited State 125: Singlet-?Sym 4.3305 eV 286.31 nm f=0.0000 <S**2>=0.000

Excited State 126: Singlet-?Sym 4.3305 eV 286.31 nm f=0.0000 <S**2>=0.000

Excited State 127: Singlet-T1U 4.3306 eV 286.30 nm f=3.4233
<S2>=0.000**

663 -> 680 0.22695
669 -> 682 0.21730
669 -> 685 -0.14604
670 -> 683 0.21730
670 -> 686 0.14604
671 -> 689 -0.18438
672 -> 680 0.10339
672 -> 689 0.17716
673 -> 687 -0.19429
674 -> 684 0.10437
676 -> 688 0.17934
677 -> 690 0.17934
678 -> 687 0.15471

Excited State 128: Singlet-?Sym 4.3306 eV 286.30 nm f=3.4236
<S2>=0.000**

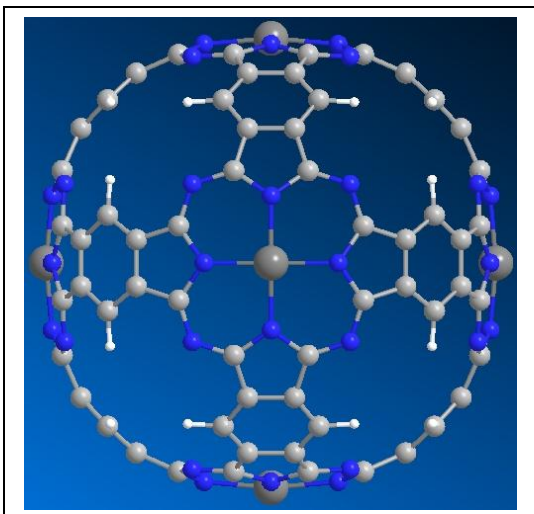
663 -> 681 0.21962
668 -> 682 0.21029
668 -> 685 0.14134
670 -> 684 0.21029
670 -> 687 0.14133
671 -> 681 -0.13473
672 -> 690 0.24025
673 -> 683 0.10412

674 -> 686 -0.19383
675 -> 688 0.17356
677 -> 689 -0.17356
678 -> 686 -0.14972

**Excited State 129: Singlet-?Sym 4.3306 eV 286.30 nm f=3.4234
<S**2>=0.000**

663 -> 679 -0.21789
668 -> 683 -0.20865
668 -> 686 0.14021
669 -> 684 -0.20865
669 -> 687 0.14021
671 -> 688 0.23583
672 -> 679 0.13225
673 -> 685 0.14655
674 -> 685 -0.13078
675 -> 690 -0.17219
676 -> 689 0.17219
678 -> 685 0.14855

Excited State 130: Singlet-T2G 4.3412 eV 285.60 nm f=0.0000 <S**2>=0.000
Excited State 131: Singlet-T2G 4.3412 eV 285.60 nm f=0.0000 <S**2>=0.000
Excited State 132: Singlet-T2G 4.3412 eV 285.60 nm f=0.0000 <S**2>=0.000
Excited State 133: Singlet-?Sym 4.4023 eV 281.64 nm f=0.0000 <S**2>=0.000
Excited State 134: Singlet-?Sym 4.4023 eV 281.64 nm f=0.0000 <S**2>=0.000
Excited State 135: Singlet-?Sym 4.4108 eV 281.09 nm f=0.0000 <S**2>=0.000
Excited State 136: Singlet-?Sym 4.4163 eV 280.74 nm f=0.0000 <S**2>=0.000
Excited State 137: Singlet-?Sym 4.4163 eV 280.74 nm f=0.0000 <S**2>=0.000
Excited State 138: Singlet-?Sym 4.4163 eV 280.74 nm f=0.0000 <S**2>=0.000
Excited State 139: Singlet-?Sym 4.4542 eV 278.36 nm f=0.0000 <S**2>=0.000
Excited State 140: Singlet-?Sym 4.4542 eV 278.36 nm f=0.0000 <S**2>=0.000



Excited State 1: Singlet-?Sym 1.1191 eV 1107.84 nm f=0.0000 <S**2>=0.000
 Excited State 2: Singlet-?Sym 1.1191 eV 1107.84 nm f=0.0000 <S**2>=0.000
 Excited State 3: Singlet-?Sym 1.1191 eV 1107.84 nm f=0.0000 <S**2>=0.000
 Excited State 4: Singlet-?Sym 1.6063 eV 771.89 nm f=0.0000 <S**2>=0.000
 Excited State 5: Singlet-?Sym 1.6063 eV 771.89 nm f=0.0000 <S**2>=0.000
 Excited State 6: Singlet-?Sym 1.6063 eV 771.89 nm f=0.0000 <S**2>=0.000
Excited State 7: Singlet-?Sym 1.8072 eV 686.07 nm f=1.0569
<S2>=0.000**

626 -> 631	0.16492
627 -> 631	-0.20537
628 -> 632	-0.16492
628 -> 633	-0.20537
629 -> 635	0.14531
629 -> 636	0.30039
630 -> 634	-0.29888
630 -> 636	-0.22405

Excited State 8: Singlet-?Sym 1.8072 eV 686.07 nm f=1.0569
<S2>=0.000**

623 -> 631	0.11002
625 -> 638	-0.10748
626 -> 633	0.26215
626 -> 642	-0.11360
627 -> 632	-0.26215
627 -> 641	0.11360
629 -> 635	0.43941
630 -> 634	0.13584
630 -> 635	0.18908

Excited State 9: Singlet-?Sym 1.8072 eV 686.07 nm f=1.0569
<S2>=0.000**

626 -> 631	-0.20993
627 -> 631	-0.17936
628 -> 632	0.20993
628 -> 633	-0.17936
629 -> 636	0.26234
630 -> 634	0.38044

	630 -> 636	-0.19567				
Excited State 10:	Singlet-?Sym	1.8647 eV	664.92 nm	f=0.0000	<S**2>=0.000	
Excited State 11:	Singlet-?Sym	1.8647 eV	664.92 nm	f=0.0000	<S**2>=0.000	
Excited State 12:	Singlet-?Sym	1.8647 eV	664.92 nm	f=0.0000	<S**2>=0.000	
Excited State 13:	Singlet-?Sym	2.5611 eV	484.10 nm	f=0.0000	<S**2>=0.000	
Excited State 14:	Singlet-?Sym	2.5611 eV	484.10 nm	f=0.0000	<S**2>=0.000	
Excited State 15:	Singlet-?Sym	2.5611 eV	484.10 nm	f=0.0000	<S**2>=0.000	
Excited State 16:	Singlet-?Sym	2.5951 eV	477.76 nm	f=0.0000	<S**2>=0.000	
Excited State 17:	Singlet-?Sym	2.5951 eV	477.76 nm	f=0.0000	<S**2>=0.000	
Excited State 18:	Singlet-?Sym	2.5951 eV	477.76 nm	f=0.0000	<S**2>=0.000	
Excited State 19:	Singlet-?Sym	2.7366 eV	453.06 nm	f=0.0000	<S**2>=0.000	
Excited State 20:	Singlet-?Sym	2.7366 eV	453.06 nm	f=0.0000	<S**2>=0.000	
Excited State 21:	Singlet-?Sym	2.7753 eV	446.74 nm	f=0.0000	<S**2>=0.000	
Excited State 22:	Singlet-?Sym	2.8294 eV	438.20 nm	f=0.0000	<S**2>=0.000	
Excited State 23:	Singlet-?Sym	2.9327 eV	422.76 nm	f=0.2196		
	<S**2>=0.000					
	627 -> 631	0.29952				
	628 -> 633	0.29952				
	629 -> 635	0.12738				
	629 -> 636	0.33382				
	629 -> 639	0.14686				
	630 -> 634	0.10188				
	630 -> 636	-0.24899				
	630 -> 639	0.19689				
Excited State 24:	Singlet-?Sym	2.9327 eV	422.76 nm	f=0.2196		
	<S**2>=0.000					
	626 -> 633	-0.30763				
	627 -> 631	-0.10232				
	627 -> 632	0.30763				
	628 -> 633	-0.10232				
	629 -> 635	0.39289				
	629 -> 636	-0.11404				
	630 -> 635	0.16906				
	630 -> 638	-0.23173				
Excited State 25:	Singlet-?Sym	2.9327 eV	422.76 nm	f=0.2196		
	<S**2>=0.000					
	626 -> 631	0.31569				
	628 -> 632	-0.31569				
	629 -> 637	0.25711				
	630 -> 634	0.43592				
Excited State 26:	Singlet-?Sym	2.9365 eV	422.21 nm	f=0.0000	<S**2>=0.000	
Excited State 27:	Singlet-?Sym	2.9365 eV	422.21 nm	f=0.0000	<S**2>=0.000	
Excited State 28:	Singlet-?Sym	2.9365 eV	422.21 nm	f=0.0000	<S**2>=0.000	
Excited State 29:	Singlet-?Sym	3.0149 eV	411.24 nm	f=0.0000	<S**2>=0.000	
Excited State 30:	Singlet-?Sym	3.0149 eV	411.24 nm	f=0.0000	<S**2>=0.000	
Excited State 31:	Singlet-?Sym	3.0609 eV	405.06 nm	f=0.0581		
	<S**2>=0.000					
	626 -> 631	0.10376				
	626 -> 633	-0.19499				
	626 -> 642	-0.11595				

627 -> 632 0.19499
627 -> 641 0.11595
628 -> 632 -0.10376
629 -> 637 -0.27205
629 -> 638 -0.20347
630 -> 638 0.47286

Excited State 32: Singlet-?Sym 3.0609 eV 405.06 nm f=0.0581

<S2>=0.000**

626 -> 631 -0.19258
626 -> 640 0.11451
628 -> 632 0.19258
628 -> 641 -0.11451
629 -> 637 0.50491
630 -> 638 0.23217
630 -> 639 -0.11773

Excited State 33: Singlet-?Sym 3.0609 eV 405.06 nm f=0.0581

<S2>=0.000**

627 -> 631 -0.21376
627 -> 640 -0.12711
628 -> 633 -0.21376
628 -> 642 0.12711
629 -> 637 0.10136
629 -> 639 0.33740
630 -> 638 0.11266
630 -> 639 0.45236

Excited State 34: Singlet-?Sym 3.0792 eV 402.64 nm f=0.0000 <S**2>=0.000

Excited State 35: Singlet-?Sym 3.0792 eV 402.64 nm f=0.0000 <S**2>=0.000

Excited State 36: Singlet-?Sym 3.0792 eV 402.64 nm f=0.0000 <S**2>=0.000

Excited State 37: Singlet-?Sym 3.3779 eV 367.04 nm f=0.0000 <S**2>=0.000

Excited State 38: Singlet-?Sym 3.3779 eV 367.04 nm f=0.0000 <S**2>=0.000

Excited State 39: Singlet-?Sym 3.3779 eV 367.04 nm f=0.0000 <S**2>=0.000

Excited State 40: Singlet-?Sym 3.3795 eV 366.88 nm f=0.0000 <S**2>=0.000

Excited State 41: Singlet-?Sym 3.3795 eV 366.88 nm f=0.0000 <S**2>=0.000

Excited State 42: Singlet-?Sym 3.3795 eV 366.88 nm f=0.0000 <S**2>=0.000

Excited State 43: Singlet-?Sym 3.6128 eV 343.18 nm f=0.0000 <S**2>=0.000

Excited State 44: Singlet-T2G 3.7527 eV 330.39 nm f=0.0000 <S**2>=0.000

Excited State 45: Singlet-T2G 3.7527 eV 330.39 nm f=0.0000 <S**2>=0.000

Excited State 46: Singlet-T2G 3.7527 eV 330.39 nm f=0.0000 <S**2>=0.000

Excited State 47: Singlet-?Sym 3.7571 eV 330.00 nm f=0.0000 <S**2>=0.000

Excited State 48: Singlet-?Sym 3.7571 eV 330.00 nm f=0.0000 <S**2>=0.000

Excited State 49: Singlet-?Sym 3.7898 eV 327.15 nm f=0.0000 <S**2>=0.000

Excited State 50: Singlet-T2U 3.7898 eV 327.15 nm f=0.0000 <S**2>=0.000

Excited State 51: Singlet-T2U 3.7898 eV 327.15 nm f=0.0000 <S**2>=0.000

Excited State 52: Singlet-?Sym 3.7900 eV 327.14 nm f=0.0000 <S**2>=0.000

Excited State 53: Singlet-?Sym 3.7900 eV 327.14 nm f=0.0000 <S**2>=0.000

Excited State 54: Singlet-?Sym 3.7900 eV 327.14 nm f=0.0000 <S**2>=0.000

Excited State 55: Singlet-?Sym 3.8841 eV 319.21 nm f=0.5596

<S2>=0.000**

623 -> 631 0.13881
625 -> 638 -0.17804

626 -> 642 -0.28476
627 -> 640 0.14820
627 -> 641 0.28476
628 -> 642 -0.14820
629 -> 635 -0.15325
630 -> 638 -0.17667

Excited State 56: Singlet-?Sym 3.8841 eV 319.21 nm f=0.5596

<S2>=0.000**

624 -> 633 0.12992
625 -> 637 0.16739
625 -> 639 0.12482
626 -> 640 -0.26772
627 -> 640 -0.19963
628 -> 641 0.26772
628 -> 642 0.19963
629 -> 637 0.17958
630 -> 634 -0.15577
630 -> 639 -0.10808

Excited State 57: Singlet-?Sym 3.8841 eV 319.21 nm f=0.5596

<S2>=0.000**

625 -> 637 -0.11076
625 -> 638 -0.10908
625 -> 639 0.13976
626 -> 640 0.17715
626 -> 642 -0.17446
627 -> 640 -0.22353
627 -> 641 0.17446
628 -> 641 -0.17715
628 -> 642 0.22353
629 -> 636 0.10498
629 -> 637 -0.11882
630 -> 634 0.10307
630 -> 638 -0.10824
630 -> 639 -0.12102

Excited State 58: Singlet-?Sym 3.9983 eV 310.09 nm f=0.0000 <S2>=0.000**

Excited State 59: Singlet-?Sym 4.0013 eV 309.86 nm f=0.0000 <S2>=0.000**

Excited State 60: Singlet-?Sym 4.0013 eV 309.86 nm f=0.0000 <S2>=0.000**

Excited State 61: Singlet-?Sym 4.0025 eV 309.76 nm f=0.0000 <S2>=0.000**

Excited State 62: Singlet-?Sym 4.0025 eV 309.76 nm f=0.0000 <S2>=0.000**

Excited State 63: Singlet-?Sym 4.0025 eV 309.76 nm f=0.0000 <S2>=0.000**

Excited State 64: Singlet-?Sym 4.0224 eV 308.24 nm f=0.0000 <S2>=0.000**

Excited State 65: Singlet-T1U 4.0283 eV 307.78 nm f=0.0091

<S2>=0.000**

588 -> 633 0.11614
589 -> 642 0.13142
591 -> 635 0.13654
591 -> 638 0.10242
592 -> 635 0.12768
593 -> 634 0.12768
593 -> 636 0.13654
593 -> 639 0.10242
599 -> 632 0.17414
599 -> 633 0.18622
601 -> 633 -0.10356

618 -> 632 -0.13554
618 -> 633 -0.14494

Excited State 66: Singlet-T1U 4.0283 eV 307.78 nm f=0.0091
<S2>=0.000**

588 -> 640 0.14438
589 -> 631 -0.12760
591 -> 634 -0.14937
591 -> 637 0.11205
592 -> 635 0.12522
592 -> 636 0.14937
592 -> 639 -0.11205
593 -> 634 0.12522
599 -> 631 0.20372
599 -> 632 0.17078
600 -> 631 0.11380
618 -> 631 -0.15857
618 -> 632 -0.13293

Excited State 67: Singlet-T1U 4.0283 eV 307.78 nm f=0.0091
<S2>=0.000**

588 -> 633 0.11832
588 -> 640 0.10865
589 -> 642 0.13388
591 -> 634 -0.11240
591 -> 635 0.13910
591 -> 638 0.10434
592 -> 636 0.11240
593 -> 636 0.13910
593 -> 639 0.10434
599 -> 631 0.15330
599 -> 632 -0.11994
599 -> 633 0.18971
601 -> 633 -0.10551
618 -> 631 -0.11932
618 -> 633 -0.14766

Excited State 68: Singlet-T1G 4.0435 eV 306.63 nm f=0.0000 <S**2>=0.000
Excited State 69: Singlet-T1G 4.0435 eV 306.63 nm f=0.0000 <S**2>=0.000
Excited State 70: Singlet-T1G 4.0435 eV 306.63 nm f=0.0000 <S**2>=0.000
Excited State 71: Singlet-?Sym 4.0592 eV 305.44 nm f=0.0000 <S**2>=0.000
Excited State 72: Singlet-?Sym 4.0592 eV 305.44 nm f=0.0000 <S**2>=0.000
Excited State 73: Singlet-?Sym 4.0592 eV 305.44 nm f=0.0000 <S**2>=0.000
Excited State 74: Singlet-?Sym 4.0837 eV 303.61 nm f=0.0000 <S**2>=0.000
Excited State 75: Singlet-?Sym 4.0837 eV 303.61 nm f=0.0000 <S**2>=0.000
Excited State 76: Singlet-?Sym 4.0837 eV 303.61 nm f=0.0000 <S**2>=0.000
Excited State 77: Singlet-T1G 4.0930 eV 302.92 nm f=0.0000 <S**2>=0.000
Excited State 78: Singlet-T1G 4.0930 eV 302.92 nm f=0.0000 <S**2>=0.000
Excited State 79: Singlet-T1G 4.0930 eV 302.92 nm f=0.0000 <S**2>=0.000
Excited State 80: Singlet-?Sym 4.0956 eV 302.73 nm f=0.0000 <S**2>=0.000
Excited State 81: Singlet-?Sym 4.0956 eV 302.73 nm f=0.0000 <S**2>=0.000
Excited State 82: Singlet-?Sym 4.0956 eV 302.73 nm f=0.0000 <S**2>=0.000

Excited State 83: Singlet-?Sym 4.1001 eV 302.39 nm f=0.0302
<S2>=0.000**

590 -> 634 -0.12724

590 -> 636	0.11150
594 -> 631	0.15796
594 -> 633	0.10031
595 -> 631	0.13842
595 -> 632	0.10031
596 -> 632	-0.15796
596 -> 633	0.13842
597 -> 636	-0.10118
597 -> 637	0.12556
598 -> 639	0.13796
601 -> 633	-0.10465
605 -> 634	-0.11246
618 -> 632	-0.10606
618 -> 633	-0.12102

Excited State 84: Singlet-?Sym 4.1001 eV 302.39 nm f=0.0302
<S2>=0.000**

590 -> 635	0.11634
590 -> 636	-0.13900
594 -> 633	0.14442
595 -> 631	-0.17255
595 -> 632	0.14442
595 -> 640	0.10300
596 -> 633	-0.17255
596 -> 642	-0.10300
597 -> 636	0.12612
597 -> 638	0.13452
598 -> 639	-0.17198
605 -> 635	0.10282
605 -> 636	-0.12285
618 -> 631	0.11065
618 -> 632	0.13221

Excited State 85: Singlet-?Sym 4.1001 eV 302.39 nm f=0.0302
<S2>=0.000**

590 -> 634	-0.12909
590 -> 635	-0.12283
594 -> 631	0.16026
594 -> 633	-0.15249
595 -> 632	-0.15249
596 -> 632	-0.16026
597 -> 637	0.12739
597 -> 638	-0.14203
598 -> 635	0.10416
600 -> 631	0.10148
601 -> 633	-0.10617
605 -> 634	-0.11409
605 -> 635	-0.10857
618 -> 631	-0.11684
618 -> 633	-0.12278

Excited State 86: Singlet-?Sym 4.1232 eV 300.70 nm f=0.0000 <S**2>=0.000
Excited State 87: Singlet-?Sym 4.1232 eV 300.70 nm f=0.0000 <S**2>=0.000
Excited State 88: Singlet-T1G 4.1371 eV 299.69 nm f=0.0000 <S**2>=0.000
Excited State 89: Singlet-T1G 4.1371 eV 299.69 nm f=0.0000 <S**2>=0.000
Excited State 90: Singlet-T1G 4.1371 eV 299.69 nm f=0.0000 <S**2>=0.000
Excited State 91: Singlet-?Sym 4.1373 eV 299.67 nm f=0.0000 <S**2>=0.000

Excited State 92: Singlet-?Sym 4.1373 eV 299.67 nm f=0.0000 <S**2>=0.000
Excited State 93: Singlet-?Sym 4.1373 eV 299.67 nm f=0.0000 <S**2>=0.000
Excited State 94: Singlet-?Sym 4.1438 eV 299.21 nm f=0.0000 <S**2>=0.000
Excited State 95: Singlet-?Sym 4.1438 eV 299.21 nm f=0.0000 <S**2>=0.000
Excited State 96: Singlet-?Sym 4.1438 eV 299.21 nm f=0.0000 <S**2>=0.000
Excited State 97: Singlet-T1U 4.1452 eV 299.10 nm f=0.0704

<S2>=0.000**

588 -> 632	-0.11386
588 -> 641	0.10012
589 -> 632	0.11206
589 -> 641	0.10173
592 -> 635	0.15749
592 -> 638	-0.11453
593 -> 634	0.15748
593 -> 637	0.11453
599 -> 632	0.25213
600 -> 632	0.17720
601 -> 632	-0.18017
603 -> 635	-0.11576
604 -> 634	-0.11576
615 -> 635	-0.13216
617 -> 634	0.13216
618 -> 632	0.19749

Excited State 98: Singlet-T1U 4.1452 eV 299.10 nm f=0.0704

<S2>=0.000**

588 -> 640	0.11064
589 -> 631	-0.12382
591 -> 634	-0.12611
592 -> 636	0.12611
599 -> 631	0.20190
599 -> 633	0.15159
600 -> 631	-0.19589
601 -> 633	0.14643
615 -> 636	-0.10583
616 -> 634	-0.10583
618 -> 631	0.15815
618 -> 633	0.11874

Excited State 99: Singlet-T1U 4.1452 eV 299.10 nm f=0.0704

<S2>=0.000**

588 -> 633	-0.12303
589 -> 642	-0.10993
591 -> 635	-0.12584
593 -> 636	-0.12584
599 -> 631	0.15191
599 -> 633	-0.20147
600 -> 631	-0.14739
601 -> 633	-0.19460
616 -> 635	-0.10561
617 -> 636	-0.10561
618 -> 631	0.11899
618 -> 633	-0.15781

Excited State 100: Singlet-?Sym 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000

Excited State 101: Singlet-?Sym 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000

Excited State 102: Singlet-T2U 4.2202 eV 293.79 nm f=0.0000 <S**2>=0.000
 Excited State 103: Singlet-T2G 4.2406 eV 292.38 nm f=0.0000 <S**2>=0.000
 Excited State 104: Singlet-T2G 4.2406 eV 292.38 nm f=0.0000 <S**2>=0.000
 Excited State 105: Singlet-T2G 4.2406 eV 292.38 nm f=0.0000 <S**2>=0.000
 Excited State 106: Singlet-?Sym 4.3137 eV 287.42 nm f=0.0000 <S**2>=0.000
 Excited State 107: Singlet-?Sym 4.3514 eV 284.93 nm f=0.0000 <S**2>=0.000
 Excited State 108: Singlet-?Sym 4.3956 eV 282.06 nm f=0.0000 <S**2>=0.000
 Excited State 109: Singlet-?Sym 4.3956 eV 282.06 nm f=0.0000 <S**2>=0.000
 Excited State 110: Singlet-?Sym 4.3956 eV 282.06 nm f=0.0000 <S**2>=0.000

Excited State 111: Singlet-?Sym 4.4237 eV 280.27 nm f=2.6106
<S2>=0.000**

619 -> 642 0.11327
 620 -> 635 0.21376
 620 -> 638 0.10935
 622 -> 636 0.21376
 622 -> 639 0.10935
 623 -> 633 0.10852
 624 -> 633 0.39204
 626 -> 640 0.19271
 628 -> 641 -0.19271

Excited State 112: Singlet-?Sym 4.4237 eV 280.27 nm f=2.6107
<S2>=0.000**

619 -> 640 -0.10679
 620 -> 634 -0.20152
 620 -> 637 0.10309
 621 -> 636 -0.20152
 621 -> 639 0.10309
 623 -> 631 0.37123
 623 -> 632 -0.13114
 624 -> 632 0.13332
 626 -> 642 0.18169
 627 -> 641 -0.18169

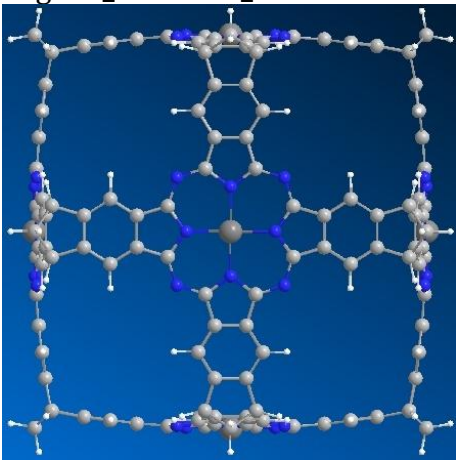
Excited State 113: Singlet-?Sym 4.4237 eV 280.27 nm f=2.6107
<S2>=0.000**

619 -> 641 0.10395
 621 -> 635 0.19617
 621 -> 638 -0.10035
 622 -> 634 0.19617
 622 -> 637 0.10035
 623 -> 631 -0.16204
 623 -> 632 -0.26178
 624 -> 632 0.26613
 624 -> 633 -0.12401
 627 -> 640 -0.17686
 628 -> 642 0.17686

Excited State 114: Singlet-?Sym 4.4579 eV 278.12 nm f=0.0000 <S**2>=0.000
 Excited State 115: Singlet-?Sym 4.4579 eV 278.12 nm f=0.0000 <S**2>=0.000
 Excited State 116: Singlet-T2U 4.4615 eV 277.90 nm f=0.0000 <S**2>=0.000
 Excited State 117: Singlet-T2U 4.4615 eV 277.90 nm f=0.0000 <S**2>=0.000
 Excited State 118: Singlet-T2U 4.4615 eV 277.90 nm f=0.0000 <S**2>=0.000
 Excited State 119: Singlet-?Sym 4.4769 eV 276.94 nm f=0.0000 <S**2>=0.000

Excited State 120: Singlet-?Sym 4.4769 eV 276.94 nm f=0.0000 <S**2>=0.000

Cage03_LC-wPBE_TDDFT



Excited State 1: Singlet-T1G 1.8446 eV 672.16 nm f=0.0000 <S**2>=0.000

Excited State 2: Singlet-T1G 1.8446 eV 672.16 nm f=0.0000 <S**2>=0.000

Excited State 3: Singlet-?Sym 1.8446 eV 672.16 nm f=0.00000 <S**2>=0.000

Excited State 4: Singlet-T2U 1.9348 eV 640.80 nm f=0.00000 <S**2>=0.000

Excited State 5: Singlet-?Sym 1.9348 eV 640.80 nm f=0.0000 <S**2>=0.000

Excited State 6: Singlet-T2U 1.9348 eV 640.80 nm f=0.0000 <S**2>=0.000

Excited State 7: Singlet-T1U 2.0199 eV 613.81 nm f=1.8247

<S2>=0.000**

985 -> 996	-0.16714
985 -> 999	-0.14729
986 -> 994	-0.10098
986 -> 996	-0.26175
987 -> 991	0.22981
987 ->1002	0.21357
988 -> 993	0.22981
988 ->1001	0.21357
990 -> 999	0.26382

Excited State 8: Singlet-?Sym 2.0199 eV 613.81 nm f=1.8247

<S2>=0.000**

985 -> 994	-0.12225
985 -> 995	0.17408
985 -> 997	0.13249
986 -> 994	0.23544
987 -> 992	-0.19631
987 ->1000	0.18244
988 -> 992	-0.12895
988 ->1000	-0.11984
989 -> 991	-0.12895
989 -> 993	0.19631
989 ->1001	-0.18244
989 ->1002	0.11984
990 -> 997	0.22536
990 -> 998	-0.14803

Excited State 9: Singlet-?Sym 2.0199 eV 613.81 nm f=1.8247

<S2>=0.000**

985 -> 995	0.28084
986 -> 994	-0.14343
986 -> 998	0.15803
987 -> 992	0.11959
987 ->1000	-0.11114
988 -> 992	-0.20802
988 ->1000	-0.19333
989 -> 991	-0.20802
989 -> 993	-0.11959
989 ->1001	0.11114
989 ->1002	0.19333
990 -> 997	-0.13729
990 -> 998	-0.23881

Excited State 10: Singlet-?Sym 2.0588 eV 602.23 nm f=0.0000 <S**2>=0.000

Excited State 11: Singlet-?Sym 2.0588 eV 602.23 nm f=0.00000 <S**2>=0.000

Excited State 12: Singlet-?Sym 2.0588 eV 602.23 nm f=0.0000 <S**2>=0.000

Excited State 13: Singlet-?Sym 3.6585 eV 338.89 nm f=0.0002

<S2>=0.000**

947 -> 992	0.12000
961 ->1000	0.20856
961 ->1001	0.12599
961 ->1002	-0.13357
962 -> 992	0.21647
963 -> 991	-0.13464

963 ->1000	0.12000
964 -> 995	-0.13923
964 -> 998	-0.13676
965 -> 994	0.13922
965 -> 997	0.13675

Excited State 14: Singlet-?Sym 3.6585 eV 338.89 nm f=0.0002

<S2>=0.000**

947 -> 992	0.10427
961 ->1000	0.18123
961 ->1001	-0.10879
961 ->1002	0.18037
962 -> 992	0.18809
962 ->1002	-0.10079
963 -> 991	0.18182
963 ->1000	0.10428
964 -> 995	-0.12097
964 -> 998	-0.11882
965 -> 994	0.12098
965 -> 996	-0.12040
965 -> 997	0.11883
965 -> 999	0.11826
966 -> 995	-0.12041
966 -> 998	0.11827

Excited State 15: Singlet-T1U 3.6585 eV 338.89 nm f=0.0002

<S2>=0.000**

948 -> 993	0.11001
955 -> 994	-0.10308
955 -> 997	0.10149
957 -> 996	-0.10308
957 -> 999	-0.10148
961 ->1001	0.22249
961 ->1002	0.16382
962 -> 993	0.15753
963 -> 991	0.16514
963 -> 993	0.17570
964 -> 996	-0.14852
964 -> 999	-0.14588
965 -> 996	-0.10937
965 -> 999	0.10742
966 -> 994	-0.14852
966 -> 995	-0.10936
966 -> 997	0.14589
966 -> 998	0.10741

Excited State 16: Singlet-T1G 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 17: Singlet-T1G 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 18: Singlet-T1G 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 19: Singlet-?Sym 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 20: Singlet-T2G 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 21: Singlet-T2G 3.6586 eV 338.88 nm f=0.00000 <S**2>=0.000

Excited State 22: Singlet-T2U 3.6587 eV 338.87 nm f=0.00000 <S**2>=0.000

Excited State 23: Singlet-T2U 3.6587 eV 338.87 nm f=0.00000 <S**2>=0.000

Excited State 24: Singlet-T2U 3.6587 eV 338.87 nm f=0.00000 <S**2>=0.000

Excited State 25: Singlet-T1G 3.8716 eV 320.24 nm f=0.00000 <S**2>=0.000

Excited State 26: Singlet-T1G 3.8716 eV 320.24 nm f=0.0000 <S**2>=0.000
 Excited State 27: Singlet-T1G 3.8716 eV 320.24 nm f=0.0000 <S**2>=0.000
 Excited State 28: Singlet-T2U 3.8726 eV 320.16 nm f=0.0000 <S**2>=0.000
 Excited State 29: Singlet-T2U 3.8726 eV 320.16 nm f=0.0000 <S**2>=0.000
 Excited State 30: Singlet-T2U 3.8726 eV 320.16 nm f=0.00000 <S**2>=0.000
 Excited State 31: Singlet-?Sym 3.8755 eV 319.92 nm f=0.0000 <S**2>=0.000
 Excited State 32: Singlet-?Sym 3.9057 eV 317.44 nm f=0.0000 <S**2>=0.000
 Excited State 33: Singlet-?Sym 3.9057 eV 317.44 nm f=0.0000 <S**2>=0.000
 Excited State 34: Singlet-?Sym 3.9227 eV 316.07 nm f=0.0000 <S**2>=0.000
 Excited State 35: Singlet-?Sym 3.9227 eV 316.07 nm f=0.0000 <S**2>=0.000
 Excited State 36: Singlet-?Sym 3.9235 eV 316.00 nm f=0.00000 <S**2>=0.000

Excited State 37: Singlet-T1U 3.9266 eV 315.75 nm f=0.0007

<S2>=0.000**

985 -> 997 -0.16917
 986 -> 994 -0.14252
 987 -> 992 0.21098
 987 ->1000 0.15197
 989 -> 993 -0.21098
 989 ->1001 -0.15197
 990 -> 997 0.43209
 990 -> 998 -0.11616
 990 -> 999 0.20106

Excited State 38: Singlet-T1U 3.9266 eV 315.75 nm f=0.0007

<S2>=0.000**

985 -> 999 0.16543
 986 -> 996 0.13937
 986 -> 999 -0.10563
 987 -> 991 -0.21725
 987 ->1002 0.15648
 988 -> 993 -0.21725
 988 ->1001 0.15648
 990 -> 997 -0.17961
 990 -> 998 0.10201
 990 -> 999 0.44492

Excited State 39: Singlet-T1U 3.9266 eV 315.75 nm f=0.0007

<S2>=0.000**

985 -> 995 0.17284
 986 -> 998 0.20517
 988 -> 992 -0.22731
 988 ->1000 0.16373
 989 -> 991 -0.22731
 989 ->1002 -0.16373
 990 -> 997 0.14718
 990 -> 998 0.46553

Excited State 40: Singlet-T2G 3.9284 eV 315.61 nm f=0.0000 <S**2>=0.000
 Excited State 41: Singlet-T2G 3.9284 eV 315.61 nm f=0.0000 <S**2>=0.000
 Excited State 42: Singlet-T2G 3.9284 eV 315.61 nm f=0.0000 <S**2>=0.000
 Excited State 43: Singlet-?Sym 3.9290 eV 315.56 nm f=0.0000 <S**2>=0.000
 Excited State 44: Singlet-?Sym 3.9290 eV 315.56 nm f=0.00000 <S**2>=0.000
 Excited State 45: Singlet-?Sym 3.9290 eV 315.56 nm f=0.00000 <S**2>=0.000

Excited State 46: Singlet-T1U 3.9400 eV 314.68 nm f=0.0756

<S2>=0.000**

985 -> 995	0.10607
985 -> 999	0.13866
986 -> 996	0.11102
986 -> 998	0.13248
987 -> 991	0.22502
987 ->1002	-0.20715
988 -> 992	0.18138
988 -> 993	0.22502
988 ->1000	-0.16697
988 ->1001	-0.20715
989 -> 991	0.18138
989 ->1002	0.16697
990 -> 998	0.19791
990 -> 999	0.24553

Excited State 47: Singlet-T1U 3.9400 eV 314.68 nm f=0.0757

<S2>=0.000**

985 -> 995	0.11804
985 -> 999	-0.11134
986 -> 998	0.14743
987 -> 991	-0.18069
987 -> 992	0.10752
987 ->1002	0.16634
988 -> 992	0.20184
988 -> 993	-0.18069
988 ->1000	-0.18582
988 ->1001	0.16634
989 -> 991	0.20184
989 -> 993	-0.10752
989 ->1002	0.18582
990 -> 997	-0.11732
990 -> 998	0.22024
990 -> 999	-0.19716

Excited State 48: Singlet-T1U 3.9400 eV 314.68 nm f=0.0756

<S2>=0.000**

985 -> 997	-0.17408
986 -> 994	-0.13938
987 -> 992	-0.26828
987 ->1000	-0.24698
988 -> 992	0.10636
989 -> 991	0.10636
989 -> 993	0.26828
989 ->1001	0.24698
990 -> 997	0.29273
990 -> 998	0.11605

Excited State 49: Singlet-?Sym 3.9631 eV 312.85 nm f=0.0000 <S2>=0.000**

Excited State 50: Singlet-?Sym 3.9633 eV 312.83 nm f=0.0000 <S2>=0.000**

Excited State 51: Singlet-?Sym 3.9633 eV 312.83 nm f=0.00000 <S2>=0.000**

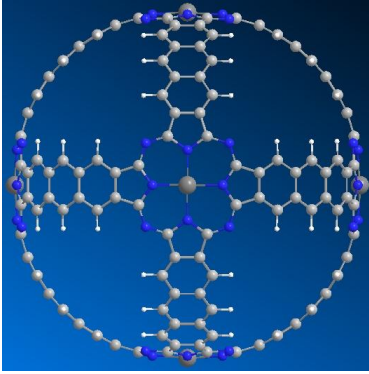
Excited State 52: Singlet-?Sym 3.9633 eV 312.83 nm f=0.00000 <S2>=0.000**

Excited State 53: Singlet-?Sym 3.9634 eV 312.83 nm f=0.0000 <S2>=0.000**

Excited State 54: Singlet-?Sym 3.9634 eV 312.83 nm f=0.0000 <S2>=0.000**

Excited State 55: Singlet-?Sym 3.9946 eV 310.38 nm f=0.00000 <S2>=0.000**

Excited State 56: Singlet-?Sym 3.9946 eV 310.38 nm f=0.0000 <S**2>=0.000
 Excited State 57: Singlet-?Sym 3.9946 eV 310.38 nm f=0.0000 <S**2>=0.000
 Excited State 58: Singlet-?Sym 3.9965 eV 310.23 nm f=0.0000 <S**2>=0.000
 Excited State 59: Singlet-?Sym 3.9965 eV 310.23 nm f=0.00000 <S**2>=0.000
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 Excited State 61: Singlet-?Sym 4.0042 eV 309.63 nm f=0.00000 <S**2>=0.000
 Excited State 62: Singlet-?Sym 4.0042 eV 309.63 nm f=0.0000 <S**2>=0.000
 Excited State 63: Singlet-?Sym 4.0087 eV 309.28 nm f=0.00000 <S**2>=0.000
 Excited State 64: Singlet-?Sym 4.0087 eV 309.28 nm f=0.00000 <S**2>=0.000
 Excited State 65: Singlet-?Sym 4.0087 eV 309.28 nm f=0.0000 <S**2>=0.000
 Excited State 66: Singlet-?Sym 4.0090 eV 309.26 nm f=0.0000 <S**2>=0.000
 Excited State 67: Singlet-?Sym 4.0090 eV 309.26 nm f=0.0000 <S**2>=0.000
 Excited State 68: Singlet-?Sym 4.0090 eV 309.26 nm f=0.0000 <S**2>=0.000
Excited State 69: Singlet-?Sym 4.0277 eV 307.83 nm f=0.0171
<S2>=0.000**
 985 -> 996 -0.22570
 985 -> 999 0.45577
 986 -> 996 -0.35347
 986 -> 999 -0.29103
 990 -> 999 -0.10583
Excited State 70: Singlet-?Sym 4.0277 eV 307.83 nm f=0.0171
<S2>=0.000**
 985 -> 995 -0.42260
 986 -> 998 0.54491
 990 -> 998 -0.10675
Excited State 71: Singlet-?Sym 4.0277 eV 307.83 nm f=0.0171
<S2>=0.000**
 985 -> 994 0.19339
 985 -> 997 0.48025
 986 -> 994 -0.37245
 986 -> 997 0.24936
 990 -> 997 0.10590
 Excited State 72: Singlet-?Sym 4.0305 eV
 307.61 nm f=0.00000 <S**2>=0.000
 Excited State 73: Singlet-?Sym 4.0305 eV 307.61 nm f=0.00000 <S**2>=0.000
 Excited State 74: Singlet-?Sym 4.0305 eV 307.61 nm f=0.0000 <S**2>=0.000
 Excited State 75: Singlet-T2U 4.0457 eV 306.46 nm f=0.0000 <S**2>=0.000



Excited State 1: Singlet-?Sym 1.2801 eV 968.58 nm f=0.0000 <S**2>=0.000
 Excited State 2: Singlet-?Sym 1.2801 eV 968.58 nm f=0.0000 <S**2>=0.000
 Excited State 3: Singlet-?Sym 1.2801 eV 968.58 nm f=0.00000 <S**2>=0.000
 Excited State 4: Singlet-?Sym 1.5102 eV 820.96 nm f=0.0000 <S**2>=0.000
 Excited State 5: Singlet-?Sym 1.5102 eV 820.96 nm f=0.00000 <S**2>=0.000
 Excited State 6: Singlet-?Sym 1.5102 eV 820.96 nm f=0.00000 <S**2>=0.000

Excited State 7: Singlet-?Sym 1.6499 eV 751.47 nm f=2.3841

<S2>=0.000**

937 -> 949 0.13509
 937 -> 951 -0.10507
 938 -> 943 -0.11081
 938 -> 945 -0.15076
 938 -> 954 -0.10767
 939 -> 943 0.19383
 939 -> 944 -0.15076
 939 -> 952 0.13843
 939 -> 953 -0.10767
 940 -> 944 0.11081
 940 -> 945 -0.19383
 940 -> 954 0.13843
 941 -> 946 -0.23343
 941 -> 947 0.18957
 941 -> 949 0.10516
 942 -> 947 -0.23710
 942 -> 948 0.16162
 942 -> 951 0.10353

Excited State 8: Singlet-?Sym 1.6499 eV 751.47 nm f=2.3840

<S2>=0.000**

937 -> 949 -0.12652
 937 -> 950 -0.11425
 938 -> 943 -0.16394
 938 -> 945 -0.11291
 938 -> 952 0.11708
 939 -> 943 -0.18153
 939 -> 944 -0.11291

939 -> 952 -0.12964
940 -> 944 0.16394
940 -> 945 0.18153
940 -> 953 -0.11708
940 -> 954 -0.12964
941 -> 946 -0.17482
941 -> 947 -0.17754
941 -> 950 0.10605
942 -> 947 0.22206
942 -> 948 0.23912

Excited State 9: Singlet-?Sym 1.6499 eV 751.47 nm f=2.3841

<S2>=0.000**

937 -> 950 0.12742
937 -> 951 -0.13424
938 -> 943 0.18282
938 -> 945 -0.19262
938 -> 952 -0.13057
938 -> 954 -0.13756
939 -> 944 -0.19262
939 -> 953 -0.13756
940 -> 944 -0.18282
940 -> 953 0.13057
941 -> 946 -0.29824
941 -> 948 -0.10427
941 -> 950 -0.11827
942 -> 948 -0.26667
942 -> 951 0.13228

Excited State 10: Singlet-?Sym 1.7722 eV 699.61 nm f=0.0000 <S**2>=0.000
Excited State 11: Singlet-?Sym 1.7722 eV 699.61 nm f=0.00000 <S**2>=0.000
Excited State 12: Singlet-?Sym 1.7722 eV 699.61 nm f=0.0000 <S**2>=0.000
Excited State 13: Singlet-?Sym 2.7209 eV 455.67 nm f=0.00000 <S**2>=0.000
Excited State 14: Singlet-?Sym 2.7209 eV 455.67 nm f=0.0000 <S**2>=0.000
Excited State 15: Singlet-?Sym 2.7209 eV 455.67 nm f=0.0000 <S**2>=0.000
Excited State 16: Singlet-?Sym 2.7612 eV 449.03 nm f=0.0000 <S**2>=0.000
Excited State 17: Singlet-?Sym 2.8079 eV 441.56 nm f=0.0000 <S**2>=0.000
Excited State 18: Singlet-?Sym 2.8079 eV 441.56 nm f=0.00000 <S**2>=0.000
Excited State 19: Singlet-?Sym 2.8287 eV 438.31 nm f=0.00000 <S**2>=0.000
Excited State 20: Singlet-?Sym 2.8287 eV 438.31 nm f=0.0000 <S**2>=0.000
Excited State 21: Singlet-?Sym 2.8287 eV 438.31 nm f=0.0000 <S**2>=0.000
Excited State 22: Singlet-?Sym 2.8301 eV 438.10 nm f=0.0000 <S**2>=0.000
Excited State 23: Singlet-?Sym 2.8703 eV 431.95 nm f=0.00000 <S**2>=0.000
Excited State 24: Singlet-?Sym 2.8703 eV 431.95 nm f=0.00000 <S**2>=0.000
Excited State 25: Singlet-?Sym 2.8703 eV 431.95 nm f=0.0000 <S**2>=0.000

Excited State 26: Singlet-?Sym 2.9115 eV 425.84 nm f=0.4458

<S2>=0.000**

939 -> 943 -0.10000

940 -> 945 0.10000
941 -> 946 -0.25387
941 -> 947 0.18276
941 -> 949 -0.22732
941 -> 964 -0.13568
942 -> 947 -0.22858
942 -> 949 -0.18175
942 -> 951 -0.25247
942 -> 966 -0.12216

Excited State 27: Singlet-?Sym 2.9115 eV 425.84 nm f=0.4459

<S2>=0.000**

941 -> 946 0.24774
941 -> 947 0.13724
941 -> 949 -0.17071
941 -> 950 -0.18639
941 -> 964 0.13240
942 -> 947 -0.17165
942 -> 948 0.18742
942 -> 949 -0.13649
942 -> 951 0.24637
942 -> 965 -0.10016

Excited State 28: Singlet-?Sym 2.9115 eV 425.84 nm f=0.4459

<S2>=0.000**

938 -> 943 -0.11389
938 -> 959 -0.10501
940 -> 944 0.11389
940 -> 958 0.10501
941 -> 946 0.14947
941 -> 948 -0.12138
941 -> 949 -0.10316
941 -> 950 0.30871
942 -> 947 -0.10373
942 -> 948 -0.31042
942 -> 950 -0.12071
942 -> 951 0.14865
942 -> 965 0.16590

Excited State 29: Singlet-?Sym 3.0164 eV 411.03 nm f=0.0000 <S**2>=0.000
Excited State 30: Singlet-?Sym 3.0164 eV 411.03 nm f=0.0000 <S**2>=0.000
Excited State 31: Singlet-?Sym 3.0164 eV 411.03 nm f=0.0000 <S**2>=0.000
Excited State 32: Singlet-?Sym 3.0489 eV 406.65 nm f=0.0000 <S**2>=0.000
Excited State 33: Singlet-?Sym 3.0489 eV 406.65 nm f=0.0000 <S**2>=0.000
Excited State 34: Singlet-?Sym 3.0582 eV 405.42 nm f=0.0000 <S**2>=0.000
Excited State 35: Singlet-?Sym 3.0582 eV 405.42 nm f=0.0000 <S**2>=0.000
Excited State 36: Singlet-?Sym 3.0693 eV 403.95 nm f=0.0000 <S**2>=0.000
Excited State 37: Singlet-?Sym 3.0693 eV 403.95 nm f=0.0000 <S**2>=0.000
Excited State 38: Singlet-?Sym 3.0693 eV 403.95 nm f=0.0000 <S**2>=0.000

Excited State 39: Singlet-?Sym 3.0967 eV 400.37 nm f=0.00000 <S**2>=0.000
Excited State 40: Singlet-?Sym 3.0967 eV 400.37 nm f=0.00000 <S**2>=0.000
Excited State 41: Singlet-?Sym 3.0967 eV 400.37 nm f=0.00000 <S**2>=0.000
Excited State 42: Singlet-?Sym 3.1036 eV 399.49 nm f=0.00000 <S**2>=0.000

Excited State 43: Singlet-?Sym 3.1036 eV 399.49 nm f=0.0001
<S2>=0.000**

938 -> 945 0.25528
938 -> 954 -0.14551
939 -> 943 -0.21007
939 -> 944 0.25528
939 -> 952 0.11974
939 -> 953 -0.14552
940 -> 945 0.21006
940 -> 954 0.11974
941 -> 949 0.20322
942 -> 949 0.16248
942 -> 951 0.31259

Excited State 44: Singlet-?Sym 3.1036 eV 399.49 nm f=0.00000 <S**2>=0.000
Excited State 45: Singlet-?Sym 3.1746 eV 390.55 nm f=0.00000 <S**2>=0.000
Excited State 46: Singlet-?Sym 3.1746 eV 390.55 nm f=0.00000 <S**2>=0.000
Excited State 47: Singlet-?Sym 3.1746 eV 390.55 nm f=0.00000 <S**2>=0.000
Excited State 48: Singlet-?Sym 3.1779 eV 390.14 nm f=0.00000 <S**2>=0.000
Excited State 49: Singlet-?Sym 3.1999 eV 387.46 nm f=0.00000 <S**2>=0.000
Excited State 50: Singlet-?Sym 3.1999 eV 387.46 nm f=0.00000 <S**2>=0.000
Excited State 51: Singlet-?Sym 3.1999 eV 387.46 nm f=0.00000 <S**2>=0.000
Excited State 52: Singlet-?Sym 3.2246 eV 384.49 nm f=0.00000 <S**2>=0.000
Excited State 53: Singlet-T2U 3.2770 eV 378.35 nm f=0.00000 <S**2>=0.000
Excited State 54: Singlet-?Sym 3.2770 eV 378.35 nm f=0.00000 <S**2>=0.000
Excited State 55: Singlet-?Sym 3.2770 eV 378.35 nm f=0.00000 <S**2>=0.000
Excited State 56: Singlet-?Sym 3.2913 eV 376.70 nm f=0.00000 <S**2>=0.000
Excited State 57: Singlet-?Sym 3.2913 eV 376.70 nm f=0.00000 <S**2>=0.000
Excited State 58: Singlet-?Sym 3.3055 eV 375.08 nm f=0.00000 <S**2>=0.000
Excited State 59: Singlet-?Sym 3.3271 eV 372.65 nm f=0.00000 <S**2>=0.000
Excited State 60: Singlet-?Sym 3.3271 eV 372.65 nm f=0.00000 <S**2>=0.000

Excited State 61: Singlet-?Sym 3.3465 eV 370.49 nm f=0.0430
<S2>=0.000**

937 -> 950 -0.13084
938 -> 943 0.14726
938 -> 959 -0.16335
938 -> 963 0.14982
940 -> 944 -0.14726
940 -> 958 0.16335
940 -> 961 -0.14983
941 -> 950 -0.21461
941 -> 965 0.11956
942 -> 948 0.13869

942 -> 965 0.30576

942 -> 966 0.10258

Excited State 62: Singlet-?Sym 3.3465 eV 370.49 nm f=0.0430

<S2>=0.000**

931 -> 956 -0.10747

937 -> 949 0.12925

939 -> 943 -0.14548

939 -> 959 0.16137

939 -> 963 0.14800

940 -> 945 0.14548

940 -> 957 -0.16137

940 -> 962 -0.14801

941 -> 949 -0.17780

941 -> 966 -0.20253

942 -> 947 -0.11490

942 -> 949 -0.14215

942 -> 965 -0.11030

942 -> 966 0.25331

Excited State 63: Singlet-?Sym 3.3465 eV 370.49 nm f=0.0430

<S2>=0.000**

930 -> 955 0.10394

937 -> 951 -0.13655

938 -> 945 0.15369

938 -> 957 -0.17049

938 -> 962 0.15637

939 -> 944 0.15370

939 -> 958 -0.17049

939 -> 961 -0.15637

941 -> 946 -0.15366

941 -> 964 0.33875

942 -> 951 -0.23777

Excited State 64: Singlet-?Sym 3.4116 eV 363.42 nm f=0.1660

<S2>=0.000**

937 -> 950 -0.19269

938 -> 952 0.27124

938 -> 954 -0.10430

939 -> 953 -0.10430

940 -> 953 -0.27124

941 -> 946 0.12533

941 -> 948 -0.12006

941 -> 950 -0.16815

942 -> 948 -0.30705

Excited State 65: Singlet-?Sym 3.4116 eV 363.42 nm f=0.1659

<S2>=0.000**

937 -> 949 -0.19617

938 -> 954 -0.10678

939 -> 952	-0.27615
939 -> 953	-0.10678
940 -> 954	-0.27615
941 -> 946	0.12831
941 -> 947	0.20961
941 -> 949	0.14357
942 -> 947	-0.26216
942 -> 949	0.11479
Excited State 66:	Singlet-?Sym 3.4116 eV 363.42 nm f=0.1660
<S**2>=0.000	
937 -> 951	0.18221
938 -> 952	0.11869
938 -> 954	0.25649
939 -> 953	0.25649
940 -> 953	-0.11869
941 -> 946	-0.30821
942 -> 948	-0.13436
942 -> 951	0.16879
Excited State 67:	Singlet-?Sym 3.4225 eV 362.26 nm f=0.0000 <S**2>=0.000
Excited State 68:	Singlet-?Sym 3.4225 eV 362.26 nm f=0.00000 <S**2>=0.000
Excited State 69:	Singlet-?Sym 3.4225 eV 362.26 nm f=0.00000 <S**2>=0.000
Excited State 70:	Singlet-?Sym 3.5521 eV 349.04 nm f=0.0000 <S**2>=0.000
Excited State 71:	Singlet-?Sym 3.5521 eV 349.04 nm f=0.00000 <S**2>=0.000
Excited State 72:	Singlet-?Sym 3.5521 eV 349.04 nm f=0.0000 <S**2>=0.000
Excited State 73:	Singlet-?Sym 3.6200 eV 342.50 nm f=0.0000 <S**2>=0.000
Excited State 74:	Singlet-?Sym 3.6200 eV 342.50 nm f=0.0000 <S**2>=0.000
Excited State 75:	Singlet-?Sym 3.6200 eV 342.50 nm f=0.0000 <S**2>=0.000
Excited State 76:	Singlet-T2G 3.6517 eV 339.52 nm f=0.0000 <S**2>=0.000
Excited State 77:	Singlet-T2G 3.6517 eV 339.52 nm f=0.0000 <S**2>=0.000
Excited State 78:	Singlet-T2G 3.6517 eV 339.52 nm f=0.0000 <S**2>=0.000
Excited State 79:	Singlet-?Sym 3.7026 eV 334.86 nm f=0.0000 <S**2>=0.000
Excited State 80:	Singlet-?Sym 3.7128 eV 333.93 nm f=0.00000 <S**2>=0.000
Excited State 81:	Singlet-?Sym 3.7128 eV 333.93 nm f=0.0000 <S**2>=0.000
Excited State 82:	Singlet-?Sym 3.7194 eV 333.34 nm f=0.0000 <S**2>=0.000
Excited State 83:	Singlet-?Sym 3.7194 eV 333.34 nm f=0.00000 <S**2>=0.000
Excited State 84:	Singlet-?Sym 3.7194 eV 333.34 nm f=0.00000 <S**2>=0.000
Excited State 85:	Singlet-?Sym 3.7632 eV 329.46 nm f=0.0000 <S**2>=0.000
Excited State 86:	Singlet-T2G 3.7947 eV 326.73 nm f=0.0000 <S**2>=0.000
Excited State 87:	Singlet-T2G 3.7947 eV 326.73 nm f=0.0000 <S**2>=0.000
Excited State 88:	Singlet-T2G 3.7947 eV 326.73 nm f=0.0000 <S**2>=0.000
Excited State 89:	Singlet-?Sym 3.8045 eV 325.88 nm f=0.0000 <S**2>=0.000
Excited State 90:	Singlet-?Sym 3.8045 eV 325.88 nm f=0.0000 <S**2>=0.000

Table S2. Optimized parameters of unit cells used for gas adsorption calculations.

<i>Structure</i>	<i>a, (nm)</i>	<i>b, (nm)</i>	<i>c, (nm)</i>
1	1.6568	1.6568	1.6568
2	1.6779	1.6779	1.6779
3	2.1381	2.1381	2.1381
4	2.3008	2.3008	2.3008
5	1.6382	1.6382	1.6382
5t	1.6629	1.6629	1.3141
6	1.7426	1.7426	1.7426
6t	1.7703	1.7703	1.3100
7	2.0611	2.0611	2.0611
7t	2.0905	2.0905	1.3126
8	2.3740	2.3740	2.3740
8t	2.4100	2.4100	1.3100
9	1.7410	1.7410	1.7410
10	1.6451	1.6451	1.6451