

Supporting information

Theoretical uncovering the chalcogen elements regulated ESDPT behaviors for 2,5-bis(2-benzoxazolyl)-hydroquinone derivatives

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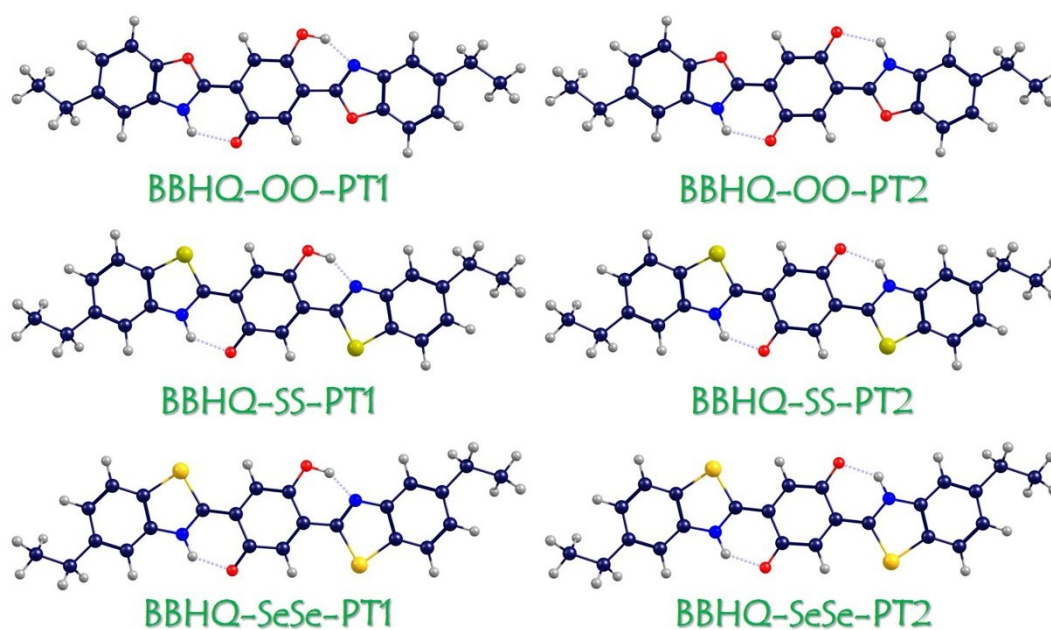


Figure S1. View of the optimized single proton-transfer BBHQ-OO-PT1, BBHQ-SS-PT1 and BBHQ SeSe-PT1 as well as the dual proton-transfer BBHQ-OO-PT2, BBHQ-SS-PT2 and BBHQ-SeSe-PT2 forms.

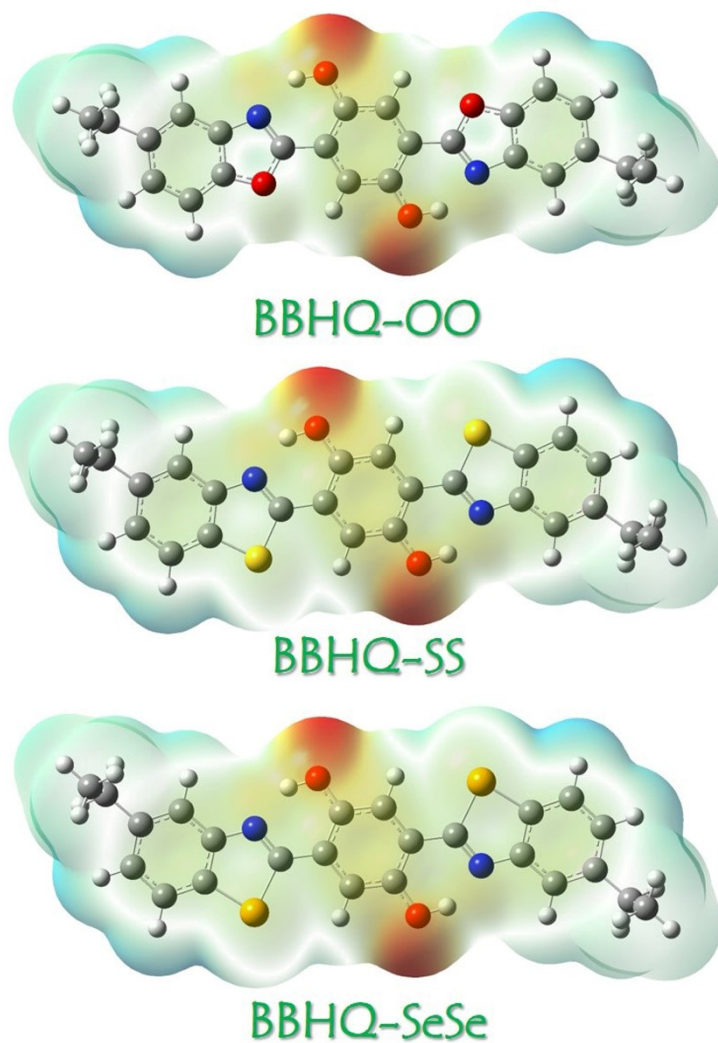


Figure S2. The MEP maps for BBHQ-OO, BBHQ-SS and BBHQ-SeSe fluorophores.

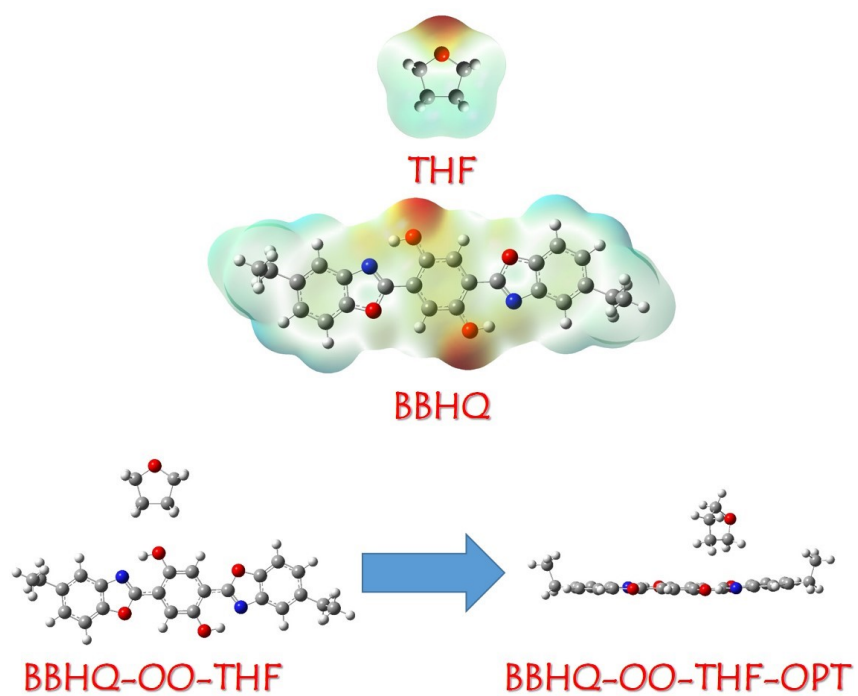


Figure S3. The MEP maps for THF and BBHQ-OO. The initial constructed structure BBHQ-OO-THF and its optimized BBHQ-OO-THF-OPT is also shown.

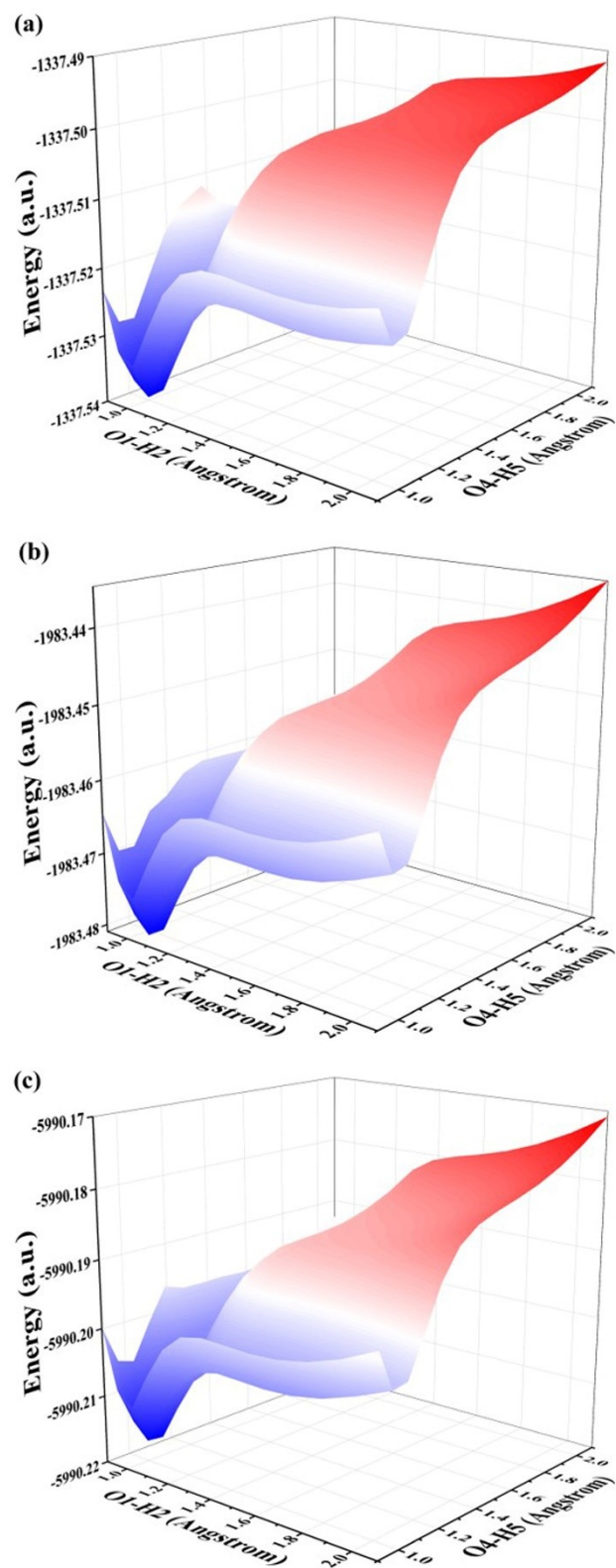


Figure S4. The constructed S_0 -state PESs for (a) BBHQ-OO, (b) BBHQ-SS and (c) BBHQ-SeSe.



Figure S5. The constructed T₁-state PES BBHQ-SS fluorophore.

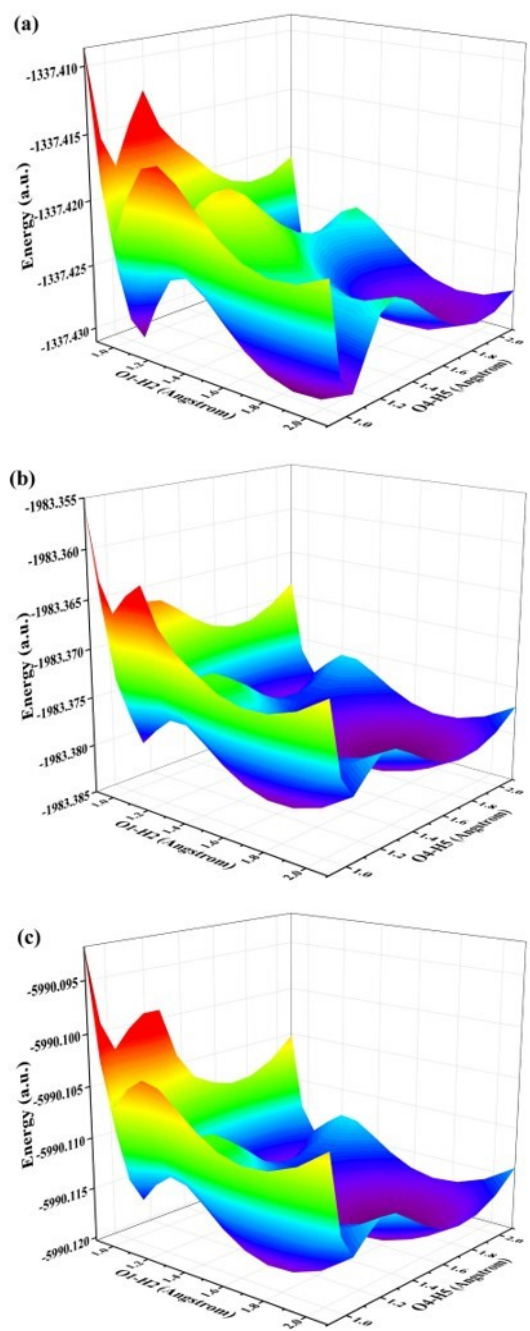


Figure S6. The constructed gas-state PES for BBHQ-OO (a), BBHQ-SS (b) and BBHQ-SeSe (c).

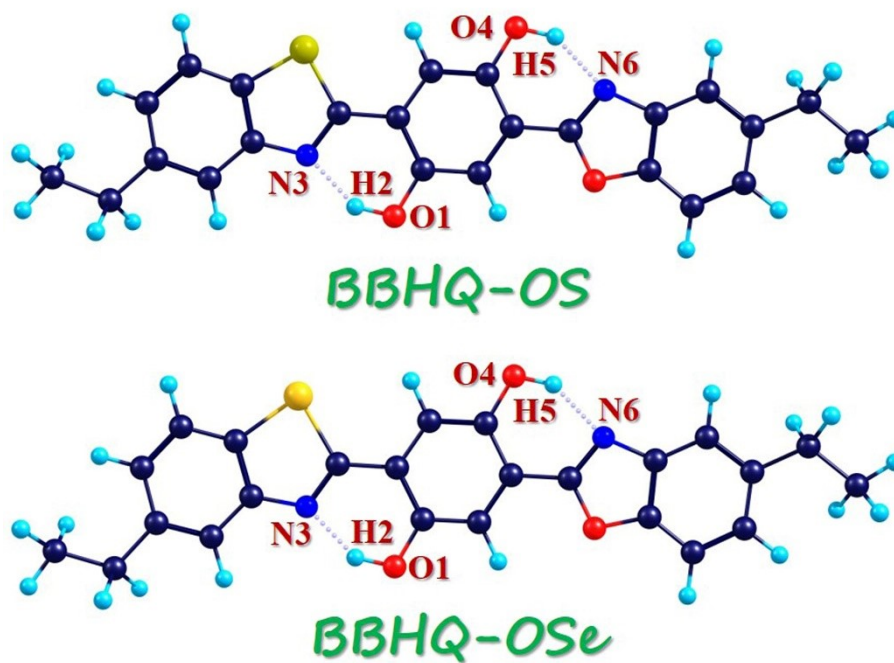


Figure S7. Structures of heterosubstituted oxygen–sulphur BBHQ-OS and oxygen-selenium BBHQ-OSe compounds.

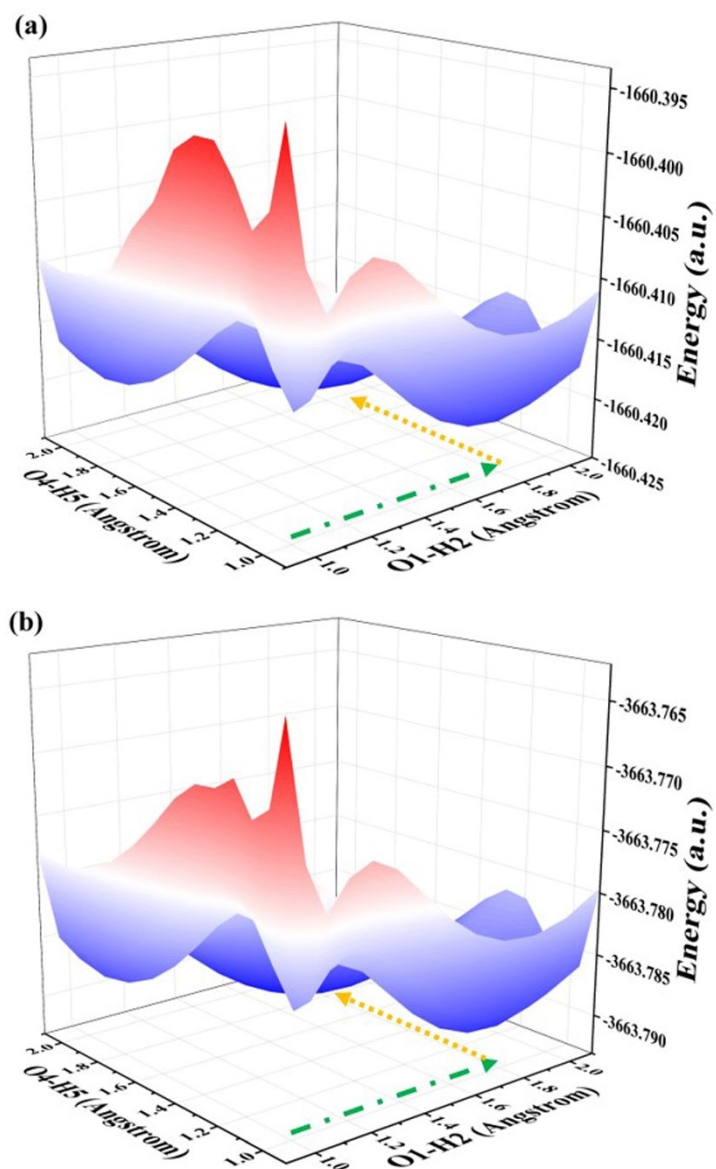


Figure S8. View of the constructed S₁-state PESs for BBHQ-OS (a) and BBHQ-OSe (b). Herein, to more clearly present the effect of heterosubstituted oxygen-sulphur and oxygen-selenium, we change the angle of the entire PESs.

Table S1. Parameters of bond lengths (Å) and bond angles (Δ°) involved in O1 \cdots H2-N3 and O4-H5 \cdots N6 for BBHQ-OO-PT1, BBHQ-SS-PT1 and BBHQ-SeSe-PT1 in S_0 and S_1 states.

	BBHQ-OO-PT1		BBHQ-SS-PT1		BBHQ-SeSe-PT1	
	S_0	S_1	S_0	S_1	S_0	S_1
O1 \cdots H2	1.7382	1.9620	1.5913	1.8707	1.5832	1.7946
H2-N3	1.0403	1.0203	1.0636	1.0211	1.0654	1.0317
O4-H5	0.9838	1.0093	0.9879	1.0153	0.9885	1.0234
H5 \cdots N6	1.7990	1.6812	1.7469	1.6567	1.7432	1.6085
Δ (O1H2N3)	132.84	124.35	141.16	130.30	142.13	134.38
Δ (O4H5N6)	146.03	148.60	146.72	148.27	146.78	149.99

Table S2. Parameters of bond lengths (Å) and bond angles (Δ°) involved in O1 \cdots H2-N3 and O4 \cdots H5-N6 for BBHQ-OO-PT2, BBHQ-SS-PT2 and BBHQ-SeSe-PT2 in S_0 and S_1 states.

	BBHQ-OO-PT2		BBHQ-SS-PT2		BBHQ-SeSe-PT2	
	S_0	S_1	S_0	S_1	S_0	S_1
O1 \cdots H2	0.9867	1.9420	0.9910	1.8070	0.9917	1.7883
H2-N3	1.7930	1.0204	1.7392	1.0296	1.7345	1.0316
O4 \cdots H5	0.9867	1.9420	0.9910	1.8070	0.9917	1.7883
H5-N6	1.7930	1.0204	1.7392	1.0296	1.7345	1.0316
Δ (O1H2N3)	145.68	125.12	146.50	133.14	146.59	134.66
Δ (O4H5N6)	145.68	125.12	146.50	133.14	146.59	134.66

Table S3. Parameters of bond lengths (Å) and bond angles (Δ°) involved in O1-H2 \cdots N3 and O4-H5 \cdots N6 for BBHQ-OO-THF-OPT complex in both S_0 and S_1 states.

	BBHQ-OO-THF-OPT	
	S_0	S_1
O1-H2	0.987	1.007
H2 \cdots N3	1.793	1.699
O4-H5	0.987	1.007
H5 \cdots N6	1.793	1.699
Δ (O1H2N3)	145.7	148.4
Δ (O4H5N6)	145.7	148.4

Table S4. The Mulliken's charge and NPA charge of O1, H2, N3, O4, H5 and N6 atoms for BBHQ-OO, BBHQ-SS and BBHQ-SeSe compounds in both S_0 and S_1 states.

	atoms	Mulliken's charge		NPA charge	
		S_0	S_1	S_0	S_1
BBHQ-OO	O1	-0.294	-0.286	-0.661	-0.659
	H2	0.300	0.300	0.506	0.504
	N3	-0.154	-0.157	-0.496	-0.498
	O4	-0.294	-0.286	-0.661	-0.659
	H5	0.300	0.300	0.506	0.504
	N6	-0.154	-0.157	-0.496	-0.498
BBHQ-SS	O1	-0.298	-0.292	-0.665	-0.663
	H2	0.308	0.308	0.503	0.499
	N3	-0.117	-0.128	-0.475	-0.480
	O4	-0.298	-0.292	-0.665	-0.663
	H5	0.308	0.308	0.503	0.499
	N6	-0.117	-0.128	-0.475	-0.480
BBHQ-SeSe	O1	-0.298	-0.292	-0.665	-0.663
	H2	0.310	0.310	0.502	0.498
	N3	-0.127	-0.138	-0.482	-0.489
	O4	-0.298	-0.292	-0.665	-0.663
	H5	0.310	0.310	0.502	0.498
	N6	-0.127	-0.138	-0.482	-0.489

The coordinates of the searched TS forms in S₁ state

BBHQ-OO (TS1 along with I → II path):

	X	Y	Z
C	-4.90114300	-0.27186500	0.21607900
C	-4.86512100	1.12796300	0.10218300
C	-5.99552600	1.91154100	0.08983600
C	-7.21260200	1.23228600	0.19973200
C	-7.28845800	-0.16786900	0.31547000
C	-6.12155400	-0.93548200	0.32457300
C	-2.81851800	0.37487300	0.07112600
H	-5.94409500	2.98816600	0.00490700
H	-8.13119800	1.80623000	0.19721200
H	-6.15986300	-2.01344300	0.41423300
C	0.81736400	1.24866700	-0.13763800
C	1.41902500	-0.06865200	-0.06825200
C	0.57198700	-1.17340600	0.06654600
C	-0.82482900	-1.03406900	0.11714200
C	-1.41285600	0.30799200	0.04516200
C	-0.57037800	1.40920900	-0.08898000
H	0.98264300	-2.17136700	0.12890700
H	-0.97205000	2.41124600	-0.15277600
C	4.93982700	0.26843300	-0.21982600
C	4.79084500	-1.12232300	-0.09328500
C	5.85191600	-1.99907900	-0.06446000
C	7.12257400	-1.42609700	-0.16910100
C	7.31607600	-0.03755400	-0.29682000
C	6.21711900	0.82234200	-0.32271600
C	2.83060600	-0.16995700	-0.09381900
H	5.71064700	-3.06718400	0.02914700
H	7.99018800	-2.07478600	-0.15381900
H	6.34666700	1.89281800	-0.42217200
N	-3.59685900	-0.70719700	0.19481300
N	3.68690300	0.83866100	-0.21870400
O	-1.59877800	-2.07258400	0.23049900
H	-2.76404300	-1.65720800	0.24244000
O	1.56745500	2.33767100	-0.25562700
H	2.54004200	2.06431200	-0.27551100
O	-3.54368500	1.52877700	0.01139400
O	3.44437500	-1.40138000	-0.01357800
C	-8.63852500	-0.84417600	0.37377300
C	-9.19559700	-1.15699300	-1.02346100
H	-9.34392900	-0.20339000	0.90880600
H	-8.55743800	-1.77088800	0.94711300

H	-10.16995300	-1.64525100	-0.95281400
H	-9.31464700	-0.24225700	-1.60821000
H	-8.52103400	-1.81919700	-1.57055400
C	8.71929300	0.52217800	-0.35010900
C	9.29894600	0.78420200	1.04815200
H	8.71863500	1.45369300	-0.92164900
H	9.36975600	-0.17444200	-0.88544500
H	10.31163800	1.18807700	0.98120400
H	8.68162300	1.50011400	1.59530400
H	9.33833700	-0.13832800	1.63156300

BBHQ-OO (TS2 along with II → III path):

	X	Y	Z
C	-4.91388900	-0.27165700	-0.22114100
C	-4.89621800	1.12531900	-0.09501500
C	-6.03703200	1.89303700	-0.06951700
C	-7.24742400	1.19901400	-0.17127700
C	-7.30436800	-0.19898100	-0.29748400
C	-6.12521000	-0.94996000	-0.32471900
C	-2.83570200	0.40399800	-0.10578900
H	-5.99891200	2.96985300	0.02110600
H	-8.17322200	1.76109000	-0.15556800
H	-6.15020700	-2.02747700	-0.42541600
C	0.82148700	1.36795300	0.12592500
C	1.40096700	0.01950500	0.01896100
C	0.56551200	-1.09613100	-0.10324100
C	-0.83341300	-0.97739200	-0.13840600
C	-1.42851200	0.35322900	-0.03107800
C	-0.60163100	1.46410200	0.08744500
H	0.98284600	-2.09177300	-0.17510800
H	-1.02643100	2.45711500	0.15872500
C	4.98960100	0.27993800	0.21866900
C	4.77785500	-1.09426200	0.09588100
C	5.80543200	-2.00823000	0.07643300
C	7.09558400	-1.48061100	0.18370800
C	7.34000000	-0.10328400	0.30891600
C	6.27143200	0.80023100	0.32838400
C	2.79611600	-0.12331800	0.09308900
H	5.62303500	-3.06991900	-0.01287900
H	7.93784600	-2.16132300	0.17339600
H	6.43724300	1.86494700	0.42735200
N	-3.60055100	-0.68902100	-0.22341700
N	3.72942800	0.84620500	0.21136100
O	-1.59151000	-2.03099200	-0.26138300

H	-2.76763100	-1.62449900	-0.27011300
O	1.55773700	2.39091200	0.24396900
H	3.41873400	1.81602900	0.27565500
O	-3.57811900	1.54617100	-0.02332000
O	3.41561300	-1.33109100	0.01963400
C	-8.64393900	-0.89738400	-0.34814100
C	-9.16148500	-1.27236700	1.04876900
H	-8.56116700	-1.80091400	-0.95750900
H	-9.37340100	-0.25065500	-0.84216300
H	-10.12858800	-1.77581700	0.98363700
H	-8.46222800	-1.94168200	1.55475900
H	-9.28198000	-0.38217100	1.67005200
C	8.75975100	0.40986100	0.36794300
C	9.33406200	0.69849300	-1.02747200
H	9.39061900	-0.32470500	0.87425400
H	8.79301000	1.32169500	0.96926900
H	10.35917000	1.06792600	-0.95574800
H	9.33960600	-0.20573200	-1.63984700
H	8.73590300	1.45109600	-1.54572100

BBHQ-SS (TS1 along with I → II path):

	X	Y	Z
C	-4.97479800	-0.08817400	-0.12016900
C	-5.19429100	1.30973500	-0.10673200
C	-6.47997900	1.83086700	-0.10361100
C	-7.55094500	0.94329100	-0.11194300
C	-7.35908400	-0.45168600	-0.12477100
C	-6.06804900	-0.96446700	-0.12948500
C	-2.81275300	0.61000300	-0.11815600
H	-6.64883300	2.89969600	-0.09850200
H	-8.56043800	1.33668200	-0.11152900
H	-5.89360000	-2.03336500	-0.14147300
C	0.91580400	1.13586000	-0.11183000
C	1.40719600	-0.23126400	-0.12458700
C	0.45077200	-1.24784700	-0.13428200
C	-0.93035600	-0.98840000	-0.13171000
C	-1.40830700	0.39674300	-0.11936700
C	-0.45667000	1.41106500	-0.10958700
H	0.74646800	-2.28889100	-0.14367900
H	-0.74890000	2.45328400	-0.10008000
C	4.99648500	0.08241200	-0.11896700
C	5.14145700	-1.32659600	-0.13250400

C	6.39634300	-1.91960600	-0.14142400
C	7.51620700	-1.09496000	-0.13461600
C	7.40334500	0.30886700	-0.12036700
C	6.14311300	0.89145400	-0.11302000
C	2.81447900	-0.46384500	-0.12729500
H	6.50510000	-2.99624200	-0.15711100
H	8.50192500	-1.54487900	-0.14374400
H	6.02897500	1.96879600	-0.10441600
N	-3.65529900	-0.43359300	-0.12658900
N	3.70594300	0.52548900	-0.11669200
O	-1.78443500	-1.97051600	-0.14027200
H	-2.87137300	-1.45999700	-0.13549400
O	1.75242700	2.16174200	-0.10183000
H	2.70475700	1.78787400	-0.10490900
C	-8.55194600	-1.37686000	-0.08013800
C	-9.05694800	-1.60832500	1.35232200
H	-8.28702000	-2.33619300	-0.53091700
H	-9.36030700	-0.95644700	-0.68422700
H	-9.92090100	-2.27633800	1.35620700
H	-8.27601100	-2.05638900	1.97051700
H	-9.35357300	-0.66593300	1.81779700
C	8.64771800	1.16346100	-0.06186700
C	9.18927900	1.31133100	1.36814300
H	8.43052800	2.15280500	-0.47162600
H	9.42157900	0.72252300	-0.69617400
H	10.08944200	1.92978800	1.38161600
H	8.44500300	1.77736200	2.01760400
H	9.44031200	0.33663500	1.79224500
S	-3.65048000	2.17149600	-0.10304800
S	3.55298000	-2.09163400	-0.14298600

BBHQ-SS (TS2 along with II → III path):

	X	Y	Z
C	4.98239300	-0.07532700	-0.19200200
C	5.21569600	1.31300900	-0.07071700
C	6.50530400	1.82394400	-0.07649000
C	7.56800800	0.93454400	-0.20345800
C	7.36185500	-0.45149200	-0.32534400
C	6.06542100	-0.95355200	-0.31960400
C	2.82603500	0.63354200	-0.04411800
H	6.68396600	2.88770700	0.01143800
H	8.58024700	1.32080400	-0.21161000
H	5.88091500	-2.01673900	-0.41434600
C	-0.92956200	1.22497900	0.15675000

C	-1.39568300	-0.16961400	0.04229100
C	-0.44652500	-1.18638100	-0.08699800
C	0.93608500	-0.94063300	-0.11693300
C	1.41830300	0.43341100	-0.00703100
C	0.48043100	1.44763300	0.12338600
H	-0.74623000	-2.22402400	-0.17133100
H	0.79326600	2.48149100	0.20820300
C	-5.04421500	0.06258500	0.19543000
C	-5.13339200	-1.33260100	0.05992600
C	-6.36840000	-1.96420100	0.04504100
C	-7.50994600	-1.17869400	0.16545700
C	-7.43867300	0.21867400	0.30101500
C	-6.19456300	0.84250400	0.31640700
C	-2.78424200	-0.44773400	0.06701900
H	-6.44418600	-3.03878800	-0.05401400
H	-8.48106800	-1.65861000	0.15760500
H	-6.11236400	1.91730100	0.42177800
N	3.65790800	-0.41147800	-0.17355400
N	-3.74186400	0.49873300	0.19485200
O	1.77769000	-1.92995900	-0.24110000
H	2.87388500	-1.42273800	-0.23665400
O	-1.74087900	2.19016100	0.27923100
H	-3.40009600	1.46636400	0.27604500
C	8.54541700	-1.38654000	-0.40858900
C	9.10323300	-1.74751800	0.97656100
H	9.33466300	-0.92126200	-1.00510400
H	8.25270500	-2.30050900	-0.93100400
H	9.95844000	-2.42110300	0.88820200
H	9.42925700	-0.85207900	1.51016500
H	8.34149700	-2.24082900	1.58426400
C	-8.70402500	1.03911600	0.37467800
C	-9.24321700	1.40254300	-1.01745800
H	-8.51344200	1.95422400	0.94032700
H	-9.46646600	0.48097300	0.92375600
H	-10.15857200	1.99234100	-0.93610600
H	-8.50944400	1.98650800	-1.57716400
H	-9.46767500	0.50332300	-1.59509900
S	3.67940200	2.18261900	0.06764300
S	-3.51881000	-2.04761400	-0.06606800

BBHQ-SeSe (TS1 along with I → II path):

	X	Y	Z
C	-4.97602700	-0.25376400	-0.10377900
C	-5.33255500	1.11617700	-0.09350100

C	-6.66463200	1.50430600	-0.09198900
C	-7.64677000	0.51959300	-0.09922200
C	-7.31934400	-0.84949800	-0.10928800
C	-5.98434000	-1.22958600	-0.11205600
C	-2.82074300	0.54492500	-0.10287600
H	-6.93994900	2.55106000	-0.08904300
H	-8.68950200	0.81419200	-0.10024800
H	-5.70592600	-2.27652200	-0.12205500
C	0.89739300	1.14511900	-0.10145200
C	1.41900200	-0.21270800	-0.10829400
C	0.48232700	-1.24706200	-0.11344000
C	-0.90339000	-1.01707500	-0.11169200
C	-1.41248100	0.35817100	-0.10427100
C	-0.47991500	1.39047400	-0.09955600
H	0.79771600	-2.28258700	-0.11897300
H	-0.79155300	2.42730800	-0.09438900
C	5.01166500	0.23608900	-0.10447200
C	5.29865900	-1.15195100	-0.10743000
C	6.60875400	-1.61022800	-0.11044400
C	7.64308500	-0.68037700	-0.10887800
C	7.38944700	0.70418500	-0.10571500
C	6.07631400	1.15285900	-0.10399100
C	2.83056300	-0.41663300	-0.10923400
H	6.82878500	-2.67001700	-0.11763700
H	8.66849500	-1.03104000	-0.11339700
H	5.85355100	2.21332700	-0.10370800
N	-3.63701800	-0.51517800	-0.10884800
N	3.69401000	0.59160200	-0.10580000
O	-1.73610400	-2.01769200	-0.11658700
H	-2.82574400	-1.52801600	-0.11406500
O	1.71264700	2.18758800	-0.09667400
H	2.67259200	1.82865700	-0.09912200
C	-8.41475700	-1.88813200	-0.06547500
C	-8.91074000	-2.15321900	1.36424700
H	-8.05083000	-2.82106100	-0.50232300
H	-9.25395600	-1.55645600	-0.68273100
H	-9.70419000	-2.90363500	1.36715900
H	-8.09636200	-2.51488800	1.99573900
H	-9.30472700	-1.24009200	1.81562500
C	8.53876800	1.68295200	-0.05226600
C	9.04587100	1.91163700	1.37972100
H	8.22582600	2.63720400	-0.48286100
H	9.36080900	1.31237700	-0.67073300
H	9.87827900	2.61872600	1.38991200

H	8.25053800	2.31137800	2.01263600
H	9.38957200	0.97555200	1.82525900
Se	-3.77159800	2.20763700	-0.09049300
Se	3.68243200	-2.15167100	-0.11345700

BBHQ-SeSe (TS2 along with II → III path):

	X	Y	Z
C	4.98328800	-0.24199100	0.19075600
C	5.35369200	1.11731400	0.07548600
C	6.68896200	1.49327900	0.07924100
C	7.66210800	0.50555400	0.19709000
C	7.32025300	-0.85337900	0.31275300
C	5.98040200	-1.22064200	0.30944200
C	2.83415200	0.57007800	0.06093400
H	6.97460000	2.53403400	-0.00427900
H	8.70720500	0.79164800	0.20301400
H	5.69139500	-2.26099900	0.39965200
C	-0.91176000	1.23810800	-0.11152500
C	-1.40927100	-0.14857400	-0.01051000
C	-0.47828600	-1.18279600	0.11253600
C	0.90851800	-0.96681800	0.13866300
C	1.42211000	0.39764700	0.03432400
C	0.50296700	1.42979300	-0.08255000
H	-0.79687400	-2.21551000	0.19261900
H	0.83440600	2.45858700	-0.16022300
C	-5.06136900	0.21835900	-0.18763600
C	-5.29323500	-1.16331600	-0.08605400
C	-6.58706400	-1.66395100	-0.10572800
C	-7.64489100	-0.76928200	-0.22595100
C	-7.43196600	0.61615800	-0.32830900
C	-6.13161900	1.10857000	-0.30902200
C	-2.80178600	-0.40165900	-0.04401800
H	-6.77393500	-2.72741500	-0.03410000
H	-8.65853300	-1.15118900	-0.24456300
H	-5.94062000	2.17194000	-0.38874100
N	3.63955900	-0.49230900	0.17982800
N	-3.73253300	0.56974400	-0.16066200
O	1.72877200	-1.97515800	0.25416800
H	2.82611400	-1.49061400	0.24440900
O	-1.70085400	2.22262100	-0.22074600
H	-3.35308400	1.52667300	-0.22428500
C	8.40385500	-1.90327200	0.38653300
C	8.91085100	-2.31829400	-1.00295700
H	8.02464100	-2.78321700	0.91180300

H	9.24096300	-1.52033500	0.97633500
H	9.69550400	-3.07368900	-0.92149700
H	8.09841500	-2.73339600	-1.60340500
H	9.31954200	-1.45982500	-1.54042700
C	-8.60715500	1.56096300	-0.40574300
C	-9.15312700	1.92573600	0.98329900
H	-9.40271900	1.10135100	-0.99770000
H	-8.30952100	2.47223800	-0.92976500
H	-10.00319300	2.60592400	0.89879800
H	-9.48336100	1.03295800	1.51859800
H	-8.38429500	2.41349900	1.58636900
Se	3.80155700	2.21829500	-0.06394100
Se	-3.64382000	-2.10947000	0.05892700