

## Supporting Information

### Excellent Ratiometric Two-Photon Fluorescent Probes for Hydrogen Sulfide Detection based on the Fluorescence Resonance Energy

#### Transfer Mechanism

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## Two-photon Absorption Cross Section

The TPA cross section can be calculated by using the TP transition matrix element  $S_{\alpha\beta}$  of the initial state  $|i\rangle$  and the final state  $|f\rangle$ . Ignoring the influence of non-resonant absorption,  $S_{\alpha\beta}$  can be expressed as<sup>1</sup>

$$S_{\alpha\beta} = \sum_s \left( \frac{\langle i | \mu_\alpha | s \rangle \langle s | \mu_\beta | f \rangle}{\omega_s - \omega} + \frac{\langle i | \mu_\beta | s \rangle \langle s | \mu_\alpha | f \rangle}{\omega_s - \omega} \right) \quad (1)$$

Where  $\mu_{\alpha(\beta)}$  is electric dipole moment operator,  $\alpha, \beta \in (x, y, z)$ .  $\omega$  is the fundamental frequency of the laser, the resonance condition can be assumed to be  $2\omega = \omega_f$ . The summation include all initial, intermediate and final electronic states. In the response theory, the TP matrix element can be calculated through the single residues of the quadratic response function.<sup>2</sup>

When a molecular material is excited by monochromatic polarized light, the microscopic TPA cross section ( $\delta$ ) can be expressed as<sup>1,3</sup>

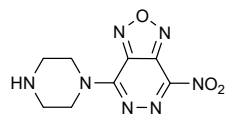
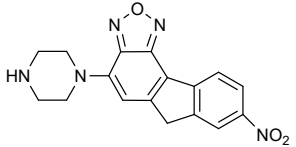
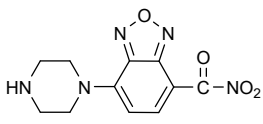
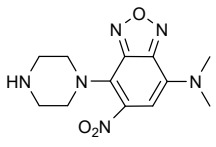
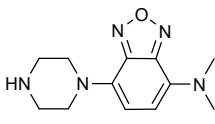
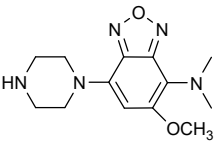
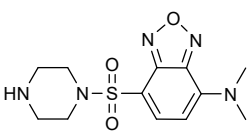
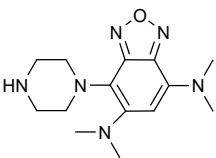
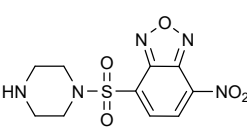
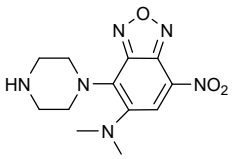
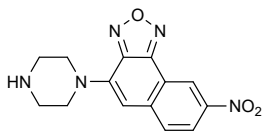
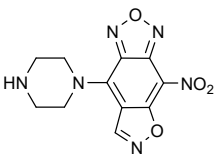
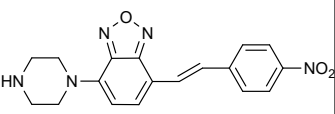
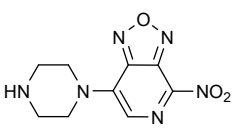
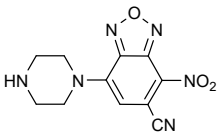
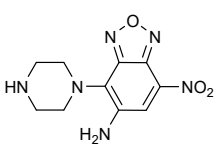
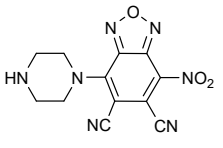
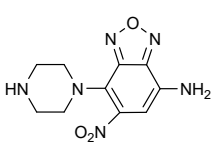
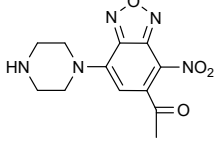
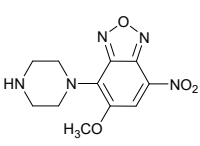
$$\delta = \sum_{\alpha\beta} (2S_{\alpha\alpha}S_{\beta\beta}^* + 4S_{\alpha\beta}S_{\alpha\beta}^*) \quad (2)$$

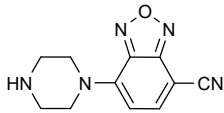
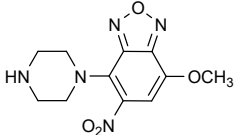
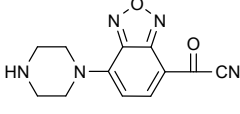
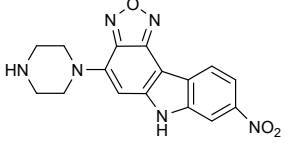
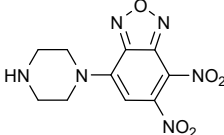
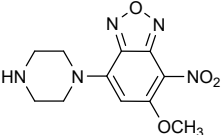
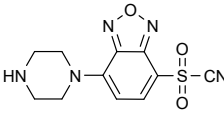
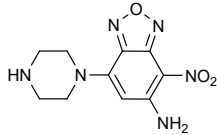
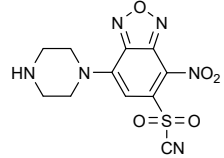
The macroscopic TPA cross section ( $\sigma$ ) can be directly compared with the experimental data. It is defined as<sup>1</sup>

$$\sigma = \frac{4\pi^2 \alpha a_0^5 \omega^2}{15c\Gamma} \delta \quad (3)$$

where  $\alpha$  is the fine structure constant,  $a_0$  is the Bohr radius,  $\omega$  is the photon energy in atomic units,  $c$  is the speed of light, and  $\Gamma$  is the broadening factor which is assumed to be 0.1 eV.<sup>4</sup>

Table S1 One-photon absorption properties of various energy acceptors.

Molecular structure	$\lambda_{op}(nm)$	$f_{op}$	Molecular structure	$\lambda_{op}(nm)$	$f_{op}$
	394	0.19		418	0.65
	399	0.58		488	0.15
	428	0.18		381	0.91
	378	0.32		442	0.15
	346	0.03		498	0.35
	385	0.60		402	0.50
	444	0.97		437	0.57
	<b>439</b>	<b>0.59</b>		<b>507</b>	<b>0.39</b>
	428	0.48		487	0.14
	413	0.59		443	0.53

	395	0.36		432	0.17
	406	0.62		389	0.67
	410	0.64		388	0.52
	389	0.46		353	0.49
	447	0.58			

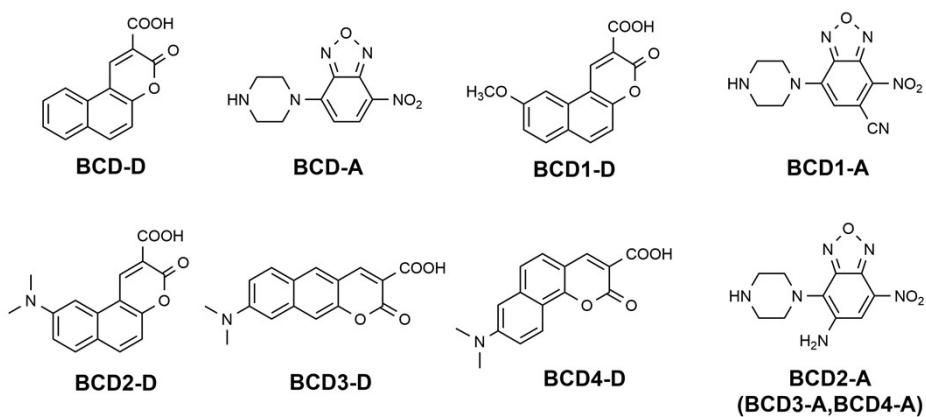


Figure S1 Chemical structures of energy donors and acceptors.

Table S2 Optimized geometries of studied molecules.

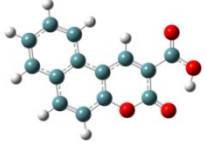
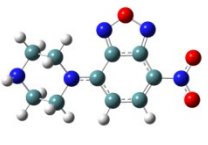
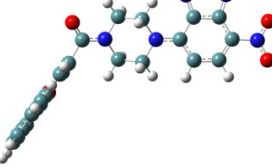
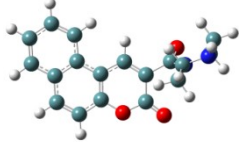
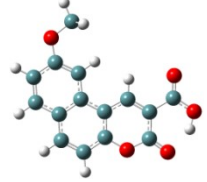
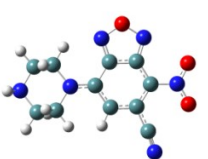
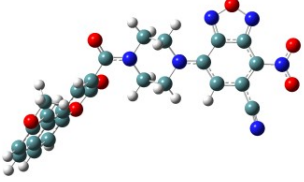
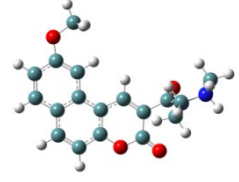
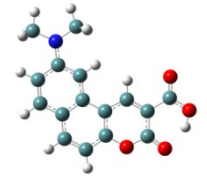
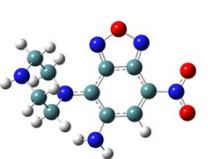
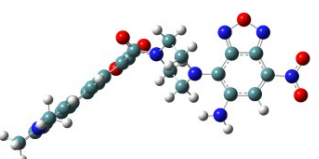
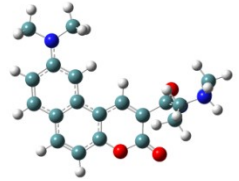
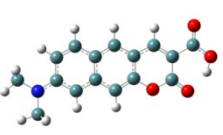
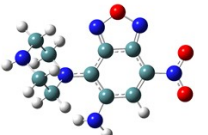
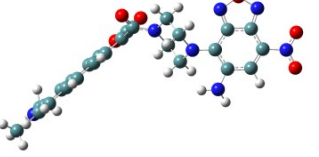
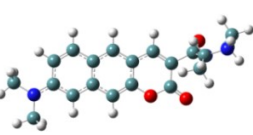
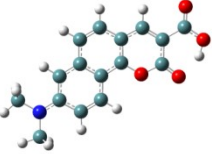
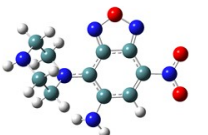
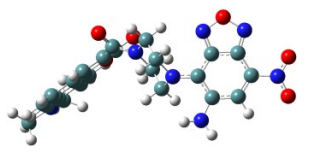
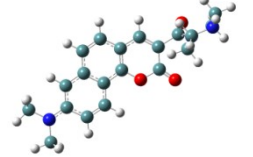
Energy donor	Energy acceptor	Probe molecule	Product molecule
 BCD-D	 BCD-A	 BCD	 BCD-H <sub>2</sub> S
 BCD1-D	 BCD1-A	 BCD1	 BCD1-H <sub>2</sub> S
 BCD2-D	 BCD2-A	 BCD2	 BCD2-H <sub>2</sub> S
 BCD3-D	 BCD3-A	 BCD3	 BCD3-H <sub>2</sub> S
 BCD4-D	 BCD4-A	 BCD4	 BCD4-H <sub>2</sub> S

Table S3 One-photon absorption and emission properties of studied molecules.

	$\lambda_{op}(nm)$	$f_{op}$	Transition	$\lambda_{em}(nm)$	$f_{em}$	Transition
BCD-D	346(360) <sup>exp</sup>	0.44	S <sub>0</sub> →S <sub>1</sub>	415(440) <sup>exp</sup>	0.67	S <sub>1</sub> →S <sub>0</sub>
BCD-A	415(490) <sup>exp</sup>	0.58	S <sub>0</sub> →S <sub>1</sub>	527(555) <sup>exp</sup>	0.65	S <sub>1</sub> →S <sub>0</sub>
BCD	405	0.67	S <sub>0</sub> →S <sub>1</sub>	477	0.72	S <sub>1</sub> →S <sub>0</sub>
	327	0.45	S <sub>0</sub> →S <sub>2</sub>			
BCD-H <sub>2</sub> S	325	0.47	S <sub>0</sub> →S <sub>1</sub>	402	0.71	S <sub>1</sub> →S <sub>0</sub>
BCD1-D	357	0.43	S <sub>0</sub> →S <sub>1</sub>	437	0.66	S <sub>1</sub> →S <sub>0</sub>
BCD1-A	439	0.59	S <sub>0</sub> →S <sub>1</sub>	587	0.62	S <sub>1</sub> →S <sub>0</sub>
BCD1	428	0.67	S <sub>0</sub> →S <sub>1</sub>	500	0.75	S <sub>1</sub> →S <sub>0</sub>
	333	0.46	S <sub>0</sub> →S <sub>2</sub>			
BCD1-H <sub>2</sub> S	330	0.49	S <sub>0</sub> →S <sub>1</sub>	414	0.75	S <sub>1</sub> →S <sub>0</sub>
BCD2-D	426	0.36	S <sub>0</sub> →S <sub>1</sub>	514	0.57	S <sub>1</sub> →S <sub>0</sub>
BCD2-A (BCD3-A, BCD4-A)	507	0.39	S <sub>0</sub> →S <sub>1</sub>	655	0.45	S <sub>1</sub> →S <sub>0</sub>
BCD2	497	0.38	S <sub>0</sub> →S <sub>1</sub>	638	0.44	S <sub>1</sub> →S <sub>0</sub>
	382	0.41	S <sub>0</sub> →S <sub>2</sub>			
BCD2-H <sub>2</sub> S	378	0.41	S <sub>0</sub> →S <sub>1</sub>	475	0.67	S <sub>1</sub> →S <sub>0</sub>
BCD3-D	410	0.83	S <sub>0</sub> →S <sub>1</sub>	489	1.19	S <sub>1</sub> →S <sub>0</sub>
BCD3	498	0.38	S <sub>0</sub> →S <sub>1</sub>	639	0.45	S <sub>1</sub> →S <sub>0</sub>
	377	0.78	S <sub>0</sub> →S <sub>2</sub>			
BCD3-H <sub>2</sub> S	375	0.77	S <sub>0</sub> →S <sub>1</sub>	463	1.20	S <sub>1</sub> →S <sub>0</sub>
BCD4-D	391	0.83	S <sub>0</sub> →S <sub>1</sub>	457	1.19	S <sub>1</sub> →S <sub>0</sub>
BCD4	491	0.41	S <sub>0</sub> →S <sub>1</sub>	639	0.44	S <sub>1</sub> →S <sub>0</sub>
	363	0.77	S <sub>0</sub> →S <sub>2</sub>			
BCD4-H <sub>2</sub> S	360	0.76	S <sub>0</sub> →S <sub>1</sub>	435	1.13	S <sub>1</sub> →S <sub>0</sub>

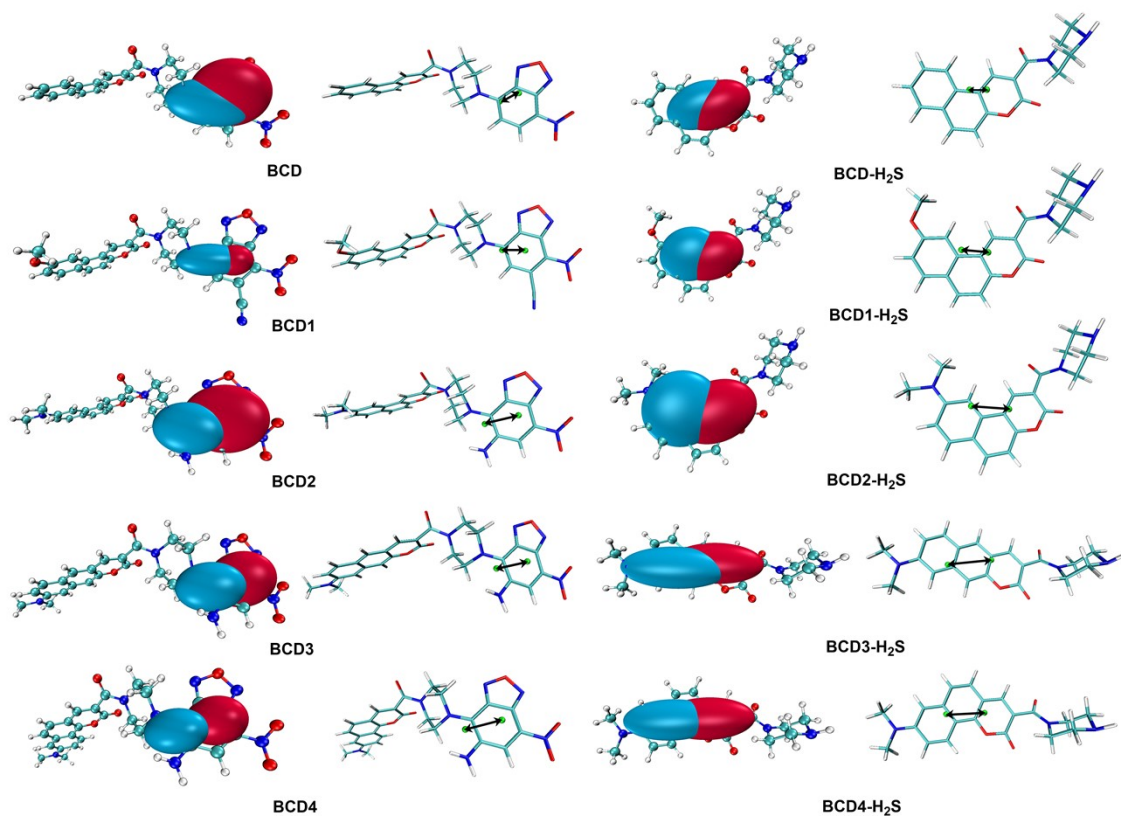


Figure S2 Contour map of the electron density difference between the ground state and the first excited state, and the barycenters of positive and negative electronic densities computed at the first excited state minimal energy structures. Blue and red indicate decrease and increase in the electron density (isocontour value 0.0007 a.u.).

Table S4 The ISC rates for spin substates.

MS	$k_{isc}^{S_1-T_1}$ (s <sup>-1</sup> )			$k_{isc}^{S_1-T_2}$ (s <sup>-1</sup> )		
	0	-1	1	0	-1	1
<b>BCD</b>	6.93×10 <sup>6</sup>	3.89×10 <sup>7</sup>	3.48×10 <sup>7</sup>	6.07×10 <sup>8</sup>	4.04×10 <sup>8</sup>	4.04×10 <sup>8</sup>
<b>BCD-H<sub>2</sub>S</b>	1.31×10 <sup>8</sup>	1.18×10 <sup>8</sup>	1.18×10 <sup>8</sup>	5.27×10 <sup>8</sup>	2.04×10 <sup>8</sup>	2.04×10 <sup>8</sup>
<b>BCD1</b>	1.11×10 <sup>6</sup>	1.55×10 <sup>7</sup>	1.55×10 <sup>7</sup>	3.09×10 <sup>7</sup>	8.43×10 <sup>7</sup>	8.45×10 <sup>7</sup>
<b>BCD1-H<sub>2</sub>S</b>	9.07×10 <sup>7</sup>	6.72×10 <sup>7</sup>	6.72×10 <sup>7</sup>	1.64×10 <sup>9</sup>	1.24×10 <sup>9</sup>	1.29×10 <sup>9</sup>
<b>BCD2</b>	7.87×10 <sup>5</sup>	2.86×10 <sup>5</sup>	3.14×10 <sup>5</sup>	4.71×10 <sup>6</sup>	2.66×10 <sup>6</sup>	2.43×10 <sup>6</sup>
<b>BCD2-H<sub>2</sub>S</b>	1.07×10 <sup>8</sup>	3.83×10 <sup>6</sup>	3.28×10 <sup>6</sup>	2.73×10 <sup>7</sup>	4.74×10 <sup>6</sup>	5.19×10 <sup>6</sup>
<b>BCD3</b>	4.98×10 <sup>4</sup>	2.43×10 <sup>5</sup>	2.36×10 <sup>5</sup>	1.89×10 <sup>6</sup>	7.43×10 <sup>6</sup>	7.51×10 <sup>6</sup>
<b>BCD3-H<sub>2</sub>S</b>	6.64×10 <sup>7</sup>	9.54×10 <sup>6</sup>	1.03×10 <sup>7</sup>	2.54×10 <sup>5</sup>	8.69×10 <sup>5</sup>	8.32×10 <sup>5</sup>
<b>BCD4</b>	4.46×10 <sup>4</sup>	3.21×10 <sup>5</sup>	3.14×10 <sup>5</sup>	1.19×10 <sup>6</sup>	4.62×10 <sup>6</sup>	4.62×10 <sup>6</sup>
<b>BCD4-H<sub>2</sub>S</b>	3.06×10 <sup>8</sup>	4.35×10 <sup>7</sup>	5.95×10 <sup>7</sup>	8.79×10 <sup>7</sup>	1.23×10 <sup>7</sup>	8.69×10 <sup>6</sup>

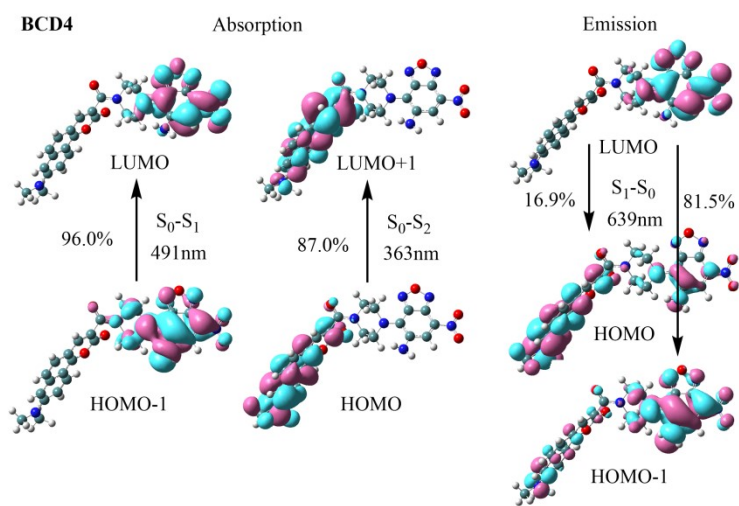


Figure S3 Absorption and emission process of **BCD4**.

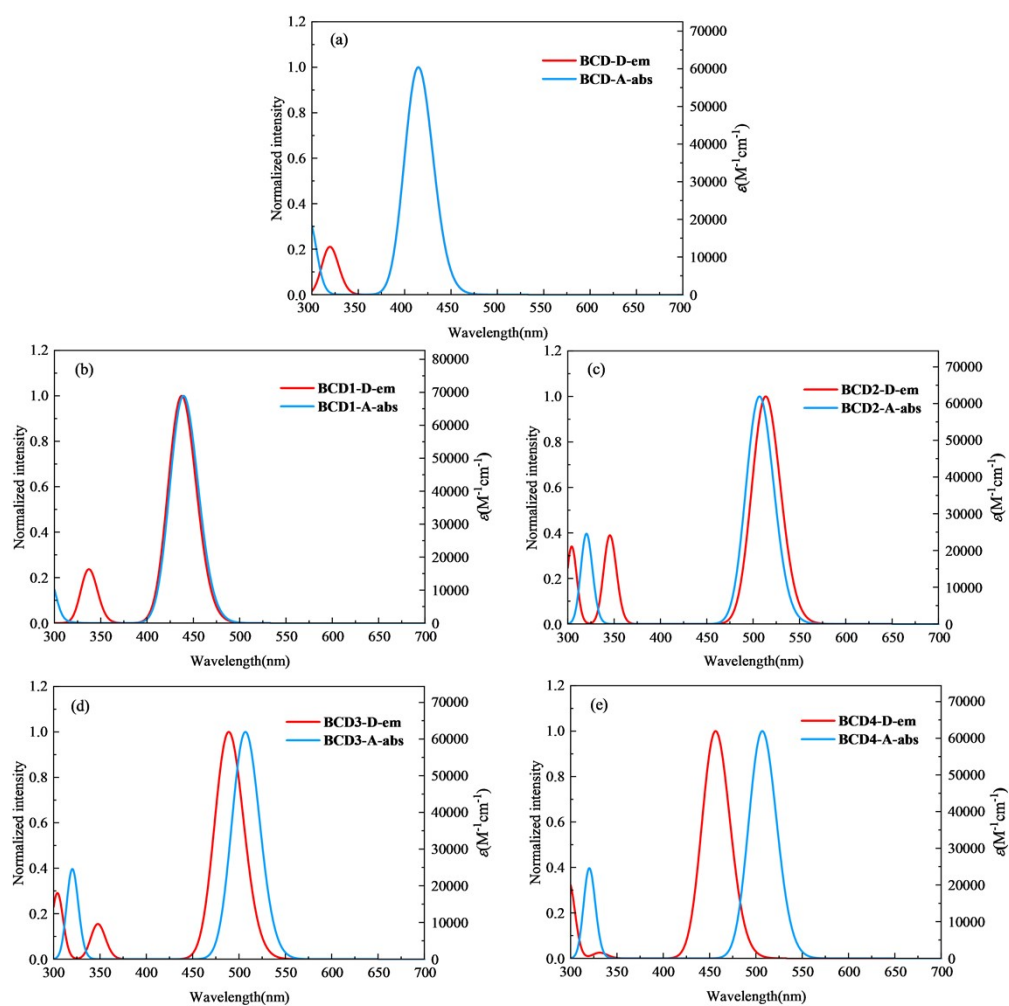


Figure S4 Spectral overlap between donor emission and acceptor absorption.



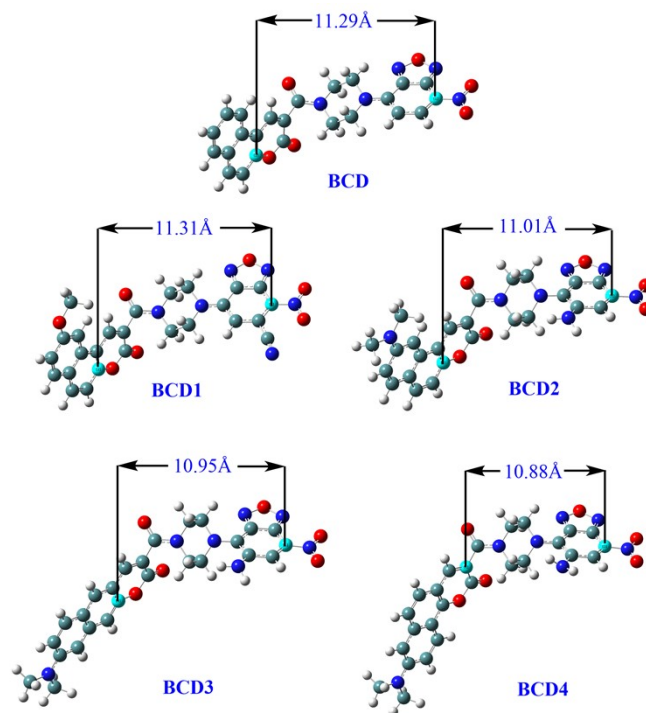


Figure S5 Distance between energy donors and acceptors.

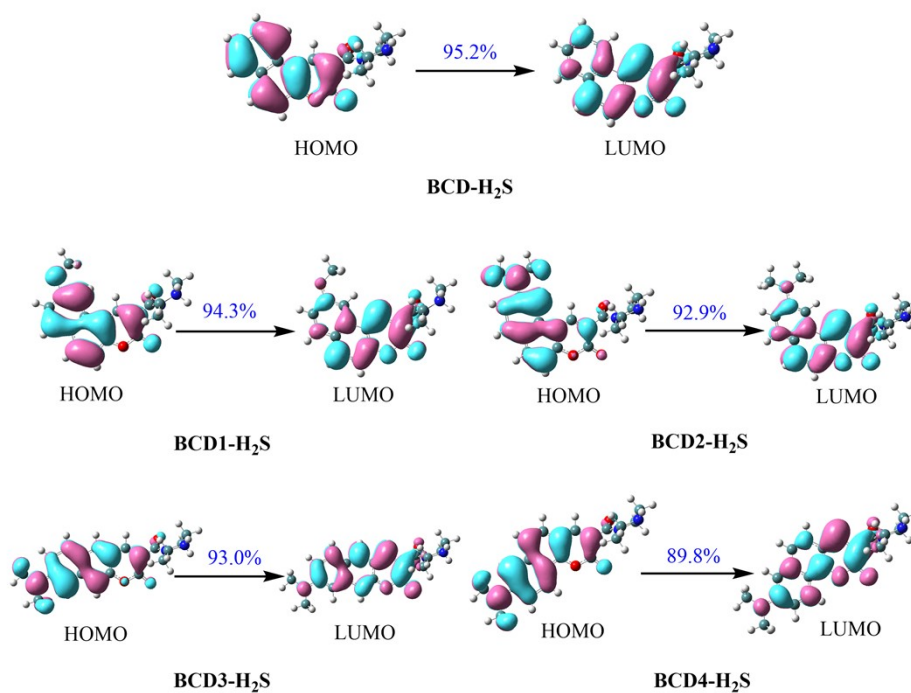


Figure S6 Molecular orbitals involved in the two-photon absorption process of product molecules.

Table S5 Two-photon absorption properties of energy donors and acceptors.

	State	$\lambda_{tp}(nm)$	$\sigma(GM)$		State	$\lambda_{tp}(nm)$	$\sigma(GM)$
BCD-D	S <sub>1</sub>	711	30	BCD-A	S <sub>1</sub>	859	35
BCD1-D	S <sub>1</sub>	730	53	BCD1-A	S <sub>1</sub>	909	46
BCD2-D	S <sub>1</sub>	862	118	BCD2-A	S <sub>1</sub>	1048	76
BCD3-D	S <sub>1</sub>	841	360	(BCD3-A,			
BCD4-D	S <sub>1</sub>	803	298	BCD4-A)			

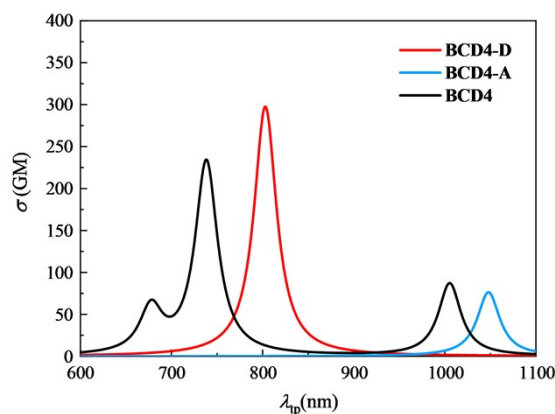


Figure S7 Two-photon absorption spectrum of **BCD4**.

Cartesian coordinates of the optimized ground state structures obtained with the PCM//CAM-B3LYP/6-31+G (d) in water solvent.

#### BCD

C	-6.51094600	2.07742300	-2.46467700
C	-5.55440600	1.26439200	-1.90278200
C	-5.66425000	0.83998100	-0.55733000
C	-6.78485500	1.27513500	0.20022400
C	-7.75396000	2.11249900	-0.40392000
C	-7.62309700	2.50816200	-1.71195400
H	-6.40759200	2.39067800	-3.49895200
H	-4.71141200	0.95139800	-2.50805800
C	-4.69248200	-0.01258400	0.07942500
C	-6.92041600	0.86428400	1.55867900
H	-8.60491400	2.43633100	0.18863900
H	-8.37013500	3.14977800	-2.16829400
C	-5.99678500	0.05728900	2.15671700
C	-4.88734200	-0.37270500	1.40113600
H	-7.78337600	1.20738900	2.12150600
H	-6.08990300	-0.26188600	3.18860900

C	-3.52033100	-0.52758100	-0.56214400
O	-4.00415500	-1.17989400	2.05353100
O	-2.16764100	-2.40678500	2.15894300
C	-2.62706000	-1.30173400	0.10012600
O	-1.66812400	-2.64522100	-1.59004100
C	-2.86977100	-1.68257700	1.47930600
N	-0.21157300	-1.59721200	-0.19905200
N	2.30332100	-0.26055500	-0.21111000
C	0.95414800	-2.24261800	-0.78676400
C	1.94445300	-1.20105000	-1.28281100
C	0.12092200	-0.66186800	0.86300600
C	1.13071100	0.38088800	0.38534500
C	-1.45611200	-1.90239900	-0.62685000
C	3.53584100	0.26809200	-0.05901200
C	4.74544200	-0.43522000	-0.47486100
C	6.06545400	0.09767600	-0.26744600
C	6.21675300	1.37197100	0.35453300
C	5.06406900	2.02275900	0.73946100
C	3.77770600	1.50438400	0.54993800
N	4.87042200	-1.61895900	-1.02186000
N	6.93836300	-0.77822200	-0.70754800
O	6.18878700	-1.82264300	-1.16645600
N	7.48759700	1.96452200	0.57055600
O	7.54758400	3.06409400	1.13051600
O	8.48744400	1.35321300	0.18661600
H	1.42636000	-2.88075900	-0.02980000
H	0.62698900	-2.86505000	-1.61766200
H	1.49303400	-0.62213300	-2.09952500
H	2.83078600	-1.69810800	-1.66172500
H	-0.77105900	-0.13567400	1.19813400
H	0.53322100	-1.21548800	1.71401000
H	1.42869200	0.96183800	1.25537000
H	0.66710100	1.05623900	-0.34545800
H	5.16063300	2.99895100	1.19997700
H	2.95130400	2.12580300	0.86162700
H	-3.32990000	-0.29603500	-1.60423700

### BCD1

C	-6.74087400	1.79810400	-1.55480400
C	-5.68888400	0.99515800	-1.16818100
C	-5.63448400	0.47862600	0.14918200
C	-6.67190100	0.79919000	1.06328300
C	-7.73843000	1.62919900	0.62895100
C	-7.77860500	2.11893600	-0.64526100
H	-4.90385900	0.76058500	-1.87287600

C	-4.56080300	-0.36537100	0.60748400
C	-6.63226700	0.29224300	2.38994100
H	-8.53100100	1.87230600	1.33070200
H	-8.59026200	2.75349800	-0.98500500
C	-5.61065200	-0.50700600	2.82237700
C	-4.58349100	-0.82433800	1.91596400
H	-7.43870500	0.55188100	3.06942700
H	-5.56976800	-0.89997200	3.83175300
C	-3.45273400	-0.77769700	-0.19819500
O	-3.59387800	-1.62777800	2.39935200
O	-1.70719700	-2.76359400	2.20502700
C	-2.45260000	-1.54676100	0.29829000
O	-1.65532600	-2.69615600	-1.60508300
C	-2.51446300	-2.03185400	1.66392700
N	-0.07775500	-1.72503800	-0.29399300
N	2.41236800	-0.34482600	-0.43397700
C	1.02587100	-2.28480900	-1.06114000
C	1.94770600	-1.17898400	-1.55285700
C	0.34872400	-0.87745800	0.80675800
C	1.29271900	0.22384200	0.32309900
C	-1.35648400	-2.03592600	-0.60577800
C	3.67673400	0.06260700	-0.25736500
C	4.82232400	-0.59527100	-0.87273600
C	6.17470100	-0.17206800	-0.63929700
C	6.45355300	0.94030300	0.20768300
C	5.34821500	1.56412900	0.78023000
C	4.02599100	1.14906600	0.56150400
N	4.85692800	-1.64466200	-1.65690200
N	6.97685400	-0.97697400	-1.29995100
O	6.15176700	-1.86795300	-1.91491000
N	7.78395900	1.37061900	0.44335500
O	7.97278900	2.32878500	1.19778900
O	8.69599500	0.76547100	-0.11952800
H	1.58318400	-2.98558700	-0.42760500
H	0.61933300	-2.82732000	-1.91282700
H	1.40440300	-0.52250600	-2.24355200
H	2.78928800	-1.61338000	-2.07985200
H	-0.51107900	-0.39664400	1.26988300
H	0.85006500	-1.48961500	1.56453700
H	1.65356200	0.74795100	1.20338400
H	0.75794800	0.93674200	-0.31522700
H	3.25600300	1.73951700	1.03239700
H	-3.39676100	-0.47234300	-1.23721300
C	5.46308100	2.71539800	1.64105400

N	5.39272100	3.63419100	2.33914200
O	-6.88038900	2.33715000	-2.79026800
C	-5.88434500	2.06651200	-3.77020500
H	-4.90769500	2.44298500	-3.44917000
H	-5.82036100	0.99326800	-3.97593600
H	-6.20152500	2.59346000	-4.66901900

**BCD2**

C	6.64986500	1.62069300	0.00403800
C	5.46586500	0.90216500	0.19890600
C	5.21825800	-0.31235800	-0.46690500
C	6.19238600	-0.83032100	-1.36471200
C	7.38839500	-0.09456100	-1.55240200
C	7.61959300	1.08356700	-0.89982300
H	4.72212400	1.29114300	0.87890600
C	4.00374600	-1.07273300	-0.28176300
C	5.96038600	-2.05144800	-2.04678200
H	8.13842400	-0.48421000	-2.23540800
H	8.54934800	1.60887700	-1.07563600
C	4.80720400	-2.76816700	-1.86908500
C	3.84263200	-2.26011300	-0.98167600
H	6.72410100	-2.41999700	-2.72596700
H	4.61909000	-3.70319500	-2.38398100
C	2.93455800	-0.69150800	0.58540000
O	2.71564900	-3.01529700	-0.83625900
O	0.73058800	-3.44969100	0.03360000
C	1.79992000	-1.42761400	0.69943800
O	1.05260900	-0.95805400	2.89008100
C	1.66980100	-2.67655700	-0.02292600
N	-0.50568000	-0.79250200	1.24595500
N	-2.68378500	0.84795700	0.45071600
C	-1.59637200	-0.54656600	2.18647700
C	-2.29109900	0.77080300	1.85437300
C	-0.91288300	-0.76051400	-0.15292500
C	-1.59043900	0.57304600	-0.47791400
C	0.74284600	-1.04077100	1.69556000
C	-4.00081300	0.84111100	0.03225200
C	-5.00848000	0.03331800	0.66638000
C	-6.37118100	-0.02701700	0.22069500
C	-6.74431400	0.76071100	-0.90839700
C	-5.79166200	1.55269100	-1.48319900
C	-4.44221300	1.63078900	-1.02835600
N	-4.87998400	-0.78632900	1.68465300
N	-7.02677300	-0.86984200	0.98238200
O	-6.10760700	-1.32531700	1.87244900

N	-8.08246000	0.75998500	-1.42751900
O	-8.33244500	1.44397900	-2.41919800
O	-8.91937200	0.07103200	-0.84945300
H	-2.31134200	-1.37360400	2.11783700
H	-1.18321200	-0.51582700	3.19337800
H	-1.60172300	1.60132400	2.05650300
H	-3.16628800	0.90317800	2.48972800
H	-0.04458200	-0.87729100	-0.79943700
H	-1.60285300	-1.58992500	-0.34569800
H	-1.97225400	0.52266500	-1.49854400
H	-0.84326300	1.37640800	-0.42012200
H	-6.08911200	2.18788400	-2.31026800
H	3.01758300	0.21439200	1.17573500
N	-3.63521100	2.58581100	-1.62144300
H	-3.80697100	2.80259200	-2.59426300
H	-2.65566300	2.59424500	-1.38134100
N	6.88714700	2.80367400	0.65040900
C	5.90414900	3.32756000	1.57950400
C	8.13872100	3.51577500	0.45569600
H	4.94321900	3.51570600	1.08451500
H	5.72931200	2.63897500	2.41645800
H	6.26358300	4.27153700	1.98681600
H	8.12559100	4.42334500	1.05770100
H	9.00294800	2.91631200	0.76731600
H	8.28056200	3.80906500	-0.59117700

**BCD3**

C	-4.55904800	-0.58524600	-1.39971700
C	-5.75693300	-0.02522000	-0.93451100
C	-3.53238600	-0.91027100	-0.52599300
C	-5.93278300	0.21885400	0.46418200
C	-4.87697700	-0.11772500	1.35140100
C	-3.72525000	-0.66132300	0.85691700
H	-4.97906900	0.05304900	2.41828900
C	-2.28398100	-1.48157900	-0.93341800
O	-2.72875600	-0.97782900	1.75266400
O	-0.73309400	-1.76191500	2.26927200
C	-1.30691800	-1.74845300	-0.03702900
O	-0.10045100	-3.56970000	-0.93993700
C	-1.53059900	-1.51181500	1.38464600
N	1.12882700	-1.76691900	-0.30880700
N	3.33267100	-0.19597900	-1.17393800
C	2.40181900	-2.42227900	-0.59890500
C	3.20677500	-1.58880500	-1.59273700
C	1.26588900	-0.39389900	0.15966200

C	2.05308700	0.43531400	-0.85757600
C	-0.03628900	-2.43129600	-0.46124500
C	4.52533600	0.36294800	-0.75339300
C	5.49280700	-0.36346100	0.02514600
C	6.71016900	0.21728300	0.51569900
C	6.97465700	1.58480800	0.20842400
C	6.07248800	2.25611200	-0.56620700
C	4.87329400	1.67428500	-1.07363700
N	5.43982900	-1.60615000	0.44735700
N	7.35926500	-0.68720600	1.20908000
O	6.57577700	-1.79536900	1.15921200
N	8.16032400	2.25147400	0.66672800
O	8.32134400	3.43651600	0.37812300
O	8.96240600	1.59905000	1.33011700
H	2.96091400	-2.53280900	0.33641000
H	2.19619200	-3.40963200	-1.00925500
H	2.69714700	-1.60042700	-2.56521500
H	4.19655600	-2.02295600	-1.73124000
H	0.28385100	0.05661600	0.29488200
H	1.78347300	-0.39435100	1.12595500
H	6.29891700	3.28037900	-0.84139100
H	-2.12658600	-1.69500400	-1.98743400
C	-8.17622400	1.11345000	0.06153800
C	-7.13862200	0.78240700	0.93257700
C	-6.82607700	0.31936400	-1.80954900
C	-7.98410700	0.86387800	-1.34198700
H	-7.23591600	0.95256500	1.99748800
H	-6.70783800	0.14078400	-2.87482000
H	-8.76921200	1.10985200	-2.04525500
H	-4.43062300	-0.76776700	-2.46348300
N	-9.34852200	1.65887700	0.50554800
C	-10.41034400	2.00824300	-0.42388500
C	-9.52973600	1.90818300	1.92303200
H	-11.24456100	2.42727000	0.13702300
H	-10.08370700	2.75938200	-1.15289700
H	-10.51759700	2.33556700	2.08905800
H	-8.78218200	2.61416200	2.30680100
H	-10.77869900	1.13175900	-0.96989400
H	-9.45590200	0.98161600	2.50604600
N	4.13345500	2.43580200	-1.96032500
H	2.22112000	1.42757600	-0.43676300
H	1.45485100	0.53749500	-1.77307600
H	3.24031900	2.07786800	-2.26275200
H	4.13952700	3.43914400	-1.83419500

**BCD4**

C	7.65798200	1.41675800	-0.22299800
C	4.60664300	-1.86499500	1.71511700
C	5.80981500	-1.22913500	1.71078400
C	5.44653800	1.09721200	-1.20554500
C	6.65804500	1.73059600	-1.19964100
H	8.07583700	0.16076700	1.48517800
C	3.61072500	-1.54745500	0.74321100
C	6.11316900	-0.22471800	0.73429500
H	4.71048900	1.35712300	-1.95843000
H	6.85573500	2.48232800	-1.95276700
C	5.13497800	0.10506700	-0.24436600
C	3.89809900	-0.57881600	-0.20514200
C	2.32898000	-2.16805500	0.68615400
O	2.98099900	-0.24913600	-1.15580400
O	1.02198200	-0.44906500	-2.15980900
C	1.40369700	-1.80907400	-0.24149900
O	0.11238000	-3.76697200	-0.52200400
C	1.73547100	-0.81758600	-1.24435700
N	-1.04896800	-1.84061000	-0.20808900
N	-3.37023900	-0.82292300	1.09287300
C	-2.34003000	-2.48586100	-0.43367700
C	-3.27079200	-2.24041800	0.75150600
C	-1.14075800	-0.42260100	0.11868200
C	-2.05764600	-0.21435800	1.32441900
C	0.09687300	-2.54397700	-0.33694300
C	-4.46928800	-0.04758600	0.79973300
C	-5.34450100	-0.30819500	-0.31595000
C	-6.46975700	0.52020000	-0.64756700
C	-6.73959900	1.65415500	0.17133500
C	-5.92702600	1.87048600	1.25263500
C	-4.83036900	1.04050000	1.59938800
N	-5.27203800	-1.26602900	-1.21199900
N	-7.04637700	0.03498300	-1.72196100
O	-6.30578000	-1.05492000	-2.05468700
N	-7.83004100	2.54095100	-0.09336300
O	-7.99973400	3.51038500	0.64753000
O	-8.55274200	2.29113400	-1.05667800
H	-2.78306100	-2.07773400	-1.34854800
H	-2.17327100	-3.55342000	-0.56810400
H	-2.87389100	-2.75748000	1.63380500
H	-4.25990600	-2.64550800	0.54423400
H	-0.15413200	-0.03080600	0.36136300
H	-1.52619300	0.12500500	-0.74923100



H	-2.16718400	0.85257600	1.51220700
H	-1.60346100	-0.67726300	2.20913500
H	-6.15680200	2.71162200	1.89751200
H	2.08921500	-2.94329300	1.40927700
H	4.38333200	-2.62477200	2.45812300
H	6.56265700	-1.47589900	2.45337200
C	7.35392400	0.43606900	0.72641700
C	9.86936700	1.72159500	0.75320800
C	9.15770700	3.06827800	-1.24108700
H	10.75484400	2.33381000	0.58820200
H	9.51163400	1.90722100	1.77362600
H	10.16434300	0.66707000	0.68013700
H	10.15845600	3.46016300	-1.06482300
H	9.13219900	2.64989200	-2.25465400
H	8.45473000	3.90833200	-1.19515600
N	-4.10269700	1.35707500	2.74550900
H	-3.71121100	0.55034800	3.22163500
H	-4.59687900	1.95148100	3.40054200
N	8.86210200	2.06348600	-0.23349800

**BCD-H<sub>2</sub>S**

C	-4.06892200	-2.66781900	0.20370100
C	-2.89480600	-1.96314600	0.33184900
C	-2.84951700	-0.57479900	0.06020000
C	-4.04613900	0.07351300	-0.34883000
C	-5.24044200	-0.67736500	-0.47295100
C	-5.25569800	-2.02315500	-0.20266400
H	-4.08110600	-3.73207700	0.41767200
H	-2.00053200	-2.48909900	0.64587500
C	-1.64728600	0.21065400	0.17939700
C	-4.03096900	1.47121500	-0.62931900
H	-6.14635000	-0.16656800	-0.78692500
H	-6.17495400	-2.59194300	-0.30001600
C	-2.88962600	2.20997800	-0.51400400
C	-1.70517900	1.56262500	-0.10760700
H	-4.95525100	1.94873100	-0.94069000
H	-2.86600700	3.27345900	-0.72348400
C	-0.37279200	-0.30936400	0.57850600
O	-0.60174900	2.35659400	-0.00712800
O	1.53500000	2.70713200	0.44000100
C	0.72833000	0.47601700	0.64504700
O	2.07793300	-0.48913800	2.32356300
C	0.63092700	1.89672700	0.36550300
C	2.03263100	-0.07226600	1.15917800
N	3.09031300	-0.09392000	0.32567800

N	5.05757900	-1.02185500	-1.47142000
C	4.40527400	-0.50844000	0.81584400
C	5.01188700	-1.55193100	-0.11156700
C	3.07325800	0.33779400	-1.07135700
C	3.71306300	-0.72638000	-1.95532300
H	5.51174600	-1.68697800	-2.09078700
H	4.28587600	-0.90111200	1.82393200
H	5.05527800	0.37494500	0.85329900
H	4.41508600	-2.47819300	-0.04848700
H	6.02838600	-1.78003900	0.22071600
H	3.77309400	-0.34812200	-2.97952700
H	3.06751700	-1.62167100	-1.95811200
H	3.62648500	1.28008100	-1.15896200
H	2.04653200	0.50803500	-1.39188000
H	-0.27447600	-1.35886700	0.83245900

**BCD1-H<sub>2</sub>S**

C	-4.06036700	1.64605600	0.08641300
C	-2.78898400	1.15136100	-0.11163100
C	-2.53176200	-0.23346700	0.03879100
C	-3.59617400	-1.10131800	0.39744200
C	-4.89174500	-0.55493000	0.59418800
C	-5.12501700	0.78210100	0.44392300
H	-1.98637900	1.82247700	-0.38235400
C	-1.22439600	-0.80452100	-0.15833900
C	-3.35691900	-2.49300500	0.55393900
H	-5.70431000	-1.22158100	0.86824900
H	-6.11207900	1.20741200	0.59181600
C	-2.11455700	-3.03179600	0.36570400
C	-1.06112900	-2.17080200	0.00928300
H	-4.18797700	-3.13552400	0.82955600
H	-1.91922100	-4.09178800	0.48088900
C	-0.05749000	-0.05695100	-0.52072500
O	0.15363100	-2.76397400	-0.17069100
O	2.30779900	-2.72908300	-0.66533200
C	1.15363200	-0.64624800	-0.66497100
O	2.29423700	0.66987400	-2.25879500
C	1.28870400	-2.08247500	-0.51135200
C	2.34197800	0.14741600	-1.13775800
N	3.40231500	0.26330400	-0.31492500
N	5.23915400	1.33069700	1.54225500
C	4.62380500	0.92355400	-0.77656500
C	5.07945300	1.96436700	0.23642900
C	3.48549400	-0.28661800	1.03744800
C	3.96928100	0.78382400	2.00869000

H	5.59706200	2.00230800	2.21536800
H	4.42096800	1.37990400	-1.74362000
H	5.40412600	0.16185500	-0.89995300
H	4.34281500	2.78584100	0.26272700
H	6.03937400	2.37969700	-0.08257100
H	4.11125200	0.33127400	2.99395600
H	3.19096800	1.56143800	2.09779600
H	4.18222600	-1.13289400	1.03517100
H	2.50602600	-0.64543600	1.34982800
H	-0.13095700	1.01269400	-0.68333100
O	-4.40367400	2.95115000	-0.03577200
C	-3.39819900	3.89137600	-0.39500900
H	-2.97324800	3.65382500	-1.37561600
H	-3.89713400	4.85861100	-0.43730000
H	-2.60338500	3.92058300	0.35738200

### BCD2-H<sub>2</sub>S

C	3.96712800	-1.12010200	0.04493100
C	2.63978600	-0.71903500	-0.13644700
C	2.24286300	0.62200900	0.02042500
C	3.20992500	1.60112200	0.37961700
C	4.54985000	1.18156800	0.56734700
C	4.92518900	-0.12300800	0.41041900
H	1.89993000	-1.45903400	-0.40451200
C	0.87931300	1.06119500	-0.16599300
C	2.82963900	2.95709600	0.54471900
H	5.29400100	1.92320000	0.84492300
H	5.96107500	-0.39475900	0.56665100
C	1.53611300	3.36886600	0.36614800
C	0.57742700	2.40373400	0.01073200
H	3.59250200	3.68021800	0.81949400
H	1.23335600	4.40247000	0.48797700
C	-0.20546900	0.20322600	-0.52631000
O	-0.69441100	2.86751300	-0.16075400
O	-2.83628400	2.61718200	-0.64641800
C	-1.47495700	0.66268200	-0.66003400
O	-2.45714400	-0.79440000	-2.23723500
C	-1.75595100	2.07464800	-0.49949300
C	-2.57094200	-0.25468900	-1.12860600
N	-3.62623000	-0.46132700	-0.31614300
N	-5.34445100	-1.71073300	1.54183300
C	-4.76801500	-1.25152500	-0.77708100
C	-5.11167800	-2.33052900	0.24021400
C	-3.77602500	0.08595300	1.03119300
C	-4.14425700	-1.02438000	2.00854000

H	-5.62815700	-2.41393900	2.21806000
H	-4.51488200	-1.68783700	-1.74152900
H	-5.62564400	-0.57888100	-0.90497900
H	-4.28994000	-3.06661400	0.27360200
H	-6.01945900	-2.84987700	-0.07912500
H	-4.33934200	-0.58359000	2.99008900
H	-3.28566600	-1.71123900	2.10612000
H	-4.56130100	0.85065300	1.01917200
H	-2.84367200	0.55238900	1.34493500
H	-0.02250300	-0.85196500	-0.69685900
N	4.35361000	-2.42348000	-0.12023100
C	3.36216100	-3.43388500	-0.43680800
C	5.72195100	-2.82899000	0.15340000
H	2.85199800	-3.21052500	-1.38144800
H	3.85574100	-4.39904700	-0.54242900
H	2.60194500	-3.52174600	0.35108500
H	5.81795000	-3.89702800	-0.03745400
H	6.43497700	-2.30821200	-0.49571000
H	6.00500500	-2.64396600	1.19751000

**BCD3-H<sub>2</sub>S**

C	1.26353800	-1.41145400	-0.54467500
C	2.59064300	-1.03944900	-0.28711300
C	0.24388400	-0.47195500	-0.55187800
C	2.90758000	0.33054800	-0.02504000
C	1.85779900	1.28572600	-0.03564300
C	0.57803300	0.88158500	-0.29186900
H	2.06525900	2.33353800	0.15643800
C	-1.13169700	-0.78319400	-0.80408900
O	-0.40843900	1.84173700	-0.30015000
O	-2.49881300	2.50250200	-0.53865300
C	-2.08688300	0.17318500	-0.76957300
O	-3.76706400	-0.55130100	-2.26437700
C	-1.72225100	1.56560100	-0.53375500
N	-4.45802900	0.01185500	-0.17304700
N	-6.33842400	-0.55369700	1.85387100
C	-5.87194600	-0.16746000	-0.50299900
C	-6.54103500	-1.08633800	0.50938300
C	-4.20704700	0.43651600	1.20317400
C	-4.91645200	-0.49726800	2.17681000
C	-3.51403300	-0.14563200	-1.12229100
H	-6.35943400	0.81579600	-0.48740600
H	-5.93867700	-0.57760100	-1.50893400
H	-6.12550300	-2.10303000	0.40061000
H	-7.61289900	-1.13368400	0.29822400

H	-3.13646500	0.42446200	1.40169900
H	-4.57411800	1.46143900	1.33243900
H	-4.79202600	-0.11250200	3.19280600
H	-4.44047200	-1.49192100	2.12646900
H	-1.40253100	-1.81345500	-1.01972900
C	5.27546700	-0.23179000	0.24429500
C	4.24347400	0.70558300	0.23291100
C	3.65730700	-1.98244100	-0.27699600
C	4.94206800	-1.60465200	-0.02545800
H	4.44541400	1.75223900	0.42301600
H	3.43348000	-3.02674400	-0.47709400
H	5.72003500	-2.35712400	-0.03092600
H	1.02831700	-2.45415500	-0.74208300
N	6.57176100	0.12050400	0.50391200
C	7.64266300	-0.85900100	0.41768500
C	6.90197300	1.51665700	0.71895000
H	8.58577000	-0.37113600	0.66029900
H	7.49841700	-1.67869200	1.13007500
H	7.96723400	1.60572200	0.92741700
H	6.35339400	1.92693400	1.57489800
H	-6.82745100	-1.12799600	2.53456400
H	7.73066300	-1.28532200	-0.58960000
H	6.67045700	2.13049500	-0.16187300

**BCD4-H<sub>2</sub>S**

C	-0.99897200	2.49565500	0.23840000
C	-2.34007500	2.34198700	0.41244200
C	-0.18404600	1.39302500	-0.15761000
C	-2.97310300	1.07316300	0.20450600
C	-2.17896400	-0.03808300	-0.19242700
C	-0.78966500	0.16412000	-0.36261100
C	1.22592400	1.47645400	-0.35486100
O	-0.05241600	-0.91398500	-0.74784100
O	1.83852400	-1.90898900	-1.31430200
C	1.96159800	0.38996600	-0.70372800
O	3.78970100	1.27407700	-1.90933900
C	1.30466100	-0.87839000	-0.94544900
C	3.43095100	0.52049200	-0.99443000
N	4.29991600	-0.17918800	-0.23753900
N	6.21611300	-0.78047600	1.74580700
C	5.72693400	-0.17585000	-0.55990100
C	6.54981700	0.15673900	0.67681700
C	3.94044000	-1.02232200	0.90136500
C	4.80620100	-0.67147800	2.10597700
H	6.79768300	-0.60341200	2.55987100

H	5.89683900	0.55177500	-1.35128200
H	6.00141100	-1.17254200	-0.92834200
H	6.35279500	1.20304700	0.96774400
H	7.61277400	0.06585300	0.43674900
H	4.58622900	-1.37063100	2.91753400
H	4.54363000	0.34448300	2.44853800
H	4.08813700	-2.07330600	0.62696800
H	2.89129600	-0.87424500	1.15202700
H	1.71832900	2.43528200	-0.21471200
C	-4.35790400	0.90869400	0.38427300
C	-2.81552100	-1.28635900	-0.39675800
C	-4.16334800	-1.42969000	-0.21768000
C	-4.98337300	-0.32540100	0.18246600
H	-4.93291200	1.77534800	0.68589500
H	-2.22214200	-2.14192200	-0.70024300
H	-4.60995100	-2.40139100	-0.38420500
H	-0.52575300	3.45989900	0.39825300
H	-2.95353600	3.18567900	0.71410900
N	-6.32930200	-0.49069100	0.35658100
C	-6.95604800	-1.78092200	0.12322300
C	-7.14559200	0.63997900	0.75671100
H	-7.10277700	1.45037200	0.01785900
H	-8.18230300	0.31907100	0.84859400
H	-6.82631500	1.04317900	1.72587300
H	-6.55709300	-2.55378000	0.79094100
H	-8.02469800	-1.69322500	0.31400100
H	-6.82470100	-2.11654200	-0.91260600

Cartesian coordinates of the optimized excited state structures obtained with the PCM//CAM-B3LYP/6-31+G (d) in water solvent.

### BCD

C	-6.87171300	1.18663700	-2.67039100
C	-5.81227600	0.61743800	-2.00285900
C	-5.79277000	0.56284700	-0.58915300
C	-6.89161700	1.11188300	0.12475800
C	-7.96841300	1.69231900	-0.58847600
C	-7.96239300	1.73041600	-1.96081000
H	-6.86700000	1.21716000	-3.75554300
H	-4.98909200	0.20909600	-2.57781400
C	-4.71068900	-0.02455800	0.16005200
C	-6.89761300	1.07188500	1.54993900
H	-8.80118200	2.10733200	-0.02783400
H	-8.79155100	2.17635400	-2.50079800
C	-5.87037700	0.51425400	2.25426800

C	-4.78337800	-0.03126100	1.54212500
H	-7.74579300	1.49792800	2.07747900
H	-5.86549000	0.47726900	3.33772000
C	-3.54718700	-0.61678600	-0.42488000
O	-3.79384400	-0.57980600	2.30078800
O	-1.86482300	-1.62706800	2.56228400
C	-2.54654800	-1.12874900	0.33366100
O	-1.62415000	-2.75187200	-1.11096900
C	-2.66376800	-1.14820000	1.78054900
N	-0.13386400	-1.41604300	-0.03972000
N	2.28734400	-0.03583400	-0.56636400
C	1.01170900	-2.14189600	-0.56605900
C	1.91551900	-1.20161000	-1.36396000
C	0.21547200	-0.24100300	0.73793900
C	1.12687800	0.69609100	-0.07126300
C	-1.39298400	-1.82774000	-0.32761900
C	3.56391400	0.36489700	-0.35189100
C	4.69125800	-0.52081900	-0.43860900
C	6.03144700	-0.05915200	-0.20160400
C	6.25684800	1.32049700	0.11278000
C	5.15342600	2.19116700	0.18664800
C	3.86929700	1.73037500	-0.03877900
N	4.72741800	-1.81480800	-0.66991400
N	6.85940400	-1.06811400	-0.29657100
O	6.06346500	-2.15865400	-0.59316300
N	7.55673900	1.81624700	0.35263700
O	7.68218700	3.02501000	0.63156700
O	8.51699000	1.03157100	0.27847300
H	1.57531500	-2.57895900	0.26587800
H	0.65395800	-2.94154600	-1.21201600
H	1.36878000	-0.83223600	-2.24229700
H	2.80334900	-1.72888900	-1.69883300
H	-0.67852500	0.31886100	1.00588600
H	0.72383500	-0.54540400	1.65855300
H	1.43501400	1.50973700	0.58041800
H	0.57240700	1.10790500	-0.92326900
H	5.32509700	3.23494900	0.40819900
H	3.06758800	2.45585500	-0.02257500
H	-3.44882800	-0.66257200	-1.50366400
<b>BCD1</b>			
C	6.87090700	1.37749800	1.71747300
C	5.76930400	0.70101000	1.23746800
C	5.64788500	0.43054300	-0.14695800
C	6.66981600	0.86466000	-1.03094400

C	7.78842900	1.55926500	-0.50027900
C	7.89283900	1.81217000	0.83752100
H	4.99718200	0.37644300	1.92047600
C	4.52071800	-0.27271000	-0.70456900
C	6.56430800	0.60251100	-2.42313300
H	8.56866500	1.89027400	-1.17947000
H	8.74434200	2.34187900	1.25143500
C	5.49345100	-0.06580200	-2.94934100
C	4.48154100	-0.49576800	-2.07335000
H	7.36038500	0.94546900	-3.07744200
H	5.40332900	-0.27229800	-4.00955200
C	3.41882400	-0.77093000	0.05676300
O	3.44153900	-1.16162200	-2.64937800
O	1.51472900	-2.24140500	-2.58701400
C	2.36503000	-1.39692500	-0.52616000
O	1.59484400	-2.73066700	1.26297400
C	2.36541300	-1.64343200	-1.95620900
N	-0.00833400	-1.65444500	0.07041600
N	-2.36004500	-0.17529700	0.62483300
C	-1.08490100	-2.26839600	0.82964200
C	-1.89338900	-1.19237100	1.56250700
C	-0.44405400	-0.61741600	-0.84447600
C	-1.26285200	0.45482400	-0.09984700
C	1.28391900	-1.97836400	0.33749500
C	-3.65978800	0.14046600	0.42369700
C	-4.75136400	-0.74397300	0.75799200
C	-6.11665800	-0.37769100	0.50546000
C	-6.43807000	0.89329400	-0.06960000
C	-5.36622600	1.77446500	-0.38340000
C	-4.04071000	1.39059100	-0.12552100
N	-4.72442900	-1.95463600	1.24889000
N	-6.89245500	-1.37442900	0.85572400
O	-6.03733800	-2.34699700	1.32191600
N	-7.77778800	1.24383800	-0.31954600
O	-8.00205800	2.35649100	-0.83246400
O	-8.67008400	0.43571800	-0.02233700
H	-1.74093600	-2.82178200	0.14897600
H	-0.65654500	-2.95880100	1.55386700
H	-1.24409400	-0.68685700	2.28884600
H	-2.73022600	-1.63926000	2.08929100
H	0.41115800	-0.12065200	-1.29762600
H	-1.05395200	-1.05595000	-1.64055400
H	-1.63688800	1.16264300	-0.83504700
H	-0.62065100	0.98220500	0.61437400



H	-3.27620900	2.12806300	-0.32609900
H	3.40738200	-0.65083400	1.13424700
C	-5.52902000	3.07805700	-0.93855500
N	-5.48860700	4.15036600	-1.37956500
O	7.07630700	1.68088900	3.02132900
C	6.10194400	1.28178200	3.97843100
H	5.13429500	1.74921100	3.76923000
H	5.99328700	0.19252000	3.99460900
H	6.47378600	1.62655200	4.94231800

## BCD2

C	6.70551700	1.57369800	-0.14362800
C	5.50791900	0.89780500	0.11126500
C	5.24446800	-0.37291000	-0.43171100
C	6.21736100	-0.99562400	-1.26163100
C	7.42934300	-0.30441700	-1.50709200
C	7.67573600	0.92925600	-0.97364300
H	4.76538900	1.36468800	0.74161500
C	4.01505800	-1.09057100	-0.18347300
C	5.96956200	-2.27512000	-1.81951800
H	8.17993000	-0.77508700	-2.13630200
H	8.61826800	1.41613900	-1.18752600
C	4.80194700	-2.95086300	-1.58368100
C	3.83894300	-2.34008000	-0.76230300
H	6.73288100	-2.72344400	-2.44932300
H	4.60216800	-3.92974400	-2.00391800
C	2.94693900	-0.60775400	0.63096600
O	2.69821500	-3.05777200	-0.55271300
O	0.70001900	-3.37232900	0.33731100
C	1.79707300	-1.30925100	0.80626600
O	1.06301500	-0.54311000	2.91641900
C	1.65122000	-2.62260000	0.21200500
N	-0.51584200	-0.63847800	1.28847000
N	-2.72223600	0.86754100	0.32504900
C	-1.59366000	-0.27927000	2.20181700
C	-2.29541100	0.98807700	1.71895300
C	-0.93249200	-0.76606100	-0.09814200
C	-1.61892300	0.52039800	-0.57637700
C	0.74649500	-0.80058400	1.75075800
C	-4.02909300	0.83624800	-0.05459300
C	-5.06162800	0.26292000	0.75961500
C	-6.41398800	0.10693600	0.29563500
C	-6.75935600	0.57766200	-1.01804900
C	-5.79137600	1.20827400	-1.78801900
C	-4.47634600	1.40762000	-1.30007200

N	-4.96002700	-0.27163500	1.95403400
N	-7.10938200	-0.51632400	1.21118700
O	-6.21690000	-0.74184500	2.24902900
N	-8.06003300	0.42252800	-1.52352900
O	-8.30778200	0.83933900	-2.67622600
O	-8.92117900	-0.12705200	-0.80780800
H	-2.31318400	-1.10380800	2.24958500
H	-1.17205800	-0.11672500	3.19223600
H	-1.59582300	1.83247100	1.76653300
H	-3.15194200	1.21211900	2.35011600
H	-0.07007300	-0.94340300	-0.73846600
H	-1.61944400	-1.61314000	-0.19910000
H	-1.99631000	0.36345100	-1.58559700
H	-0.88984700	1.33911300	-0.58980900
H	-6.06511500	1.60404100	-2.75666100
H	3.04098200	0.35002400	1.13090000
N	-3.63477400	2.18220300	-2.01290900
H	-3.96431500	2.65497800	-2.84443400
H	-2.78285500	2.54462900	-1.60681100
N	6.95499000	2.81585200	0.37605700
C	5.99370500	3.42582100	1.27530400
C	8.24796600	3.45086500	0.18271700
H	5.02070200	3.55792000	0.78775300
H	5.84419100	2.82609000	2.18344600
H	6.35564800	4.40933100	1.57204800
H	8.23781200	4.42557600	0.66871600
H	9.06587200	2.86202400	0.61772200
H	8.46325900	3.61025900	-0.87954700

### BCD3

C	-4.62985400	-0.74559500	-1.33250500
C	-5.83160800	-0.15729600	-0.91662300
C	-3.57870800	-0.93222300	-0.44668500
C	-5.98614100	0.26225200	0.44279400
C	-4.90542700	0.06670600	1.34259100
C	-3.75098200	-0.51187200	0.89713200
H	-4.99179600	0.37112700	2.38068800
C	-2.32798300	-1.52740700	-0.80360200
O	-2.73070500	-0.69116100	1.80336300
O	-0.71467400	-1.37430800	2.37824300
C	-1.32602300	-1.65759000	0.09763900
O	-0.13031700	-3.53133800	-0.70280200
C	-1.52900200	-1.24821000	1.48288300
N	1.11760500	-1.72113500	-0.14079800
N	3.36979100	-0.26330800	-1.06904200

C	2.37622000	-2.41790600	-0.37458200
C	3.20416500	-1.67377800	-1.41965200
C	1.27373100	-0.32107700	0.21671600
C	2.09133800	0.42087800	-0.84909900
C	-0.06077000	-2.37409300	-0.27709100
C	4.57188200	0.28879600	-0.74847300
C	5.60908400	-0.44004500	-0.07675400
C	6.81903200	0.18639900	0.38374300
C	7.01978000	1.58698600	0.12951100
C	6.06196300	2.28956600	-0.58917400
C	4.90133700	1.65004100	-1.08958400
N	5.61444100	-1.69761800	0.29906900
N	7.53688600	-0.69602400	1.02908700
O	6.80184000	-1.87101900	0.96840900
N	8.17433500	2.24585000	0.58103000
O	8.29710400	3.46788900	0.34584900
O	9.03552100	1.59081100	1.20149400
H	2.93434500	-2.47661700	0.56610800
H	2.15753900	-3.42599300	-0.72231500
H	2.68314200	-1.70376500	-2.38533500
H	4.17819500	-2.14231200	-1.53702100
H	0.30093600	0.16253800	0.28954400
H	1.77361800	-0.24391700	1.18845500
H	6.23654300	3.33180200	-0.81917600
H	-2.18648600	-1.87576500	-1.82321200
C	-8.25983900	1.04331500	-0.02089400
C	-7.19636900	0.85362300	0.86159500
C	-6.92665000	0.04516700	-1.80422700
C	-8.08924700	0.61769200	-1.38444900
H	-7.27737100	1.15790000	1.89756400
H	-6.82455200	-0.26746300	-2.83983800
H	-8.89445400	0.75156600	-2.09518100
H	-4.51712800	-1.06172100	-2.36628600
N	-9.43668200	1.61375300	0.37563000
C	-10.52966000	1.80439500	-0.56395300
C	-9.59429900	2.04641200	1.75140400
H	-11.36640600	2.26516000	-0.04089800
H	-10.24542800	2.46425100	-1.39229500
H	-10.58694200	2.47515200	1.88151000
H	-8.85362700	2.81022600	2.02004800
H	-10.87765100	0.85252900	-0.98188800
H	-9.48962800	1.20746800	2.45080100
N	4.10434800	2.33124300	-1.93653700
H	2.26755800	1.44086500	-0.51094600

H	1.52608300	0.44682200	-1.78830400
H	3.40954900	1.85843200	-2.49842700
H	4.37292800	3.25458000	-2.25107600
<b>BCD4</b>			
C	7.71943300	1.39090200	-0.24238500
C	4.63249800	-1.80401100	1.78212700
C	5.83997100	-1.17720200	1.76472500
C	5.51338000	1.05314900	-1.23075300
C	6.72886900	1.67863500	-1.23661100
H	8.11648000	0.18939400	1.50956600
C	3.64549700	-1.51195300	0.79287900
C	6.15701700	-0.20786500	0.75724500
H	4.78462100	1.29253700	-1.99740100
H	6.93722800	2.40364100	-2.01270900
C	5.18810100	0.09567800	-0.23928900
C	3.94663100	-0.57808600	-0.18640900
C	2.36062500	-2.12357700	0.74786000
O	3.03914100	-0.27615000	-1.15471300
O	1.08956300	-0.50029900	-2.17115300
C	1.44213000	-1.78878500	-0.19729100
O	0.14399000	-3.75713400	-0.33001800
C	1.78987900	-0.83868700	-1.23436300
N	-1.01439500	-1.80759300	-0.24439400
N	-3.35497400	-0.72267700	0.94453600
C	-2.29650700	-2.47129500	-0.44606300
C	-3.24056600	-2.16267400	0.71372600
C	-1.11661700	-0.37594300	-0.01508300
C	-2.05464800	-0.08113800	1.16301200
C	0.13544000	-2.52362400	-0.26467500
C	-4.50379100	-0.02232400	0.73904100
C	-5.45411300	-0.36641600	-0.27920000
C	-6.59115500	0.45969100	-0.58449200
C	-6.81070700	1.65584800	0.18200800
C	-5.94770000	1.95940400	1.22616000
C	-4.86395100	1.10919100	1.55631900
N	-5.42377400	-1.37211100	-1.12206300
N	-7.23099800	-0.05462700	-1.60249100
O	-6.51997200	-1.19932300	-1.93246000
N	-7.89002900	2.50751300	-0.10140800
O	-8.03342200	3.54212100	0.58608800
O	-8.66571300	2.20423500	-1.02981800
H	-2.73884200	-2.12129800	-1.38513300
H	-2.12670600	-3.54460300	-0.51140700
H	-2.84023800	-2.60258600	1.63628700

H	-4.22382000	-2.58706100	0.52610100
H	-0.13935500	0.03976300	0.22440000
H	-1.49046200	0.11629500	-0.91943100
H	-2.17970600	0.99700700	1.25043400
H	-1.61035400	-0.46667700	2.08835800
H	-6.14187200	2.83295800	1.83368300
H	2.10942700	-2.87284600	1.49395000
H	4.39842000	-2.53689400	2.54841000
H	6.58620500	-1.40422300	2.52011700
C	7.40190600	0.44390700	0.73676300
C	9.92496800	1.71393200	0.74087600
C	9.23635400	3.00073900	-1.30053200
H	10.81564600	2.31466400	0.56235500
H	9.56061600	1.93587500	1.75163100
H	10.21342200	0.65576000	0.70517100
H	10.23814500	3.39199700	-1.12900200
H	9.21557400	2.55150900	-2.30084600
H	8.53801600	3.84573600	-1.28534700
N	-4.17357600	1.35508000	2.68728700
H	-3.55459400	0.66198700	3.08525700
H	-4.47265300	2.09273100	3.31175100
N	8.92752500	2.02895200	-0.26477900

### **BCD-H<sub>2</sub>S**

C	4.28491600	-2.59086100	0.08669500
C	3.06146700	-1.93759200	-0.10379500
C	2.95192600	-0.54949100	0.01349100
C	4.12020200	0.20578300	0.33526200
C	5.34081400	-0.47354000	0.52520800
C	5.42364900	-1.85708100	0.40193800
H	4.33603900	-3.66979000	-0.01261000
H	2.19190000	-2.53632700	-0.34724500
C	1.68547500	0.14137700	-0.18176300
C	4.04458100	1.61110400	0.45885600
H	6.22778200	0.10288400	0.77152900
H	6.37468000	-2.35712300	0.55202700
C	2.83594600	2.28538700	0.26184600
C	1.69752200	1.57830000	-0.05097600
H	4.93987000	2.17281100	0.70597100
H	2.77942400	3.36501700	0.34642900
C	0.47305400	-0.47630200	-0.46941500
O	0.56318200	2.30225600	-0.26250300
O	-1.58745400	2.49553100	-0.71498600
C	-0.71857300	0.28050500	-0.56898800
O	-1.87270100	-1.28928400	-1.86459600

C	-0.67289100	1.70621900	-0.52375900
C	-1.96071500	-0.42882500	-0.96745100
N	-3.13475300	-0.14254800	-0.35916900
N	-5.31763400	-0.63407600	1.36686400
C	-4.38423400	-0.69693100	-0.87719800
C	-5.11025900	-1.48934900	0.20133400
C	-3.28757500	0.63185900	0.86958600
C	-4.03984600	-0.18841700	1.91302600
H	-5.84431600	-1.13363800	2.07785700
H	-4.15121000	-1.32497900	-1.73499200
H	-5.01898700	0.13602200	-1.20642400
H	-4.51742000	-2.38735100	0.44737200
H	-6.08061600	-1.81743300	-0.18210100
H	-4.22235200	0.43656000	2.79197100
H	-3.40456500	-1.03658800	2.22285400
H	-3.83508100	1.55473500	0.64833100
H	-2.30593400	0.89816600	1.25685500
H	0.40053900	-1.54748900	-0.59837500

#### BCD1-H<sub>2</sub>S

C	-4.23079900	1.56151800	0.16875100
C	-2.91057300	1.09846800	-0.03495800
C	-2.61416000	-0.25682900	0.04226800
C	-3.65640900	-1.18810800	0.33304200
C	-4.97695400	-0.68610400	0.53418500
C	-5.26412900	0.65129600	0.45504700
H	-2.13106500	1.81454700	-0.25157300
C	-1.24789100	-0.74356400	-0.16859200
C	-3.37581900	-2.55459600	0.41593100
H	-5.76997000	-1.39423000	0.75530500
H	-6.26892200	1.02876300	0.60812900
C	-2.06617700	-3.03098400	0.20742200
C	-1.04667900	-2.15460700	-0.07625600
H	-4.17232100	-3.25646900	0.63998700
H	-1.85030400	-4.09237900	0.26373500
C	-0.14706700	0.06171000	-0.43799200
O	0.19468500	-2.69667900	-0.29682500
O	2.34756800	-2.55340000	-0.75985500
C	1.14669600	-0.50232900	-0.55996400
O	2.02928500	1.27810000	-1.80206700
C	1.31992000	-1.91876900	-0.54715200
C	2.25720600	0.40296300	-0.94324300
N	3.47332000	0.27846700	-0.35908300
N	5.57159600	1.06412700	1.36483800
C	4.61432800	1.03486700	-0.87008900

C	5.21902700	1.90473400	0.22359500
C	3.76047100	-0.49345500	0.84623800
C	4.38585300	0.40785500	1.90678200
H	6.01935100	1.62334500	2.08547700
H	4.27642800	1.64016200	-1.70911300
H	5.36912200	0.32104800	-1.22533400
H	4.49475900	2.69136600	0.49780000
H	6.12124700	2.39175500	-0.15746400
H	4.67440100	-0.20280300	2.76726900
H	3.62844600	1.13712600	2.24399900
H	4.44430100	-1.31229400	0.59681700
H	2.83775000	-0.92214500	1.23217800
H	-0.23688400	1.13440400	-0.54090300
O	-4.57813600	2.84708300	0.10734900
C	-3.59717700	3.84958400	-0.17771400
H	-3.15032400	3.68121800	-1.16092800
H	-4.13991100	4.79262300	-0.17494400
H	-2.82574500	3.86307400	0.59665000

#### BCD2-H<sub>2</sub>S

C	4.09900500	-1.07519000	0.11997900
C	2.73332900	-0.69228600	-0.06364900
C	2.32031600	0.62612400	0.02520800
C	3.28004500	1.64752400	0.31097500
C	4.64467600	1.24910400	0.49443800
C	5.05159600	-0.04683900	0.40573300
H	2.00724400	-1.46100100	-0.27898500
C	0.91527600	0.98651800	-0.16944500
C	2.88401300	2.98386200	0.40327300
H	5.37577300	2.02223300	0.71275100
H	6.09479500	-0.29012200	0.55357500
C	1.53564000	3.33216200	0.20892500
C	0.59375500	2.36074300	-0.06927500
H	3.61680300	3.75314400	0.62127900
H	1.21840200	4.36798900	0.27114600
C	-0.11599800	0.08670200	-0.43368300
O	-0.69850600	2.79014300	-0.27003600
O	-2.83231900	2.46941900	-0.73360900
C	-1.45333100	0.52777200	-0.55294400
O	-2.17642900	-1.35327500	-1.76742100
C	-1.75233800	1.92041100	-0.52772200
C	-2.47549000	-0.47538800	-0.93234900
N	-3.70840300	-0.44098500	-0.36230400
N	-5.72452000	-1.42258200	1.36332300
C	-4.77876300	-1.29335800	-0.87284200

C	-5.29902800	-2.22147900	0.21651800
C	-4.06559800	0.29822800	0.84382400
C	-4.60376700	-0.65886800	1.90365200
H	-6.11321800	-2.02513500	2.08335800
H	-4.39242300	-1.86097800	-1.71714000
H	-5.59746100	-0.64862100	-1.21924700
H	-4.50476300	-2.93958000	0.48527700
H	-6.15400900	-2.78755600	-0.16458800
H	-4.94662800	-0.07981800	2.76625500
H	-3.78133600	-1.31540900	2.23845300
H	-4.82349700	1.05029500	0.59713100
H	-3.18761300	0.81142700	1.22995900
H	0.06993200	-0.97369400	-0.54040200
N	4.46542700	-2.36560000	0.02550800
C	3.48668000	-3.41103500	-0.25942700
C	5.86120000	-2.75043900	0.21062000
H	3.00781300	-3.24447000	-1.22915100
H	3.99577300	-4.37127200	-0.28712900
H	2.71780200	-3.44908200	0.51837400
H	5.95164700	-3.82662500	0.08596500
H	6.50052600	-2.25890900	-0.52902100
H	6.20763600	-2.48456100	1.21413600

### BCD3-H<sub>2</sub>S

C	1.37579100	-1.57730200	-0.12821400
C	2.67896500	-1.12460500	-0.00224300
C	0.28374900	-0.67767300	-0.34365300
C	2.95491700	0.28327600	-0.08749700
C	1.86097600	1.19172500	-0.30564700
C	0.58875700	0.71581100	-0.42772600
H	2.04869800	2.25805300	-0.37744800
C	-1.05485800	-1.05696900	-0.47348000
O	-0.40800400	1.62221300	-0.64746300
O	-2.50637400	2.21889100	-1.02284500
C	-2.07514800	-0.10186700	-0.63831700
O	-3.62297800	-1.55175600	-1.65688900
C	-1.75297200	1.27766200	-0.77689900
N	-4.50283100	-0.00408500	-0.24729000
N	-6.58561900	0.14631100	1.65909100
C	-5.87428200	-0.35102600	-0.61233100
C	-6.64304600	-0.85834600	0.60012600
C	-4.40296000	0.92145400	0.87681900
C	-5.20414000	0.39169300	2.06229500
C	-3.45790100	-0.59223200	-0.87948100
H	-6.36573300	0.55012200	-1.00222400



H	-5.84035000	-1.10407900	-1.39732200
H	-6.21115500	-1.82219600	0.92114900
H	-7.68721100	-1.02965200	0.32284100
H	-3.35936300	1.03454000	1.16319200
H	-4.78526600	1.90205300	0.57211600
H	-5.19064700	1.13678500	2.86315800
H	-4.71591900	-0.52407000	2.43960200
H	-1.32289100	-2.10719200	-0.43275000
C	5.35467300	-0.14017500	0.24943700
C	4.25172500	0.74857500	0.03583700
C	3.79585100	-1.99935900	0.21431300
C	5.07615600	-1.53819400	0.33571100
H	4.42510300	1.81479000	-0.03311900
H	3.60639000	-3.06681500	0.28264000
H	5.87886500	-2.24499100	0.49752400
H	1.16332000	-2.64051400	-0.06326200
N	6.61026200	0.34076700	0.36271200
C	7.72615300	-0.56951900	0.58252200
C	6.88192800	1.77143200	0.27105100
H	8.64677900	0.00529400	0.65052300
H	7.59515300	-1.13008100	1.51435500
H	7.95186900	1.93355800	0.37886400
H	6.36724700	2.32159300	1.06536800
H	-7.13233300	-0.15858900	2.45955400
H	7.81887300	-1.28064900	-0.24550300
H	6.56872500	2.17014800	-0.69901100

#### **BCD4-H<sub>2</sub>S**

C	-1.10260000	2.54802000	0.39034200
C	-2.43762800	2.34760700	0.53243100
C	-0.23138000	1.49173900	-0.03582200
C	-3.03256600	1.06144000	0.25693000
C	-2.18405700	-0.01257900	-0.18019600
C	-0.82693100	0.22241300	-0.31608600
C	1.14872400	1.63344200	-0.17320400
O	-0.05090200	-0.81883100	-0.76609800
O	1.88110900	-1.72582300	-1.32414800
C	1.94633400	0.52303000	-0.52964300
O	3.75863300	1.78457300	-1.33243000
C	1.33584100	-0.71746100	-0.88588000
C	3.39732800	0.74623000	-0.74379400
N	4.30013500	-0.15887300	-0.28890400
N	6.33938600	-1.10732200	1.42557300
C	5.70623900	-0.04898700	-0.66978500
C	6.59550200	0.04318200	0.56270300

C	4.02138700	-1.23386700	0.65785200
C	4.94751100	-1.12091400	1.86510800
H	6.95781900	-1.08388500	2.23149600
H	5.82210700	0.82949900	-1.30175600
H	5.97838600	-0.94303200	-1.24656200
H	6.39618000	0.99869900	1.07835700
H	7.64513500	0.03584500	0.25484600
H	4.78579700	-1.98223500	2.51986600
H	4.68476000	-0.20891500	2.42953800
H	4.16476500	-2.20034100	0.16177200
H	2.98635100	-1.16833000	0.98746900
H	1.62193000	2.58927100	0.01883500
C	-4.39201800	0.85401300	0.40325000
C	-2.79904100	-1.28037000	-0.45785800
C	-4.14121400	-1.47184900	-0.31050700
C	-4.99438100	-0.40990600	0.12773700
H	-5.00415400	1.68351900	0.73416900
H	-2.17331400	-2.10050900	-0.79066000
H	-4.55881400	-2.44538100	-0.53034300
H	-0.66443200	3.51859500	0.60215200
H	-3.08362200	3.15712100	0.85858400
N	-6.32654500	-0.59143900	0.27594000
C	-6.92996800	-1.88366000	-0.01790800
C	-7.18298700	0.49723000	0.72855900
H	-7.14827500	1.34239400	0.03267100
H	-8.20898500	0.14015300	0.78334700
H	-6.88499700	0.84560000	1.72328700
H	-6.51515500	-2.66741100	0.62552500
H	-8.00147100	-1.82380400	0.15916100
H	-6.76614600	-2.16529800	-1.06398400

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