



Supporting Information

for

Novel route to enhance the thermo-optical performance of bicyclic diene photoswitches for solar thermal batteries

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Beilstein J. Org. Chem. **2024**, *20*, 1053–1068. [doi:10.3762/bjoc.20.93](https://doi.org/10.3762/bjoc.20.93)

Additional tables, figures and Cartesian coordinates

S1. Optimized geometries of the transition states along the displacement vectors.

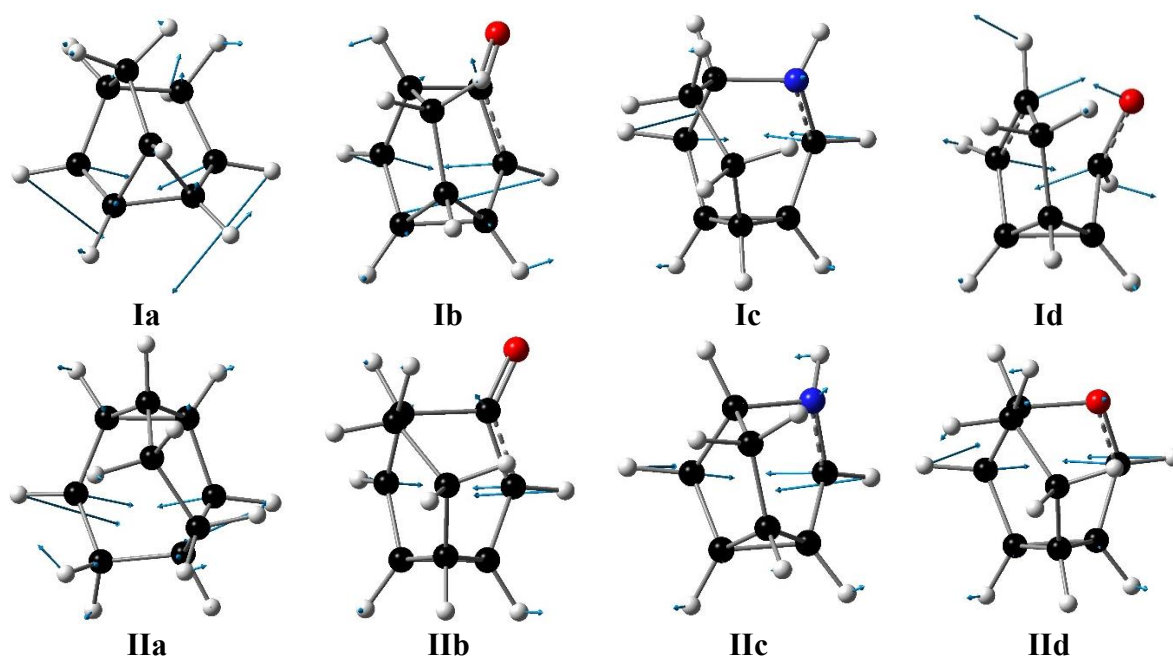


Figure S1: Optimized geometries of TS involved in the back isomerization of the photoproducts to the parent bicyclic dienes illustrating the displacement vectors at the PBE/6-311++G** level of theory (TS for type Id photoswitch is associated with the thermal degradation to carbonyl compound).

S2. Solar energy conversion efficiencies and the reality check for the energy storage efficiencies of the studied BBD-based photoswitches in gas phase.

Table S1: The calculated energy of the photon involved for the first important electronic excitation (with oscillatory strength higher than 0.01), sum of storage energy (SE) and the TBR barrier, and the solar energy conversion efficiency of the studied BBD-based photoswitches.

System	E_{photon} (kJ/mol)	SE + TBR barrier (kJ/mol)	$\eta_{\text{efficiency}}$
Ia	562.15	290.79	10.06
Ib	483.97	248.29	7.78
Ic	479.18	313.57	10.08
IIa	579.08	293.49	9.36
IIb	507.19	280.26	7.99
IIc	475.43	305.76	10.31
IIId	497.66	282.86	8.89

S3. Effect of solvation on the thermochemical properties

Table S2: Effect of solvation on the thermochemical properties of the studied BBD-based photoswitches. The energy storage capacities were calculated at DLPNO-CCSD(T)/Def2TZVP level for the geometries optimized with the M062X/6-311++G**. The TBR barrier were calculated at (8,8)-CASPT2/6-311++G** level for the geometries optimized with the PBE/6-311++G** (SMD solvation model).

Medium	Ia	Ic	IIa	IIc
	Storage energy (kJ/mol)			
Gas	141.15	158.38	156.35	165.74
Cyclohexane	143.57	158.61	158.95	167.31
Toluene	143.96	158.60	159.35	167.49
Dichloromethane	145.72	158.56	161.05	168.32
Ethanol	146.14	158.81	161.46	168.88
Acetonitrile	146.22	158.57	161.55	168.72
	ESD (MJ/kg)			
Gas	1.33	1.48	1.30	1.37
Cyclohexane	1.35	1.48	1.32	1.38
Toluene	1.36	1.48	1.33	1.38
Dichloromethane	1.37	1.48	1.34	1.39
Ethanol	1.38	1.48	1.34	1.39
Acetonitrile	1.38	1.48	1.35	1.39
	TBR barrier (kJ/mol)			
Gas	149.64	155.19	137.14	140.02
Cyclohexane	148.27	160.99	137.44	139.83
Toluene	148.17	153.44	137.23	139.83
Dichloromethane	145.26	162.67	137.05	139.89
Ethanol	145.93	139.14	135.82	139.81
Acetonitrile	146.12	136.36	137.50	139.70

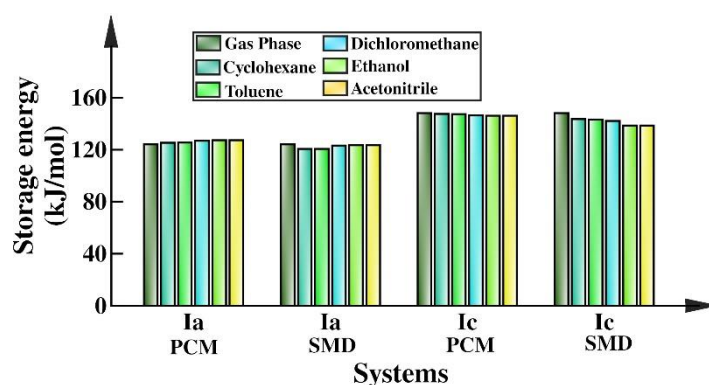


Figure S2: Effect of solvation model on storage energies of type Ia and Ic photoswitches in different polarity solvents calculated at the M062X/6-311++G** level of theory

S4. Effect of solvation on the photophysical properties of the studied BBD-based photoswitches

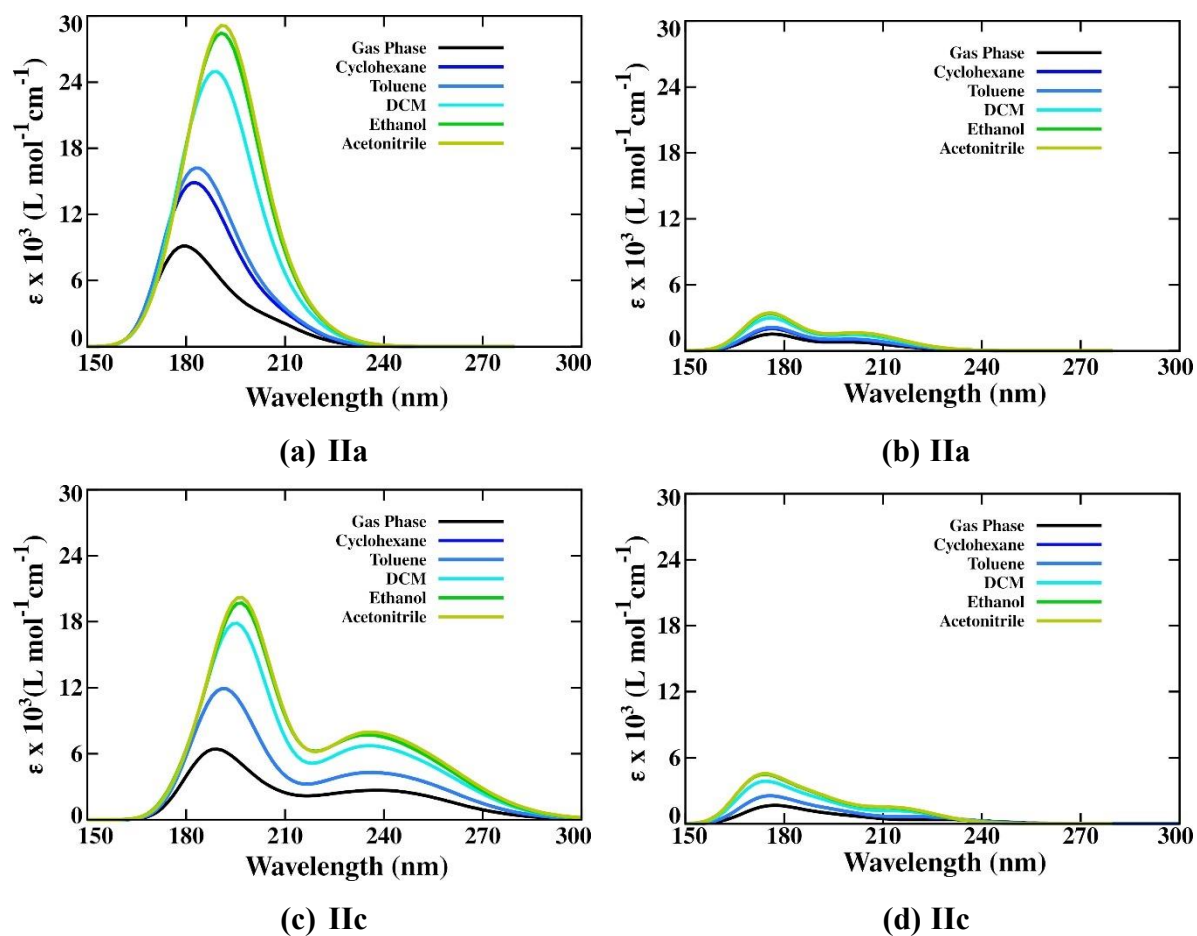


Figure S3: Effect of different polarity solvents on the optical absorption spectra of dienes and photoproducts of IIa and IIc photoswitches (M062X/6-311++G**).

Table S3: Spectral data for the optical absorption of the diene and photoproducts of Ia and Ic photoswitches in the presence of different polarity solvents (M062X/6-311++G** considering SMD solvation model).

Systems	Medium	λ_{onset}	f	λ (nm)	ϵ	λ_{onset}	f	λ	ϵ
		(nm)			(Lmol ⁻¹ cm ⁻¹)	(nm)		(nm)	(Lmol ⁻¹ cm ⁻¹)
		Diene				Photoproduct			
Ia	Gas	241.12	0.029	212.80	2151.00	216.48	0.010	185.09	1377.58
	Cyclohexane	244.72	0.022	217.36	2481.97	218.40	0.013	184.90	1812.15
	Toluene	245.44	0.026	217.68	2631.70	218.72	0.010	193.87	1198.71
	Dichloromethane	250.40	0.044	219.75	3758.86	220.00	0.015	194.01	1579.31
	Ethanol	252.00	0.050	220.51	4228.76	220.64	0.017	194.07	1751.84
	Acetonitrile	252.00	0.051	220.64	4380.79	220.96	0.018	194.17	1790.76
Ic	Gas	295.60	0.043	249.65	2375.97	251.20	0.011	177.38	1669.30
	Cyclohexane	299.00	0.061	250.45	3608.89	247.60	0.014	224.13	609.59
	Toluene	299.50	0.061	250.52	3620.59	247.60	0.014	224.08	609.70
	Dichloromethane	303.50	0.023	262.01	3659.86	244.00	0.024	218.04	1105.17
	Ethanol	303.50	0.034	260.50	4404.56	242.20	0.030	215.68	1398.38
	Acetonitrile	305.00	0.034	261.16	4784.67	242.92	0.031	216.08	1425.70

Table S4: Spectral data for the optical absorption of the diene and photoproducts of IIa and IIc photoswitches in the presence of different polarity solvents (M062X/6-311++G** considering SMD solvation model).

Systems	Medium	λ_{onset}	f	λ (nm)	ϵ	λ_{onset}	f	λ	ϵ
		(nm)			(Lmol ⁻¹ cm ⁻¹)	(nm)		(nm)	(Lmol ⁻¹ cm ⁻¹)
		Diene				Photoproduct			
IIa	Gas	233.92	0.022	206.58	2697.24	229.96	0.010	172.85	1376.49
	Cyclohexane	236.08	0.031	208.27	3564.67	232.12	0.013	204.69	951.39
	Toluene	236.80	0.034	208.56	3833.06	232.48	0.013	204.81	1008.82
	Dichloromethane	240.04	0.057	210.62	6334.85	234.28	0.020	205.20	1383.39
	Ethanol	241.12	0.062	211.16	7580.02	235.00	0.023	205.36	1546.73
	Acetonitrile	241.48	0.063	211.30	7982.72	235.00	0.024	205.39	1578.63
IIc	Gas	292.20	0.029	251.62	2162.12	247.40	0.013	202.79	1292.60
	Cyclohexane	296.20	0.042	252.51	2994.26	247.60	0.016	200.60	1758.85
	Toluene	297.40	0.045	252.57	3211.26	247.60	0.016	200.05	1877.45
	Dichloromethane	302.50	0.066	252.98	4787.90	246.00	0.014	222.39	913.87
	Ethanol	303.00	0.014	263.95	3286.29	245.20	0.019	220.07	1273.94
	Acetonitrile	304.50	0.014	264.66	3444.76	245.60	0.020	220.24	1283.45

CARTESIAN COORDINATES

Ia-R₁

C	-1.65384700	0.30952200	-0.36945100
C	-0.86544900	1.35879000	-0.13630600
C	0.55044300	1.13653100	0.37408700
H	0.97655600	2.04517700	0.79899500
C	1.36368600	0.53603700	-0.77272200
C	1.19356200	-0.78466400	-0.78795500
C	0.26307400	-1.19946400	0.34095100
H	0.47589600	-2.19208500	0.74137300
C	0.51102700	-0.05891200	1.34469000
H	1.89579400	1.12486900	-1.50960800
H	1.56900000	-1.46648400	-1.54159300
H	1.47713500	-0.18845000	1.83629600
H	-0.27525200	0.03593200	2.09611700
H	-1.21216600	2.36828000	-0.33139800
H	-2.65939100	0.45705300	-0.75210100
C	-1.20441100	-1.11625000	-0.13954100
H	-1.33464800	-1.69103800	-1.06446200
H	-1.86143100	-1.58279700	0.60386800

Ia-P₁

C	-0.53969300	-1.20081000	-0.27611800
C	0.88156100	-0.83572200	-0.74300900
C	1.23518100	0.60099400	-0.42303900
H	2.17410200	0.94163200	-0.84271400
C	1.28845800	-0.42165500	0.66665200
C	-0.19618800	-0.51626800	1.07260100
C	-0.96097300	0.74578500	0.50384400
H	-1.61290100	1.30409500	1.17434400
C	0.12366800	1.59879100	-0.15916700
H	2.16401900	-0.67820900	1.24605500
H	-0.49576500	-0.93063100	2.03075100
H	0.49097300	2.37544900	0.51855600
H	-0.24906200	2.08417000	-1.06511200
H	1.45852600	-1.38726200	-1.47387700
H	-0.75566600	-2.26705300	-0.33022400
C	-1.63780200	-0.16334100	-0.55425200
H	-2.61033300	-0.52736000	-0.21627700
H	-1.72916500	0.23853400	-1.56658100

Ib-R₁

C	-0.83172800	1.34779900	-0.28197800
C	0.47054300	1.63343500	-0.17476200
C	1.45256600	0.56189000	0.25971500
H	2.40039300	0.99489300	0.57777300
C	1.58664200	-0.47191700	-0.86574500
C	0.60851400	-1.36530000	-0.76140300
C	-0.26750000	-1.03603600	0.44518200
H	-0.75948000	-1.89435400	0.90053600
C	0.74948800	-0.29380600	1.33453800
H	2.32497700	-0.40858500	-1.65423600
H	0.39110100	-2.17079900	-1.45003200
H	1.44445700	-1.00697700	1.78090000
H	0.28787300	0.31021000	2.11707700
H	0.83939700	2.62659400	-0.41288900
H	-1.57013600	2.07375800	-0.60238100
C	-1.33278200	-0.02888400	0.00214400
O	-2.49663000	-0.32597800	-0.12536200

Ib-P₁

C	-0.34223600	-1.20636700	-0.05625500
C	0.95525600	-0.88121900	-0.83722800
C	1.39550300	0.55574500	-0.65946800
H	2.22123800	0.85265500	-1.29448400
C	1.67212500	-0.43328400	0.42503600
C	0.31469400	-0.46851700	1.15881600
C	-0.51962300	0.80754400	0.75173100
H	-1.01134000	1.40868300	1.51424800
C	0.38769200	1.59573100	-0.21170100

Ia-TS

C	0.64726900	1.45624500	-0.10263600
C	-0.81347000	1.15146300	-0.21558100
C	-1.18890800	-0.28735700	-0.76710100
H	-2.05519000	-0.35711500	-1.43394800
C	-1.29023100	0.13880600	0.72508300
C	-0.06771200	-0.46287800	1.37215800
C	0.88725700	-0.89689900	0.28701300
H	1.55158500	-1.72374900	0.57525200
C	-0.04832600	-1.26658500	-0.91261200
H	-2.24740500	0.22600600	1.24469100
H	-0.16457200	-1.05751000	2.28636100
H	-0.42145200	-2.29582500	-0.78910200
H	0.45717700	-1.20350400	-1.89140300
H	-1.48004600	1.95526000	-0.53773900
H	0.95702200	-2.42272100	-0.52426900
C	1.66616600	0.36740000	-0.12579200
H	2.45714100	0.53860100	0.61958100
H	2.19346500	0.29394800	-1.11260700

Ia-P₂

C	1.64982300	-0.32722400	0.48076900
C	0.63039000	-1.06482000	-0.31162000
C	-0.80886900	-1.15328900	0.12588400
H	-1.28956000	-2.12192300	0.09426900
C	-0.44885700	-0.42514100	-1.16076400
C	-0.79224100	1.00352600	-0.90458200
C	-1.25350300	1.18908800	0.33050900
H	-1.51394100	2.14814900	0.76147400
C	-1.32102600	-0.10397300	1.11011600
H	-0.64398900	-0.85901200	-2.13343000
H	-0.65152900	1.78469800	-1.64177200
H	-2.34091900	-0.32535900	1.43738000
H	-0.69908200	-0.05227100	2.01209100
H	1.00469700	-1.99882600	-0.72246900
H	1.94579400	-0.80643900	1.41306400
C	2.22198300	0.81841500	0.13165700
H	1.94726300	1.32511300	-0.78714700
H	2.97506600	1.28637200	0.75471700

Ib-TS

C	-0.52377500	-1.25650600	-0.33774200
C	0.98758400	-1.13320500	-0.47256000
C	1.59595500	0.27108200	-0.59100800
H	2.56584600	0.33872300	-1.08718400
C	1.48870500	-0.44287500	0.75368000
C	0.16834300	0.06685100	1.31301600
C	-0.43749400	1.04394500	0.39160000
H	-1.06370400	1.84086400	0.80425700
C	0.63627300	1.44310900	-0.63306300
H	2.32608500	-0.74977600	1.38234100
H	-0.20534200	-0.13972100	2.31662100
H	1.15070500	2.36638200	-0.31808800
H	0.20579900	1.61927600	-1.63132400
H	1.53270800	-1.96259800	-0.92473600
H	-0.99143300	-2.21051600	-0.61163600
C	-1.36897800	-0.12104400	-0.16644000
O	-2.60004100	-0.04134700	-0.18439400

Ib-P₂

C	1.05844100	1.05904500	-0.53794600
C	-0.14834300	1.33928600	0.29203400
C	-1.51256500	0.81435600	-0.08510700
H	-2.34609900	1.50116700	-0.02342100
C	-0.82824700	0.30873100	1.17154500
C	-0.52992500	-1.12881300	0.90405600
C	-0.91596200	-1.49012400	-0.31874500
H	-0.75144900	-2.46523500	-0.76083800
C	-1.57978700	-0.35404200	-1.06297400

H	2.64678500	-0.69687100	0.80883000
H	0.21960800	-0.84832200	2.17041600
H	0.89801000	2.40727600	0.31402300
H	-0.18390000	2.02824200	-1.03606300
H	1.32918000	-1.47649600	-1.65856500
H	-0.61929700	-2.25842600	-0.04089300
C	-1.40155300	-0.12273300	-0.08325800
O	-2.53393000	-0.06226800	-0.46294400

Ic_R1

C	-1.62877900	0.15117700	-0.34387200
C	-0.94317800	1.28487500	-0.13012100
C	0.49073800	1.16324000	0.36264400
H	0.87887900	2.09871800	0.76291900
C	1.27429900	0.59367800	-0.81317300
C	1.18343200	-0.73923100	-0.81268700
C	0.30609400	-1.17030400	0.35202000
H	0.50851800	-2.16204600	0.75540000
C	0.54193300	-0.02250500	1.34364500
H	1.70752800	1.20259800	-1.59785200
H	1.52531000	-1.40472200	-1.59614900
H	1.53072200	-0.11980900	1.79311400
H	-0.22388300	0.02642000	2.11793700
H	-1.39300100	2.24581500	-0.33760300
H	-2.63591100	0.15195300	-0.74421500
N	-1.11436500	-1.10609600	-0.04021700
H	-1.44484700	-1.86183900	-0.62276900

Ic-P1

C	-0.54660200	-1.16248100	-0.28332200
C	0.88335000	-0.82574100	-0.73433900
C	1.23123800	0.60710700	-0.39879400
H	2.17375900	0.95282800	-0.80515200
C	1.27046900	-0.42095000	0.68715900
C	-0.21784800	-0.51610600	1.07628300
C	-0.98140700	0.71496300	0.44872300
H	-1.72079500	1.24715500	1.04616300
C	0.10317600	1.59531900	-0.16031300
H	2.13570600	-0.68779600	1.27598600
H	-0.54104600	-0.92679200	2.02863300
H	0.43436400	2.36690700	0.54157500
H	-0.26403500	2.06756500	-1.07236800
H	1.46068900	-1.37607400	-1.46507200
H	-0.82848500	-2.20867200	-0.39621200
N	-1.54808100	-0.13183300	-0.65540500
H	-2.46784800	-0.46496000	-0.37810400

Id-R1

C	-1.60763500	0.05407000	-0.37589100
C	-0.99334500	1.21980600	-0.15349200
C	0.42866400	1.17574400	0.37862400
H	0.75611600	2.12640900	0.79559100
C	1.28321900	0.64064800	-0.76631800
C	1.22233300	-0.69204000	-0.78643000
C	0.31496300	-1.14851200	0.33899200
H	0.48815300	-2.15265400	0.71861000
C	0.47934400	-0.01599500	1.35348200
H	1.75046700	1.27112000	-1.51335600
H	1.61774400	-1.34737700	-1.55096000
H	1.45364600	-0.09613000	1.83628700
H	-0.31375400	0.00324100	2.10102900
H	-1.50042400	2.14806200	-0.37771600
H	-2.61032100	-0.03694800	-0.77392000
O	-1.05086000	-1.16475700	-0.14617000

Id-P1

C	-0.47331400	-1.17745200	-0.30505700
C	0.93873900	-0.74941200	-0.73569100
C	1.17341900	0.69942800	-0.36897200
H	2.09167700	1.12471500	-0.75416700
C	1.27137500	-0.34147200	0.69966800
C	-0.20941900	-0.55296500	1.06950900

H	-1.13290900	0.62397600	2.16109500
H	-0.03133000	-1.77137700	1.61907400
H	-2.61384300	-0.59644400	-1.32396400
H	-1.05175700	-0.13353100	-1.99782900
H	-0.16730800	2.33967700	0.71211100
H	1.25327400	1.62773600	-1.43908800
C	1.94969800	0.14641200	-0.22944900
O	2.73519500	-0.66188500	0.03154600

Ic-TS

C	-0.77742700	-1.30832600	-0.17010400
C	0.70058900	-1.14126200	-0.40465500
C	1.22749500	0.30686700	-0.67629700
H	2.10688800	0.37319500	-1.32401000
C	1.24822900	-0.31663500	0.70760800
C	-0.01537600	0.16900800	1.42918400
C	-0.85843500	0.87211000	0.32309100
H	-1.56960200	1.63585000	0.66520700
C	0.19048300	1.40874300	-0.70268000
H	2.16150400	-0.59432400	1.23676000
H	0.17833900	0.79190700	2.31855000
H	0.62921800	2.35119200	-0.33900600
H	-0.25200900	1.58562400	-1.69541500
H	1.24653500	-1.97240400	-0.85834100
H	-1.23079800	-2.29211000	-0.34439800
N	-1.57255000	-0.21367500	-0.36671800
H	-2.55557200	-0.32623800	-0.12919800

Ic-P2

C	-1.55315600	0.43771900	0.09221300
C	-0.76458600	-0.80332600	-0.02737900
C	0.53296800	-0.87437700	-0.80414700
H	0.65716900	-1.73663100	-1.44477700
C	0.56057200	-1.01655200	0.69686000
C	1.26530700	0.20198900	1.19221200
C	1.63495000	0.99841100	0.18955000
H	2.12207500	1.95935200	0.30263600
C	1.26145500	0.41974300	-1.15773400
H	0.70380300	-1.96895000	-1.19025200
H	1.42483000	0.40382500	2.24408200
H	2.15174200	0.21476900	-1.75976100
H	0.63767500	1.10608600	-1.74051700
H	-1.39041500	-1.68381700	-0.11096700
H	-0.99824600	1.36197300	0.28002100
N	-2.81780600	0.40326300	-0.01992300
H	-3.20904700	1.33891100	0.08903600

Id-TS

C	-0.92467000	-0.91409800	-0.15081200
C	0.50732200	-1.05633400	-0.69294200
C	1.28342800	0.23638500	-0.61031600
H	2.21925800	0.29555900	-1.16686500
C	1.19903300	-0.66507000	0.61103400
C	-0.06349100	-0.16730100	1.30256500
C	-0.55375800	0.99354900	0.60634700
H	-1.41129600	1.57941600	0.93471900
C	0.45897500	1.49278600	-0.36989500
H	2.04858200	-1.14247200	1.09781300
H	-0.42948700	-0.47715700	2.28021600
H	1.07135700	2.26320600	0.14417600
H	0.00787600	1.94172700	-1.26422200
H	0.78258100	-1.83168100	-1.41324800
H	-1.31375700	-1.91300200	0.15884900
O	-1.80201800	-0.02938600	-0.61841600

Id-P2

C	-1.56265000	0.48588800	0.08286800
C	-0.80334500	-0.78021500	-0.01816700
C	0.50153500	-0.88933800	-0.78799200
H	0.59657200	-1.76347100	-1.41712100
C	0.52061200	-1.00913000	0.70902500
C	1.24866300	0.20267400	1.19189200

C	-1.04909500	0.60984500	0.43637700
H	-1.87891100	1.04627800	0.99031200
C	-0.03808400	1.58854600	-0.14060600
H	2.14422200	-0.55874200	1.29706800
H	-0.52008600	-1.00538700	2.00495400
H	0.20749000	2.37786500	0.57614500
H	-0.43123300	2.03958800	-1.05314000
H	1.56465100	-1.24709100	-1.46388400
H	-0.73687800	-2.22101100	-0.46863000
O	-1.51533300	-0.25191500	-0.63250300

IIa-R₁

C	1.35589900	1.24658900	-0.08575900
C	0.11128000	1.71622300	-0.01736500
C	-1.13461400	0.86578600	0.15866500
H	-1.99126600	1.53037400	0.28310100
C	-1.01363900	-0.04772300	1.36013100
C	-0.17407000	-1.07506200	1.27451600
C	0.64001000	-1.22769900	0.01205700
H	1.10217600	-2.21776000	-0.00836200
C	-0.25754300	-1.08136900	-1.24207600
C	-1.36829900	-0.01955400	-1.08583300
H	-1.60652300	0.14190500	2.24838000
H	-0.03909800	-1.77314900	2.09402800
H	-0.71440000	-2.04888800	-1.46006700
H	0.38224300	-0.83838000	-2.09492500
H	-2.33940300	-0.50767300	-0.97178300
H	-1.42257400	0.61032200	-1.97689800
H	-0.03678700	2.78934900	-0.09586500
H	2.16440300	1.96407000	-0.20235000
C	1.78371300	-0.19591800	-0.01018100
H	2.41971700	-0.32919500	0.87445600
H	2.42508800	-0.40861200	-0.87463900

IIa-P₁

C	-1.24326800	0.82093200	-0.41256000
C	-1.36456300	-0.70597900	-0.55902600
C	-0.12215700	-1.49494000	-0.23344100
H	-0.31885700	-2.55571200	-0.36062100
C	-0.91269500	-0.90710500	0.89410200
C	-0.65037800	0.60998900	0.99795700
C	0.72654400	1.13541600	0.47091100
H	1.10415500	1.98684800	1.04014500
C	1.78973000	0.05250800	0.36340700
C	1.31883300	-1.10177800	-0.52566700
H	-1.36845200	-1.51292700	1.66720900
H	-1.07124400	1.11205300	1.86681400
H	1.99680100	-0.32935500	1.36985500
H	2.72417100	0.46931600	-0.02438400
H	1.95770800	-1.97238900	-0.35386800
H	1.42938800	-0.84265200	-1.58276900
H	-2.18139100	-1.19626800	-1.07458900
H	-2.19648700	1.33372000	-0.53769700
C	0.04400600	1.54053200	-0.87358700
H	-0.10441100	2.61969200	-0.94700400
H	0.51231300	1.19022200	-1.79566000

IIb-R₁

C	0.90104300	1.44906200	-0.04935800
C	-0.40637700	1.71849200	0.01819400
C	-1.50833600	0.69461900	0.16726700
H	-2.45565600	1.22113100	0.28731600
C	-1.27692600	-0.23033400	1.34489100
C	-0.29093200	-1.11541400	1.25482000
C	0.55912600	-1.11611600	0.00608600
H	1.20755200	-1.99106600	-0.02813400
C	-0.33635800	-1.07305200	-1.26685100
C	-1.58641700	-0.18708500	-1.10957200
H	-1.92433600	-0.16797600	2.21201400
H	-0.06819600	-1.81741500	2.04966100
H	-0.64049800	-2.09708000	-1.48862800
H	0.27292500	-0.73762100	-2.10899900
H	-2.48013000	-0.80755400	-1.02029000

C	1.64713100	0.96996100	0.17827700
H	2.15733200	1.92012700	0.27732500
C	1.26731300	0.37798200	-1.16097400
H	0.63413000	-1.95646900	-1.21934400
H	1.40242700	0.41802100	2.24164300
H	2.15633700	0.13089400	-1.74888300
H	0.67335600	1.07138200	-1.76486300
H	-1.45016400	-1.64591200	-0.09492700
H	-0.97951800	1.40693100	0.25797600
O	-2.76325400	0.53394700	-0.01750800

IIa-TS

C	-1.00851600	1.29174000	-0.65538900
C	-1.60285000	-0.04506200	-0.29854700
C	-0.70931000	-1.33172300	-0.31763700
H	-1.27341100	-2.25575500	-0.49400300
C	-1.09069400	-0.53559500	0.97584400
C	-0.03869200	0.40888000	1.47666000
C	1.07548700	0.75131400	0.51924100
H	1.84402700	1.35046700	1.03284800
C	1.72215700	-0.57567200	0.03523900
C	0.72214700	-1.36804700	-0.83235500
H	-1.75458700	-1.01788500	1.69743600
H	0.25385100	0.30264000	2.52994800
H	2.00688300	-1.17494300	0.91716800
H	2.64658300	-0.38171000	-0.53451700
H	1.04601100	-2.41936100	-0.90331800
H	0.74744700	-0.97595100	-1.86539200
H	-2.65246700	-0.20078400	-0.55979600
H	-1.58275100	1.88089800	-1.38369900
C	0.45618700	1.55339900	-0.63187300
H	0.62601500	2.62573100	-0.43608300
H	0.93689900	1.37124900	-1.62769400

IIa-P₂

C	-1.64548800	-0.21514800	-0.75004500
C	-0.91305500	-1.11585100	0.18227800
C	0.55658600	-1.40747400	0.09330900
H	0.83507000	-2.43448000	0.30300000
C	0.03046000	-0.61913400	1.27382700
C	0.43156800	0.80442200	1.36282700
C	1.00787400	1.46149600	0.35575400
H	1.27315200	2.50641100	0.48008900
C	1.27742100	0.81753200	-0.97359700
C	1.49877300	-0.70012000	-0.86070700
H	-0.05160100	-1.13784600	2.22115700
H	0.24351100	1.31389100	2.30283300
H	2.15324200	1.27423300	-1.44181000
H	0.43343100	1.02121600	-1.64162800
H	2.51620300	-0.87424200	-0.49622300
H	1.43771900	-1.15410100	-1.85397200
H	-1.50515600	-1.97542900	0.48548800
H	-1.63840700	-0.50443500	-1.80028200
C	-2.32479300	0.86158900	-0.37298000
H	-2.33979700	1.17678700	0.66487000
H	-2.87344600	1.46412400	-1.08752100

IIb-TS

C	-0.62613100	-1.33125200	-0.51656200
C	0.90496000	-1.38111200	-0.47458600
C	1.71431000	-0.09934200	-0.47438900
H	2.76208300	-0.25666300	-0.74489400
C	1.33344900	-0.79230600	0.83838600
C	-0.00690200	-0.38412900	1.39256700
C	-0.68925000	0.76929100	0.80024600
H	-1.47595300	1.18893000	1.43899600
C	0.20066800	1.84264600	0.16888000
C	1.12447500	1.24090300	-0.89922000
H	2.08780200	-1.22840400	1.49620800
H	-0.40165300	-0.88029400	2.28221800
H	0.79870500	2.32412200	0.96270500
H	-0.43668800	2.62430800	-0.27334700
H	1.94152800	1.94284100	-1.12689600

H	-1.71709900	0.45135400	-1.98556200
H	-0.71570900	2.75811700	-0.05201100
H	1.62690700	2.24929400	-0.14758100
C	1.49640200	0.08798000	0.00544100
O	2.69836100	-0.05376200	0.00708800

I**b**-P₁

C	-0.29549100	-1.43368200	-0.08160500
C	1.06439200	-1.12475900	-0.74946500
C	1.50784400	0.31240300	-0.66574600
H	2.46593100	0.42940800	-1.16172900
C	1.60969000	-0.54708600	0.55690900
C	0.21799500	-0.72389900	1.20240600
C	-0.80904700	0.43505700	0.99020100
H	-1.51400800	0.57001600	1.81263700
C	-0.19151900	1.75290600	0.53492600
C	0.61009300	1.54034100	-0.75149400
H	2.54918900	-0.75872800	1.04893600
H	0.18486600	-1.23501900	2.16003700
H	0.46826100	2.12149700	1.32687600
H	-0.97441600	2.49717500	0.37596300
H	1.23089200	2.41723700	-0.94627400
H	-0.07335200	1.44254300	-1.60103800
H	1.54415600	-1.80359500	-1.44097000
H	-0.58117500	-2.48378200	-0.09928600
C	-1.40253800	-0.38339600	-0.17605900
O	-2.39610700	-0.27050800	-0.82944900

I**c**-R₁

C	1.44560000	1.06735200	-0.21467200
C	0.25513000	1.67804100	-0.13832300
C	-1.05259000	0.95209200	0.13428300
H	-1.84296800	1.69422900	0.25624200
C	-0.89729900	0.14546100	1.40623000
C	-0.12738000	-0.94118500	1.36065300
C	0.56436700	-1.23953300	0.05035800
H	1.01670200	-2.23217100	0.06726800
C	-0.42741700	-1.17206300	-1.12608800
C	-1.43323800	-0.00252200	-1.01164500
H	-1.36845500	0.47790300	2.32566400
H	0.06838300	-1.55191900	2.23567500
H	-0.96978300	-2.11925000	-1.16387600
H	0.15861800	-1.09597300	-2.04434900
H	-2.43747100	-0.39031400	-0.81936400
H	-1.47175000	0.55759900	-1.94863300
H	0.23692200	2.75542100	-0.24307700
H	2.34774400	1.65762000	-0.33924200
N	1.67914500	-0.30252100	-0.19295700
H	2.54500700	-0.56135400	0.25961300

I**c**-P₁

C	-1.11961000	0.92245300	-0.42727600
C	-1.42012900	-0.57933500	-0.55581700
C	-0.25571500	-1.47013700	-0.20650500
H	-0.54367500	-2.51073900	-0.31970400
C	-0.99651600	-0.79883400	0.90729600
C	-0.58996400	0.68516600	0.99310800
C	0.80647800	1.07593300	0.41615200
H	1.24151400	1.95363600	0.89887300
C	1.79054000	-0.07741400	0.34919000
C	1.21327000	-1.20495400	-0.51065400
H	-1.51574500	-1.34281800	1.68472400
H	-0.95552000	1.25015700	1.84690700
H	1.97037500	-0.43453300	1.36956200
H	2.74736200	0.25600500	-0.06052400
H	1.77601200	-2.12402000	-0.32881300
H	1.32654800	-0.95106700	-1.56562900
H	-2.27672700	-0.99158600	-1.07355500
H	-1.97137500	1.57183800	-0.62668800
N	0.20396700	1.37633700	-0.92817000
H	0.20334500	2.37149600	-1.12092500

I**d**-R₁

H	0.55932100	1.10444400	-1.83739100
H	1.36122800	-2.29839300	-0.84964400
H	-1.12786000	-2.16899900	-1.01709900
C	-1.44028300	-0.19134200	-0.24654400
O	-2.64503600	-0.04900400	-0.48294000

I**b**-P₂

C	1.48935900	0.96277600	-0.55400400
C	0.47450000	1.46085200	0.41540600
C	-1.01498700	1.30559100	0.15410200
H	-1.62215500	2.15198800	0.45177500
C	-0.36213300	0.52967300	1.26580000
C	-0.30461400	-0.94917700	1.11539400
C	-1.08914400	-1.59293400	0.25251300
H	-1.04650100	-2.67598400	0.19391500
C	-2.05110300	-0.86553100	-0.65356400
C	-1.51116200	0.51639700	-1.04782900
H	-0.53152200	0.87661100	2.27939600
H	0.37736900	-1.50185500	1.75478400
H	-3.01573300	-0.76170300	-0.14190900
H	-2.24136900	-1.45992200	-1.55028700
H	-2.28340400	1.08822800	-1.56642500
H	-0.68928500	0.37220300	-1.75434900
H	0.75336900	2.38665400	0.90727200
H	1.75467600	1.54497000	-1.42889700
C	2.14703600	-0.16450300	-0.40742000
O	2.73475500	-1.15500700	-0.29845700

I**c**-TS

C	1.16694400	-1.09133200	-0.60515200
C	1.52343900	0.36438500	-0.37919500
C	0.39798300	1.43860900	-0.28153800
H	0.78408600	2.44251600	-0.49111300
C	0.98372700	0.73499700	0.94792600
C	0.24075700	-0.50647900	1.42193900
C	-0.85806000	-0.96302500	0.45496600
H	-1.40563800	-1.82045000	0.87687900
C	-1.81042100	0.19873900	0.11076700
C	-1.03706700	1.22675800	-0.73931400
H	1.58261700	1.30383300	1.66330500
H	-0.12773400	-0.43747200	2.45857700
H	-2.16004600	0.65345300	1.05238700
H	-2.70193300	-0.14814500	-0.43786700
H	-1.56096400	2.19716200	-0.72418700
H	-1.03891800	0.88206900	-1.78921500
H	2.50016200	0.69351600	-0.74462400
H	1.88311800	-1.70027500	-1.17175100
N	-0.15221500	-1.43981400	-0.75035300
H	-0.33305600	-2.40341700	-1.02230600

I**c**-P₂

C	-1.79328000	-0.09492900	0.54755800
C	-1.17908500	0.09238800	-0.77940000
C	0.13286000	0.84273300	-0.95242800
H	0.17637900	1.44089700	-1.85410000
C	0.10519100	-0.64072200	-1.14600000
C	0.83489700	-1.46484600	-0.14601400
C	1.77449800	-0.93584200	0.63655200
H	2.31593500	-1.56962100	1.33196300
C	2.13019400	0.52985900	0.57977400
C	0.90786500	1.39505900	0.24037200
H	0.13099900	-1.01712300	-2.16268200
H	0.59689000	-2.52247000	-0.08540600
H	2.91050600	0.67734000	-0.17667900
H	2.56096300	0.84975200	1.53123700
H	1.22418600	2.41626000	0.01940300
H	0.26588700	1.45942800	1.12192000
H	-1.90834300	0.21766700	-1.57014200
H	-1.11666800	-0.36102400	1.36652100
N	-3.04740500	0.03018300	0.70297700
H	-3.30374700	-0.14458600	1.67464300

I**d**-TS

C	-1.39602000	1.09566400	0.12448200
C	-0.18609200	1.65742000	0.07108200
C	1.10574000	0.88742300	-0.13924400
H	1.92648700	1.59524900	-0.25931600
C	0.96947000	0.02323300	-1.37590400
C	0.12834500	-1.00578200	-1.31308800
C	-0.64078800	-1.18301700	-0.02910300
H	-1.17357700	-2.13244000	-0.01718100
C	0.26424600	-1.08181800	1.20856000
C	1.39111500	-0.03638000	1.05808200
H	1.52030600	0.26479500	-2.27900300
H	-0.06018900	-1.66223100	-2.15421600
H	0.69150000	-2.06942200	1.39472700
H	-0.37718900	-0.84738400	2.06130600
H	2.35153700	-0.53291900	0.89577300
H	1.47654600	0.56047700	1.96889400
H	-0.14780600	2.73559000	0.16180100
H	-2.29266900	1.69420100	0.23393900
O	-1.71638100	-0.21829600	0.04550900

IId-P₁

C	1.08789700	-0.90963600	-0.47683900
C	1.40674800	0.58955400	-0.55187800
C	0.25222600	1.46587700	-0.14212100
H	0.53737100	2.51082600	-0.21046400
C	1.00751900	0.74291800	0.92759400
C	0.60153500	-0.74304100	0.96135200
C	-0.78268000	-1.10258500	0.36477000
H	-1.20713200	-2.02963900	0.75603200
C	-1.78483900	0.03102200	0.34193000
C	-1.21607500	1.20856500	-0.45328800
H	1.54371600	1.25064900	1.71748000
H	0.97904800	-1.34934800	1.77901100
H	-1.98018500	0.32616200	1.37905000
H	-2.73112800	-0.29977600	-0.09207300
H	-1.78522600	2.11207500	-0.22227600
H	-1.33091000	1.01455700	-1.52126900
H	2.25924600	1.01346000	-1.06619800
H	1.89535200	-1.58063600	-0.76733600
O	-0.20176700	-1.33304700	-0.94763400

C	0.99187200	-1.17203600	-0.71816700
C	1.54677300	0.18170100	-0.35769100
C	0.56074900	1.39287900	-0.22667700
H	1.05372900	2.35452000	-0.41141400
C	1.06922400	0.57336100	0.97488900
C	0.16224100	-0.54918200	1.43714300
C	-0.92747200	-0.88624400	0.46456900
H	-1.56113400	-1.70790500	0.83154400
C	-1.76865200	0.33788600	0.06633800
C	-0.88358900	1.34267600	-0.70151000
H	1.74549100	1.04672900	1.69034100
H	-0.21936900	-0.45886800	2.46432100
H	-2.16439200	0.78776000	0.99131600
H	-2.63309700	0.04567300	-0.55159100
H	-1.31544500	2.35431300	-0.62646500
H	-0.90125300	1.08120200	-1.77414700
H	2.55875100	0.39096000	-0.71523500
H	1.52167500	-1.75066700	-1.48728700
O	-0.32397900	-1.43374600	-0.75559400

IId-P₂

C	-1.64627900	0.41007600	0.45971100
C	-1.10852400	-0.69098900	-0.37435400
C	0.13757600	-0.58491400	-1.23635000
H	0.03313300	-1.11974800	-2.17346000
C	0.18104100	-1.43129500	-0.00685000
C	1.03202900	-0.94459700	1.11043800
C	1.60882200	0.25753700	1.11807900
H	2.21857600	0.54847300	1.96737400
C	1.42142400	1.26436400	0.01625700
C	1.05047100	0.62114200	-1.32851500
H	0.12819000	-2.50671700	-0.12215000
H	1.18392100	-1.62124800	1.94475700
H	2.33464500	1.85199500	-0.10664700
H	0.65107600	1.98606900	0.31230200
H	1.97066200	0.27079500	-1.80639700
H	0.61615100	1.37170000	-1.99290600
H	-1.90152200	-1.28965300	-0.80709400
H	-0.96284700	0.86981400	1.19339900
O	-2.79141800	0.77882200	0.38004100