

## **Supporting Information**

**For**

### **The Impact of the Different Geometrical Restrictions on the Nonadiabatic Photoisomerization of Biliverdin Chromophore**

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## 1. Bond lengths of key structures

**Table S1.** Bond lengths (Å) of BV in different optimized geometries.

Geometries	C <sub>4</sub> C <sub>5</sub>	C <sub>5</sub> C <sub>6</sub>	C <sub>9</sub> C <sub>10</sub>	C <sub>10</sub> C <sub>11</sub>	C <sub>14</sub> C <sub>15</sub>	C <sub>15</sub> C <sub>16</sub>
S <sub>0_min</sub>	1.364	1.446	1.404	1.389	1.441	1.364
S <sub>1_min</sub>	1.373	1.435	1.380	1.456	1.402	1.396
CI <sub>1</sub>	1.373	1.432	1.378	1.456	1.401	1.396
CI <sub>2</sub>	1.394	1.402	1.449	1.379	1.439	1.367
CI <sub>3</sub>	1.364	1.453	1.438	1.366	1.378	1.427
CI <sub>4</sub>	1.446	1.378	1.380	1.416	1.443	1.366

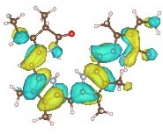
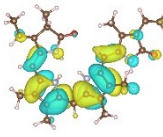
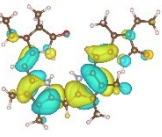
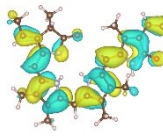
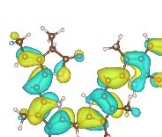
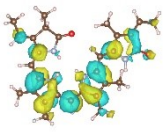
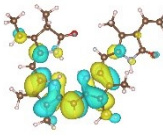
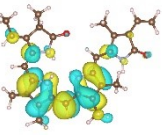
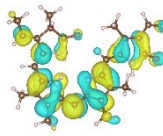
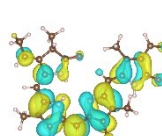
## 2. Dihedral angles of key structures

**Table S2.** Dihedral angles (degree) of BV in different optimized geometries

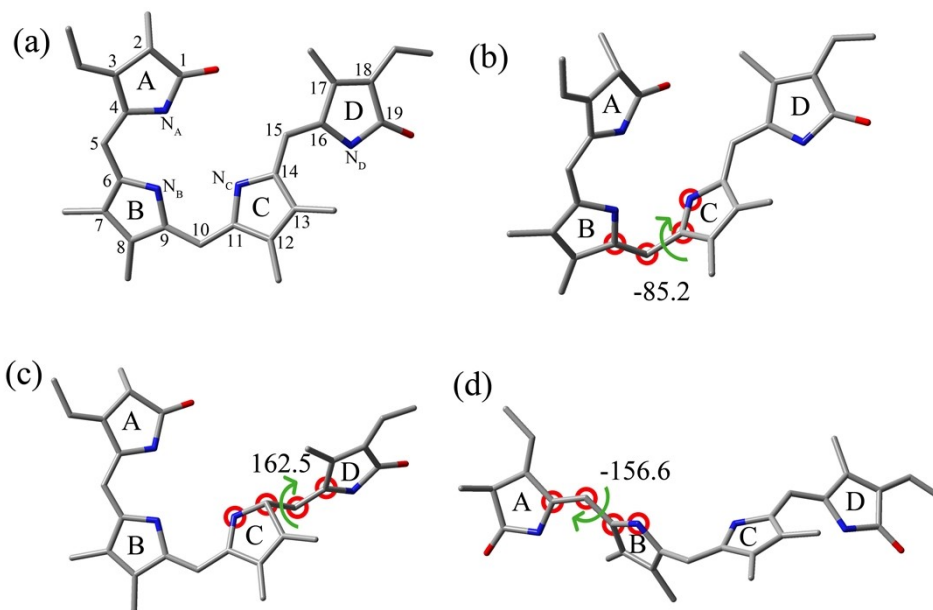
Geometries	N <sub>A</sub> C <sub>4</sub> C <sub>5</sub> C <sub>6</sub>	C <sub>4</sub> C <sub>5</sub> C <sub>6</sub> N <sub>B</sub>	N <sub>B</sub> C <sub>9</sub> C <sub>10</sub> C <sub>1</sub>	C <sub>9</sub> C <sub>10</sub> C <sub>11</sub> N		N <sub>C</sub> C <sub>14</sub> C <sub>15</sub> C <sub>16</sub>	C <sub>14</sub> C <sub>15</sub> C <sub>16</sub> N <sub>B</sub>
				1	c		
S <sub>0_min</sub>	5.3	28.2	-16.5	-12.4	-144.2	6.4	
S <sub>1_min</sub>	5.4	27.0	7.6	-85.2	-163.8	18.9	
CI <sub>1</sub>	5.4	24.4	7.8	-85.4	-164.5	19.0	
CI <sub>2</sub>	12.1	17.6	-93.4	1.8	-143.0	7.6	
CI <sub>3</sub>	2.6	35.1	-24.8	-2.7	177.0	95.0	
CI <sub>4</sub>	89.6	-4.2	-8.4	-20.1	-141.2	6.3	

### 3. Excitation energy at different levels

**Table S3.** Excitation energy at different levels.

	OM2/MRCI (16, 12)	SA(2)- CASSCF (6,6)	MS- CASPT2 (6,6)	TDDFT/ B3LYP	TDDFT/ M06-2X
Vertical Excited Energy/ eV	2.31	2.46	2.37	1.96	2.11
HOMO					
LUMO					

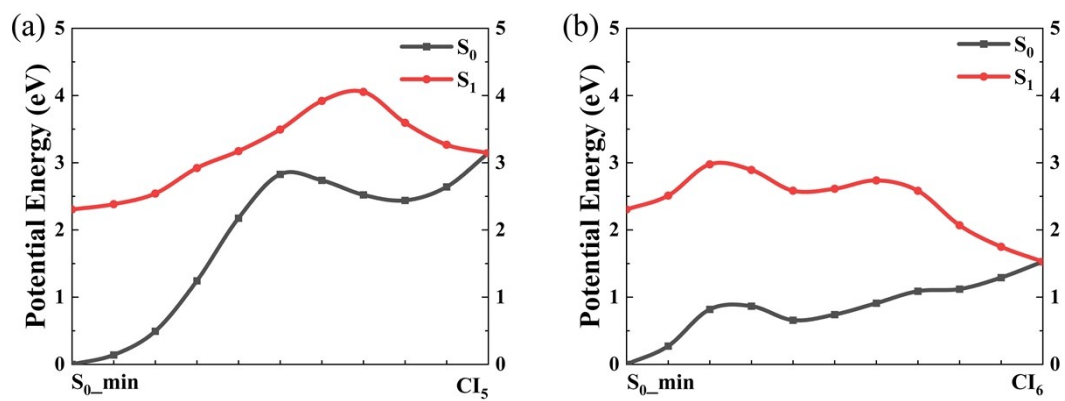
#### 4. The structures of $S_{0\_min}$ , $S_{1\_min}$ and $CI_{5/6}$



**Figure S1.** The structure of  $S_{0/1\_min}$  and  $CI_{5/6}$  and their major rotating dihedral angles

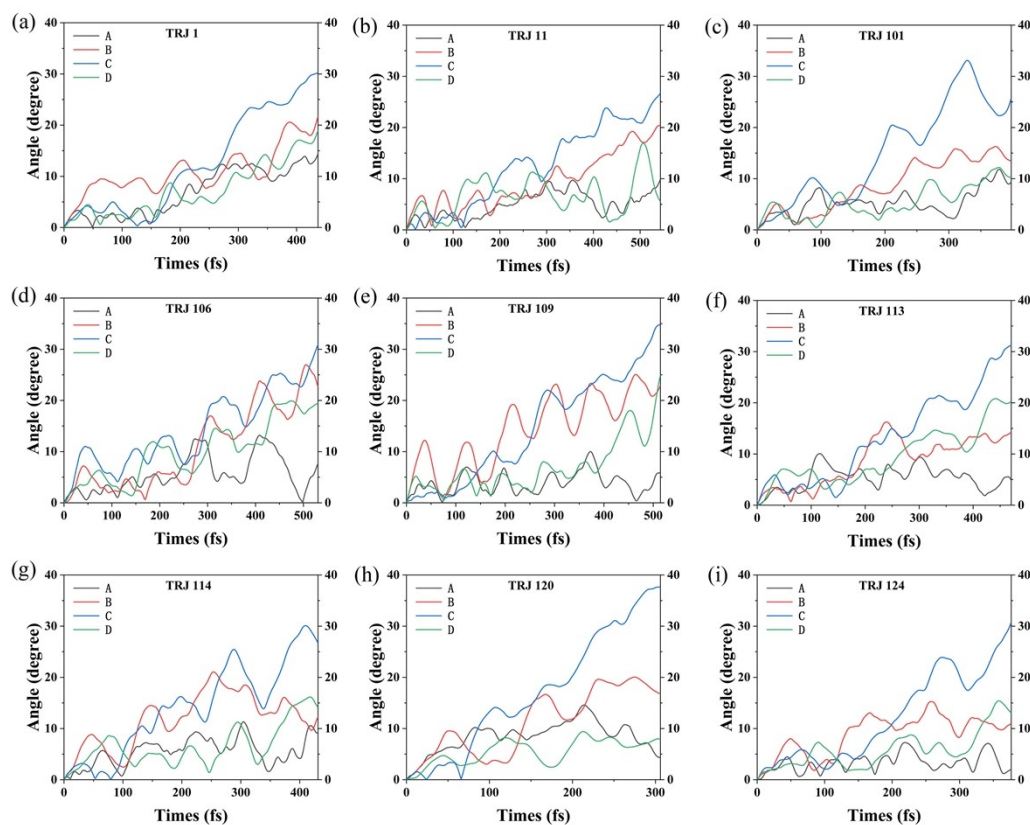
(marked by red circles) (a)  $S_{0\_min}$ ; (b)  $S_{1\_min}$ ; (c)  $CI_5$ ; (d)  $CI_6$ .

## 5. PE curves of CI<sub>5/6</sub>



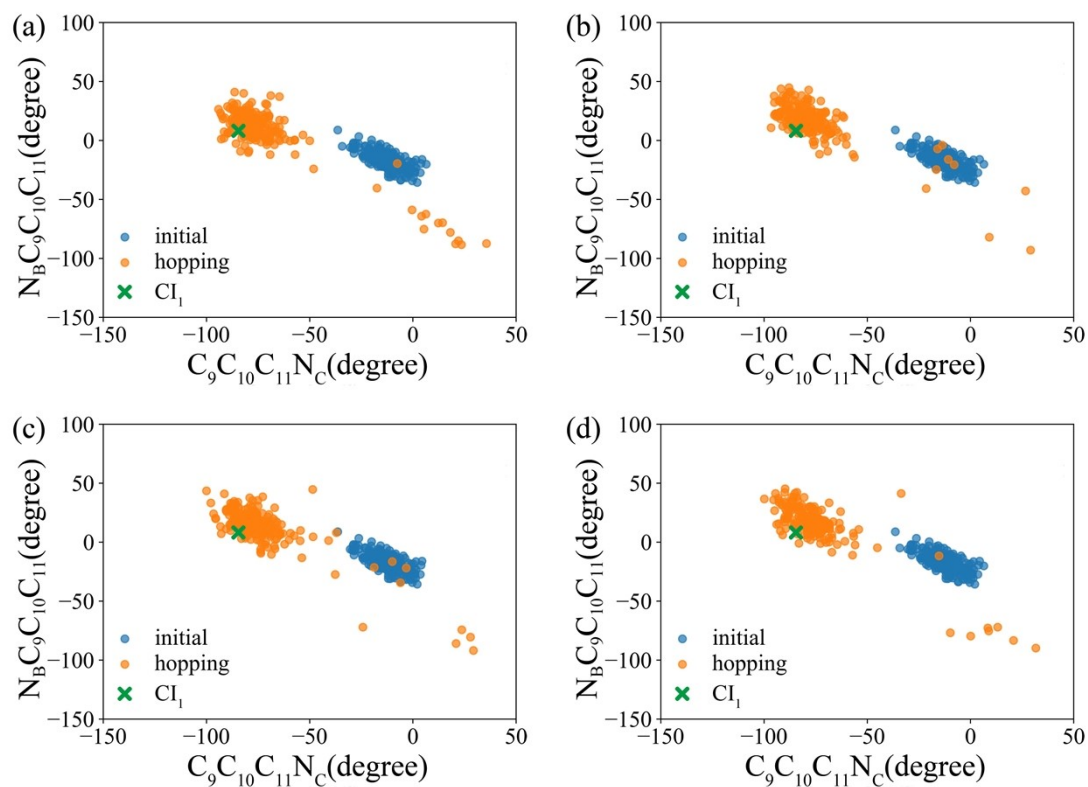
**Figure S2.** Potential energy curves along the linear interpolated pathways from S<sub>0\_min</sub> to the two conical intersections (a) CI<sub>5</sub>, (b) CI<sub>6</sub>.

## 6. The time evolution of the normal vector



**Figure S3.** The time evolution of the normal vector of the four rings in the typical trajectories of **Model 0** through the  $CI_1$  channel. In order to analyze the contributions of the ring motions to photoisomerization in detail, we employed the method proposed by Böckmann et al. (*J. Phys. Chem. A*, 2010, **114**, 745-754) to describe the torsional motions of the A, B, C, D rings by examining their normal vectors perpendicular to the ring planes. The torsional motion of the ring plane is characterized by the angle between the normal vector and its corresponding initial one. Figure S3 shows the time evolution of these angles along several typical trajectories in the TSH dynamics of the original BV. Here, in the  $C_{10}C_{11}$  isomerization channel, the twisting motion of Ring C contributes play the dominant role and the motion of Ring B is also present, while the motions of Rings A and D give very minor contributions.

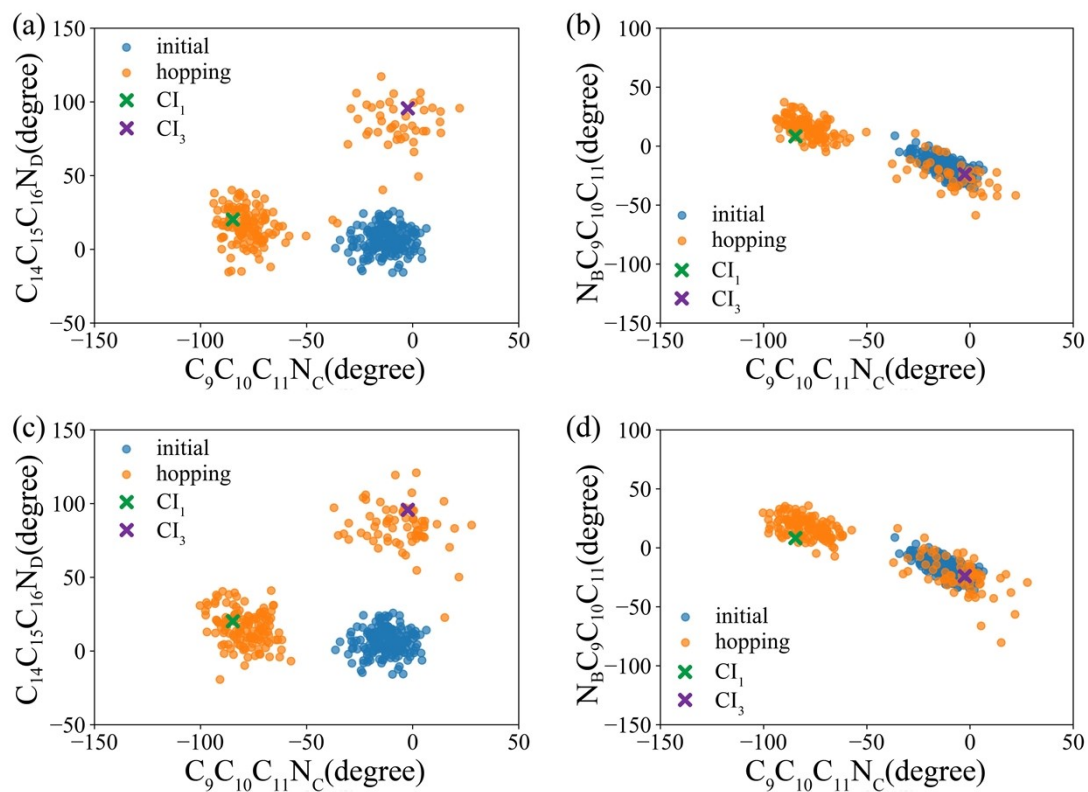
## 7. Distributions of key dihedral angles at the initial, hopping and CI geometries



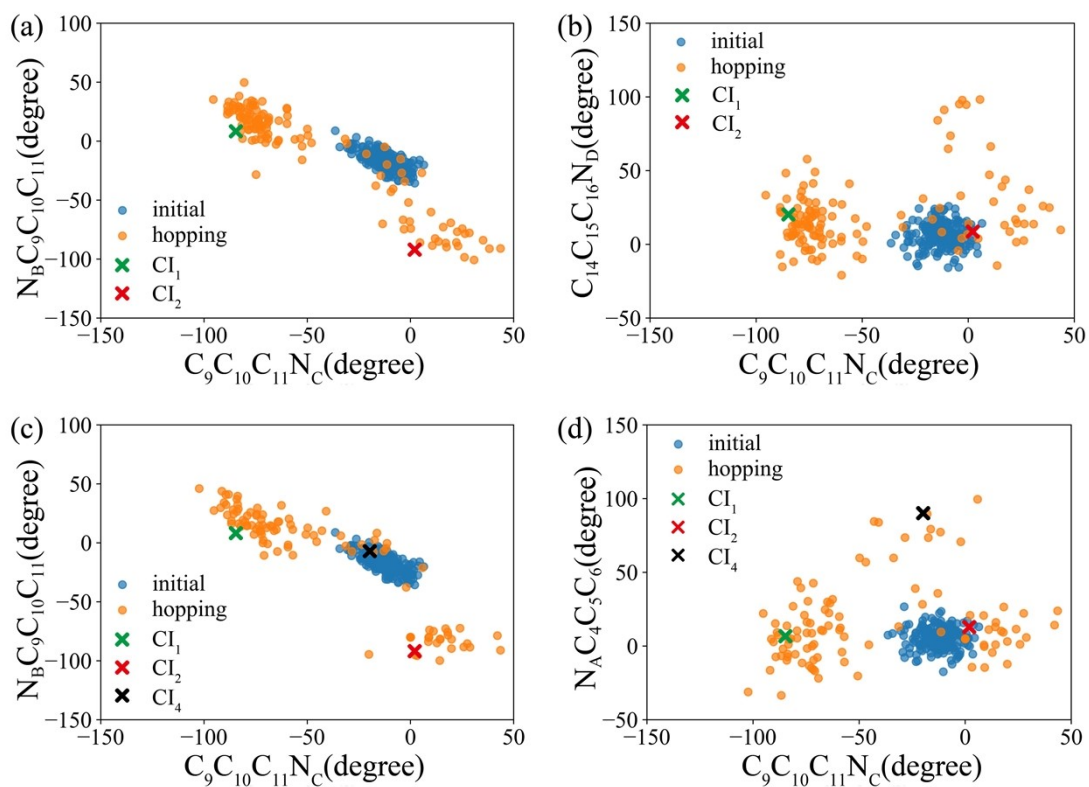
**Figure S4.** Distributions of key dihedral angles at the initial, hopping and CI geometries

of the four models (a) **Model 0**; (b) **Model I**; (c) **Model IV**; (d) **Model VIII**.

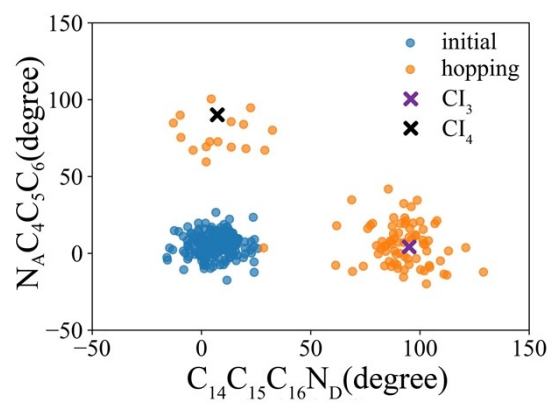




**Figure S5.** Distributions of key dihedral angles at the initial, hopping and CI geometries of the two models (a) and (b) **Model II**; (c) and (d) **Model V**.



**Figure S6.** Distributions of key dihedral angles at the initial, hopping and CI geometries of the two models (a) and (b) **Model III**; (c) and (d) **Model VII**.



**Figure S7.** Distributions of key dihedral angles at the initial, hopping and CI geometries of **Model VI**.

## 8. Cartesian coordinates

Cartesian coordinates of the  $S_0$  min structure

Atom	x	y	z
C	5.1467488792	-4.6291439917	1.3019979238
C	4.8734739420	-3.2580807716	0.8074524817
C	3.6430940521	-2.8197182360	0.4822566544
C	3.3600317575	-1.4279154772	0.0414261421
N	1.9787813138	-1.3109432220	-0.1626169090
C	1.3133530873	-2.5136423506	0.1336226871
O	0.0851184968	-2.5861617519	0.0542093217
C	2.3385163402	-3.5782849668	0.5508307556
C	2.2573067625	-4.7095595936	-0.4562868804
C	4.2381783217	-0.3903923970	-0.0739729537
C	3.7626655788	0.9540979530	-0.3140627796
N	2.5225198432	1.3726455996	0.1102530295
C	2.3690363957	2.7390333392	-0.1847177413
C	3.5688350702	3.1651358118	-0.8511399083
C	3.7985989569	4.5161479512	-1.4033406063
C	4.4234240190	2.0480845533	-0.9505440660
C	5.7537674455	1.9878395350	-1.5940104658
C	1.2070531134	3.4736792191	0.1025063929
C	-0.0127410852	2.8771528350	0.3953260421
C	-1.2013564769	3.4724204693	0.9758243463
C	-1.3332924684	4.8793518792	1.4063831160
C	-2.1659613526	2.4676518486	1.1152556643
C	-3.4778170912	2.6103881834	1.7854110698
C	-1.6036544173	1.2567007633	0.5707074521
N	-0.3114484278	1.5118159635	0.2046152342
C	-2.1343995487	-0.0748830777	0.4222730216
C	-3.4264150156	-0.3306017972	0.0674002984
C	-4.0246043061	-1.7004257351	-0.0663556290
C	-3.2823677610	-2.9231839718	0.3063369579
C	-5.2997564307	-1.5681460948	-0.5329324578
C	-6.2798174224	-2.5962919266	-0.8187496089
C	-7.5043114917	-2.2874588809	-1.2632700137
C	-5.5679134168	-0.0944874711	-0.7306854589
O	-6.5608945895	0.4957050280	-1.1470258336
N	-4.3923777251	0.5837384143	-0.3233342373
H	5.5644329420	-5.2271520860	0.4782562656
H	5.7472233781	-2.5991519004	0.7026111842
H	1.5905532973	-0.6348356641	-0.8069080490
H	2.5369433434	-4.3554915517	-1.4576560451
H	2.9440484761	-5.5143310434	-0.1648943186

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H	1.2348952825	-5.1057016156	-0.4861644659
H	5.3110669980	-0.5364322269	0.0039028693
H	2.0152478772	0.9118202681	0.8598504646
H	4.8760741750	4.7299367345	-1.4235417795
H	3.2923270743	5.2786590618	-0.7920807866
H	5.6424897798	1.6712720334	-2.6433726883
H	6.4005575090	1.2674198723	-1.0696301009
H	6.2293828529	2.9800512542	-1.5686100444
H	1.2691187477	4.5710756942	0.0871688740
H	-0.4495371451	5.4700233333	1.1245858358
H	-1.4551974827	4.9137567648	2.4989690977
H	-4.1888395742	3.1404538295	1.1286938880
H	-3.3506144969	3.2023214864	2.7057320690
H	-3.8855375967	1.6274834270	2.0523649483
H	0.2338133571	0.8851554690	-0.3744593898
H	-1.4485942814	-0.9038383510	0.5801555186
H	-3.2550559687	-3.0060855694	1.4043545515
H	-2.2547161701	-2.8852081716	-0.0759907944
H	-3.7888281585	-3.8080342557	-0.1047530828
H	-5.9599422189	-3.6310090236	-0.6499625378
H	-7.8207987243	-1.2681500139	-1.4293111281
H	-8.2309176341	-3.0647942576	-1.4749964449
H	-4.2535253138	1.5764630970	-0.4117005242
H	4.2356869469	-5.1178629342	1.6755724605
H	2.1158842648	-3.9317764534	1.5880542404
H	5.8846058597	-4.5844296430	2.1152388483
H	3.4082777290	4.5605740642	-2.4310173748
H	-2.2242958429	5.3187630712	0.9369896566

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Cartesian coordinates of the S<sub>1</sub> min structure

Atom	x	y	z
C	4.3738320351	-4.5264919901	1.8918987022
C	4.3282512681	-3.1395963422	1.3675845340
C	3.2873416400	-2.6524709258	0.6640076763
C	3.2044978841	-1.2536094174	0.1846245275
N	1.9451604919	-1.0808864043	-0.4092231598
C	1.1967476305	-2.2573804978	-0.3902760955
O	0.0582742518	-2.2904052906	-0.8749723415
C	2.0137330129	-3.3694789496	0.2807633233
C	2.2408229379	-4.4600366814	-0.7502251881
C	4.1454569992	-0.2600027648	0.2974331560
C	3.8349711942	1.0828393213	-0.1005667097
N	2.5306565218	1.5666364854	-0.0780693672
C	2.5032501576	2.8535953131	-0.6389680106
C	3.8727858794	3.1895096107	-1.0043115007
C	4.2589161235	4.4621799796	-1.6454421821
C	4.6807813746	2.0984484530	-0.6597608654
C	6.1382714697	1.9460364333	-0.8649009871
C	1.3117636396	3.4852770995	-0.9331366237
C	0.1131876741	2.8039380834	-0.4663423024
C	-0.5280433696	2.8741667120	0.8215824083
C	-0.1509207261	3.8295949140	1.8864973906
C	-1.5595805326	1.9289126318	0.8383720105
C	-2.4031778289	1.6105949579	2.0094368362
C	-1.5201784240	1.2198880717	-0.4366917448
N	-0.4961185566	1.8133439403	-1.1899130879
C	-2.1119578438	0.0351314205	-0.8975234691
C	-3.3242730212	-0.4953489123	-0.4528010182
C	-3.7743601477	-1.8845507783	-0.7301787009
C	-2.9308318651	-2.8736696088	-1.4334930634
C	-5.0373122779	-2.0379919083	-0.2034803175
C	-5.8864553973	-3.1988504179	-0.1891604047
C	-7.1208964755	-3.1571996874	0.3382630208
C	-5.4381962038	-0.7149251319	0.3997142607
O	-6.4623546891	-0.3406403682	0.9555921745
N	-4.3211140243	0.1629443797	0.2153389098
H	4.9978431083	-5.1392362742	1.2237502323
H	5.2086855362	-2.5147638966	1.5690143313
H	1.7298778120	-0.3045315155	-1.0167360576
H	2.8236871098	-4.0721815416	-1.5966788681
H	2.7950300139	-5.2900427759	-0.2946107920
H	1.2753214412	-4.8297571663	-1.1180135120

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H	5.1507716927	-0.4726240327	0.6534989298
H	1.8338034377	1.2359568751	0.5783859573
H	5.3541646259	4.5428203893	-1.6979818736
H	3.8637809796	5.3105100288	-1.0653211219
H	6.3244865161	1.2152902564	-1.6673738860
H	6.6131214941	1.5910031155	0.0630005122
H	6.5847794830	2.9104443274	-1.1482710975
H	1.2419108541	4.4303854078	-1.4452054723
H	0.8570157814	4.2219607625	1.7018466987
H	-0.1741109539	3.3287343480	2.8667660237
H	-3.3482038070	2.1759196585	1.9574261064
H	-1.8775288520	1.9124596738	2.9272577301
H	-2.6110638900	0.5342410005	2.0621776027
H	-0.2614670262	1.5695509401	-2.1448653825
H	-1.5629638905	-0.5479509499	-1.6413523426
H	-3.3235953756	-3.8853713936	-1.2577317031
H	-1.8950872299	-2.8217796343	-1.0849888933
H	-2.9627917700	-2.6685443411	-2.5160899653
H	-5.4715903136	-4.1101313594	-0.6318724853
H	-7.5396277631	-2.2621769675	0.7757154807
H	-7.7514759590	-4.0394360898	0.3386321410
H	-4.3234898302	1.1416990911	0.4576681452
H	3.3697972397	-4.9712882133	1.9545574481
H	1.4690147325	-3.7582722407	1.1771688741
H	4.8241874514	-4.5257849794	2.8946946781
H	3.8482934930	4.5034453758	-2.6674490824
H	-0.8674203284	4.6638933985	1.8952322509

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Cartesian coordinates of the Cl<sub>1</sub> structure

Atom	x	y	z
C	4.2902145792	-4.3543459095	2.2479704314
C	4.2106903318	-3.0165921650	1.6118928403
C	3.1518928669	-2.6003423206	0.8904816003
C	3.0405518330	-1.2501969623	0.2937957061
N	1.7674645053	-1.1453899867	-0.2892992508
C	1.0410088345	-2.3242588242	-0.1627261575
O	-0.1027663063	-2.4274262038	-0.6258594796
C	1.8800717130	-3.3642068799	0.5972600176
C	2.1037578540	-4.5453529231	-0.3266100549
C	3.9747918399	-0.2434753780	0.2977237744
C	3.6562356955	1.0560461702	-0.2115075579
N	2.3418726570	1.5236094017	-0.2592897136
C	2.3234235336	2.7722560881	-0.9053595651
C	3.6962997596	3.0896284774	-1.2701900090
C	4.0908340620	4.3095371981	-2.0020761072
C	4.5043284374	2.0338390875	-0.8258741454
C	5.9663586630	1.8829700524	-0.9989218213
C	1.1397028594	3.3853622999	-1.2539325360
C	-0.0669178926	2.7424476143	-0.7521243805
C	-0.7158799932	2.9086703018	0.5332524384
C	-0.3328747328	3.9408752424	1.5218620613
C	-1.7451097412	1.9730555956	0.6166252599
C	-2.5948460929	1.7435013968	1.8063017967
C	-1.7068028347	1.1759376459	-0.6021685826
N	-0.6772652019	1.7147716621	-1.4026196815
C	-2.2956927937	-0.0383933510	-0.9775398429
C	-3.5010790083	-0.5446751017	-0.4877079494
C	-3.9388533360	-1.9538590471	-0.6612643975
C	-3.0817761924	-2.9858837214	-1.2808583808
C	-5.2021766613	-2.0783453686	-0.1247344396
C	-6.0427724950	-3.2384999664	-0.0235647589
C	-7.2734202907	-3.1695551540	0.5117999163
C	-5.6107881077	-0.7161922053	0.3838996022
O	-6.6360184259	-0.3103025716	0.9135254003
N	-4.4968857954	0.1528519233	0.1418859225
H	4.9135003920	-5.0103961893	1.6215504161
H	5.0841701663	-2.3640358557	1.7459062960
H	1.5322457236	-0.4276079880	-0.9587799563
H	2.6760198630	-4.2370021286	-1.2119234546
H	2.6665862640	-5.3269397472	0.1995995392
H	1.1368999592	-4.9545037555	-0.6468706259



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H	4.9872683414	-0.4209496390	0.6562129525
H	1.6615769018	1.2743528398	0.4506346279
H	3.7897622557	4.2215415337	-3.0589099942
H	5.1813473018	4.4435511027	-1.9527685120
H	6.4217788283	2.8554150494	-1.2379942246
H	6.1695153136	1.1804505438	-1.8224082150
H	6.4184509815	1.4935029327	-0.0734694822
H	1.0772016827	4.2977720701	-1.8210259528
H	-1.0403267444	4.7803922131	1.4622136240
H	0.6797159745	4.3068515382	1.3107666045
H	-3.5437536762	2.2951115634	1.7040632324
H	-2.0756037332	2.1226928313	2.6987706689
H	-2.7927997988	0.6729929437	1.9461163625
H	-0.4416229092	1.3992991880	-2.3355132980
H	-1.7505211590	-0.6687303813	-1.6853983113
H	-3.4907741068	-3.9834296470	-1.0664401744
H	-2.0593248910	-2.9243203219	-0.8958476529
H	-3.0711955479	-2.8393144922	-2.3736441394
H	-5.6268714691	-4.1752912482	-0.4075364416
H	-7.6955574224	-2.2501233807	0.8918316549
H	-7.8965048961	-4.0544352681	0.5782562801
H	-4.5147707184	1.1506142166	0.2909854894
H	3.2953154827	-4.8086980499	2.3659542334
H	1.3494819017	-3.6685728693	1.5340032886
H	4.7573623567	-4.2630530430	3.2388756767
H	3.6003580805	5.1914071494	-1.5613005677
H	-0.3643415837	3.5179922993	2.5377970976

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Cartesian coordinates of the Cl<sub>2</sub> structure

Atom	x	y	z
C	7.9444701763	-3.8131995901	0.8684492548
C	6.8243569443	-2.9063165932	0.5320494545
C	5.6018438121	-2.9883066797	1.1148620587
C	4.4905912562	-2.0591407038	0.8246744944
N	3.4378561057	-2.3552814239	1.6578258224
C	3.7321903815	-3.4645923979	2.4948174333
O	2.9125458929	-3.8866248210	3.2949970414
C	5.1513413246	-3.9652091566	2.1738901675
C	5.0270730346	-5.3841376090	1.6587827856
C	4.4999667470	-1.0657342039	-0.1532842299
C	3.5326812268	-0.0594497998	-0.2807167493
N	2.6128643123	0.3438621799	0.7034800581
C	1.9038911737	1.4259305117	0.2433226675
C	2.3142762381	1.7020748057	-1.1226276626
C	1.7276388058	2.7657834235	-1.9653274897
C	3.3352001527	0.8130654234	-1.4367681202
C	4.0675327444	0.6909868602	-2.7144181134
C	0.9800955554	2.1660143914	1.0787968287
C	-0.3649872428	1.8659826074	1.1109185603
C	-1.4010320628	2.5041450522	1.9081287594
C	-1.1742239653	3.6251838454	2.8412607603
C	-2.6179927800	1.8721515273	1.6068428027
C	-3.9191651316	2.1444346544	2.2594553922
C	-2.3489531664	0.8532306929	0.6402665486
N	-0.9790344893	0.8295979677	0.4015758236
C	-3.2192142811	-0.1075917308	0.0155079152
C	-4.4748655099	0.2066344038	-0.4236762301
C	-5.4650218576	-0.7403656685	-1.0014307366
C	-5.2213534471	-2.1963960171	-1.0793899221
C	-6.5709142098	-0.0308394592	-1.3908193890
C	-7.7955898994	-0.5092137880	-1.9939384261
C	-8.7835062312	0.3338723363	-2.3186351120
C	-6.3102242950	1.4216128869	-1.0823875796
O	-7.0089516909	2.4161793750	-1.2834661988
N	-5.0409332792	1.4790050819	-0.4790283518
H	8.0693129804	-4.5361356790	0.0493988285
H	7.0307046958	-2.1421822947	-0.2325306499
H	2.5115187601	-1.9587757639	1.5889447355
H	4.4481991030	-5.4109647104	0.7261533974
H	6.0255886411	-5.7926872724	1.4626197705
H	4.5291786551	-6.0072367025	2.4100310802

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H	5.3130299750	-1.0629651261	-0.8822754116
H	2.6535684994	0.0906503746	1.6844613652
H	1.1431222135	2.3105546729	-2.7794848850
H	2.5308926340	3.3777078128	-2.4024219409
H	3.5693713277	-0.0560028575	-3.3499252126
H	5.1087391369	0.3792931458	-2.5395261140
H	4.0664588927	1.6586806724	-3.2327378892
H	1.3770923103	3.0142666144	1.6191980510
H	-0.1693115968	3.5630913749	3.2883229683
H	-1.9258497135	3.5999832103	3.6445738118
H	-4.3823240912	3.0475678664	1.8270555319
H	-3.7549454727	2.3215948863	3.3351345467
H	-4.5993193265	1.2912730462	2.1387254255
H	-0.5419109155	0.2999204727	-0.3373130342
H	-2.8393207872	-1.1242106821	-0.1039814903
H	-5.0773524797	-2.6021785037	-0.0664842132
H	-4.3193924697	-2.3926985059	-1.6813996635
H	-6.0783773339	-2.6995267692	-1.5477323596
H	-7.8675041929	-1.5905658579	-2.1656377369
H	-8.7125147885	1.3974767858	-2.1467019817
H	-9.7002288790	-0.0299676268	-2.7716087732
H	-4.5657827549	2.3301541958	-0.2289308616
H	7.7675276318	-4.3584654562	1.8050572433
H	5.7760468116	-3.9037046922	3.0935276610
H	8.8688881755	-3.2286412248	0.9662213688
H	1.0709432943	3.4038040656	-1.3618024003
H	-1.2669757579	4.5802113624	2.2978926507

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Cartesian coordinates of the Cl<sub>3</sub> structure

Atom	x	y	z
C	4.6743756851	-4.8367120925	1.0245380486
C	4.5628934142	-3.4148333321	0.6217952674
C	3.4106944725	-2.8488012600	0.2048794014
C	3.2777027899	-1.4141005562	-0.1360102280
N	1.9350740487	-1.2014706409	-0.5193186820
C	1.1617553851	-2.3316965454	-0.3652701166
O	-0.0656540597	-2.3092130639	-0.5630094231
C	2.0566761442	-3.5052472372	0.0685182498
C	2.0123743418	-4.5456953321	-1.0345121421
C	4.1901202133	-0.4078705446	-0.0152380634
C	3.7929630511	0.9736861953	-0.2281976956
N	2.5323279797	1.4190768975	0.1483120553
C	2.4030434039	2.7708239670	-0.1765321923
C	3.6075374102	3.1827030025	-0.7928753159
C	3.8885090970	4.5240513138	-1.3474983927
C	4.4770916664	2.0481625627	-0.8314646207
C	5.8310141498	1.9976355783	-1.4245849006
C	1.1766448649	3.4888426725	0.0444794047
C	-0.0200112399	2.8311841733	0.0937838235
C	-1.3498643990	3.3346269778	0.4588250932
C	-1.6081603474	4.7479115739	0.8151968618
C	-2.2374847486	2.2775882854	0.4486567808
C	-3.6823240154	2.2927677735	0.7549035842
C	-1.4977656198	1.0762590522	0.0368360621
N	-0.1602096106	1.4285403463	-0.1190570932
C	-1.9117164297	-0.2232157851	-0.1609962444
C	-3.2652455247	-0.6206441911	0.0549818525
C	-3.8363078235	-1.1312112109	1.3468639630
C	-3.0274147484	-1.2078619880	2.5786282686
C	-5.1327263059	-1.5127088166	1.1312788406
C	-6.1065054399	-2.0643245113	2.0336238127
C	-7.3433561479	-2.3914618827	1.6258905690
C	-5.4372062396	-1.2423020987	-0.3374880093
O	-6.4252506566	-1.3945223756	-1.0243535347
N	-4.2027943410	-0.6901560708	-0.8990676265
H	5.1184815243	-5.4107797050	0.1955756531
H	5.4866289588	-2.8235841308	0.6640019055
H	1.6221320777	-0.3515382443	-0.9583895447
H	2.4270480137	-4.1342075394	-1.9643292672
H	2.6084496083	-5.4192605921	-0.7428769882
H	0.9752367268	-4.8597462749	-1.2092795662

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H	5.2348788702	-0.6074340976	0.2164595402
H	1.9674166128	0.9671429895	0.8564042128
H	4.9535068556	4.7651053318	-1.2104725082
H	3.2784878276	5.2891670185	-0.8406347498
H	5.7524809998	1.8371005798	-2.5124939331
H	6.4145952888	1.1748527709	-0.9826487132
H	6.3537616904	2.9494596891	-1.2410350729
H	1.2268767514	4.5765382217	0.1377247008
H	-0.9978349720	5.0217227428	1.6860718724
H	-2.6693359572	4.9002893236	1.0595915347
H	-4.2621578569	2.0610361875	-0.1544061405
H	-3.9835048601	3.2865254411	1.1139746970
H	-3.9104333214	1.5542731417	1.5404791999
H	0.3656836279	1.0122240219	-0.8842442645
H	-1.2140719767	-1.0249213676	-0.4053420295
H	-2.1902403925	-0.5047881458	2.5216197230
H	-2.6324756197	-2.2292006810	2.6792339866
H	-3.6488152044	-0.9751085241	3.4539179059
H	-5.7777830607	-2.2044771282	3.0651738920
H	-7.6843630092	-2.2633481194	0.6067928553
H	-8.0593753624	-2.8091469649	2.3237047454
H	-4.0806734773	-0.4361555249	-1.8709075586
H	3.6930542293	-5.2682827465	1.2740701974
H	1.6911277506	-3.9212920523	1.0419170184
H	5.3318229513	-4.9204534415	1.9026264862
H	3.6560911757	4.5350628467	-2.4248486826
H	-1.3412771351	5.3910697992	-0.0344017543

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Cartesian coordinates of the Cl<sub>4</sub> structure

Atom	x	y	z
C	4.2147674600	-2.2189845400	3.2571964400
C	4.1769510100	-1.7331812200	1.8622338600
C	3.3627579700	-2.2661116700	0.9122398800
C	3.3236027500	-1.7701618500	-0.4565130900
N	2.3788392900	-2.4357022000	-1.1676448200
C	1.7111582900	-3.4028791300	-0.3475413800
O	0.7704816700	-4.0547716500	-0.7800341000
C	2.3795484100	-3.4069713700	1.0367477800
C	3.0583007800	-4.7500634700	1.2240892600
C	4.1334484600	-0.7012826100	-0.9975986100
C	3.6772685900	0.5955821200	-0.9069328000
N	2.4286445900	0.9533164000	-0.3943328500
C	2.3232947500	2.3562095600	-0.4021435100
C	3.5387720600	2.8826167000	-1.0318428400
C	3.7638180000	4.3251237400	-1.2854700700
C	4.3486665400	1.8200605600	-1.3600402800
C	5.6637537900	1.8200421800	-2.0385075800
C	1.2438363400	3.0763739700	0.0669144800
C	0.0220453000	2.4808940300	0.4644168200
C	-1.0003477700	3.0373595900	1.3009140600
C	-0.9460182300	4.3421684500	1.9938662100
C	-2.0458749700	2.0925241100	1.3868238600
C	-3.2485192800	2.2117769800	2.2415193400
C	-1.6802855800	0.9818626600	0.5684247500
N	-0.4050388000	1.2059777000	0.0786916300
C	-2.3763825200	-0.2484126900	0.2784468600
C	-3.7156348200	-0.2873719800	0.0134007500
C	-4.5243728500	-1.5130737500	-0.2391684200
C	-3.9557413600	-2.8737814700	-0.1406628500
C	-5.8057639100	-1.1332318100	-0.5396167400
C	-6.9523050600	-1.9563289100	-0.8514928300
C	-8.1437397000	-1.4110379500	-1.1292529200
C	-5.8541433200	0.3750299900	-0.5007758500
O	-6.7839609500	1.1494424300	-0.7216249200
N	-4.5613114500	0.8065833300	-0.1398224000
H	3.3565719500	-2.8615215700	3.4945155200
H	4.8576932200	-0.9121459400	1.5989238900
H	2.1800287600	-2.2817473600	-2.1481222100
H	3.8432888800	-4.8958999400	0.4706965300
H	3.5149006900	-4.7951054100	2.2210116400
H	2.3181960000	-5.5531132900	1.1329842800

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H	5.0943276500	-0.9429653300	-1.4326020900
H	1.9607487600	0.3955280000	0.3114542800
H	4.7979309900	4.4950147700	-1.6162017000
H	3.5859701100	4.8991297200	-0.3647792600
H	5.5667418600	1.3482878900	-3.0272446500
H	6.3970925400	1.2609935000	-1.4380132100
H	6.0219067500	2.8507673600	-2.1689374000
H	1.3253675000	4.1633111000	0.1476946400
H	-0.0697836800	4.9258805800	1.6735121400
H	-0.8883593400	4.1760833900	3.0806837100
H	-3.9498252700	2.9451719700	1.8100938900
H	-2.9469123100	2.5653326700	3.2402129500
H	-3.7510714700	1.2415266100	2.3447889600
H	-0.0052438000	0.6868119000	-0.6915179500
H	-1.7912782700	-1.1683533500	0.2694262800
H	-3.5958231100	-3.0516372600	0.8845839900
H	-3.1160470700	-2.9820693800	-0.8444755100
H	-4.7222528700	-3.6218786500	-0.3840465200
H	-6.7914172800	-3.0410728000	-0.8468141200
H	-8.3036131700	-0.3429165100	-1.1337666300
H	-8.9999943100	-2.0352875200	-1.3629434400
H	-4.2707027500	1.7696293700	-0.1029844500
H	4.2226965300	-1.3615048400	3.9438233300
H	1.6076762700	-3.2202150400	1.8221504400
H	5.1423133400	-2.7914237300	3.4028510300
H	3.0764628700	4.6678276400	-2.0704644300
H	-1.8592565400	4.9117118300	1.7689144000

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Cartesian coordinates of the Cl<sub>5</sub> structure

Atom	x	y	z
C	6.1805452977	-4.4592453084	1.1308152950
C	5.6598217715	-3.1256677522	0.7446208846
C	4.4380036830	-2.9386353060	0.2065030587
C	3.8857499953	-1.6061576660	-0.1363196265
N	2.5699752926	-1.7645970056	-0.5438619054
C	2.2048548385	-3.1346546031	-0.5699731423
O	1.0902966132	-3.4850863523	-0.9444153615
C	3.3891610333	-3.9834742999	-0.0910874824
C	3.7832571056	-4.9093886194	-1.2261225249
C	4.5547329800	-0.4026766908	-0.0643362330
C	3.9108929028	0.8534875953	-0.2313654651
N	2.5507156845	1.0706477432	-0.0739985758
C	2.2875645403	2.4424291513	-0.2093534373
C	3.5519973126	3.0938154519	-0.5340628307
C	3.6848555422	4.5357708592	-0.8299707629
C	4.5423057608	2.1157703244	-0.5469772001
C	5.9826800252	2.2693130107	-0.8479045023
C	1.0581732867	3.0676604195	-0.0489622447
C	-0.1769837561	2.3951352101	0.1069816281
C	-1.3999005504	3.0110906135	0.5987479600
C	-1.5093942776	4.3940934217	1.1103102055
C	-2.3755222896	2.0112011031	0.7440730910
C	-3.6726224308	2.2671698881	1.4103841243
C	-1.7466191825	0.6629664805	0.3433512727
N	-0.4364149884	1.0804510228	-0.1233582640
C	-2.7297030887	0.8131004137	-0.7600350813
C	-3.9623923893	0.1410417671	-0.6814825529
C	-4.3841325365	-0.8387502776	0.3279193586
C	-3.5482339737	-1.2418920533	1.4796328063
C	-5.6151304045	-1.3447556409	-0.0610501001
C	-6.4191405870	-2.3476573771	0.5772251150
C	-7.6034870660	-2.7227502663	0.0629401442
C	-6.0052930583	-0.6568489580	-1.3425882821
O	-7.0049416466	-0.7579877509	-2.0461616056
N	-4.9335377463	0.2267840767	-1.6573635047
H	6.8765959853	-4.8062478303	0.3528357158
H	6.3374478759	-2.2752955769	0.9097112440
H	2.0828896242	-1.0791358576	-1.1044155367
H	4.1269786676	-4.3308892648	-2.0944863876
H	4.5961988754	-5.5714556702	-0.9010784924
H	2.9201016545	-5.5185459162	-1.5190644405



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H	5.6269683067	-0.3872415257	0.1196676900
H	1.9658696964	0.4537819742	0.4804969316
H	4.7464399599	4.8170658694	-0.8683616474
H	3.1865177377	5.1306633631	-0.0490690729
H	6.2092786068	1.7982324483	-1.8162079321
H	6.5856172142	1.7885748930	-0.0615095720
H	6.2477961464	3.3352589857	-0.8977715190
H	1.0459582668	4.1591451142	-0.0135972469
H	-2.4594429748	4.8329294043	0.7716808598
H	-0.6774072317	5.0174906739	0.7508306726
H	-4.2260873225	3.0586896169	0.8817302357
H	-3.4700435905	2.6023584621	2.4391947152
H	-4.2859609427	1.3599490065	1.4503122933
H	0.2026695795	0.4255889772	-0.5444135395
H	-2.5193816365	1.3965866941	-1.6762469395
H	-2.5465348853	-0.8056985655	1.3713740629
H	-3.4904090996	-2.3402691435	1.5153253257
H	-4.0116122526	-0.8837826461	2.4134764471
H	-6.0183028958	-2.7863659886	1.4963367182
H	-8.0049999917	-2.2944396954	-0.8445389779
H	-8.2045167380	-3.4818494261	0.5526481469
H	-4.8970617144	0.8070446496	-2.4803733966
H	5.3722567235	-5.1949667775	1.2444451717
H	3.0975826341	-4.5545371105	0.8245210044
H	6.7245582892	-4.3790110607	2.0822062403
H	3.2218062584	4.7549878563	-1.8036563949
H	-1.4957624467	4.3808376250	2.2103027408

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Cartesian coordinates of the Cl<sub>6</sub> structure

Atom	x	y	z
C	0.4075767142	-3.0613227836	-1.1804713527
C	-0.3058148894	-1.7946349292	-0.9033104115
C	-1.3814528519	-1.3779595730	-1.6164958807
C	-2.1391792546	-0.1407483480	-1.3177349858
N	-3.2274873481	-0.0813376153	-2.1490294930
C	-3.2724125812	-1.1873642717	-3.0355884009
O	-4.1705312959	-1.3116766750	-3.8540762098
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