Supporting Information for:

Anabaena sensory rhodopsin is a light-driven unidirectional rotor

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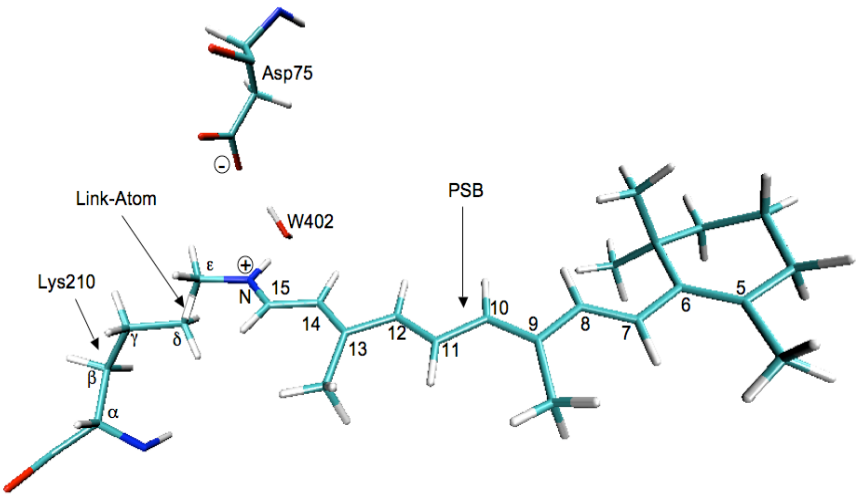
SI Computational Methods

Methodology. The QM/MM method has been fully described elsewhere (1). Briefly, the method is based on the hydrogen link-atom (HLA) approach (2). The QM part is treated at the CASPT2//CASSCF level of theory, employing the 6-31G(d) basis set and an active space comprising the full π-system (12 electrons in 12 π-orbitals) of the protonated Schiff base (PSB) retinal chromophore. The MM part is described by the AMBER96 force field (3). The QM and MM segments interact in the following way: (a) all QM atoms experience the electrostatic potential due to the MM point charges, (b) stretching, bending and torsional potentials involving at least one MM atom are modeled using the corresponding MM potential, and (c) QM and MM atom pairs separated by more than two bonds interact via either standard or reparameterized (4, 5) van der Waals potentials. The CASSCF/AMBER geometry optimizations are carried out by linking the GAUSSIAN 03 (6) and TINKER (7) programs, whereas the CASPT2 single point energy calculations are carried out with the MOLCAS 6.2 program (8).

The QM/MM Scheme. The QM/MM scheme is defined by the following Hamiltonian (in atomic units):

$$\hat{H} = \hat{H}_{QM} + \hat{H}_{MM} - \sum_A \sum_i \frac{Q_A}{|\bar{R}_A - \bar{r}_i|} + \sum_A \sum_j \frac{Q_A Z_j}{|\bar{R}_A - \bar{R}_j|} + E^{vdW}_{QM/MM} + E^{bonded}_{QM/MM}$$

where $\hat{H}_{QM}$ describes the QM segment, $\hat{H}_{MM}$ the MM segment, and the remaining terms account for interactions between the QM and MM segments. In turn, these terms represent electrostatic interaction between MM point charges and QM electrons, electrostatic interaction between MM point charges and QM nuclei, short-range van der Waals interactions, and additional parameterized potentials required to correctly describe the QM/MM frontier geometry, respectively. Note that the QM wave function is explicitly polarized by the MM point charges. In contrast, the MM point charges remain constant during the QM/MM calculations. On the other hand, the MM point charges include polarization effects in a mean-field way.

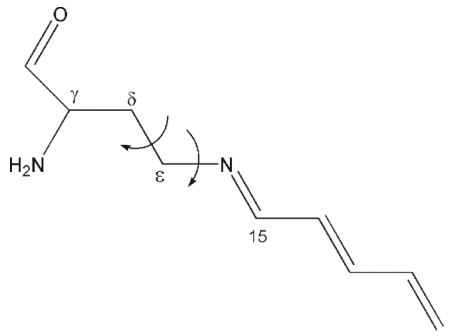


Scheme 1

The QM/MM frontier is placed at the C_ε-C_δ bond of the Lys210 side-chain (see Scheme 1 above). This choice ensures that the QM segment (comprising the full retinal chromophore and the last bond of the Lys210

side-chain) is of feasible size and that the QM/MM frontier is well separated from the "reactive" π-backbone. The QM C_ε atom is capped with a hydrogen atom (the HLA approach), to restore full valence. The link atom is throughout all calculations held fixed along the C_ε-C_δ axis, at 1 Å distance from C_ε.

A number of AMBER96 MM parameters for atoms close to the QM/MM frontier have been modified, as further detailed in previous studies (1, 4, 5). First, the charges assigned to Lys210 (totaling +1) have been reparameterized, since our QM/MM scheme requires the MM part of Lys210 to have a net charge of zero (the positive charge of Lys210 is included in the QM system). Furthermore, the charge of the C_δ atom is set to zero, to ensure that the QM wave function is not over-polarized by the HLA. This procedure is motivated by the small value of the default AMBER96 charge for this atom, and makes it possible to use standard MM bonded potentials for the description of the QM/MM frontier geometry. Second, van der Waals parameters for retinal and the C_{15}-N-C_ε-C_δ torsion potential, which are not included in AMBER96, have been determined in such a way that the CASSCF N-C_ε-C_δ-C_γ and C_{15}-N-C_ε-C_δ torsional energy profiles (both S_0 and S_1) of the model system shown in Scheme 2 below is best reproduced by the QM/MM calculations.



Scheme 2

The protein models. The models of ASR_{AT} and ASR_{13C} were built starting from the 2.0 Å resolution X-ray crystal structure reported by Vogeley et al., with PDB entry 1XIO (9). All amino acid residues were included, but neither solvent nor lipidic molecules used in the crystallization process were retained. The crystal structure includes two forms of the retinal chromophore; coordinates for both 13-*cis* (set A) and all-*trans* (set B) retinal are provided. Moreover, a specific set of Lys210 coordinates is provided for both chromophore forms. Thus, the model of ASR_{13C} includes 13-*cis* retinal and Lys210-setA, whereas the model of ASR_{AT} includes all-*trans* retinal and Lys210-setB. For all other residues the crystal structure reports only one set of coordinates. The only charged residue of the chromophore binding domain is the anionic aspartate residue (Asp75) that acts as a counterion to retinal. In order to obtain an overall uncharged QM+MM system, the protonation states of residues His21, Lys96, Lys167 and His219 were set to neutral. Finally, the protein models also include a water molecule (W402), located between retinal and Asp75, which was modeled using the TIP3P method (10).

References

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Table S1. QM/MM energies ($E_{QM/MM}$, in a.u.), oscillator strengths (f), and dipole moments (μ, in Debye) of different states of computed molecular structures

Structure	State	$E_{QM/MM}$		f	μ[c]
		CASPT2[a]	CASSCF[b]		
ASR_{AT}	S_0	-871.315886 (0.557)	-868.611579		29.5
	S_1	-871.234717 (0.549)	-868.492563	1.29	15.3
	S_2	-871.196438 (0.550)	-868.460953	0.42	23.8
ASR_{AT}-CI	S_0	-871.243612 (0.553)	-868.532199		31.8
	S_1	-871.260840 (0.550)	-868.517812	0.09	12.3
	S_2	-871.179816 (0.542)	-868.454822	0.01	33.5
ASR_{AT}-K	S_0	-871.270362 (0.556)	-868.562245		28.0
	S_1	-871.190724 (0.549)	-868.449540	1.18	13.7
	S_2	-871.151389 (0.548)	-868.410935	0.23	22.4
ASR_{AT}-L	S_0	-871.317898 (0.557)	-868.614171		29.7
	S_1	-871.234479 (0.549)	-868.491005	1.11	15.4
	S_2	-871.194118 (0.549)	-868.459061	0.29	25.6
ASR_{13C}	S_0	-871.320286 (0.557)	-868.618306		19.5
	S_1	-871.235341 (0.548)	-868.490899	1.05	35.3
	S_2	-871.194602 (0.549)	-868.460393	0.30	22.9
ASR_{13C}-CI	S_0	-871.248880 (0.554)	-868.542687		17.00
	S_1	-871.266968 (0.550)	-868.524325	0.03	37.3
	S_2	-871.184867 (0.548)	-868.466460	<0.00	16.5
ASR_{13C}-K	S_0	-871.285944 (0.556)	-868.582218		20.7
	S_1	-871.205669 (0.548)	-868.459669	1.10	34.7
	S_2	-871.164260 (0.548)	-868.427788	0.31	24.2
ASR_{13C}-L	S_0	-871.320816 (0.557)	-868.620053		19.2
	S_1	-871.237541 (0.549)	-868.494543	1.17	35.1

	S_2	-871.197913 (0.549)	-868.463985	0.43	24.5
ASR_{AT}-(-161)	S_0	-871.304296 (0.553)	-868.581666		23.5
	S_1	-871.249935 (0.550)	-868.515559	1.30	15.6
	S_2	-871.220704 (0.548)	-868.483898	0.58	25.2
ASR_{AT}-(-140)	S_0	-871.298160 (0.553)	-868.573336		22.5
	S_1	-871.245823 (0.550)	-868.510660	1.27	16.2
	S_2	-871.212987 (0.547)	-868.475189	0.52	25.5
ASR_{AT}-(-125)	S_0	-871.282503 (0.552)	-868.555613		23.2
	S_1	-871.249295 (0.549)	-868.512895	0.84	17.9
	S_2	-871.197932 (0.547)	-868.464473	0.32	28.7
ASR_{AT}-(-110)	S_0	-871.248661 (0.553)	-868.534581		31.4
	S_1	-871.259582 (0.549)	-868.515912	0.14	12.7
	S_2	-871.178620 (0.548)	-868.457161	0.01	33.8
ASR_{13C}-(21)	S_0	-871.308126 (0.553)	-868.586465		24.6
	S_1	-871.252243 (0.549)	-868.518045	1.21	32.8
	S_2	-871.222645 (0.547)	-868.486350	0.50	23.5
ASR_{13C}-(30)	S_0	-871.306761 (0.553)	-868.583735		25.0
	S_1	-871.254432 (0.549)	-868.520283	1.16	32.1
	S_2	-871.221173 (0.547)	-868.484673	0.50	23.4
ASR_{13C}-(40)	S_0	-871.302842 (0.552)	-868.578926		25.1
	S_1	-871.254982 (0.549)	-868.520979	1.07	31.1
	S_2	-871.217094 (0.547)	-868.481319	0.48	22.8
ASR_{13C}-(50)	S_0	-871.300591 (0.552)	-868.575875		25.1
	S_1	-871.255915 (0.549)	-868.521284	1.01	30.8
	S_2	-871.214900 (0.547)	-868.479634	0.44	22.2
ASR_{13C}-(60)	S_0	-871.286991 (0.552)	-868.562238		23.9
	S_1	-871.260275 (0.549)	-868.523478	0.69	30.9
	S_2	-871.202668 (0.546)	-868.473150	0.22	19.4

ASR_{13C}-(70)	S_0	-871.282818 (0.552)	-868.558731		23.3
	S_1	-871.262033 (0.549)	-868.524016	0.58	31.5
	S_2	-871.200521 (0.545)	-868.472099	0.15	18.6

[a] CASPT2(12,12)/6-31G(d) calculations with a real level shift of 0.2, reference weights in parentheses
[b] CASSCF(12,12)/6-31G(d) three-root state-average calculations with equal weights (1/3) for S_0, S_1 and S_2
[c] Obtained using CASSCF wavefunctions and standard Mulliken population analysis

Table S2. CASSCF/AMBER vibrational frequencies (in cm^{-1}) for Schiff base N-D stretching in different states of ASR[a]

State	Scheme A[b]	Scheme B[c]	Exp[d]
ASR_{AT}	2654	2609	2163, 2125
ASR_{AT}-K	2754	2720	2483
ASR_{AT}-L	2692	2622	
ASR_{13C}	2702	2632	2165
ASR_{13C}-K	2751	2689	2351
ASR_{13C}-L	2655	2605	

[a] Note that no empiric scaling parameters have been used in the calculations to, as often done, improve the agreement with the experimental data
[b] Obtained by fitting CASSCF/AMBER energies of structures distorted from equilibrium (with respect to the N-H bond length) to a second-order polynomial, using CASSCF(12,12)/6-31G(d) for the QM system
[c] Obtained by performing numerical CASSCF/AMBER frequency calculations, using CASSCF(8,8)/3-21G(d) for the QM system
[d] Experimental data from (24)

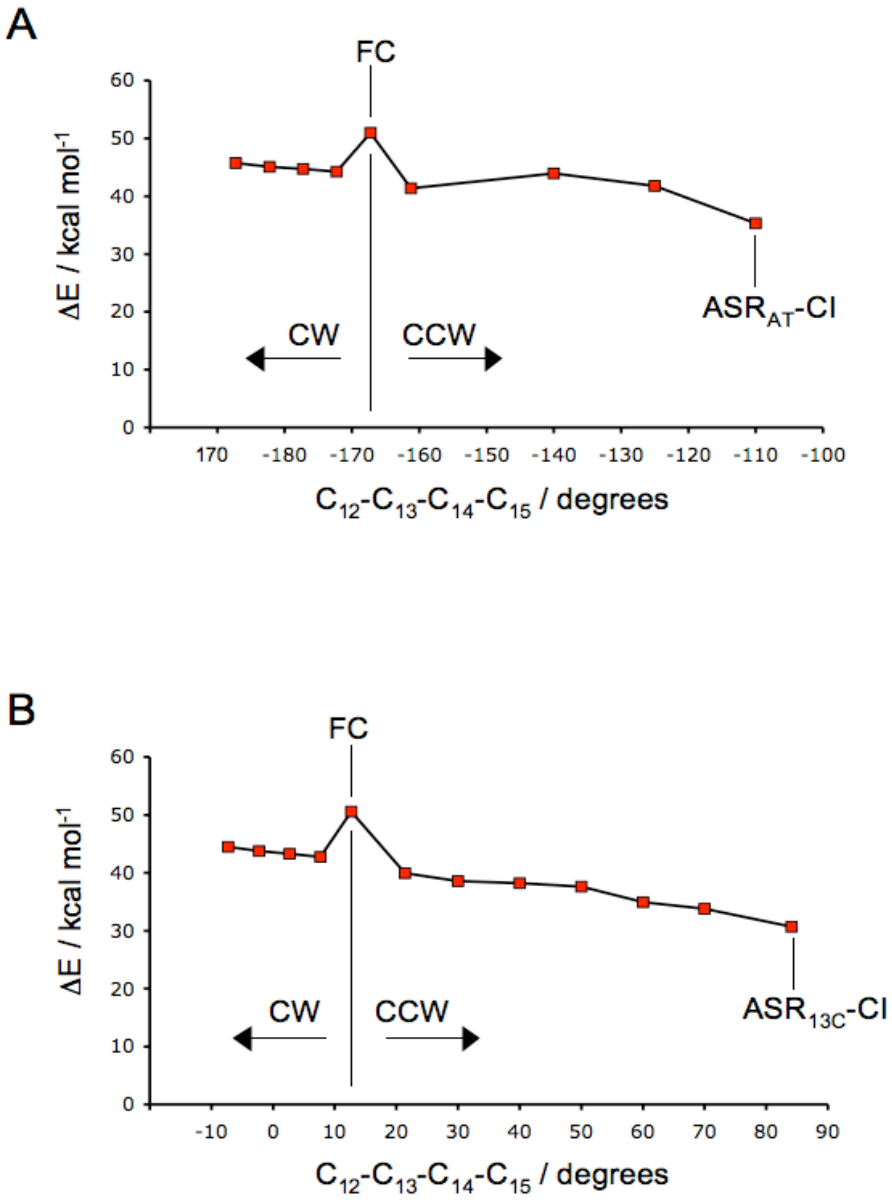

Fig. S1 (*A*) CASPT2//CASSCF/AMBER S_1 energy profile for CCW and limited CW C13=C14 torsional motion starting from the Franck-Condon (FC) point of ASR_{AT}. (*B*) The corresponding energy profile for ASR_{13C}. Notably, for both ASR_{AT} and ASR_{13C}, the CW motion is energetically less favorable.

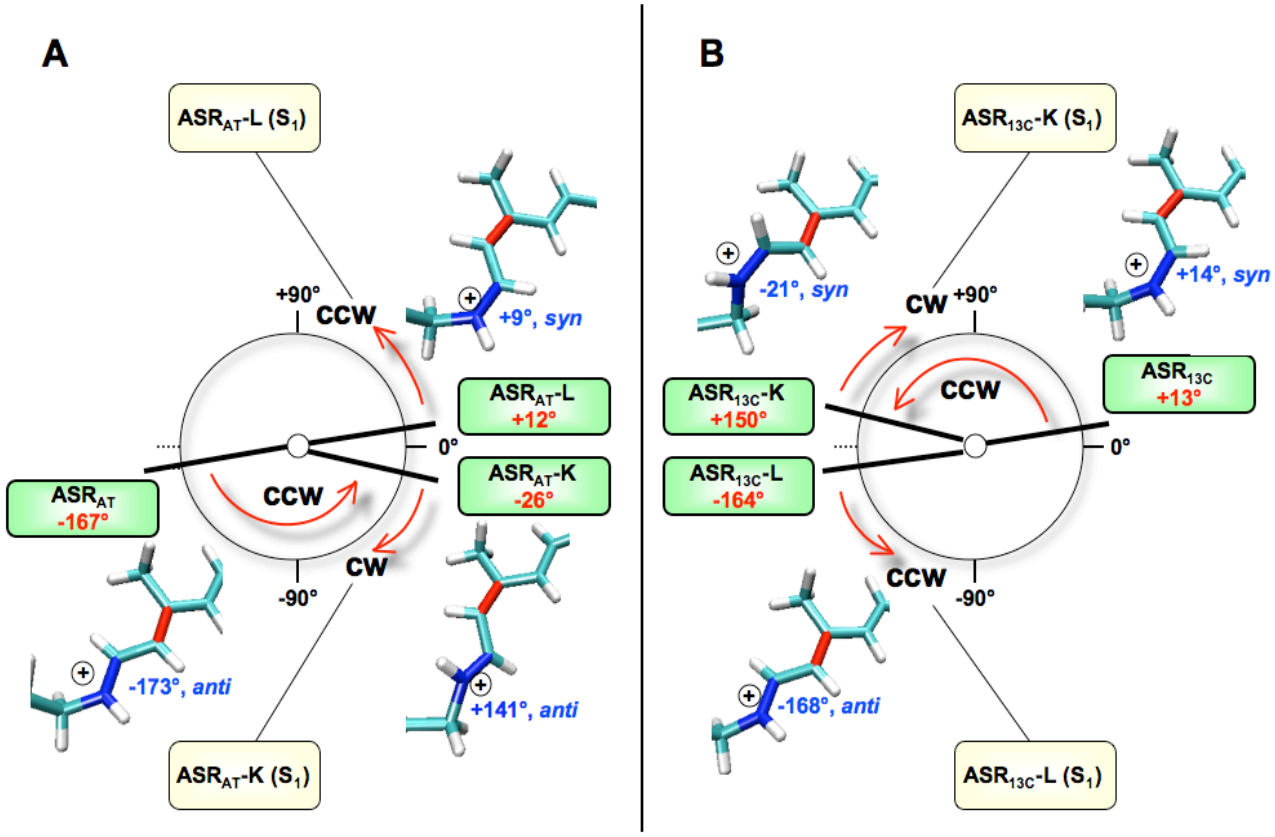

Fig. S2 (*A*) C13=C14 Newman projections highlighting the influence of C15=N geometry (*syn* or *anti*) on the direction (CCW or CW) of C13=C14 photoisomerization in the parent, K and L states of ASR_{AT}. Isomerization directions are determined by excited state geometry optimizations and are indicated by red curly arrows. Structural data are also reported: C15=N dihedrals in blue font and C13=C14 dihedrals in red font. Notably, photoisomerization in the K state (C15=N *anti* with M helicity) would occur in a direction opposite (i.e., CW) to that in the parent state, whereas photoisomerization in the L state (C15=N *syn* with P helicity) would occur in the same direction (i.e., CCW). (*B*) The corresponding data for ASR_{13C}. Notably, photoisomerization in the K state (C15=N *syn* with M helicity) would occur in a direction opposite (i.e., CW) to that in the parent state, whereas photoisomerization in the L state (C15=N *anti* with P helicity) would occur in the same direction (i.e., CCW). Taken together, this data (panels A and B) show that the thermal K→L transition is required for the molecular rotor function of ASR.

SI Molecular Structures

Cartesian coordinates (in Å) of computed molecular structures obtained at the CASSCF(12,12)/6-31G(d)/AMBER level of theory, together with AMBER charges of the MM atoms. Atoms in bold font have been kept frozen in the calculations. Atom HLA denotes the hydrogen link atom.

ASR_{AT}

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.775051	-1.194053	7.880010	.22455
H	-5.999425	-3.108739	9.267852	.14260
C	-6.505648	-1.248707	10.244308	-.00940
C	-5.086848	-0.692040	10.079462	.01870
C	-4.904893	0.329141	8.963841	.00000
C	-3.438499	0.776910	8.996314	
N	-3.072447	1.460917	7.756612	
H	-6.551699	-1.593702	11.279825	.03620
H	-7.241183	-0.450359	10.154021	.03620
H	-4.403551	-1.521131	9.901933	.01030
H	-4.807042	-0.208359	11.017243	.01030
H	-5.556087	1.188550	9.127664	.06210
H	-5.145156	-0.144018	8.009407	.06210
H	-2.792494	-0.080227	9.110551	
H	-3.267867	1.445995	9.824446	
H	-3.041752	2.474565	7.776553	
C	2.540743	5.211347	-1.831143	
C	3.172906	6.214507	-2.820007	
C	4.396674	5.663855	-3.535128	
C	3.974632	4.477798	-4.383851	
C	3.076545	3.509052	-3.646378	
C	2.441859	3.809400	-2.479220	

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C    1.668216    2.737042   -1.821504
C    1.181298    2.710416   -0.564673
C    0.448208    1.611647    0.057930
C    0.012059    1.857067    1.320043
C   -0.779254    1.012576    2.175397
C   -1.205887    1.488720    3.368851
C   -1.967674    0.753581    4.351076
C   -2.267164    1.426585    5.500918
C   -2.771359    0.818807    6.678633
C    3.409569    5.173525   -0.554989
C    1.148419    5.788837   -1.493606
C    2.984677    2.169323   -4.352137
C    0.176650    0.335307   -0.701244
C   -2.372342   -0.668090    4.046421
H    3.455950    4.830620   -5.272887
H    4.845362    3.946254   -4.758195
H    4.838325    6.430614   -4.162578
H    5.160511    5.364288   -2.823124
H    3.406682    7.130384   -2.286606
H    2.432263    6.482334   -3.570201
H    0.667374    5.316719   -0.647950
H    1.246531    6.845388   -1.268012
H    0.477142    5.703956   -2.341005
H    3.013902    4.527475    0.216128
H    4.415286    4.827638   -0.766272
H    3.476443    6.173574   -0.132761
H    2.059392    1.632551   -4.195274
H    3.077874    2.331779   -5.421188
H    3.802800    1.511742   -4.061516
H    1.507950    1.854730   -2.405220
H    1.319607    3.550900    0.079520
H    0.248796    2.818062    1.744940
H   -1.033048    0.020474    1.856717
H   -0.927173    2.492064    3.641655
H   -1.985561    2.460894    5.578029
H   -0.175813   -0.455231   -0.052850
H   -0.572485    0.487433   -1.472446
H    1.076946   -0.020500   -1.189175
H   -2.884018   -1.160444    4.862138
H   -3.037940   -0.668560    3.191425
H   -1.508576   -1.265095    3.782721
H   -2.872215   -0.248472    6.735849
O   -3.319321    4.290919    8.208171     -.83400
H   -3.920111    5.034593    8.374465      .41700
H   -2.794977    4.341844    9.055608      .41700
HLA -4.394685    0.484917    8.975142
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ASR_{AT}-CI

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.780978	-1.197009	7.881732	.22455
H	-6.002977	-3.113063	9.263052	.14260
C	-6.482521	-1.252505	10.246469	-.00940
C	-5.060627	-0.682256	10.084406	.01870
C	-4.906580	0.372979	8.994624	.00000
C	-3.461379	0.907385	8.942929	
N	-3.204123	1.462535	7.616318	
H	-6.521305	-1.606944	11.278811	.03620
H	-7.220591	-0.454155	10.171461	.03620
H	-4.370824	-1.497829	9.873363	.01030
H	-4.772769	-0.218423	11.029996	.01030
H	-5.588927	1.202526	9.189623	.06210
H	-5.172012	-0.089431	8.041768	.06210
H	-2.759772	0.104109	9.125506	
H	-3.322344	1.673462	9.696607	
H	-3.642810	2.364152	7.424476	
C	2.411036	5.256052	-1.707421	
C	2.934851	6.297242	-2.722368	
C	4.211284	5.851073	-3.419136	
C	3.901002	4.617382	-4.250288	
C	3.064287	3.594182	-3.515183	
C	2.406613	3.847345	-2.343127	
C	1.700028	2.725086	-1.708931	
C	1.289386	2.587932	-0.406530	
C	0.629863	1.459642	0.166834	
C	0.203556	1.596560	1.508577	
C	-0.550294	0.704892	2.241124	
C	-1.091022	1.079488	3.520108	
C	-2.083325	0.423514	4.175122	

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C   -2.744717    1.123056    5.294141
C   -2.576487    0.816061    6.657198
C    3.304727    5.303895   -0.450206
C    0.983278    5.701879   -1.335485
C    3.041013    2.244209   -4.206431
C    0.316430    0.217847   -0.626081
C   -2.681034   -0.865968    3.656861
H    3.372158    4.909446   -5.155871
H    4.817444    4.148555   -4.598386
H    4.595657    6.642164   -4.054302
H    4.990710    5.628062   -2.696499
H    3.070403    7.245927   -2.214810
H    2.173022    6.465030   -3.480461
H    0.571024    5.155756   -0.496747
H    0.992204    6.755310   -1.079162
H    0.306438    5.575808   -2.173465
H    2.913802    4.710641    0.365692
H    4.304951    4.939278   -0.654468
H    3.379553    6.328266   -0.095572
H    2.043405    1.830333   -4.299187
H    3.438521    2.344500   -5.208373
H    3.655174    1.512563   -3.688286
H    1.521495    1.887628   -2.344922
H    1.456621    3.390630    0.276799
H    0.455027    2.523852    1.990827
H   -0.822096   -0.235949    1.819014
H   -0.756413    2.027031    3.903492
H   -3.514427    1.844869    5.028839
H    0.351524   -0.664208    0.000195
H   -0.675532    0.277116   -1.063166
H    1.018835    0.074811   -1.434837
H   -3.398327   -1.291567    4.346181
H   -3.173110   -0.710337    2.701732
H   -1.912094   -1.616282    3.496928
H   -1.980133   -0.031116    6.965805
O   -3.392940    4.343830    8.179262     -.83400
H   -3.893618    5.157027    8.351952      .41700
H   -2.848939    4.325791    9.012455      .41700
HLA -4.398775    0.560738    8.976467
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ASR_{AT}-K

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.779231	-1.196158	7.882159	.22455
H	-6.008673	-3.120059	9.257130	.14260
C	-6.452698	-1.263089	10.253543	-.00940
C	-5.037499	-0.662139	10.071104	.01870
C	-4.989395	0.449886	9.026292	.00000
C	-3.609289	1.108171	8.780917	
N	-3.462444	1.240582	7.321395	
H	-6.467379	-1.635748	11.279913	.03620
H	-7.201705	-0.472249	10.211346	.03620
H	-4.339488	-1.452138	9.795945	.01030
H	-4.722127	-0.230891	11.022924	.01030
H	-5.685936	1.232675	9.325086	.06210
H	-5.359014	0.001878	8.099541	.06210
H	-2.815931	0.477646	9.153705	
H	-3.564757	2.075945	9.262840	
H	-4.333808	1.359720	6.839805	
C	2.380712	5.245430	-1.655581	
C	2.875165	6.249842	-2.718545	
C	4.151917	5.792314	-3.409032	
C	3.857341	4.517532	-4.182579	
C	3.016282	3.524191	-3.410610	
C	2.369833	3.819876	-2.252663	
C	1.614315	2.728660	-1.583546	
C	1.445710	2.527584	-0.259658	
C	0.650791	1.454321	0.343957	
C	0.330413	1.587995	1.662594	
C	-0.604693	0.741165	2.357128	
C	-1.122056	0.964979	3.593992	
C	-2.233130	0.165528	4.072680	

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C   -2.883750    0.329583    5.258403
C   -2.500558    0.873238    6.538727
C    3.301100    5.342381   -0.418341
C    0.960779    5.692545   -1.259485
C    2.987337    2.150461   -4.058370
C    0.179919    0.303323   -0.525476
C   -2.800400   -0.904455    3.171805
H    3.342133    4.760708   -5.109914
H    4.778758    4.033367   -4.493380
H    4.520050    6.559096   -4.082540
H    4.942146    5.618584   -2.684220
H    3.000750    7.222040   -2.255503
H    2.101363    6.373929   -3.472948
H    0.552832    5.125887   -0.430934
H    0.981070    6.739756   -0.973466
H    0.274867    5.600034   -2.095737
H    2.880465    4.863644    0.456327
H    4.273127    4.894844   -0.597370
H    3.449590    6.387592   -0.158096
H    1.988176    1.739494   -4.154019
H    3.402172    2.213521   -5.058050
H    3.586317    1.428000   -3.511011
H    1.166956    2.005877   -2.239491
H    1.876259    3.209460    0.444338
H    0.698680    2.443751    2.202461
H   -0.971869   -0.100041    1.809617
H   -0.782816    1.795899    4.189941
H   -3.833848   -0.166462    5.342597
H   -0.031997   -0.588751    0.050059
H   -0.714843    0.555952   -1.089249
H    0.946294    0.040935   -1.244755
H   -3.692384   -1.341519    3.601416
H   -3.049412   -0.539923    2.184810
H   -2.069122   -1.694249    3.055307
H   -1.505958    0.818599    6.946861
O   -3.382647    4.490300    8.182292     -.83400
H   -3.898940    5.280573    8.396371      .41700
H   -2.846470    4.411432    9.011230      .41700
HLA -4.500463    0.683082    8.939374
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ASR_{AT}-L

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.773032	-1.192766	7.881745	.22455
H	-6.014515	-3.127104	9.254645	.14260
C	-6.427503	-1.246085	10.199406	-.00940
C	-5.001572	-0.734239	9.911078	.01870
C	-4.833806	0.282055	8.774951	.00000
C	-3.337661	0.623689	8.655109	
N	-3.096329	1.681301	7.666140	
H	-6.416546	-1.579088	11.239099	.03620
H	-7.148463	-0.431471	10.142871	.03620
H	-4.359972	-1.590371	9.708036	.01030
H	-4.637737	-0.255558	10.821756	.01030
H	-5.404313	1.183045	9.011559	.06210
H	-5.192931	-0.147343	7.838096	.06210
H	-2.775857	-0.257828	8.390343	
H	-2.967611	0.992037	9.600862	
H	-3.135073	2.630256	8.013858	
C	2.298192	5.203132	-1.522183	
C	2.817682	6.203600	-2.579108	
C	4.079317	5.723906	-3.279462	
C	3.765835	4.448944	-4.046458	
C	2.916246	3.463402	-3.267692	
C	2.268441	3.771364	-2.108319	
C	1.520722	2.688343	-1.419959	
C	1.113595	2.626775	-0.129395	
C	0.346333	1.537952	0.488527	
C	-0.142603	1.749029	1.745213	
C	-1.001963	0.841576	2.475333	
C	-1.509482	1.090730	3.711569	
C	-2.347202	0.135785	4.424573	

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C   -2.823990    0.313371    5.694704
C   -2.795549    1.551658    6.410502
C    3.215884    5.278155   -0.282021
C    0.882720    5.687846   -1.143710
C    2.867169    2.090358   -3.921132
C    0.087846    0.268565   -0.295222
C   -2.692113   -1.161208    3.740721
H    3.249819    4.695479   -4.973378
H    4.685585    3.955977   -4.352906
H    4.449491    6.485213   -3.958337
H    4.871160    5.539764   -2.559335
H    2.972824    7.167593   -2.105155
H    2.045109    6.357800   -3.329292
H    0.469657    5.185908   -0.278830
H    0.917118    6.750244   -0.924442
H    0.188983    5.551722   -1.967309
H    2.850779    4.689032    0.549076
H    4.216337    4.924176   -0.503485
H    3.288027    6.308051    0.059685
H    1.862330    1.689529   -3.998285
H    3.262241    2.153188   -4.928812
H    3.472005    1.362441   -3.387094
H    1.294684    1.838484   -2.034069
H    1.319322    3.440689    0.533819
H    0.092152    2.681089    2.232610
H   -1.256286   -0.079962    1.992510
H   -1.231892    2.006676    4.202846
H   -3.338798   -0.502248    6.166533
H   -0.113417   -0.573755    0.352708
H   -0.752643    0.380759   -0.974979
H    0.954035    0.007867   -0.890247
H   -3.358636   -1.759324    4.348747
H   -3.187589   -0.972123    2.795638
H   -1.810833   -1.755408    3.528541
H   -2.531133    2.457826    5.914060
O   -3.359973    4.443087    8.218378     -.83400
H   -3.928414    5.215416    8.375793      .41700
H   -2.840380    4.460982    9.069092      .41700
HLA -4.309605    0.401735    8.732961
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ASR_{13C}

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.526994	-4.764040	10.942348	.22455
H	-8.717293	-6.739851	12.229213	.14260
C	-9.020249	-4.801072	13.095634	-.00940
C	-7.754722	-4.271344	12.395425	.01870
C	-7.173001	-3.032185	13.076270	.00000
C	-5.808295	-2.656026	12.470445	
N	-5.934708	-1.766408	11.310702	
H	-8.774089	-5.078928	14.120593	.03620
H	-9.784904	-4.024371	13.128730	.03620
H	-7.974232	-4.030049	11.354771	.01030
H	-7.000501	-5.054168	12.424523	.01030
H	-7.031278	-3.259586	14.135365	.06210
H	-7.876537	-2.207862	12.990814	.06210
H	-5.270108	-3.543764	12.183710	
H	-5.217772	-2.111465	13.195329	
H	-6.016190	-0.780912	11.524685	
C	-0.867829	1.527060	1.809426	
C	-0.380480	2.418064	0.644926	
C	0.841517	1.858908	-0.066471	
C	0.486942	0.515797	-0.686636	
C	-0.362137	-0.371522	0.202844	
C	-0.958188	0.053195	1.353605	
C	-1.702802	-0.958270	2.145970	
C	-2.105065	-0.950737	3.440731	
C	-2.850804	-2.046120	4.084587	
C	-3.336845	-1.839747	5.342470	
C	-4.115829	-2.782993	6.120628	
C	-4.581405	-2.542854	7.374950	
C	-5.263901	-3.551692	8.180774	

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C   -5.698260   -3.338620    9.460595
C   -5.770779   -2.037370   10.059954
C    0.106724    1.675093    2.997469
C   -2.252195    2.079235    2.208857
C   -0.489538   -1.789969   -0.336013
C   -3.064224   -3.323901    3.302084
C   -5.441272   -4.934738    7.602249
H   -0.189686    3.418112    1.021278
H   -1.185332    2.516946   -0.080927
H    1.176146    2.543641   -0.838385
H    1.668567    1.741466    0.627435
H    1.390357   -0.027653   -0.954615
H   -0.044412    0.674630   -1.624925
H    0.196230    2.722786    3.275013
H   -0.228146    1.132132    3.873313
H    1.096037    1.307029    2.751526
H   -2.181139    3.154200    2.346310
H   -2.985271    1.905661    1.426948
H   -2.635559    1.656425    3.128280
H   -0.037222   -1.854404   -1.318927
H    0.018486   -2.513802    0.293889
H   -1.520164   -2.113628   -0.439845
H   -1.933540   -1.848801    1.597008
H   -1.913182   -0.106732    4.073820
H   -3.137614   -0.890417    5.811833
H   -4.318098   -3.736071    5.676580
H   -4.355165   -1.592150    7.825402
H   -6.064500   -4.167751   10.036429
H   -5.747454   -1.174960    9.423096
H   -5.921045   -5.593382    8.314263
H   -6.055134   -4.896437    6.708812
H   -4.493050   -5.375061    7.317020
H   -3.504717   -4.113853    3.891881
H   -3.707813   -3.153155    2.444071
H   -2.115773   -3.696757    2.931992
O   -6.026424    1.029935   11.433211     -.83400
H   -6.561891    1.840148   11.461837      .41700
H   -5.534945    1.122580   12.289983      .41700
HLA -6.694584   -2.900317   12.863909
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ASR_{13C}-CI

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.531088	-4.766266	10.943138	.22455
H	-8.716379	-6.738875	12.229024	.14260
C	-9.033525	-4.818940	13.134787	-.00940
C	-7.751130	-4.278528	12.485561	.01870
C	-7.133648	-3.108288	13.261365	.00000
C	-5.905581	-2.535740	12.527623	
N	-6.325443	-1.831918	11.317948	
H	-8.814716	-5.120240	14.159640	.03620
H	-9.795827	-4.039279	13.164641	.03620
H	-7.979397	-3.963435	11.467560	.01030
H	-7.014878	-5.077888	12.447555	.01030
H	-6.824586	-3.464537	14.245451	.06210
H	-7.883725	-2.332156	13.405103	.06210
H	-5.225697	-3.336383	12.282599	
H	-5.378353	-1.833356	13.165611	
H	-6.774167	-0.925385	11.471072	
C	-0.838579	1.520072	1.810042	
C	-0.352668	2.450778	0.675774	
C	0.875937	1.921653	-0.046951	
C	0.524601	0.602978	-0.718016	
C	-0.308027	-0.321400	0.141306	
C	-0.907816	0.059285	1.309719	
C	-1.620953	-0.986330	2.062192	
C	-2.049934	-1.029534	3.362230	
C	-2.752610	-2.139299	3.944295	
C	-3.189442	-2.000742	5.273321	
C	-3.979071	-2.880878	5.993060	
C	-4.304668	-2.642676	7.365789	
C	-5.130507	-3.412070	8.127504	

```
C   -5.237339   -3.150122    9.574988
C   -6.115507   -2.157586   10.064777
C    0.124511    1.642757    3.010279
C   -2.233793    2.043318    2.212126
C   -0.411618   -1.724485   -0.435244
C   -3.023228   -3.381972    3.136659
C   -5.880765   -4.600679    7.570338
H   -0.172456    3.439466    1.084341
H   -1.154667    2.564786   -0.050525
H    1.214823    2.634155   -0.790283
H    1.697405    1.776125    0.647860
H    1.426458    0.074288   -1.015822
H   -0.019616    0.793678   -1.642209
H    0.205093    2.682031    3.317713
H   -0.215884    1.072803    3.866958
H    1.116859    1.285158    2.762492
H   -2.180950    3.115182    2.373169
H   -2.957832    1.873714    1.421340
H   -2.616537    1.593636    3.119629
H    0.012132   -1.746016   -1.431242
H    0.134871   -2.448452    0.161372
H   -1.435282   -2.074510   -0.516340
H   -1.806059   -1.874828    1.502321
H   -1.892415   -0.197791    4.016594
H   -2.890807   -1.102176    5.780974
H   -4.354636   -3.761363    5.526021
H   -3.821274   -1.794863    7.817986
H   -4.527967   -3.635678   10.241813
H   -6.633368   -1.549253    9.337576
H   -6.516715   -5.062016    8.314761
H   -6.496317   -4.326271    6.720032
H   -5.193215   -5.365097    7.218279
H   -3.368891   -4.198107    3.751615
H   -3.763335   -3.197624    2.364821
H   -2.115271   -3.714643    2.648757
O   -6.174193    0.978861   11.458840     -.83400
H   -6.594821    1.853247   11.490658      .41700
H   -5.616418    1.024657   12.274639      .41700
HLA -6.702561   -2.907303   13.003819
```

ASR_{13C}-K

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.541469	-4.772058	10.944915	.22455
H	-8.731347	-6.755630	12.221219	.14260
C	-8.999256	-4.855939	13.167860	-.00940
C	-7.637761	-4.442711	12.594133	.01870
C	-7.002167	-3.213951	13.284022	.00000
C	-6.062167	-2.421550	12.345171	
N	-6.842767	-2.021040	11.171712	
H	-8.869126	-5.162242	14.207214	.03620
H	-9.700701	-4.021585	13.141201	.03620
H	-7.785191	-4.269982	11.531115	.01030
H	-6.946368	-5.274941	12.679937	.01030
H	-6.443601	-3.548786	14.159819	.06210
H	-7.795278	-2.551350	13.639610	.06210
H	-5.236968	-3.040875	12.029209	
H	-5.665532	-1.550463	12.852424	
H	-7.795138	-1.786298	11.384025	
C	-0.726279	1.534774	1.591517	
C	-0.289624	2.491214	0.459517	
C	0.971860	2.027539	-0.253017	
C	0.709379	0.687210	-0.924431	
C	-0.103957	-0.272930	-0.080303	
C	-0.743890	0.077783	1.067760	
C	-1.497473	-0.988142	1.786272	
C	-1.734222	-1.097248	3.112706	
C	-2.549982	-2.128319	3.772586	
C	-2.815257	-1.928396	5.094247	
C	-3.750944	-2.639482	5.943174	
C	-3.967153	-2.253993	7.230194	
C	-5.060504	-2.714002	8.068327	

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C   -5.242389   -2.173802    9.310448
C   -6.549035   -2.083801    9.920126
C    0.247936    1.696974    2.780188
C   -2.130103    1.998933    2.029810
C   -0.162173   -1.680467   -0.654207
C   -3.070251   -3.295603    2.963732
C   -5.972026   -3.808766    7.575252
H   -0.161819    3.488688    0.868035
H   -1.093324    2.562884   -0.270888
H    1.277698    2.756562   -0.995283
H    1.793681    1.936123    0.450892
H    1.648764    0.208960   -1.191444
H    0.186985    0.845881   -1.867429
H    0.336785    2.748841    3.040988
H   -0.091622    1.175869    3.666790
H    1.237121    1.321378    2.546003
H   -2.102177    3.063293    2.245313
H   -2.860555    1.852439    1.239681
H   -2.488594    1.491407    2.916922
H    0.393054   -1.729919   -1.583638
H    0.271669   -2.413306    0.018481
H   -1.177835   -2.000300   -0.870333
H   -1.880789   -1.771718    1.158965
H   -1.358030   -0.347886    3.779812
H   -2.349540   -1.077828    5.562333
H   -4.335087   -3.430137    5.511972
H   -3.362582   -1.461895    7.638545
H   -4.487650   -1.557921    9.757345
H   -7.385474   -1.930915    9.261037
H   -6.836402   -3.932284    8.219542
H   -6.311473   -3.637624    6.564388
H   -5.430461   -4.748479    7.589247
H   -3.531346   -4.052643    3.583716
H   -3.793883   -2.985417    2.215512
H   -2.251936   -3.772325    2.433632
O   -6.014478    0.996942   11.337905     -.83400
H   -6.517557    1.815645   11.449616      .41700
H   -5.516344    0.978569   12.187722      .41700
HLA -6.669823   -2.933787   12.952104
```

ASR_{13C}-L

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.529580	-4.765354	10.942442	.22455
H	-8.703206	-6.724529	12.239344	.14260
C	-9.078787	-4.797987	13.116266	-.00940
C	-7.791551	-4.264384	12.478745	.01870
C	-7.440135	-2.877920	13.013612	.00000
C	-5.966678	-2.579924	12.710074	
N	-5.783686	-2.068077	11.349706	
H	-8.877145	-5.062757	14.155348	.03620
H	-9.856565	-4.033841	13.105087	.03620
H	-7.897793	-4.197771	11.395444	.01030
H	-6.985415	-4.961577	12.704303	.01030
H	-7.599200	-2.855472	14.095204	.06210
H	-8.090454	-2.145320	12.535341	.06210
H	-5.381038	-3.477120	12.833496	
H	-5.582990	-1.825998	13.379779	
H	-5.772604	-1.056889	11.265796	
C	-0.641728	1.596666	1.403898	
C	-0.163834	2.541832	0.279094	
C	1.112012	2.064122	-0.397393	
C	0.861756	0.718728	-1.061803	
C	0.031475	-0.232068	-0.225373	
C	-0.655258	0.136920	0.890452	
C	-1.429223	-0.922782	1.589412	
C	-1.786581	-0.992684	2.890478	
C	-2.562072	-2.072999	3.518095	
C	-2.983665	-1.843511	4.790412	
C	-3.827877	-2.659454	5.639671	
C	-4.188967	-2.186612	6.859890	
C	-4.939434	-2.880693	7.890681	

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C   -5.133878   -2.204158    9.061038
C   -5.543586   -2.779932   10.302795
C    0.301547    1.748998    2.617548
C   -2.049809    2.086350    1.800480
C   -0.006026   -1.647328   -0.782029
C   -2.883373   -3.324245    2.733890
C   -5.430813   -4.285552    7.645454
H   -0.037939    3.539968    0.686674
H   -0.947269    2.616381   -0.472735
H    1.439300    2.782779   -1.140432
H    1.916332    1.977115    0.326909
H    1.806534    0.239588   -1.305651
H    0.357966    0.868051   -2.016294
H    0.369987    2.796639    2.900958
H   -0.049379    1.201344    3.483909
H    1.300310    1.390536    2.397544
H   -2.018796    3.159993    1.960698
H   -2.772826    1.902555    1.012024
H   -2.424907    1.628899    2.707384
H    0.699267   -1.747862   -1.598230
H    0.258692   -2.391647   -0.039276
H   -0.987800   -1.909323   -1.169715
H   -1.715988   -1.751339    0.969814
H   -1.526341   -0.195880    3.558293
H   -2.688986   -0.909632    5.238348
H   -4.166053   -3.618429    5.293540
H   -3.814010   -1.217557    7.140478
H   -4.811882   -1.180222    9.114873
H   -5.599023   -3.844774   10.426877
H   -5.877176   -4.735171    8.523429
H   -6.182160   -4.282650    6.862253
H   -4.618754   -4.919467    7.313583
H   -3.257979   -4.115080    3.370262
H   -3.624905   -3.135501    1.962262
H   -1.992243   -3.700447    2.242750
O   -5.967892    0.762315   11.447103     -.83400
H   -6.601568    1.490791   11.534507      .41700
H   -5.463368    0.897582   12.291912      .41700
HLA -6.927443   -2.774223   12.908011
```

ASR_{AT}-(-161) Structure along the photoisomerization path of ASR_{AT} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of -161°

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.762119	-1.187748	7.878728	.22455
H	-5.997793	-3.106321	9.266548	.14260
C	-6.502454	-1.248131	10.243021	-.00940
C	-5.082233	-0.688876	10.081239	.01870
C	-4.901988	0.342803	8.973921	.00000
C	-3.448480	0.828267	9.007722	
N	-3.099880	1.523888	7.787061	
H	-6.550027	-1.592622	11.278361	.03620
H	-7.237710	-0.449625	10.153035	.03620
H	-4.396646	-1.514416	9.897479	.01030
H	-4.803528	-0.212238	11.023064	.01030
H	-5.568270	1.189728	9.138455	.06210
H	-5.128130	-0.125138	8.013815	.06210
H	-2.785934	-0.017624	9.133345	
H	-3.302756	1.492000	9.846914	
H	-3.102684	2.528169	7.798362	
C	2.512512	5.362729	-1.710517	
C	3.128468	6.423024	-2.652503	
C	4.388413	5.945605	-3.355946	
C	4.028468	4.783902	-4.266318	
C	3.160688	3.746600	-3.594450	
C	2.495568	3.968899	-2.391218	
C	1.831632	2.849525	-1.806964	
C	1.228115	2.761508	-0.533066	
C	0.579336	1.669332	0.010860	
C	0.033501	1.879719	1.353396	
C	-0.728466	1.038562	2.086146	
C	-1.226161	1.474116	3.398381	

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C   -1.973208    0.760960    4.278601
C   -2.351560    1.452386    5.507112
C   -2.772998    0.863808    6.670480
C    3.342195    5.323509   -0.411150
C    1.083828    5.861763   -1.410553
C    3.106945    2.436505   -4.352172
C    0.350009    0.357450   -0.695553
C   -2.434286   -0.652225    3.996304
H    3.498329    5.154136   -5.144668
H    4.920674    4.302099   -4.659464
H    4.821138    6.753653   -3.936644
H    5.146375    5.640511   -2.639856
H    3.312687    7.327147   -2.081940
H    2.396487    6.695252   -3.409116
H    0.586859    5.334303   -0.607971
H    1.129233    6.908973   -1.133658
H    0.453227    5.793953   -2.290097
H    2.935371    4.662365    0.341678
H    4.359768    4.996678   -0.596596
H    3.380504    6.319084    0.023278
H    2.122709    1.983857   -4.372658
H    3.401406    2.610624   -5.380863
H    3.804825    1.708478   -3.940221
H    1.816808    1.948154   -2.386391
H    1.266743    3.619138    0.099910
H    0.247942    2.841093    1.786386
H   -0.993556    0.064801    1.724492
H   -0.955494    2.477368    3.674879
H   -2.193081    2.516405    5.517977
H    0.408799   -0.468786    0.004727
H   -0.639423    0.336376   -1.148582
H    1.074000    0.179874   -1.479409
H   -2.756501   -1.170468    4.891154
H   -3.274560   -0.636682    3.309144
H   -1.651505   -1.249108    3.545479
H   -2.842040   -0.202041    6.754862
O   -3.329645    4.404312    8.192374     -.83400
H   -3.933563    5.131281    8.401808      .41700
H   -2.815355    4.381769    9.044407      .41700
HLA -4.396739    0.511535    8.985673
```

ASR_{AT}-(-140) Structure along the photoisomerization path of ASR_{AT} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of -140°

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.762150	-1.187771	7.878616	.22455
H	-6.003542	-3.113588	9.262860	.14260
C	-6.485726	-1.253520	10.241221	-.00940
C	-5.053463	-0.731139	10.071276	.01870
C	-4.858493	0.289912	8.961160	.00000
C	-3.382286	0.708872	8.957139	
N	-3.055012	1.391721	7.728337	
H	-6.539673	-1.592588	11.277650	.03620
H	-7.203302	-0.440019	10.146310	.03620
H	-4.390992	-1.573635	9.880515	.01030
H	-4.752673	-0.256670	11.006752	.01030
H	-5.486241	1.164073	9.136895	.06210
H	-5.131332	-0.169429	8.007348	.06210
H	-2.754214	-0.169296	9.035808	
H	-3.166981	1.349308	9.799341	
H	-3.161047	2.394595	7.690161	
C	2.386473	5.292878	-1.641217	
C	2.917563	6.339435	-2.645878	
C	4.187650	5.892638	-3.353194	
C	3.871846	4.678573	-4.211231	
C	3.058403	3.637466	-3.485695	
C	2.425650	3.878200	-2.274366	
C	1.843169	2.746944	-1.631608	
C	1.320077	2.658021	-0.335166	
C	0.741238	1.534413	0.222080	
C	0.167465	1.726142	1.537981	
C	-0.645276	0.868876	2.187663	
C	-1.285486	1.306497	3.420991	

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C   -2.114742    0.577241    4.193276
C   -2.612999    1.253855    5.389584
C   -2.770728    0.691388    6.626742
C    3.250937    5.354631   -0.364534
C    0.942350    5.725010   -1.305739
C    3.042817    2.295225   -4.189545
C    0.572109    0.210580   -0.475213
C   -2.489693   -0.841454    3.856182
H    3.323413    4.986472   -5.101597
H    4.781975    4.213936   -4.582860
H    4.575498    6.691512   -3.974887
H    4.967357    5.652262   -2.636003
H    3.064471    7.278859   -2.124201
H    2.154033    6.531007   -3.396457
H    0.514126    5.206080   -0.457976
H    0.938103    6.784697   -1.073335
H    0.278242    5.581462   -2.151209
H    2.880782    4.726680    0.434691
H    4.273191    5.048503   -0.556484
H    3.264807    6.374041    0.010933
H    2.090278    1.782343   -4.135536
H    3.269796    2.443315   -5.238655
H    3.804988    1.628822   -3.789300
H    1.828029    1.834884   -2.190409
H    1.342567    3.520051    0.293325
H    0.331871    2.687858    1.991549
H   -0.867791   -0.102808    1.796615
H   -1.085897    2.321323    3.709383
H   -2.698987    2.321927    5.320923
H    0.573079   -0.599409    0.243467
H   -0.371356    0.181044   -1.015327
H    1.366108    0.021275   -1.183459
H   -3.114093   -1.277157    4.624121
H   -3.049814   -0.871172    2.927172
H   -1.609946   -1.460709    3.726300
H   -2.651954   -0.366700    6.781387
O   -3.336771    4.266828    8.196687     -.83400
H   -3.943986    4.983533    8.431189      .41700
H   -2.791643    4.263707    9.030281      .41700
HLA -4.344285    0.435831    8.959763
```

ASR_{AT}-(-125) Structure along the photoisomerization path of ASR_{AT} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of -125°

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.765246	-1.189321	7.878867	.22455
H	-6.004646	-3.115018	9.262248	.14260
C	-6.477424	-1.250143	10.237772	-.00940
C	-5.040710	-0.725712	10.082858	.01870
C	-4.829845	0.304602	8.983782	.00000
C	-3.358100	0.742513	8.986594	
N	-3.050021	1.421262	7.746250	
H	-6.539380	-1.585836	11.274913	.03620
H	-7.191872	-0.434420	10.137761	.03620
H	-4.376295	-1.566126	9.891099	.01030
H	-4.748959	-0.257678	11.024803	.01030
H	-5.467770	1.173138	9.154929	.06210
H	-5.086752	-0.153795	8.025874	.06210
H	-2.717931	-0.125164	9.072091	
H	-3.160641	1.399208	9.823138	
H	-3.350135	2.384504	7.659530	
C	2.391807	5.294941	-1.647820	
C	2.929017	6.340503	-2.649938	
C	4.199148	5.893547	-3.356579	
C	3.878402	4.678780	-4.210596	
C	3.064322	3.637987	-3.479992	
C	2.423065	3.881679	-2.282761	
C	1.808089	2.750756	-1.632162	
C	1.297581	2.657338	-0.343835	
C	0.727198	1.520277	0.233631	
C	0.196746	1.709484	1.552797	
C	-0.554335	0.828801	2.259760	
C	-1.160089	1.252441	3.507989	

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C   -2.069709    0.563024    4.223526
C   -2.627478    1.278959    5.399636
C   -2.597677    0.769769    6.678093
C    3.259461    5.352434   -0.372112
C    0.946452    5.732966   -1.322529
C    3.051306    2.298190   -4.193303
C    0.560458    0.196881   -0.468607
C   -2.615684   -0.781693    3.793375
H    3.327274    4.988963   -5.097503
H    4.787695    4.217327   -4.587431
H    4.583469    6.692933   -3.980333
H    4.981406    5.652750   -2.642382
H    3.073367    7.281323   -2.130215
H    2.168335    6.526896   -3.404164
H    0.505968    5.215197   -0.480211
H    0.937809    6.793696   -1.095659
H    0.294171    5.584707   -2.176269
H    2.892839    4.723396    0.428300
H    4.277748    5.039597   -0.573989
H    3.285701    6.371404    0.005082
H    2.092756    1.794379   -4.163970
H    3.297664    2.453746   -5.237154
H    3.797566    1.616011   -3.790101
H    1.779841    1.845988   -2.199290
H    1.312444    3.514868    0.291771
H    0.363941    2.673893    2.000078
H   -0.768879   -0.146019    1.874846
H   -0.875677    2.230606    3.856090
H   -3.108796    2.231659    5.235443
H    0.578402   -0.619237    0.242349
H   -0.389818    0.161487   -0.994153
H    1.341218    0.017835   -1.195556
H   -3.268883   -1.211060    4.542361
H   -3.183162   -0.681451    2.873165
H   -1.821519   -1.494768    3.601550
H   -2.180922   -0.203546    6.867407
O   -3.383475    4.281145    8.203109    -.83400
H   -3.940677    5.040475    8.432130     .41700
H   -2.813439    4.274662    9.019044     .41700
HLA -4.316565    0.457308    8.984767
```

ASR_{AT}-(-110) Structure along the photoisomerization path of ASR_{AT} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of -110°

Atom	x	y	z	charge
N	2.593000	5.425000	10.766000	-.51630
C	1.598000	4.397000	11.015000	.03810
C	1.894000	3.247000	10.041000	.53660
O	2.171000	2.124000	10.461000	-.58190
H	2.294660	6.326150	10.418160	.29360
H	1.652250	4.029300	12.031930	.08800
C	0.200000	4.985000	10.779000	-.03030
C	-0.894000	3.935000	10.722000	.79940
O	-0.622000	2.724000	10.890000	-.80140
O	-2.054000	4.344000	10.493000	-.80140
H	0.168790	5.536590	9.849410	-.01220
H	-0.022330	5.685980	11.579840	-.01220
N	-7.314000	-2.087000	8.008000	-.39805
C	-6.874000	-2.459000	9.345000	-.24000
C	-7.932000	-3.320000	10.048000	.68395
O	-7.826000	-4.547000	10.085000	-.63955
H	-7.773576	-1.193416	7.879944	.22455
H	-6.004582	-3.115159	9.263441	.14260
C	-6.483977	-1.252684	10.243006	-.00940
C	-5.043703	-0.733525	10.098883	.01870
C	-4.816253	0.301157	9.004732	.00000
C	-3.342841	0.757718	9.013995	
N	-3.049570	1.453161	7.767157	
H	-6.555057	-1.592001	11.278875	.03620
H	-7.198275	-0.436728	10.142058	.03620
H	-4.385048	-1.578094	9.907782	.01030
H	-4.757511	-0.273011	11.045945	.01030
H	-5.468431	1.160053	9.171799	.06210
H	-5.067487	-0.158414	8.045618	.06210
H	-2.693696	-0.105076	9.087288	
H	-3.153487	1.407269	9.859698	
H	-3.429119	2.401042	7.668751	
C	2.403441	5.296612	-1.668265	
C	2.939981	6.347929	-2.666329	
C	4.214115	5.903514	-3.366020	
C	3.885078	4.692610	-4.220271	
C	3.073025	3.650633	-3.487290	
C	2.434387	3.883724	-2.296931	
C	1.799341	2.743185	-1.633719	
C	1.288596	2.652485	-0.357773	
C	0.705454	1.508033	0.250233	
C	0.204530	1.686678	1.565795	
C	-0.504694	0.787899	2.325095	
C	-1.067296	1.195196	3.587125	

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C   -2.055085    0.556262    4.259453
C   -2.658029    1.255002    5.411153
C   -2.471812    0.857661    6.743290
C    3.267486    5.353724   -0.391946
C    0.959569    5.730852   -1.340404
C    3.065151    2.318568   -4.210857
C    0.557552    0.193722   -0.469171
C   -2.698644   -0.724541    3.775988
H    3.332072    5.008845   -5.102947
H    4.790283    4.228218   -4.601612
H    4.608594    6.701449   -3.985828
H    4.988626    5.655435   -2.646208
H    3.076054    7.288067   -2.143703
H    2.184227    6.531713   -3.426150
H    0.528100    5.204425   -0.499520
H    0.947429    6.790436   -1.110968
H    0.307110    5.577042   -2.192718
H    2.891488    4.722894    0.402249
H    4.283449    5.032691   -0.591761
H    3.296555    6.372470   -0.015077
H    2.101975    1.823273   -4.199338
H    3.329519    2.482133   -5.248939
H    3.799714    1.630232   -3.799120
H    1.777327    1.844976   -2.208242
H    1.316650    3.511068    0.274099
H    0.347978    2.661865    1.995592
H   -0.716448   -0.188630    1.950655
H   -0.734134    2.148849    3.957508
H   -3.428915    1.990731    5.203645
H    0.615898   -0.634904    0.223487
H   -0.394736    0.137338   -0.987459
H    1.333204    0.060970   -1.210563
H   -3.373173   -1.139611    4.513825
H   -3.258278   -0.558182    2.862381
H   -1.955375   -1.482390    3.551701
H   -1.904429   -0.034914    6.968242
O   -3.391731    4.267649    8.208476     -.83400
H   -3.943773    5.040521    8.408192      .41700
H   -2.825919    4.289466    9.028501      .41700
HLA -4.298012    0.461724    9.007993
```

ASR_{13C}-(21) Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 21°

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.505711	-4.753602	10.939592	.22455
H	-8.714974	-6.736936	12.229175	.14260
C	-9.028379	-4.807144	13.104314	-.00940
C	-7.759252	-4.278904	12.415771	.01870
C	-7.193209	-3.054662	13.129808	.00000
C	-5.862068	-2.617049	12.497669	
N	-6.049093	-1.747168	11.346985	
H	-8.790613	-5.090277	14.129914	.03620
H	-9.792600	-4.029858	13.133184	.03620
H	-7.973394	-4.023127	11.376802	.01030
H	-7.002852	-5.059816	12.441384	.01030
H	-7.014575	-3.318128	14.175195	.06210
H	-7.921287	-2.249048	13.092761	.06210
H	-5.292489	-3.486204	12.210412	
H	-5.277258	-2.067475	13.222764	
H	-6.119573	-0.765841	11.545029	
C	-0.869799	1.525923	1.819657	
C	-0.386044	2.412857	0.649599	
C	0.836401	1.856269	-0.063056	
C	0.487804	0.515197	-0.690956	
C	-0.361980	-0.377766	0.183533	
C	-0.957751	0.047078	1.365353	
C	-1.622655	-0.963687	2.130941	
C	-2.140198	-0.948464	3.442579	
C	-2.800497	-2.033008	4.006167	
C	-3.317740	-1.885478	5.365609	
C	-4.071902	-2.793419	6.028153	
C	-4.574387	-2.582680	7.394939	

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C   -5.227485   -3.529571    8.122052
C   -5.646952   -3.292033    9.511546
C   -5.820269   -2.040815   10.065026
C    0.105884    1.669711    3.006627
C   -2.253753    2.080673    2.217861
C   -0.491832   -1.790551   -0.362862
C   -3.033944   -3.309935    3.232843
C   -5.485380   -4.916455    7.565580
H   -0.194622    3.412888    1.024784
H   -1.193540    2.513844   -0.073526
H    1.168395    2.542914   -0.832976
H    1.665648    1.738826    0.627892
H    1.390660   -0.033174   -0.951585
H   -0.041326    0.670340   -1.632820
H    0.198269    2.716845    3.281943
H   -0.231481    1.131939    3.885762
H    1.095920    1.301137    2.764830
H   -2.175384    3.154010    2.358615
H   -2.988592    1.917907    1.435813
H   -2.642959    1.665984    3.138425
H   -0.043512   -1.843943   -1.347018
H    0.025787   -2.515160    0.258330
H   -1.522485   -2.116756   -0.460551
H   -1.718633   -1.911270    1.642215
H   -2.049538   -0.070502    4.048284
H   -3.080877   -0.960164    5.859553
H   -4.320603   -3.721765    5.561317
H   -4.343939   -1.628862    7.835069
H   -5.795638   -4.160357   10.127867
H   -5.794449   -1.178563    9.427303
H   -5.977370   -5.543089    8.299130
H   -6.119076   -4.886068    6.685088
H   -4.563903   -5.414177    7.280965
H   -3.441972   -4.094802    3.848756
H   -3.724662   -3.140969    2.412294
H   -2.102300   -3.685660    2.828838
O   -5.998753    1.089884   11.394614     -.83400
H   -6.575181    1.861947   11.498409      .41700
H   -5.500006    1.128745   12.248217      .41700
HLA -6.728002   -2.901726   12.908907
```

ASR_{13C}-(30) Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 30°

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.512295	-4.756722	10.940988	.22455
H	-8.715295	-6.737126	12.228312	.14260
C	-9.024091	-4.808977	13.110116	-.00940
C	-7.754473	-4.267600	12.429664	.01870
C	-7.162485	-3.070600	13.174578	.00000
C	-5.872331	-2.561818	12.507902	
N	-6.140896	-1.752070	11.327895	
H	-8.786592	-5.097372	14.134393	.03620
H	-9.788911	-4.032579	13.144751	.03620
H	-7.980988	-3.974769	11.404059	.01030
H	-7.005962	-5.056273	12.416562	.01030
H	-6.925169	-3.383607	14.193359	.06210
H	-7.901763	-2.275490	13.226875	.06210
H	-5.241448	-3.396216	12.246359	
H	-5.321321	-1.941945	13.204130	
H	-6.293471	-0.772797	11.495194	
C	-0.854533	1.524152	1.812996	
C	-0.370549	2.424198	0.652535	
C	0.854523	1.879511	-0.063966	
C	0.502546	0.545467	-0.704019	
C	-0.338238	-0.362240	0.165927	
C	-0.932991	0.047112	1.352538	
C	-1.597674	-0.971963	2.115012	
C	-2.106803	-0.970098	3.430412	
C	-2.779666	-2.049885	3.995070	
C	-3.286034	-1.897299	5.360017	
C	-4.069793	-2.784309	6.019343	
C	-4.528859	-2.590259	7.405775	

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C   -5.208558   -3.524534    8.119871
C   -5.607318   -3.299886    9.522336
C   -5.893371   -2.060119   10.052592
C    0.115205    1.668006    3.003828
C   -2.245619    2.065243    2.204519
C   -0.458514   -1.769140   -0.397310
C   -3.023184   -3.331129    3.227351
C   -5.572128   -4.876009    7.539862
H   -0.185229    3.420936    1.038951
H   -1.175584    2.528745   -0.072402
H    1.185495    2.573765   -0.828317
H    1.683556    1.756279    0.626230
H    1.402028    0.004477   -0.989645
H   -0.039027    0.714871   -1.635432
H    0.199364    2.714277    3.285280
H   -0.222254    1.121730    3.877372
H    1.107655    1.305960    2.761065
H   -2.179514    3.139637    2.344555
H   -2.973050    1.892586    1.417293
H   -2.634479    1.644054    3.122592
H   -0.039172   -1.799956   -1.395438
H    0.091166   -2.492547    0.197762
H   -1.485457   -2.111782   -0.471139
H   -1.708816   -1.906590    1.605073
H   -1.992715   -0.102536    4.048333
H   -3.018512   -0.984255    5.864062
H   -4.378772   -3.687303    5.536685
H   -4.234052   -1.672045    7.882391
H   -5.644819   -4.167855   10.156696
H   -5.967153   -1.223366    9.385618
H   -6.080219   -5.485035    8.277915
H   -6.224997   -4.777099    6.678689
H   -4.699287   -5.428899    7.212743
H   -3.356511   -4.132576    3.868533
H   -3.770209   -3.187302    2.451592
H   -2.112936   -3.674952    2.752389
O   -6.051362    1.070508   11.401588     -.83400
H   -6.583460    1.875727   11.492016      .41700
H   -5.544511    1.091762   12.250720      .41700
HLA -6.710756   -2.892457   12.941170
```

ASR_{13C}-(40) **Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 40°**

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.515473	-4.758285	10.941540	.22455
H	-8.715370	-6.737321	12.228687	.14260
C	-9.026205	-4.808075	13.110501	-.00940
C	-7.751782	-4.271567	12.435966	.01870
C	-7.166115	-3.067264	13.175828	.00000
C	-5.875032	-2.563595	12.507773	
N	-6.158507	-1.769835	11.324585	
H	-8.795055	-5.094564	14.136619	.03620
H	-9.789268	-4.029488	13.139507	.03620
H	-7.971797	-3.989486	11.405401	.01030
H	-7.002871	-5.059703	12.434536	.01030
H	-6.938289	-3.364684	14.201270	.06210
H	-7.908329	-2.273590	13.205660	.06210
H	-5.246483	-3.400104	12.248635	
H	-5.320940	-1.937211	13.195366	
H	-6.370708	-0.798638	11.478562	
C	-0.856041	1.526597	1.813473	
C	-0.372679	2.421777	0.649778	
C	0.850586	1.873554	-0.066787	
C	0.498875	0.537142	-0.701637	
C	-0.342548	-0.364547	0.172006	
C	-0.936719	0.050363	1.353252	
C	-1.609222	-0.967525	2.115952	
C	-2.114269	-0.968224	3.426674	
C	-2.787661	-2.052922	3.989062	
C	-3.284017	-1.901865	5.350748	
C	-4.049299	-2.795740	6.024525	
C	-4.475476	-2.605326	7.418707	

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C   -5.158470   -3.529014    8.136121
C   -5.501849   -3.306354    9.558826
C   -5.919252   -2.090602   10.053447
C    0.113758    1.671672    3.005115
C   -2.246122    2.072442    2.203750
C   -0.468885   -1.773579   -0.385370
C   -3.022542   -3.331716    3.215821
C   -5.598057   -4.856843    7.557401
H   -0.187645    3.421026    1.029851
H   -1.178852    2.520662   -0.074444
H    1.177993    2.564738   -0.835059
H    1.680600    1.752580    0.622545
H    1.398759   -0.004949   -0.983616
H   -0.042608    0.702730   -1.633421
H    0.201719    2.718396    3.283756
H   -0.225450    1.129271    3.880615
H    1.105648    1.306024    2.765579
H   -2.176663    3.147238    2.338514
H   -2.974491    1.899699    1.417429
H   -2.636927    1.655917    3.123308
H   -0.040670   -1.814061   -1.379127
H    0.067444   -2.499760    0.218166
H   -1.498353   -2.106768   -0.467551
H   -1.722814   -1.899840    1.604244
H   -2.001163   -0.104117    4.049271
H   -3.017142   -0.985576    5.849231
H   -4.355238   -3.703072    5.548656
H   -4.141399   -1.703503    7.901099
H   -5.377813   -4.142828   10.224038
H   -6.113892   -1.293228    9.365458
H   -6.156441   -5.425700    8.290831
H   -6.237126   -4.717192    6.693146
H   -4.756482   -5.462974    7.240755
H   -3.385342   -4.127313    3.847597
H   -3.742134   -3.183025    2.415508
H   -2.098680   -3.683292    2.772636
O   -6.057612    1.052176   11.398846     -.83400
H   -6.559332    1.876991   11.483058      .41700
H   -5.545222    1.066526   12.244696      .41700
HLA -6.714227   -2.890976   12.942023
```

ASR_{13C}-(50) **Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 50°**

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.514499	-4.757820	10.941346	.22455
H	-8.715339	-6.737293	12.228688	.14260
C	-9.026626	-4.809989	13.112622	-.00940
C	-7.752408	-4.272935	12.439697	.01870
C	-7.167717	-3.072367	13.185842	.00000
C	-5.885071	-2.558406	12.510866	
N	-6.183234	-1.771614	11.324971	
H	-8.794604	-5.098095	14.138065	.03620
H	-9.790177	-4.031934	13.142487	.03620
H	-7.972863	-3.986485	11.410728	.01030
H	-7.003287	-5.061133	12.434074	.01030
H	-6.928260	-3.379249	14.205575	.06210
H	-7.912756	-2.281922	13.231905	.06210
H	-5.250433	-3.390989	12.253967	
H	-5.333956	-1.925858	13.195922	
H	-6.397474	-0.799293	11.479223	
C	-0.855243	1.525583	1.810191	
C	-0.371805	2.423645	0.648773	
C	0.852857	1.876349	-0.066656	
C	0.501050	0.541380	-0.705357	
C	-0.340226	-0.362067	0.167875	
C	-0.934596	0.050557	1.347823	
C	-1.609779	-0.968043	2.112666	
C	-2.110517	-0.966594	3.422000	
C	-2.782337	-2.053048	3.989499	
C	-3.271773	-1.906949	5.349444	
C	-4.034536	-2.805430	6.021757	
C	-4.451598	-2.617014	7.415150	

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C   -5.190843   -3.506792    8.118129
C   -5.466844   -3.290015    9.560603
C   -5.952197   -2.097662   10.052597
C    0.113887    1.670044    3.002221
C   -2.245374    2.068567    2.203424
C   -0.465589   -1.771760   -0.388124
C   -3.022581   -3.330214    3.216416
C   -5.629916   -4.839298    7.548059
H   -0.186635    3.421570    1.032150
H   -1.177426    2.524546   -0.075986
H    1.184441    2.569677   -0.831316
H    1.680472    1.752469    0.625197
H    1.401476    0.000503   -0.987942
H   -0.039571    0.709296   -1.637289
H    0.199734    2.716779    3.281620
H   -0.226045    1.126072    3.876378
H    1.105849    1.304869    2.762279
H   -2.177308    3.142930    2.342045
H   -2.974714    1.895393    1.418078
H   -2.632774    1.648264    3.122548
H   -0.040107   -1.813607   -1.383112
H    0.072328   -2.495904    0.216500
H   -1.495010   -2.105988   -0.466264
H   -1.725539   -1.900039    1.601033
H   -1.997817   -0.101221    4.043129
H   -3.004697   -0.994055    5.854339
H   -4.344792   -3.709665    5.542710
H   -4.100580   -1.724090    7.901942
H   -5.296653   -4.125702   10.217974
H   -6.164434   -1.309142    9.356635
H   -6.181449   -5.410751    8.285100
H   -6.266631   -4.716611    6.679165
H   -4.778757   -5.438599    7.240265
H   -3.381468   -4.126894    3.848796
H   -3.747282   -3.179107    2.421561
H   -2.102539   -3.681967    2.766275
O   -6.066477    1.054483   11.404001     -.83400
H   -6.567151    1.880407   11.488761      .41700
H   -5.544731    1.074081   12.244062      .41700
HLA -6.719125   -2.892614   12.949795
```

ASR_{13C}-(60) **Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 60°**

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.519826	-4.760491	10.941987	.22455
H	-8.715507	-6.737527	12.228561	.14260
C	-9.028403	-4.812868	13.121758	-.00940
C	-7.755992	-4.264466	12.454572	.01870
C	-7.145248	-3.087603	13.222847	.00000
C	-5.894322	-2.528585	12.518814	
N	-6.254304	-1.789160	11.316368	
H	-8.795598	-5.109176	14.144708	.03620
H	-9.794425	-4.037335	13.159131	.03620
H	-7.990364	-3.951036	11.437064	.01030
H	-7.014132	-5.058169	12.415876	.01030
H	-6.863934	-3.430786	14.220397	.06210
H	-7.891877	-2.304521	13.333337	.06210
H	-5.222786	-3.335501	12.275981	
H	-5.365495	-1.853404	13.181941	
H	-6.551033	-0.832893	11.461970	
C	-0.839563	1.514684	1.816710	
C	-0.354173	2.443730	0.680606	
C	0.875917	1.918493	-0.041149	
C	0.524510	0.600228	-0.711620	
C	-0.309679	-0.329431	0.142956	
C	-0.910936	0.050249	1.322773	
C	-1.599274	-0.988697	2.075516	
C	-2.074729	-1.009193	3.383577	
C	-2.760102	-2.098590	3.964256	
C	-3.219899	-1.953087	5.321593	
C	-3.998690	-2.838188	6.011572	
C	-4.395144	-2.635608	7.401562	

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C   -5.161044   -3.496032    8.115217
C   -5.422048   -3.267695    9.567114
C   -6.050970   -2.130965   10.044753
C    0.125626    1.637090    3.014030
C   -2.233948    2.041424    2.215518
C   -0.410433   -1.726510   -0.448275
C   -3.033431   -3.359467    3.177907
C   -5.779694   -4.743127    7.516232
H   -0.176783    3.432582    1.089776
H   -1.155278    2.557803   -0.046944
H    1.210565    2.630363   -0.787302
H    1.700708    1.778042    0.650822
H    1.424416    0.070924   -1.015066
H   -0.021571    0.793420   -1.634752
H    0.205460    2.677061    3.318783
H   -0.211499    1.069388    3.873468
H    1.118860    1.282233    2.764946
H   -2.176002    3.113274    2.375178
H   -2.957874    1.875473    1.423781
H   -2.621053    1.598831    3.124005
H    0.003530   -1.728649   -1.449254
H    0.152980   -2.453270    0.129242
H   -1.431823   -2.083957   -0.524806
H   -1.736119   -1.901449    1.536102
H   -1.942472   -0.155164    4.015348
H   -2.924727   -1.051368    5.830413
H   -4.336978   -3.730275    5.529851
H   -3.987539   -1.768923    7.892019
H   -4.996219   -3.982231   10.256248
H   -6.432383   -1.422860    9.331274
H   -6.368063   -5.272862    8.255951
H   -6.428935   -4.502292    6.680683
H   -5.025571   -5.431122    7.146499
H   -3.345233   -4.174334    3.812537
H   -3.803260   -3.196668    2.429147
H   -2.140705   -3.689576    2.661542
O   -6.124959    1.035661   11.432432     -.83400
H   -6.587768    1.886215   11.492003      .41700
H   -5.586411    1.067056   12.261599      .41700
HLA -6.706369   -2.891472   12.975861
```

ASR_{13C}-(70) **Structure along the photoisomerization path of ASR_{13C} with a C_{12}-C_{13}-C_{14}-C_{15} dihedral angle of 70°**

Atom	x	y	z	charge
N	-0.148460	1.918457	13.830959	-.51630
C	-1.141273	0.868683	13.996030	.03810
C	-0.829445	-0.264696	13.024035	.53660
O	-0.506618	-1.374576	13.452660	-.58190
H	-0.441152	2.826564	13.494348	.29360
H	-1.084336	0.477914	15.003524	.08800
C	-2.531083	1.469594	13.808052	-.03030
C	-3.686501	0.474778	13.858206	.79940
O	-3.520987	-0.755942	13.744513	-.80140
O	-4.830315	0.965505	13.840200	-.80140
H	-2.582850	1.971263	12.848148	-.01220
H	-2.676768	2.229116	14.572980	-.01220
N	-10.064218	-5.661172	11.035740	-.39805
C	-9.548768	-6.042577	12.353772	-.24000
C	-10.604227	-6.832861	13.125663	.68395
O	-10.477992	-8.050757	13.253906	-.63955
H	-10.519292	-4.760239	10.941867	.22455
H	-8.715949	-6.738076	12.228516	.14260
C	-9.027979	-4.813291	13.121073	-.00940
C	-7.755281	-4.268451	12.453053	.01870
C	-7.147837	-3.089052	13.219124	.00000
C	-5.898058	-2.537041	12.509322	
N	-6.265708	-1.793205	11.313173	
H	-8.795748	-5.108705	14.144406	.03620
H	-9.792654	-4.036400	13.156508	.03620
H	-7.988327	-3.959614	11.433566	.01030
H	-7.012872	-5.061857	12.418920	.01030
H	-6.864964	-3.428626	14.217240	.06210
H	-7.896796	-2.307129	13.326055	.06210
H	-5.236544	-3.349781	12.256347	
H	-5.359232	-1.867616	13.170474	
H	-6.569550	-0.838271	11.462227	
C	-0.843976	1.514730	1.823157	
C	-0.359317	2.441168	0.685215	
C	0.870219	1.911905	-0.035362	
C	0.519453	0.593200	-0.706822	
C	-0.315569	-0.332956	0.149850	
C	-0.913805	0.051015	1.327509	
C	-1.603445	-0.987080	2.081875	
C	-2.075247	-1.005302	3.385220	
C	-2.761048	-2.100042	3.962094	
C	-3.216926	-1.957853	5.311183	
C	-3.994835	-2.847638	5.999522	
C	-4.367549	-2.645697	7.387333	

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C   -5.189475   -3.458780    8.094070
C   -5.381270   -3.230718    9.553076
C   -6.074850   -2.133598   10.042393
C    0.122490    1.638070    3.020390
C   -2.238909    2.041831    2.223333
C   -0.422103   -1.734005   -0.432245
C   -3.030245   -3.359925    3.174780
C   -5.791701   -4.723996    7.519042
H   -0.180629    3.431636    1.090313
H   -1.161405    2.552737   -0.041621
H    1.208004    2.623871   -0.779837
H    1.692608    1.768836    0.659073
H    1.420687    0.063712   -1.006484
H   -0.024621    0.784843   -1.631459
H    0.203220    2.678181    3.324763
H   -0.213006    1.070845    3.880940
H    1.115558    1.283022    2.770876
H   -2.180905    3.113879    2.382899
H   -2.963965    1.876046    1.432399
H   -2.625906    1.599179    3.132054
H   -0.013856   -1.746150   -1.435302
H    0.141692   -2.458260    0.148181
H   -1.444716   -2.089864   -0.500198
H   -1.743385   -1.900267    1.545210
H   -1.944882   -0.153424    4.020522
H   -2.925574   -1.055756    5.821190
H   -4.342485   -3.735246    5.516811
H   -3.934380   -1.790389    7.875739
H   -4.921306   -3.941366   10.223679
H   -6.466573   -1.425109    9.334587
H   -6.367297   -5.258003    8.265848
H   -6.437642   -4.527007    6.670210
H   -5.010373   -5.395509    7.175356
H   -3.347996   -4.173297    3.808253
H   -3.793506   -3.197634    2.419369
H   -2.132014   -3.690283    2.668810
O   -6.121122    1.029523   11.427392     -.83400
H   -6.585234    1.878949   11.492214      .41700
H   -5.576826    1.061610   12.252582      .41700
HLA -6.709788   -2.895569   12.970356
```