



Supporting Information

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Toward Fast and Efficient Visible-Light-Driven Molecular Motors: A Minimal Design

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Computational details

Light-absorption features. The light absorption of motors **1a–4d** was investigated in the following way, using Dunning’s correlation-consistent polarized valence triple- ζ (cc-pVTZ) basis set^[1] for all steps and considering each of the E_{out} , Z_{in} , E_{in} and Z_{out} isomers (although being enantiomers, the results for E_{out} and E_{in} are identical, as are the results for Z_{out} and Z_{in}). First, the ground-state (S_0) equilibrium geometries of the motors were optimized with the complete active space self-consistent field (CASSCF) method.^[2] Based on the resulting geometries, the same method was then used to calculate the wave function at the vertical Franck-Condon (FC) point in the bright and photoactive first excited singlet $\pi\pi^*$ state (S_1) of each species. Finally, from these wave functions, single-point calculations were performed with complete active space second-order perturbation theory (CASPT2)^[3] to obtain vertical $S_0 \rightarrow S_1$ excitation energies. The corresponding oscillator strengths were obtained with the complete active space state-interaction (CASSI) method.^[4] All CASSCF and CASPT2 calculations were carried out with active spaces comprising the full π -systems of the motors, i.e., utilizing CAS(6,6), CAS(8,8) and CAS(10,10) for **1a–1d**, **2a–2d/3a–3d** and **4a–4d**, respectively. As a complement to the CASPT2//CASSCF results, vertical excitation energies (both $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$) were also calculated using the approximate coupled-cluster singles and doubles (CC2) method^[5] within the resolution-of-the-identity (RI) approximation.^[6,7] These calculations were based on S_0 equilibrium geometries optimized with Møller-Plesset second-order perturbation theory (MP2).

Enantiomerization barriers. The $E_{\text{out}} \leftrightarrow E_{\text{in}}$ and $Z_{\text{out}} \leftrightarrow Z_{\text{in}}$ enantiomerization free-energy barriers of motors **1a–4d** were calculated in the gas phase and in non-polar (cyclohexane) and polar (water) solvents using both MP2 and density functional theory (DFT) methods in

combination with the cc-pVTZ basis set. The solvents were described with the SMD continuum solvation model^[8] and the DFT calculations were carried out with the B3LYP and M06-2X^[9] global and the ω B97X-D^[10] range-separated hybrid functionals. Following S_0 equilibrium geometry optimization of the four motor isomers and the enantiomerization transition structures that connect them, frequency calculations were performed to obtain Gibbs free energies (at room temperature) of the resulting geometries and to ensure that these do correspond to minima (real vibrational frequencies only) or transition structures (one imaginary vibrational frequency). Throughout, the MP2/B3LYP/M06-2X/ ω B97X-D geometries were subjected to MP2/B3LYP/M06-2X/ ω B97X-D frequency calculations, respectively. Thereby, the enantiomerization free-energy barriers predicted by any of the methods stem exclusively from calculations with that very method.

MEP calculations. The photoisomerization minimum energy path (MEP) calculations on motors **1d/2d/3d/4d** were started from the S_1 FC points at the CASSCF S_0 equilibrium geometries of the E_{out} , Z_{in} , E_{in} and Z_{out} isomers, and were performed using state-averaged CASSCF (SA-CASSCF) in combination with Dunning's correlation-consistent polarized valence double- ζ (cc-pVDZ) basis set.^[11] Employing equal (0.5) weights for S_0 and S_1 in the state-averaging, the MEP calculations were done with the same active spaces as the light-absorption calculations (i.e., with CAS(6,6), CAS(8,8) and CAS(10,10) for **1d**, **2d/3d** and **4d**, respectively). For **4d** (MEPs in Figure 3), the S_0 and S_1 energies of the S_1 MEP geometries were refined through CASPT2 single-point calculations with the cc-pVDZ basis set, so as to account for dynamic electron correlation effects. For **1d/2d/3d** (MEPs in Figures S3–S5), on the other hand, no such refinement was deemed necessary, based on

a comparison in Figure S6 of the MEPs of **4d** obtained with and without CASPT2 single-point calculations. Indeed, as can be seen from Figure S6, the two sets of MEPs are very similarly shaped.

NAMD simulations. The non-adiabatic molecular dynamics (NAMD) simulations of the photoisomerizations of motor **4d** were carried out using SA-CASSCF(10,10), with equal weights for S_0 and S_1 , in combination with Ahlrich’s split valence plus polarization double- ζ (SVP) basis set.^[11] First, for each of the E_{out} , Z_{in} , E_{in} and Z_{out} isomers, 10 different initial nuclear configurations and velocities were generated from a harmonic-oscillator Wigner distribution^[12,13] of the corresponding S_0 vibrational normal modes calculated at the MP2/SVP level of theory. For each isomer, these initial conditions were then used to start 10 photoisomerization trajectories from the S_1 FC points. Evaluating nuclear forces “on the fly”, the trajectories were propagated classically for a maximum of 700 fs employing the velocity Verlet algorithm^[14] with a fixed integration time step of 1 fs.

During the simulations, the non-adiabatic coupling $\langle \Psi_1 | \frac{\partial}{\partial \mathbf{R}} \Psi_0 \rangle$ between the S_1 and S_0 states was evaluated in the framework of Landau-Zener theory,^[15,16] using the algorithm by Robb and co-workers^[17,18] as implemented in the MOLCAS 8.0 suite of programs.^[19] In this framework/algorithm, the coupling is large when $\langle \Psi_1 | \frac{\partial}{\partial t} \Psi_0 \rangle$ is large, as calculated using the numerical approximation

$$\langle \Psi_1(t) | \frac{\partial}{\partial t} \Psi_0(t) \rangle \approx \frac{\langle \Psi_1(t) | \Psi_0(t + \Delta t) \rangle}{\Delta t}.$$

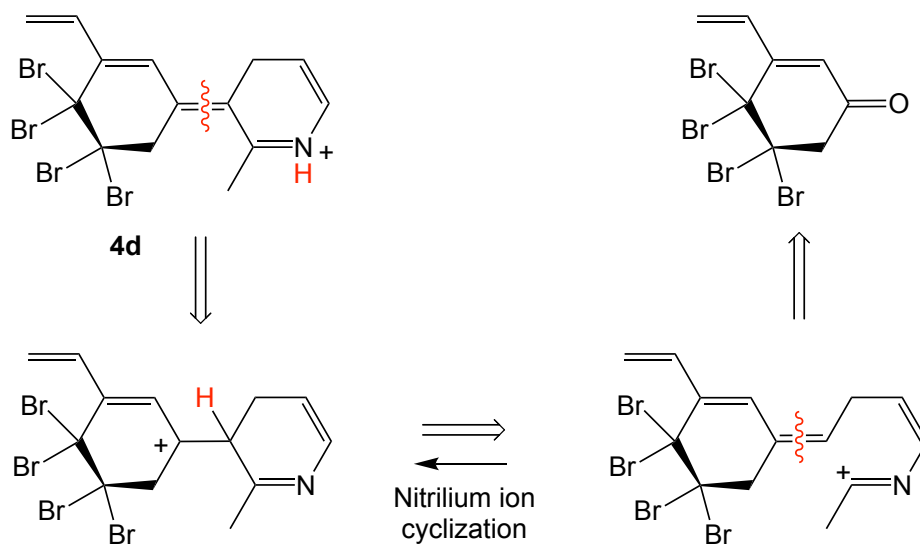
Performing this calculation at each step along the trajectories for which the energy gap between the two states is smaller than 0.03 a.u., a trajectory was allowed to hop from the S_1 state to the S_0 state subject to the condition that $\langle \Psi_1(t) | \Psi_0(t + \Delta t) \rangle$ exceeds a default value (0.25) signaling the

proximity of a S_1/S_0 conical intersection region (by virtue of the associated deviation of the S_1 and S_0 wave functions from orthogonality). Qualitatively, the procedure to only allow a single hop between the two states (from S_1 to S_0) has been validated in previous NAMD simulations of motor **1a**, which showed that increasing the number of allowed hops does not affect the predictions of key quantities like photoisomerization times and quantum yields by more than 10%.^[20]

Software used. The MP2 and DFT calculations were done with Gaussian 09.^[21] The CC2 calculations were done with TURBOMOLE 6.6.^[22,23] All other calculations were done with MOLCAS 8.0.^[19]

Retrosynthetic analysis and Scheme S1

As shown by Lumento et al.^[24] who built on earlier work by Gawley and Chemburkar,^[25] photoisomerizable Schiff-base systems can be synthesized through nitrilium ion cyclization onto an indanylidene moiety. Thus, using a nitrilium ion that upon cyclization yields a dihydropyridinium motif and replacing indanylidene with a tetrabrominated cyclohexenylidene, a retrosynthetic analysis for the preparation of motor **4d** can be summarized as in Scheme S1.



Scheme S1. Retrosynthetic analysis for the preparation of motor **4d**.

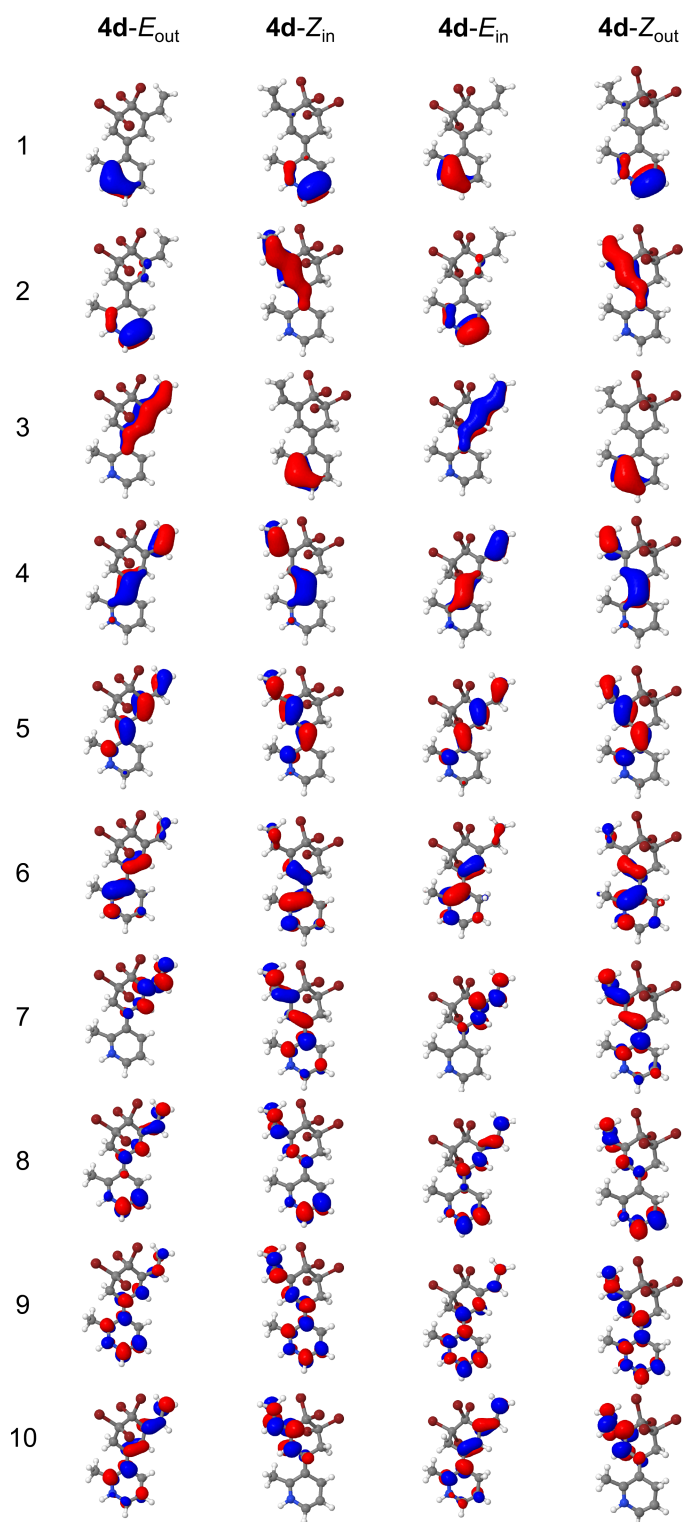


Figure S1. Active CASSCF molecular orbitals 1–10 at the CASSCF S_0 equilibrium geometries of the E_{out} , Z_{in} , E_{in} and Z_{out} isomers of motor **4d**.

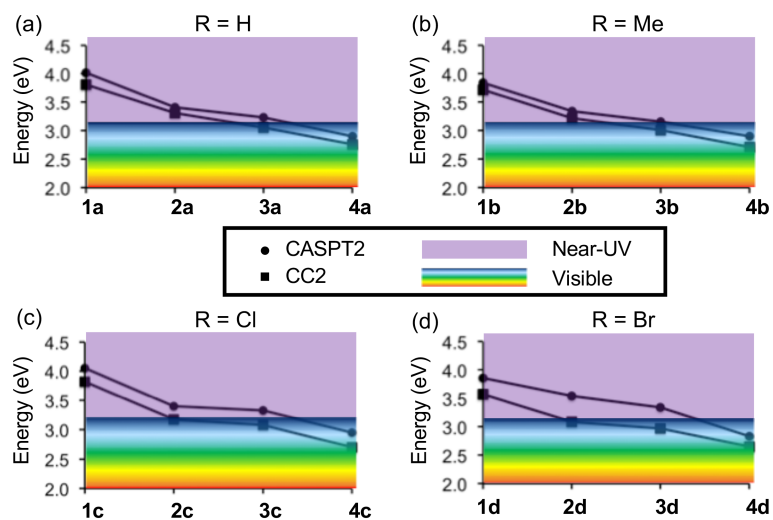


Figure S2. Vertical $S_0 \rightarrow S_1$ excitation energies of the Z_{out} and Z_{in} isomers of motors (a) **1a–4a**, (b) **1b–4b**, (c) **1c–4c** and (d) **1d–4d** in the near-UV (<400 nm, >3.1 eV) or visible (>400 nm, <3.1 eV) regime calculated with CASPT2 and CC2.

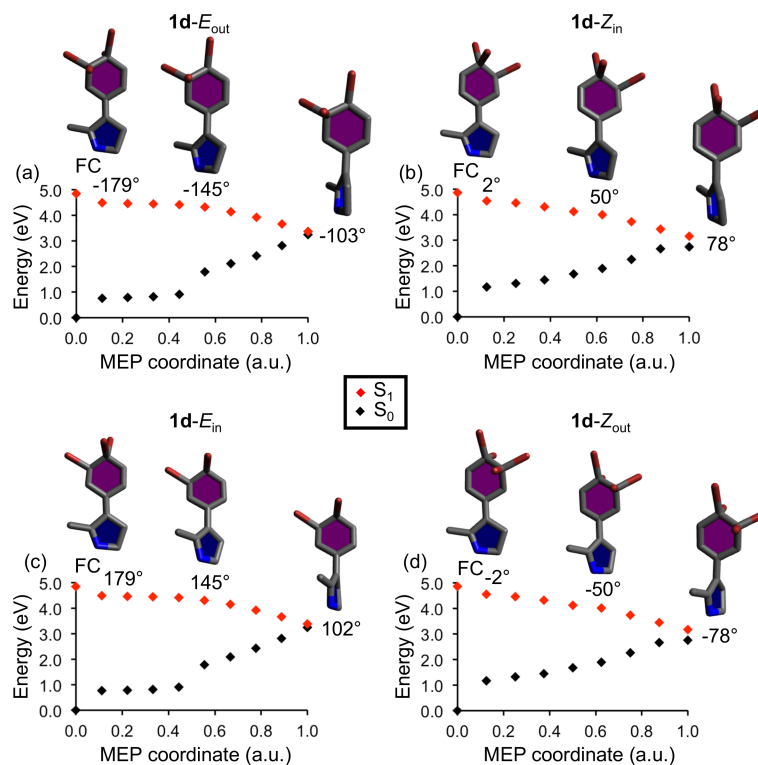


Figure S3. SA-CASSCF photoisomerization MEPs from the S_1 FC points of the (a) E_{out} , (b) Z_{in} , (c) E_{in} and (d) Z_{out} isomers of motor **1d**. Shown are also molecular geometries along the respective path and the corresponding ω dihedral angles.

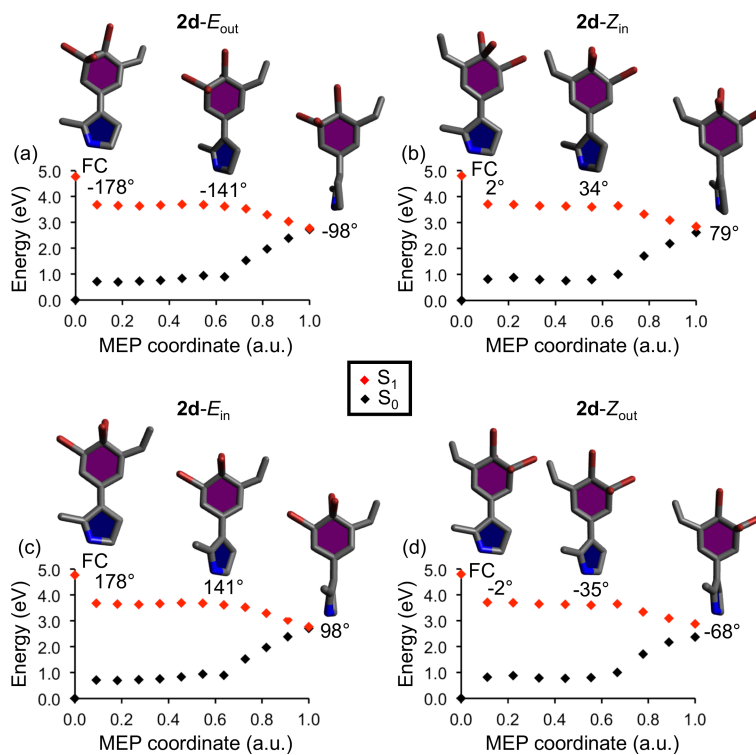


Figure S4. SA-CASSCF photoisomerization MEPs from the S_1 FC points of the (a) E_{out} , (b) Z_{in} , (c) E_{in} and (d) Z_{out} isomers of motor **2d**. Shown are also molecular geometries along the respective path and the corresponding ω dihedral angles.

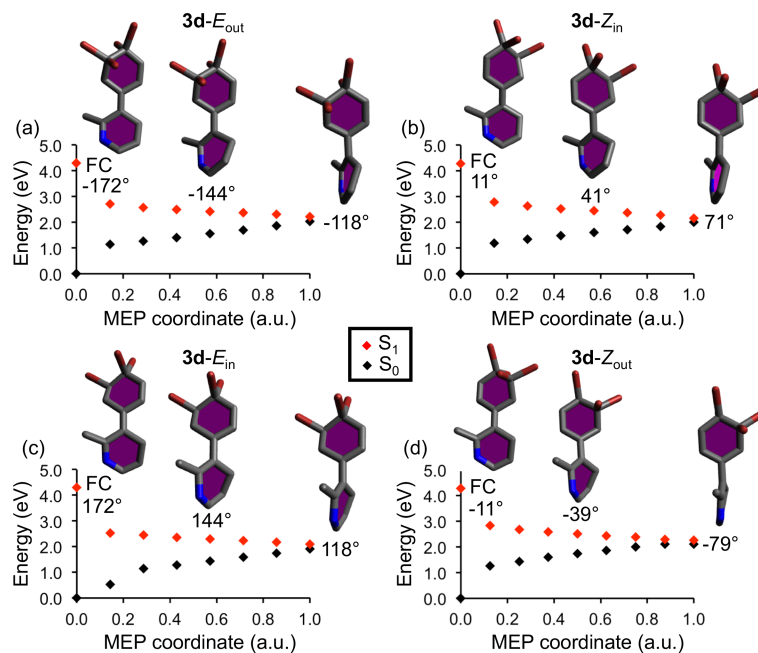


Figure S5. SA-CASSCF photoisomerization MEPs from the S_1 FC points of the (a) E_{out} , (b) Z_{in} , (c) E_{in} and (d) Z_{out} isomers of motor **3d**. Shown are also molecular geometries along the respective path and the corresponding ω dihedral angles.

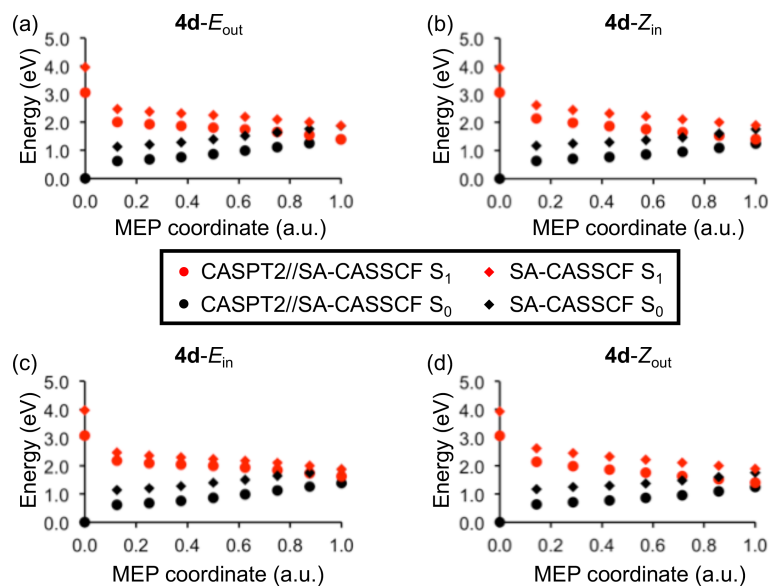


Figure S6. Comparison of CASPT2//SA-CASSCF and SA-CASSCF photoisomerization MEPs from the S_1 FC points of the (a) E_{out} , (b) Z_{in} , (c) E_{in} and (d) Z_{out} isomers of motor **4d**.

Table S1. CASSCF occupation numbers for active molecular orbitals 1–10 in the S ₀ and S ₁ states of the <i>E</i> _{out} / <i>E</i> _{in} and <i>Z</i> _{out} / <i>Z</i> _{in} isomers of motor 4d ^[a]											
Isomer	State	Active molecular orbital									
		1	2	3	4	5	6	7	8	9	10
<i>E</i> _{out} / <i>E</i> _{in}	S ₀	1.97	1.96	1.94	1.92	1.88	0.07	0.05	0.03	0.04	0.13
	S ₁	1.97	1.95	1.94	1.90	1.02	0.98	0.05	0.06	0.03	0.10
<i>Z</i> _{out} / <i>Z</i> _{in}	S ₀	1.97	1.96	1.92	1.94	1.88	0.03	0.13	0.04	0.05	0.07
	S ₁	1.97	1.95	1.89	1.93	1.10	0.90	0.11	0.03	0.05	0.06

[a] All calculations carried out with the cc-pVTZ basis set and CASSCF/cc-pVTZ S₀ equilibrium geometries.

Table S2. Vertical CC2 excitation energies (in eV) of the E_{out}/E_{in} and Z_{out}/Z_{in} isomers of motors 1a–4d ^[a]						
Isomer	Excitation	4' and 5' substituents	Motor			
			1	2	3	4
E_{out}/E_{in}	$S_0 \rightarrow S_1$	R = H (a)	3.82 (0.70)	3.32 (1.05)	3.09 (0.42)	2.79 (0.72)
	$S_0 \rightarrow S_2$	R = H (a)	5.32 (0.03)	4.85 (0.06)	4.35 (0.18)	3.94 (0.24)
	$S_0 \rightarrow S_1$	R = Me (b)	3.73 (0.73)	3.23 (0.95)	3.05 (0.47)	2.74 (0.71)
	$S_0 \rightarrow S_2$	R = Me (b)	4.86 (0.03)	4.61 (0.10)	4.17 (0.12)	3.79 (0.16)
	$S_0 \rightarrow S_1$	R = Cl (c)	3.81 (0.71)	3.17 (0.89)	3.08 (0.45)	2.71 (0.71)
	$S_0 \rightarrow S_2$	R = Cl (c)	4.67 (0.02)	4.46 (0.13)	4.13 (0.10)	3.65 (0.13)
	$S_0 \rightarrow S_1$	R = Br (d)	3.55 (0.52)	3.08 (0.78)	2.97 (0.50)	2.65 (0.69)
	$S_0 \rightarrow S_2$	R = Br (d)	3.85 (0.01)	3.75 (0.01)	3.55 (0.01)	3.45 (0.04)
Z_{out}/Z_{in}	$S_0 \rightarrow S_1$	R = H (a)	3.81 (0.62)	3.31 (0.88)	3.06 (0.42)	2.76 (0.68)
	$S_0 \rightarrow S_2$	R = H (a)	5.39 (0.05)	4.96 (0.09)	4.39 (0.05)	4.03 (0.05)
	$S_0 \rightarrow S_1$	R = Me (b)	3.72 (0.65)	3.22 (0.81)	3.01 (0.46)	2.71 (0.67)
	$S_0 \rightarrow S_2$	R = Me (b)	4.90 (0.06)	4.66 (0.12)	4.22 (0.03)	3.87 (0.02)
	$S_0 \rightarrow S_1$	R = Cl (c)	3.82 (0.66)	3.18 (0.77)	3.08 (0.45)	2.70 (0.67)
	$S_0 \rightarrow S_2$	R = Cl (c)	4.70 (0.02)	4.52 (0.14)	4.17 (0.04)	3.74 (0.02)
	$S_0 \rightarrow S_1$	R = Br (d)	3.57 (0.50)	3.09 (0.69)	2.97 (0.49)	2.65 (0.65)
	$S_0 \rightarrow S_2$	R = Br (d)	3.87 (0.02)	3.76 (0.01)	3.60 (0.01)	3.51 (0.01)

[a] All calculations carried out with the cc-pVTZ basis set and MP2/cc-pVTZ S_0 equilibrium geometries. Oscillator strengths in parentheses.

Table S3. Vertical CASPT2 excitation energies (in eV) of the E_{out}/E_{in} and Z_{out}/Z_{in} isomers of motors 1a–4d ^[a]						
Isomer	Excitation	4' and 5' substituents	Motor			
			1	2	3	4
E_{out}/E_{in}	$S_0 \rightarrow S_1$	R = H (a)	4.00 (0.82)	3.45 (1.12)	3.30 (0.66)	2.94 (0.97)
	$S_0 \rightarrow S_1$	R = Me (b)	3.91 (0.56)	3.53 (0.86)	3.18 (0.68)	2.93 (0.94)
	$S_0 \rightarrow S_1$	R = Cl (c)	4.01 (0.74)	3.41 (0.82)	3.36 (0.57)	2.98 (0.81)
	$S_0 \rightarrow S_1$	R = Br (d)	3.82 (0.66)	3.32 (0.84)	3.33 (0.25)	2.81 (0.85)
Z_{out}/Z_{in}	$S_0 \rightarrow S_1$	R = H (a)	4.02 (0.60)	3.41 (0.81)	3.23 (0.55)	2.90 (0.73)
	$S_0 \rightarrow S_1$	R = Me (b)	3.84 (0.61)	3.34 (0.77)	3.16 (0.57)	2.90 (0.71)
	$S_0 \rightarrow S_1$	R = Cl (c)	4.05 (0.54)	3.40 (0.63)	3.33 (0.50)	2.95 (0.60)
	$S_0 \rightarrow S_1$	R = Br (d)	3.86 (0.49)	3.54 (0.42)	3.34 (0.29)	2.83 (0.62)

[a] All calculations carried out with the cc-pVTZ basis set and CASSCF/cc-pVTZ S_0 equilibrium geometries. Oscillator strengths in parentheses.

Table S4. Enantiomerization free-energy barriers (in kJ mol ⁻¹) for motors 1a–4d at different levels of theory ^[a]							
Motor	Enantiomerization	Gas phase	B3LYP		M06-2X	ωB97X-D	MP2
			Water	Cyclohex.	Gas phase	Gas phase	Gas phase
1a	$E_{out} \leftrightarrow E_{in}$	17.7	24.5	26.8	27.8	26.8	25.2
	$Z_{out} \leftrightarrow Z_{in}$	20.1	23.4	23.9	23.6	24.2	25.9
1b	$E_{out} \leftrightarrow E_{in}$	46.3	43.3	47.3	48.7	45.7	51.1
	$Z_{out} \leftrightarrow Z_{in}$	43.3	42.0	39.9	43.2	46.5	46.8
1c	$E_{out} \leftrightarrow E_{in}$	64.2	66.2	65.5	68.4	62.8	71.9
	$Z_{out} \leftrightarrow Z_{in}$	62.8	59.3	62.1	66.5	58.0	68.8
1d	$E_{out} \leftrightarrow E_{in}$	73.5	71.6	73.4	78.3	72.9	84.2
	$Z_{out} \leftrightarrow Z_{in}$	73.1	74.2	68.8	76.8	73.9	81.8
2a	$E_{out} \leftrightarrow E_{in}$	22.6	25.2	28.1	28.1	26.6	29.3
	$Z_{out} \leftrightarrow Z_{in}$	24.5	23.7	24.2	25.6	27.7	29.6
2b	$E_{out} \leftrightarrow E_{in}$	55.6	52.8	56.5	57.1	58.3	61.2
	$Z_{out} \leftrightarrow Z_{in}$	52.6	51.2	49.6	52.8	54.9	56.4
2c	$E_{out} \leftrightarrow E_{in}$	73.6	74.3	70.2	78.2	71.0	83.8
	$Z_{out} \leftrightarrow Z_{in}$	73.0	71.7	69.4	77.4	68.6	80.3
2d	$E_{out} \leftrightarrow E_{in}$	85.1	89.0	82.3	91.3	84.4	96.6
	$Z_{out} \leftrightarrow Z_{in}$	84.3	83.8	79.4	88.2	83.5	93.1
3a	$E_{out} \leftrightarrow E_{in}$	24.5	26.1	26.2	27.9	25.3	30.1
	$Z_{out} \leftrightarrow Z_{in}$	21.2	22.3	21.6	23.7	24.2	26.9
3b	$E_{out} \leftrightarrow E_{in}$	44.6	43.1	43.4	48.2	44.6	49.2
	$Z_{out} \leftrightarrow Z_{in}$	41.9	41.3	38.3	44.3	43.0	44.7
3c	$E_{out} \leftrightarrow E_{in}$	63.4	64.1	63.9	67.4	60.2	69.3
	$Z_{out} \leftrightarrow Z_{in}$	61.6	63.6	59.1	65.4	58.1	65.3
3d	$E_{out} \leftrightarrow E_{in}$	72.4	77.6	77.8	81.3	71.7	79.9
	$Z_{out} \leftrightarrow Z_{in}$	71.5	75.9	72.3	76.4	71.4	77.5
4a	$E_{out} \leftrightarrow E_{in}$	26.4	26.6	27.3	28.1	26.9	32.0
	$Z_{out} \leftrightarrow Z_{in}$	21.4	23.3	22.0	24.4	25.7	26.5
4b	$E_{out} \leftrightarrow E_{in}$	53.0	54.8	51.9	56.4	55.5	58.5
	$Z_{out} \leftrightarrow Z_{in}$	50.9	48.3	43.7	53.4	47.5	54.1
4c	$E_{out} \leftrightarrow E_{in}$	72.5	72.2	72.0	77.7	69.4	76.0
	$Z_{out} \leftrightarrow Z_{in}$	70.3	69.1	69.5	75.0	69.0	75.0
4d	$E_{out} \leftrightarrow E_{in}$	83.4	84.9	81.9	90.1	85.0	93.0
	$Z_{out} \leftrightarrow Z_{in}$	82.4	84.4	83.5	86.7	81.9	89.3

[a] All calculations carried out with the cc-pVTZ basis set in the gas phase or in combination with an SMD description of the solvent (water or cyclohexane).

Table S5. α and α' pyramidalization dihedral angles along the photoisomerization MEPs of the different isomers of motor **4d**

Isomer	MEP point	α [deg.]	α' [deg.]
E_{out}	1	0	0
	2	1	-3
	3	2	-3
	4	1	-2
	5	1	-3
	6	1	-3
	7	1	-2
	8	1	-2
	9	1	-2
Z_{in}	1	-1	3
	2	-1	4
	3	-1	3
	4	-1	3
	5	-1	2
	6	-1	2
	7	-1	3
	8	-1	3
E_{in}	1	0	0
	2	-2	-3
	3	-2	-3
	4	-1	-3
	5	-1	-3
	6	-1	-3
	7	-1	-3
	8	-1	-2
	9	-1	-2
Z_{out}	1	1	-3
	2	1	-4
	3	1	-3
	4	0	-3
	5	1	-2
	6	1	-2
	7	1	-3
	8	1	-3

Description of multimedia files

4d-e-out-z-in.mov

This movie from the NAMD simulations of motor **4d** shows two representative trajectories merged together to illustrate a full 360° CCW $E_{\text{out}} \rightarrow Z_{\text{in}} \rightarrow E_{\text{out}}$ rotation around the central olefinic bond.

4d-e-in-z-out.mov

This movie from the NAMD simulations of motor **4d** shows two representative trajectories merged together to illustrate a full 360° CW $E_{\text{in}} \rightarrow Z_{\text{out}} \rightarrow E_{\text{in}}$ rotation around the central olefinic bond.

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Cartesian coordinates (in Å) for CASSCF S_0 equilibrium geometries of motors

1a–4d

1a- E_{out}

C	-3.02385830	-1.22029694	0.23365109
C	-1.82841062	0.76053164	-0.05572181
C	-0.81037590	-0.27614444	-0.03305658
C	-1.55389879	-1.60755317	0.03089133
C	0.54100527	-0.13762017	-0.09478952
C	1.37845939	-1.36303431	-0.17350957
C	1.30425357	1.16898098	-0.14543547
C	2.72115919	-1.31861580	-0.19337078
C	2.66705510	1.06053058	0.53940291
H	1.44762669	1.43365569	-1.19012785
H	0.75048239	1.96923153	0.31366115
C	3.51310116	-0.05274780	-0.06181498
H	3.17927260	2.01033717	0.46068643
H	2.51836166	0.86740981	1.59672983
H	4.38832118	-0.23446023	0.54922534
H	3.88383629	0.23503522	-1.04251414
H	-3.68994987	-1.65491540	-0.49496667
H	3.26330983	-2.23779851	-0.31467389
H	0.88789688	-2.31128609	-0.25793876
H	-1.20190022	-2.22589488	0.84163905
H	-1.43069620	-2.16427446	-0.88764628
H	-3.39210356	-1.45176937	1.22219284
H	-3.82461336	0.78434010	0.05929865
C	-1.70254404	2.23857374	-0.21392635
H	-1.26855928	2.66203781	0.68188484
H	-1.06083607	2.47562034	-1.04829543
H	-2.67263358	2.68616679	-0.37250699
N	-2.99461043	0.23471113	0.06227360

1a-Z_{in}

C	3.01297533	-1.25587278	-0.11010099
C	1.52304520	-1.60980863	-0.03306226
C	0.80649784	-0.26286216	-0.03826220
C	1.84228573	0.75167394	0.07906262
H	3.60620753	-1.70806266	0.66895833
H	3.45710103	-1.49178974	-1.06590911
H	1.22764946	-2.22706415	-0.86706780
H	1.30977227	-2.15814905	0.87405675
C	-0.54086492	-0.10169572	-0.12138252
C	-1.24819990	1.20099462	-0.22175675
C	-1.43704886	-1.31960254	-0.19828606
C	-2.58971071	1.28255023	-0.22786665
C	-2.77340948	-1.09497321	0.50593987
H	-1.61121148	-1.53466995	-1.25007495
H	-0.94580234	-2.18473569	0.22025518
C	-3.50764970	0.10802315	-0.06984630
H	-3.37965320	-1.98655318	0.41795456
H	-2.59576211	-0.93686465	1.56474390
H	-4.34184229	0.38411096	0.56306585
H	-3.93293130	-0.13319269	-1.04087557
H	3.84030600	0.72909691	0.14593821
H	-3.03965541	2.24818086	-0.36613840
C	1.73667790	2.23163806	0.22976997
H	1.37068148	2.66338254	-0.69205536
H	1.04656427	2.47869980	1.02224103
H	2.70275266	2.65996297	0.45254112
H	-0.68763694	2.10092419	-0.34370008
N	3.00153695	0.19888059	0.06562560

1a- E_{in}

C	3.02421004	-1.22022846	0.23256306
C	1.82840349	0.76073795	-0.05491008
C	0.81039310	-0.27595945	-0.03250930
C	1.55386348	-1.60736077	0.03225454
C	-0.54097071	-0.13759624	-0.09497187
C	-1.37824595	-1.36317434	-0.17329480
C	-1.30447113	1.16878264	-0.14707563
C	-2.72094250	-1.31897745	-0.19314120
C	-2.66726506	1.06078487	0.53784439
H	-0.75095511	1.96970734	0.31108256
H	-1.44783713	1.43219377	-1.19207782
C	-3.51314538	-0.05321311	-0.06227236
H	-3.88427509	0.23371355	-1.04305868
H	-4.38810690	-0.23472896	0.54918227
H	3.39445709	-1.45264103	1.22011404
H	-3.26293499	-2.23832089	-0.31390435
H	-0.88755674	-2.31141860	-0.25701737
H	1.42932281	-2.16544661	-0.88523905
H	1.20275929	-2.22438991	0.84440734
H	3.68887689	-1.65410596	-0.49780216
H	3.82461046	0.78459197	0.05945933
C	1.70248142	2.23889605	-0.21200802
H	1.06229031	2.47644839	-1.04742099
H	1.26668267	2.66147230	0.68331247
H	2.67273466	2.68689155	-0.36837654
H	-3.17964019	2.01042049	0.45817279
H	-2.51853684	0.86875090	1.59535776
N	2.99464396	0.23491800	0.06256470

1a-Z_{out}

C	-3.01320385	-1.25626889	-0.10722256
C	-1.84211036	0.75148754	0.07819498
C	-0.80646053	-0.26302456	-0.04040806
C	-1.52291034	-1.61004075	-0.03559279
C	0.54088066	-0.10174374	-0.12352432
C	1.24819558	1.20107791	-0.22321540
C	1.43746158	-1.31931953	-0.20034484
C	2.58969846	1.28279339	-0.22694425
C	2.77224793	-1.09490966	0.50698022
H	0.94573200	-2.18524203	0.21595745
H	1.61393573	-1.53285173	-1.25205858
C	3.50754677	0.10852404	-0.06656286
H	3.93549960	-0.13235187	-1.03650630
H	4.33998369	0.38478264	0.56859811
H	-3.46124390	-1.49360413	-1.06083158
H	3.03978115	2.24841159	-0.36489424
H	0.68768962	2.10077320	-0.34721579
H	-1.30667496	-2.16044491	0.86953062
H	-1.23000176	-2.22533543	-0.87196279
H	-3.60318583	-1.70745748	0.67491142
H	-3.84000324	0.72890702	0.14842754
C	-1.73633463	2.23150350	0.22836954
H	-1.04476329	2.47881296	1.01947049
H	-1.37209876	2.66308261	-0.69424543
H	-2.70202187	2.65978290	0.45290891
H	3.37885698	-1.98632633	0.41983082
H	2.59221071	-0.93746431	1.56548858
N	-3.00137117	0.19868104	0.06669615

1b- E_{out}

C	-4.11530796	-1.05756363	0.35095198
C	-2.75591437	0.76686299	-0.15972272
C	-1.83765799	-0.35740513	-0.08051863
C	-2.69941378	-1.60100766	0.12572719
C	-0.48363186	-0.36133977	-0.20257419
C	0.22525416	-1.63877323	-0.19312321
C	0.39807900	0.84753100	-0.40720339
C	1.56250620	-1.71749310	-0.19896565
C	1.77230193	0.75472249	0.29694600
H	0.54439744	0.96418989	-1.47566112
H	-0.07912157	1.74633006	-0.05857930
C	2.53376295	-0.52024319	-0.19363869
H	-4.85395965	-1.48814240	-0.30665607
H	2.01672935	-2.69175420	-0.22930009
H	-0.34564887	-2.54513667	-0.19794031
H	-2.36992734	-2.18292132	0.97203639
H	-2.67201682	-2.23979045	-0.74611126
H	-4.45446523	-1.16404092	1.37084720
H	-4.73381902	0.99218016	0.02669236
C	-2.50461191	2.20779654	-0.45291203
H	-1.98354421	2.66049440	0.37971134
H	-1.89186406	2.31146234	-1.33502947
H	-3.43723355	2.73149239	-0.60338108
N	-3.95948494	0.36690305	0.04532187
C	2.53330725	2.04712870	-0.03206706
H	2.02270914	2.89972097	0.40144130
H	3.53436980	2.03400129	0.37737039
H	2.61080498	2.21981112	-1.09703144
C	1.53689980	0.72768865	1.81836581
H	2.46239355	0.85434418	2.36131945
H	0.88671334	1.54665104	2.10662641
H	1.08015646	-0.19334252	2.15707638
C	3.07464296	-0.38120300	-1.63077341
H	3.89642994	0.32044042	-1.67343182
H	3.44898115	-1.33732495	-1.97528223
H	2.31786141	-0.06090991	-2.33515501
C	3.71740975	-0.89217692	0.71494423
H	4.25937117	-1.72645120	0.28654380
H	4.41523255	-0.07093716	0.81136997
H	3.40133083	-1.18484335	1.70651010

1b-Z_{in}

C	3.92237923	-1.36034806	-0.21449377
C	2.40572284	-1.58360620	-0.22555244
C	1.80529679	-0.18329992	-0.13043208
C	2.92127873	0.72735278	0.10494340
H	4.44189684	-1.91862581	0.54808307
H	4.39216328	-1.55112161	-1.16771652
H	2.09954848	-2.09424854	-1.12505247
H	2.10782018	-2.19219786	0.61651014
C	0.48249296	0.10104724	-0.23633901
C	-0.10853126	1.43738728	-0.21714512
C	-0.51265263	-1.01242415	-0.46693385
C	-1.43656640	1.62224898	-0.20232053
C	-1.86044426	-0.81398767	0.25984485
H	-0.67777457	-1.07797673	-1.53737528
H	-0.10059530	-1.96318168	-0.16346020
C	-2.49775485	0.54418467	-0.18950543
H	4.91123351	0.52070730	0.22417018
H	-1.79977434	2.63435609	-0.22881724
C	2.93840915	2.19724842	0.37220943
H	2.62731662	2.73446149	-0.51291134
H	2.26064703	2.43886654	1.17689240
H	3.93320254	2.52304330	0.64074823
H	0.51811374	2.30121273	-0.24308554
N	4.03116738	0.07388592	0.08121295
C	-2.74661800	-2.01912844	-0.08463381
H	-2.31274599	-2.92501241	0.32282673
H	-3.73684776	-1.92017519	0.33968205
H	-2.85260756	-2.16044308	-1.15164601
C	-1.60214382	-0.84488976	1.77764860
H	-2.52716966	-0.89968063	2.33350445
H	-1.02407709	-1.72529595	2.03544751
H	-1.05897671	0.02339919	2.12895968
C	-3.62472296	1.00689028	0.75149228
H	-4.09383351	1.89717554	0.35047518
H	-4.39418544	0.25244191	0.84680569
H	-3.26306791	1.24748876	1.74150956
C	-3.08801753	0.48122570	-1.61465757
H	-3.97417302	-0.13756841	-1.64377019
H	-3.37703260	1.47455612	-1.93557289
H	-2.38349714	0.10053886	-2.34249713

1b- E_{in}

C	4.11451329	-1.05705123	0.35437949
C	2.75582161	0.76698939	-0.15970072
C	1.83759224	-0.35748305	-0.08146635
C	2.69930748	-1.60094146	0.12578593
C	0.48361590	-0.36146607	-0.20427089
C	-0.22538787	-1.63891548	-0.19538148
C	-0.39819479	0.84731844	-0.40873293
C	-1.56270424	-1.71730086	-0.20074761
C	-1.77191847	0.75463728	0.29653683
H	0.07925382	1.74639856	-0.06112785
H	-0.54546780	0.96336008	-1.47714982
C	-2.53384780	-0.52021238	-0.19369852
H	4.45101802	-1.16311274	1.37522707
H	-2.01721481	-2.69145326	-0.23133411
H	0.34541795	-2.54536109	-0.20136632
H	2.67400882	-2.23912439	-0.74659750
H	2.36825876	-2.18363138	0.97095426
H	4.85492165	-1.48780288	-0.30116220
H	4.73348304	0.99258741	0.02954268
C	2.50489366	2.20773806	-0.45446394
H	1.89285029	2.31069358	-1.33715035
H	1.98327618	2.66138218	0.37731256
H	3.43774694	2.73111810	-0.60470148
N	3.95909686	0.36735667	0.04778812
C	-3.71630658	-0.89281108	0.71620489
H	-4.41432215	-0.07187300	0.81382594
H	-4.25847754	-1.72718242	0.28823223
H	-3.39889437	-1.18580937	1.70725507
C	-3.07654586	-0.38061964	-1.63009955
H	-3.45144434	-1.33652938	-1.97462790
H	-3.89829828	0.32113530	-1.67148212
H	-2.32062629	-0.06021958	-2.33536474
C	-1.53545536	0.72734759	1.81780177
H	-0.88475049	1.54598300	2.10583388
H	-2.46057282	0.85433484	2.36132179
H	-1.07892526	-0.19392972	2.15615039
C	-2.53293993	2.04727221	-0.03177655
H	-2.02180772	2.89965935	0.40152814
H	-2.61101219	2.22019144	-1.09666306
H	-3.53378458	2.03437493	0.37822499

1b-Z_{out}

C	-3.92255903	-1.35956788	-0.21774634
C	-2.92061904	0.72678684	0.10696454
C	-1.80516455	-0.18388812	-0.13087407
C	-2.40608415	-1.58397009	-0.22575508
C	-0.48251992	0.10047983	-0.23821660
C	0.10823859	1.43700358	-0.22114157
C	0.51284681	-1.01285020	-0.46825748
C	1.43624183	1.62206052	-0.20629642
C	1.85999290	-0.81362921	0.25959697
H	0.10086365	-1.96366629	-0.16484074
H	0.67882374	-1.07849011	-1.53855284
C	2.49759875	0.54417885	-0.19051754
H	-4.38991965	-1.54650310	-1.17294508
H	1.79938279	2.63413457	-0.23501472
H	-0.51863465	2.30061065	-0.24991936
H	-2.11021310	-2.19172315	0.61768182
H	-2.09857605	-2.09589424	-1.12403664
H	-4.44457431	-1.92011167	0.54143265
H	-4.91063828	0.52065075	0.22673029
C	-2.93665814	2.19593638	0.37837872
H	-2.25563970	2.43530694	1.18096289
H	-2.62911313	2.73564683	-0.50647929
H	-3.93038399	2.52097015	0.65176323
N	-4.03077879	0.07379453	0.08258964
C	1.60028451	-0.84304574	1.77719613
H	1.02179186	-1.72307991	2.03531944
H	2.52479832	-0.89748205	2.33394045
H	1.05700402	0.02570533	2.12718994
C	2.74659324	-2.01903394	-0.08284674
H	2.85339154	-2.16155030	-1.14961793
H	3.73649934	-1.91945036	0.34208758
H	2.31254113	-2.92451103	0.32532620
C	3.08996704	0.47952362	-1.61472125
H	3.37919458	1.47250399	-1.93652537
H	3.97632965	-0.13906906	-1.64171086
H	2.38662737	0.09767446	-2.34309536
C	3.62308758	1.00836681	0.75154177
H	4.39246937	0.25412397	0.84915019
H	4.09273902	1.89811144	0.34995869
H	3.25987387	1.25037041	1.74064815

1c- E_{out}

C	-4.70881214	-1.04745868	0.33701521
C	-3.31218597	0.72147808	-0.29234157
C	-2.40970326	-0.41861085	-0.10420422
C	-3.29323932	-1.62216355	0.21213996
C	-1.05893862	-0.45533797	-0.19681912
C	-0.35958546	-1.73080239	-0.02105262
C	-0.17171501	0.72706544	-0.51733247
C	0.97412674	-1.84076599	-0.00123005
C	1.18089083	0.64604997	0.19629914
H	0.01276865	0.75664372	-1.58299214
H	-0.61141985	1.66109507	-0.22880350
C	1.90707446	-0.67323909	-0.17490735
H	-5.42856656	-1.51037131	-0.31922880
H	1.44438807	-2.79812713	0.09059848
H	-0.93712289	-2.62467269	0.09135926
H	-2.99480756	-2.10613461	1.12878066
H	-3.25058867	-2.35463638	-0.58125182
H	-5.09325161	-1.06358425	1.34545105
H	-5.29097955	0.98571391	-0.14613771
C	-3.02783860	2.13352763	-0.69081974
H	-2.49690234	2.63906749	0.10427107
H	-2.42042873	2.16031669	-1.58279757
H	-3.94863812	2.66618310	-0.88023720
N	-4.52345589	0.35212540	-0.06921827
Cl	2.13206501	2.07626991	-0.22698814
Cl	2.38032680	-0.64627794	-1.90473087
Cl	0.86995538	0.69135413	1.95917284
Cl	3.36877021	-0.92321067	0.78879648

1c-Z_{in}

C	-4.47101991	1.33517290	-0.43285887
C	-2.95031592	1.52348183	-0.44615820
C	-2.38212138	0.12978773	-0.19855599
C	-3.52585088	-0.73539535	0.10972063
H	-4.98483180	1.97289255	0.26863590
H	-4.92788919	1.44367972	-1.40481278
H	-2.62192322	1.93227749	-1.38909303
H	-2.64692192	2.20610570	0.33509546
C	-1.06520757	-0.18394561	-0.24089865
C	-0.49554441	-1.51821088	-0.04881047
C	-0.06339586	0.90367527	-0.56867511
C	0.82332795	-1.74621565	-0.01261332
C	1.26595393	0.71280801	0.16278134
H	0.12952678	0.89945454	-1.63368903
H	-0.43531746	1.87856121	-0.30661400
C	1.86658826	-0.67519270	-0.18163200
H	-5.50922640	-0.47183205	0.17143517
H	1.20113046	-2.74293963	0.08810781
C	-3.57685917	-2.16896902	0.52704017
H	-3.23752537	-2.80063916	-0.28224369
H	-2.93982674	-2.33002646	1.38421306
H	-4.58683056	-2.45384712	0.78427331
H	-1.13775645	-2.36364912	0.05029322
N	-4.61566323	-0.06268754	-0.00348353
Cl	2.35412918	2.03922879	-0.26186828
Cl	0.93737225	0.80729353	1.92172146
Cl	3.28274642	-1.05613842	0.80706255
Cl	2.36458322	-0.71986054	-1.90399614

1c- E_{in}

C	4.70888653	-1.04740180	0.33703385
C	3.31221750	0.72151344	-0.29228210
C	2.40974128	-0.41855937	-0.10398312
C	3.29330180	-1.62210675	0.21230675
C	1.05896811	-0.45526655	-0.19646662
C	0.35961870	-1.73072890	-0.02068958
C	0.17177747	0.72716422	-0.51696684
C	-0.97409005	-1.84072358	-0.00105089
C	-1.18095067	0.64606258	0.19642220
H	0.61140546	1.66116179	-0.22820483
H	-0.01258946	0.75693893	-1.58264045
C	-1.90702907	-0.67321922	-0.17494352
H	5.09339541	-1.06344182	1.34544497
H	-1.44434673	-2.79808810	0.09076432
H	0.93716381	-2.62457882	0.09184495
H	3.25057187	-2.35458769	-0.58107438
H	2.99495574	-2.10606723	1.12898022
H	5.42859103	-1.51037781	-0.31921930
H	5.29104397	0.98570469	-0.14642114
C	3.02784879	2.13349826	-0.69097663
H	2.42026204	2.16013095	-1.58283676
H	2.49708779	2.63922415	0.10411346
H	3.94863259	2.66607828	-0.88068262
N	4.52351145	0.35215016	-0.06931470
Cl	-0.87024766	0.69127452	1.95934689
Cl	-2.13208962	2.07626267	-0.22700523
Cl	-3.36894687	-0.92325416	0.78842785
Cl	-2.37985222	-0.64629584	-1.90487874

1c-Z_{out}

C	4.47125797	1.33393096	-0.43676248
C	3.52550118	-0.73465938	0.11160775
C	2.38218656	0.13034068	-0.19776121
C	2.95070720	1.52396912	-0.44493904
C	1.06544923	-0.18381072	-0.24230951
C	0.49598672	-1.51871550	-0.05384357
C	0.06327566	0.90371361	-0.56871419
C	-0.82291595	-1.74664994	-0.01727223
C	-1.26520021	0.71193673	0.16420626
H	0.43519903	1.87866141	-0.30689928
H	-0.13090823	0.89958220	-1.63349988
C	-1.86639478	-0.67512191	-0.18186497
H	4.92433446	1.43837200	-1.41096510
H	-1.20075179	-2.74381190	0.07871667
H	1.13819068	-2.36460663	0.04146741
H	2.65054613	2.20541647	0.33865397
H	2.61976415	1.93482672	-1.38604301
H	4.98865368	1.97353287	0.26033716
H	5.50904484	-0.47166924	0.17253653
C	3.57573638	-2.16713159	0.53270225
H	2.93574659	-2.32647462	1.38797487
H	3.23965371	-2.80103456	-0.27620993
H	4.58497463	-2.45087489	0.79406216
N	4.61561454	-0.06260243	-0.00329110
Cl	-3.28017069	-1.05872896	0.80947519
Cl	-2.36850500	-0.71519925	-1.90295292
Cl	-2.35404892	2.03883049	-0.25688716
Cl	-0.93425877	0.80284827	1.92285138

1d- E_{out}

C	5.44070177	-1.01868737	-0.67180483
C	4.04382809	0.30209759	0.65186482
C	3.13654186	-0.60693580	-0.04804391
C	4.01600210	-1.55359417	-0.85916618
C	1.78175179	-0.64655188	-0.01048215
C	1.07461115	-1.68645705	-0.75924682
C	0.89976087	0.28237856	0.79517760
C	-0.26050299	-1.74897821	-0.84707157
C	-0.44279068	0.55976255	0.10636901
H	0.69650584	-0.17366565	1.75550726
H	1.36130213	1.23291940	0.96987641
C	-1.18267639	-0.76608839	-0.18801924
H	6.12903403	-1.75046026	-0.27923186
H	-0.73053534	-2.55755289	-1.36780385
H	1.64512433	-2.44454981	-1.25398067
H	3.73975768	-1.55602928	-1.90200113
H	3.93776744	-2.56667577	-0.49114210
H	5.85918376	-0.59509486	-1.57229140
H	6.02197814	0.56051916	0.68992242
C	3.76079801	1.38608037	1.63616603
H	3.25884392	2.20425755	1.13656984
H	3.12168989	1.02199898	2.42638919
H	4.67946993	1.75610948	2.06654939
N	5.25334547	0.04909368	0.31536430
Br	-1.46016528	1.77353699	1.22205375
Br	-0.04268456	1.50117301	-1.57255910
Br	-2.78445642	-0.54047350	-1.24591751
Br	-1.73652259	-1.66533544	1.53902630

1d-Z_{in}

C	-5.21996319	0.83192500	-1.04571578
C	-3.70091246	1.02274816	-1.11211416
C	-3.12620580	-0.12955283	-0.29467359
C	-4.26852747	-0.81090135	0.32192062
H	-5.75336393	1.69395209	-0.67793868
H	-5.65762433	0.52271106	-1.98273055
H	-3.35574848	1.00452752	-2.13426878
H	-3.42018747	1.97483195	-0.68424345
C	-1.80521667	-0.40397400	-0.17306099
C	-1.22677792	-1.52363256	0.56752454
C	-0.80791784	0.47041646	-0.90572074
C	0.09440508	-1.69423551	0.71161664
C	0.51466370	0.61992220	-0.14705095
H	-0.59984825	0.03056660	-1.87300746
H	-1.19979429	1.45740695	-1.07470202
C	1.13086775	-0.77402690	0.12971345
H	-6.25536999	-0.58294453	0.23265425
H	0.47297356	-2.55602171	1.22119205
C	-4.31610875	-1.94356177	1.29483121
H	-3.94334498	-2.84539093	0.82935003
H	-3.70476975	-1.71910489	2.15651877
H	-5.33032732	-2.12040068	1.62264535
H	-1.86124215	-2.26190770	1.00269761
N	-5.36191023	-0.26621085	-0.07979712
Br	0.10219611	1.52948460	1.54807636
Br	1.68240026	1.78677338	-1.15948563
Br	2.67521044	-0.70989911	1.29870387
Br	1.70161240	-1.63355867	-1.54801086

1d- E_{in}

C	-5.44068344	-1.01871346	-0.67181396
C	-4.04379802	0.30199901	0.65187235
C	-3.13655743	-0.60691149	-0.04799257
C	-4.01595442	-1.55362139	-0.85917441
C	-1.78173883	-0.64647814	-0.01040092
C	-1.07462298	-1.68629300	-0.75920982
C	-0.89969191	0.28236457	0.79514718
C	0.26046189	-1.74883611	-0.84719090
C	0.44281271	0.55977882	0.10636533
H	-0.69642852	-0.17353500	1.75560161
H	-1.36117476	1.23294927	0.96991973
C	1.18261909	-0.76616807	-0.18785534
H	-6.12899170	-1.75053740	-0.27929029
H	0.73035726	-2.55735152	-1.36812251
H	-1.64521718	-2.44432213	-1.25393902
H	-3.73967393	-1.55607808	-1.90199850
H	-3.93771453	-2.56669181	-0.49111885
H	-5.85915032	-0.59512320	-1.57231169
H	-6.02196485	0.56044571	0.68995070
C	-3.76085915	1.38605134	1.63619549
H	-3.25873048	2.20418403	1.13670435
H	-3.12198534	1.02202237	2.42664858
H	-4.67962837	1.75617045	2.06629468
N	-5.25334887	0.04901566	0.31537355
Br	1.46035456	1.77363239	1.22179688
Br	0.04275365	1.50101180	-1.57259578
Br	2.78452598	-0.54076130	-1.24594817
Br	1.73636687	-1.66540633	1.53916531

1d-Z_{out}

C	5.22020941	0.83218097	-1.04535181
C	4.26841650	-0.81069688	0.32201827
C	3.12627436	-0.12951079	-0.29496716
C	3.70110523	1.02266133	-1.11253654
C	1.80529248	-0.40407736	-0.17374537
C	1.22650263	-1.52294705	0.56804781
C	0.80748705	0.47064453	-0.90572801
C	-0.09451592	-1.69364388	0.71256485
C	-0.51491544	0.62016265	-0.14702590
H	1.19971325	1.45730933	-1.07573801
H	0.59930414	0.03010282	-1.87269426
C	-1.13086814	-0.77400238	0.12956320
H	5.65842488	0.52310790	-1.98215727
H	-0.47257577	-2.55531977	1.22281310
H	1.86076945	-2.26075765	1.00427252
H	3.41993348	1.97484790	-0.68521166
H	3.35645386	1.00381315	-2.13485889
H	5.75325202	1.69428791	-0.67722815
H	6.25535053	-0.58271165	0.23317046
C	4.31583429	-1.94403188	1.29412248
H	3.70384177	-1.72074290	2.15561494
H	3.94379113	-2.84557649	0.82745955
H	5.32991514	-2.12068195	1.62248684
N	5.36191512	-0.26603278	-0.07945447
Br	-1.68284767	1.78716054	-1.15829211
Br	-0.10156865	1.52938716	1.54816724
Br	-2.67571081	-0.71057776	1.29778530
Br	-1.69995033	-1.63441102	-1.54817298

2a- E_{out}

C	-3.23064278	-1.79731671	0.25078070
C	-2.62240779	0.43121229	-0.10486473
C	-1.35629595	-0.28160066	-0.00313430
C	-1.70409367	-1.76389027	0.11337106
C	-0.09207091	0.21870794	-0.04201510
C	1.03479717	-0.70786126	-0.03352637
C	0.26921926	1.68449427	-0.14349808
C	2.33419638	-0.32928011	-0.03126917
C	1.58095525	1.98174167	0.57712389
H	0.37177270	1.93693418	-1.19585822
H	-0.50275570	2.31371188	0.26375690
C	2.72104552	1.12492218	0.04796495
H	1.82003621	3.03131645	0.46613961
H	1.45340028	1.79687423	1.63870640
H	3.58534992	1.23783175	0.68753804
H	3.02245155	1.46330157	-0.93961050
H	-3.72179289	-2.42413584	-0.47660341
H	0.81910959	-1.75643514	-0.07771261
H	-1.23235735	-2.22163117	0.96871758
H	-1.39204386	-2.30757088	-0.76732254
H	-3.56750794	-2.07803813	1.23741340
C	-2.91092035	1.88015020	-0.33363270
H	-2.64421078	2.45138054	0.54459030
H	-2.33931022	2.25160314	-1.16984884
H	-3.96245476	2.02950437	-0.53353682
N	-3.60292993	-0.39803014	0.00901052
C	3.37324754	-1.35950142	-0.13008789
H	3.02166003	-2.37541733	-0.15341887
C	4.69217602	-1.13872314	-0.21425597
H	5.12110107	-0.15620026	-0.20879770
H	5.37650244	-1.95972231	-0.29878473
H	-4.55407706	-0.10273192	-0.03999780

2a-Z_{in}

C	3.86521829	-0.54187063	-0.23988254
C	2.54554481	-1.31432746	-0.13416386
C	1.47028620	-0.23476717	-0.04074221
C	2.17456203	1.03348579	0.10786564
H	4.60400637	-0.83438772	0.48925134
H	4.30954026	-0.58323272	-1.22316258
H	2.40470685	-1.95359390	-0.99156530
H	2.54535931	-1.94058517	0.74716776
C	0.13220196	-0.47386623	-0.07744812
C	-0.90744059	0.54917679	-0.07677695
C	-0.36319741	-1.89858004	-0.19757846
C	-2.23309301	0.27656378	-0.04787000
C	-1.67368124	-2.09634962	0.55514183
H	-0.51256109	-2.11232148	-1.25336126
H	0.37590461	-2.59770811	0.16300836
C	-2.74674019	-1.13592875	0.06386888
H	-2.00708552	-3.11912281	0.43936862
H	-1.50320189	-1.93816529	1.61514994
H	-3.59367512	-1.16198718	0.73559509
H	-3.11613482	-1.44866709	-0.90888144
C	1.65629346	2.41357046	0.35241697
H	1.13752279	2.77178852	-0.52599897
H	0.96694820	2.41283956	1.18307327
H	2.46940131	3.09098965	0.57113890
H	-0.62262556	1.57477496	-0.15935821
N	3.44613440	0.83992545	0.02586038
C	-3.18424652	1.38884304	-0.15648227
H	-2.75011972	2.37141257	-0.21112627
C	-4.51827811	1.27956696	-0.21411474
H	-5.02867770	0.33760767	-0.17718606
H	-5.13187110	2.15370495	-0.30845348
H	4.10154273	1.58694619	0.10868571

2a- E_{in}

C	3.23160527	-1.79836866	0.24372519
C	2.62222538	0.43108189	-0.10477938
C	1.35627025	-0.28192684	0.00020047
C	1.70431008	-1.76432094	0.11482874
C	0.09194937	0.21842252	-0.03672850
C	-1.03492247	-0.70814959	-0.02557656
C	-0.26865276	1.68429660	-0.14071631
C	-2.33432599	-0.32960222	-0.02677937
C	-1.58272846	1.98391483	0.57462000
H	0.50224961	2.31317469	0.26929282
H	-0.36659047	1.93602078	-1.19375186
C	-2.72148808	1.12482082	0.04615281
H	-3.02135346	1.45958361	-0.94319274
H	-3.58699223	1.23964364	0.68392692
H	3.57395096	-2.08260400	1.22748366
H	-0.81904362	-1.75691963	-0.06471076
H	1.38707437	-2.30796560	-0.76402954
H	1.23714968	-2.22188729	0.97283803
H	3.71851867	-2.42286160	-0.48855812
C	2.91035657	1.88057516	-0.33041601
H	2.33850410	2.25401061	-1.16562104
H	2.64364778	2.44963439	0.54923057
H	3.96183118	2.03067606	-0.53009539
H	-1.82167543	3.03300099	0.45860871
H	-1.45820084	1.80359452	1.63737350
N	3.60306456	-0.39841030	0.00462986
C	-3.37328267	-1.36003667	-0.12436096
H	-3.02210982	-2.37629892	-0.13954518
C	-4.69140556	-1.13875710	-0.21941873
H	-5.11937192	-0.15575122	-0.22472535
H	-5.37580327	-1.95968078	-0.30427217
H	4.55408922	-0.10330978	-0.04829930

2a-Z_{out}

C	-3.86534294	-0.54199896	-0.23888504
C	-2.17449340	1.03347687	0.10753672
C	-1.47028289	-0.23480062	-0.04112120
C	-2.54555246	-1.31439359	-0.13411480
C	-0.13220151	-0.47388839	-0.07807983
C	0.90743902	0.54917693	-0.07721628
C	0.36333229	-1.89853995	-0.19838199
C	2.23306893	0.27657917	-0.04789037
C	1.67343834	-2.09625741	0.55501916
H	-0.37589589	-2.59787445	0.16153176
H	0.51334840	-2.11190227	-1.25415015
C	2.74668141	-1.13592410	0.06398806
H	3.11625096	-1.44870065	-0.90868526
H	3.59347149	-1.16199705	0.73589467
H	-4.31056903	-0.58363293	-1.22174660
H	0.62264096	1.57476712	-0.15981911
H	-2.54478372	-1.94082570	0.74708816
H	-2.40519667	-1.95350107	-0.99171481
H	-4.60346152	-0.83437447	0.49099385
C	-1.65614341	2.41358755	0.35177507
H	-0.96719534	2.41301277	1.18277725
H	-1.13689823	2.77149042	-0.52647488
H	-2.46925294	3.09118746	0.56991189
H	2.00688910	-3.11905997	0.43965466
H	1.50245299	-1.93778619	1.61490628
N	-3.44611272	0.83987520	0.02621473
C	3.18426942	1.38886842	-0.15613370
H	2.75017459	2.37146375	-0.21048625
C	4.51828942	1.27954665	-0.21354282
H	5.02862433	0.33754356	-0.17685522
H	5.13194839	2.15367501	-0.30753496
H	-4.10148137	1.58694187	0.10898100

2b- E_{out}

C	4.18316834	1.52328906	0.40919638
C	3.19946988	-0.49015280	-0.23351589
C	2.07998885	0.41128822	-0.04000538
C	2.67883900	1.78270974	0.26155669
C	0.74794764	0.14494310	-0.14044846
C	-0.20053928	1.23591197	-0.02024685
C	0.12983408	-1.19678451	-0.42245218
C	-1.54854767	1.09821376	-0.04708530
C	-1.22055474	-1.39835046	0.29277127
H	-0.00475399	-1.28116327	-1.49518378
H	0.77673303	-2.00307703	-0.12432471
C	-2.23870557	-0.27147081	-0.12293481
H	4.79359016	2.14758468	-0.22420577
H	0.19710078	2.22710475	0.05431484
H	2.27043600	2.21024291	1.16387564
H	2.49016141	2.47495213	-0.54730027
H	4.53215611	1.61571971	1.42715368
C	3.23206141	-1.92300750	-0.64853721
H	2.85564366	-2.54072763	0.15554806
H	2.61126236	-2.07919006	-1.51693968
H	4.24331212	-2.22816065	-0.87422934
N	4.30658901	0.12667786	-0.01491765
C	-2.29128878	2.40736928	-0.01700565
H	-1.66713817	3.23424462	0.27071976
C	-3.55598242	2.70284637	-0.34669273
H	-4.27886381	1.99023219	-0.68018145
H	-3.88687166	3.72178504	-0.29448292
C	-3.45839112	-0.30692528	0.82228035
H	-3.23384434	0.10642405	1.79540892
H	-4.28859733	0.24743435	0.41919797
H	-3.80116267	-1.32196804	0.96085468
C	-2.74003559	-0.47584198	-1.56937073
H	-3.37587260	-1.34734596	-1.63843524
H	-3.32047455	0.37385397	-1.89518572
H	-1.92911142	-0.59262466	-2.27655957
C	-1.70903399	-2.80295611	-0.09807244
H	-1.75770025	-2.93889952	-1.16978688
H	-1.02461159	-3.54721215	0.29301442
H	-2.68402860	-3.02594486	0.31073232
C	-0.96706487	-1.40458882	1.81328093
H	-1.83345083	-1.75250722	2.35609959
H	-0.15414279	-2.08288052	2.04881001
H	-0.70693206	-0.42880772	2.20169096
H	5.18930883	-0.32376924	-0.10598984

2b-Z_{in}

C	4.41123161	-0.91561115	-0.37027362
C	2.96177853	-1.41453974	-0.35477174
C	2.12105944	-0.16040278	-0.12948434
C	3.05977830	0.91790770	0.15253006
H	5.05775898	-1.42628716	0.32570510
H	4.86404112	-0.94110315	-1.35019016
H	2.71469704	-1.90597360	-1.28281614
H	2.81720565	-2.12845634	0.44400595
C	0.76275184	-0.12458680	-0.18423805
C	-0.05695579	1.06614318	-0.05215696
C	-0.00668459	-1.38444588	-0.47496990
C	-1.41221901	1.07270153	-0.05544666
C	-1.35806195	-1.45223831	0.25712591
H	-0.15949543	-1.43452259	-1.54775802
H	0.56987381	-2.25777317	-0.20872948
C	-2.24988407	-0.21436404	-0.13277415
C	2.82249932	2.33991914	0.54592485
H	2.38319196	2.88135851	-0.28031054
H	2.14695161	2.38737403	1.38661223
H	3.75263379	2.81946167	0.81576710
H	0.42902197	2.01408421	0.00746363
N	4.26940359	0.48573490	0.04329272
C	-2.01027546	2.42956907	0.00291052
H	-1.31685682	3.18201273	0.33518830
C	-3.22633722	2.86955701	-0.34484609
H	-4.01175485	2.25015381	-0.72060077
H	-3.44902229	3.91559387	-0.26220684
C	-3.45450005	-0.12360261	0.82764573
H	-3.17216936	0.24426825	1.80408814
H	-4.21974704	0.53017285	0.44503505
H	-3.90976363	-1.09491683	0.95508264
C	-2.78850306	-0.35035809	-1.57431033
H	-3.52020712	-1.14345821	-1.63814929
H	-3.27216258	0.56060150	-1.89152497
H	-2.00474154	-0.55651179	-2.29120268
C	-1.08661723	-1.50363108	1.77370523
H	-1.97810606	-1.76184274	2.32619606
H	-0.34821035	-2.26782308	1.98926530
H	-0.71751329	-0.56562809	2.16783633
C	-2.00309355	-2.79021104	-0.13984833
H	-2.08021528	-2.90821275	-1.21190854
H	-1.39741561	-3.60799743	0.23308778
H	-2.99098900	-2.91036197	0.28156131
H	5.05802270	1.07476144	0.20252067

2b- E_{in}

C	-4.18930629	1.49955209	0.43016414
C	-3.19632099	-0.51042536	-0.20949961
C	-2.08118678	0.39781977	-0.02277087
C	-2.68638033	1.76614229	0.28041066
C	-0.74815315	0.13924644	-0.13075330
C	0.19436537	1.23589867	-0.01555809
C	-0.12471798	-1.19929540	-0.41711155
C	1.54285737	1.10743523	-0.05772917
C	1.23603987	-1.39147906	0.28082285
H	-0.76296427	-2.00850108	-0.10822986
H	-0.00379757	-1.28620947	-1.49126461
C	2.24089750	-0.25731339	-0.14718300
H	-4.53827832	1.59453425	1.44786101
H	-0.20897336	2.22412430	0.06703420
H	-2.50210127	2.45988910	-0.52810364
H	-2.27872414	2.19494215	1.18250716
H	-4.80320446	2.11810838	-0.20554581
C	-3.22240294	-1.94442262	-0.62099767
H	-2.60696389	-2.09804230	-1.49371534
H	-2.83580058	-2.55805464	0.18133441
H	-4.23318655	-2.25685637	-0.83868132
N	-4.30609145	0.10070684	0.01172384
C	2.27713330	2.42169219	-0.03237049
H	1.65142386	3.24310475	0.26752944
C	3.53441520	2.72667795	-0.38108457
H	4.25580026	2.01975150	-0.72961019
H	3.85953873	3.74760116	-0.33154511
H	-5.18656241	-0.35502141	-0.07484835
C	3.47484682	-0.28713753	0.77954092
H	4.29530812	0.27356710	0.36537889
H	3.26228810	0.12246124	1.75694583
H	3.82620983	-1.30023480	0.91045217
C	2.72168852	-0.45518641	-1.60148201
H	3.29152613	0.39898900	-1.93428910
H	3.36210482	-1.32234215	-1.68206453
H	1.90096468	-0.57587889	-2.29659167
C	1.72922313	-2.79257763	-0.11686506
H	1.05375986	-3.54150122	0.28083469
H	1.76726597	-2.92732528	-1.18915184
H	2.70985482	-3.00982331	0.28136119
C	1.00187297	-1.40053514	1.80444387
H	0.19776365	-2.08584095	2.04965372
H	1.87795860	-1.74145771	2.33605283
H	0.73832425	-0.42726821	2.19679194

2b-Z_{out}

C	-4.41043961	-0.91370878	-0.38169655
C	-3.06108735	0.91834342	0.15118332
C	-2.12137335	-0.16050815	-0.12639132
C	-2.96182755	-1.41424655	-0.35488898
C	-0.76304178	-0.12483034	-0.17827644
C	0.05692419	1.06566688	-0.04535719
C	0.00594431	-1.38542790	-0.46741833
C	1.41212846	1.07234262	-0.05180564
C	1.35942743	-1.45218842	0.26072618
H	-0.57009864	-2.25815444	-0.19806543
H	0.15607470	-1.43808090	-1.54043946
C	2.24960464	-0.21467044	-0.13367766
H	-4.85442714	-0.93619922	-1.36573340
H	-0.42905605	2.01345634	0.01741330
H	-2.82370199	-2.12641040	0.44667156
H	-2.70886760	-1.90822190	-1.27997917
H	-5.06383652	-1.42522241	0.30717833
C	-2.82470519	2.33963744	0.54756237
H	-2.15238059	2.38542447	1.39093479
H	-2.38181571	2.88194247	-0.27622201
H	-3.75561168	2.81938391	0.81432552
N	-4.27029923	0.48673804	0.03596243
C	2.01038121	2.42890464	0.00738902
H	1.31770268	3.18115266	0.34164004
C	3.22551176	2.86904390	-0.34278442
H	4.01008066	2.25003654	-0.72094562
H	3.44868095	3.91490661	-0.25905207
C	3.45934002	-0.12448120	0.82033176
H	4.22516604	0.52475956	0.43127020
H	3.18322252	0.24824811	1.79670317
H	3.91170109	-1.09687004	0.94947082
C	2.78053841	-0.35024080	-1.57813822
H	3.26054498	0.56169713	-1.89833089
H	3.51345271	-1.14196509	-1.64562438
H	1.99337224	-0.55819311	-2.29071069
C	1.09319485	-1.50220240	1.77822269
H	0.35779023	-2.26830979	1.99708305
H	1.98731391	-1.75712029	2.32797075
H	0.72258051	-0.56482397	2.17236613
C	2.00319731	-2.79060060	-0.13722471
H	1.39854946	-3.60797163	0.23828773
H	2.07683427	-2.90946963	-1.20944703
H	2.99240519	-2.91071014	0.28105682
H	-5.05949374	1.07565881	0.19249260

2c- E_{out}

C	4.74830480	1.38967642	0.35759385
C	3.59692300	-0.52569347	-0.33386933
C	2.55137788	0.46825713	-0.08678692
C	3.26540384	1.76837974	0.27093013
C	1.20540345	0.31865798	-0.16467316
C	0.34319967	1.47215780	0.05468727
C	0.49341902	-0.96271333	-0.51718966
C	-1.00862469	1.46227102	0.05476272
C	-0.84972670	-1.06257014	0.20019445
H	0.31193072	-0.99632520	-1.58304838
H	1.05232155	-1.83589653	-0.24432776
C	-1.76225038	0.15224437	-0.14468137
H	5.38761627	1.97557293	-0.28352525
H	0.81556629	2.42292772	0.18813822
H	2.91749884	2.16945927	1.20996932
H	3.11042797	2.51960288	-0.49046481
H	5.14152064	1.41593747	1.36247250
C	3.50281297	-1.94522450	-0.79251873
H	3.06766441	-2.55490973	-0.01248685
H	2.88335768	-2.01847163	-1.67341025
H	4.48411456	-2.33413798	-1.02335123
N	4.75098085	-0.00325832	-0.10878503
C	-1.69387359	2.76463577	0.16601607
H	-1.06469163	3.53882240	0.56495291
C	-2.92475449	3.10454747	-0.23180995
H	-3.62174833	2.41960689	-0.66567914
H	-3.25072573	4.12008646	-0.12156585
Cl	-3.24338181	0.06835300	0.82274338
Cl	-0.52276728	-1.09864680	1.96158565
Cl	-1.60373412	-2.60277684	-0.24173863
Cl	-2.21308946	0.07327962	-1.88190669
H	5.59647978	-0.52105588	-0.22263047

2c-Z_{in}

C	4.78339469	-1.05211413	-0.52059014
C	3.29744872	-1.42612144	-0.51722152
C	2.56877945	-0.12232231	-0.20767955
C	3.60185366	0.85801641	0.13291534
H	5.38851065	-1.65634614	0.13625833
H	5.22602339	-1.05387617	-1.50522485
H	3.00281096	-1.83932578	-1.46933916
H	3.09642606	-2.16829635	0.24278420
C	1.22083360	0.02821338	-0.23024795
C	0.50015930	1.27100757	0.00195297
C	0.36099737	-1.15998675	-0.58537254
C	-0.84547047	1.40380762	0.02849908
C	-0.96756327	-1.12596725	0.16028182
H	0.16065339	-1.15531644	-1.64884000
H	0.84318791	-2.09119493	-0.34499775
C	-1.74565491	0.18642886	-0.15441529
C	3.48553658	2.26483549	0.62236311
H	3.07818907	2.89359406	-0.15737034
H	2.83126424	2.30762032	1.48047659
H	4.45516479	2.65067077	0.90240128
H	1.05959863	2.17183449	0.11202133
N	4.76466370	0.32923750	-0.02047022
C	-1.38295045	2.77398389	0.14952832
H	-0.66688335	3.47560446	0.53679014
C	-2.57698953	3.24724529	-0.22313853
H	-3.35329133	2.64314691	-0.64194085
H	-2.78786379	4.29210750	-0.10646627
Cl	-2.24702983	0.17199062	-1.87935867
Cl	-3.20164242	0.26610113	0.85119520
Cl	-1.89781331	-2.56766885	-0.27144560
Cl	-0.60658170	-1.21048097	1.91476732
H	5.60404920	0.83483523	0.16874920

2c- E_{in}

C	-4.76631800	1.36834934	0.34970317
C	-3.60264695	-0.53666169	-0.32929086
C	-2.56361193	0.45786143	-0.07858976
C	-3.28418663	1.75480780	0.27557808
C	-1.21577812	0.30878644	-0.15125278
C	-0.35917217	1.46601509	0.06796703
C	-0.49912513	-0.97100175	-0.49906356
C	0.99302652	1.46121952	0.06771809
C	0.84638048	-1.06398179	0.21498282
H	-1.05378668	-1.84540388	-0.22175022
H	-0.32050183	-1.00687394	-1.56545051
C	1.74965314	0.15541858	-0.12557635
H	-5.16600160	1.40266415	1.35202788
H	-0.83650286	2.41424114	0.20069508
H	-3.12434339	2.50725661	-0.48366995
H	-2.94277635	2.15492747	1.21750995
H	-5.39878087	1.95581507	-0.29702607
C	-3.49830391	-1.95351302	-0.78379874
H	-2.86504231	-2.02650913	-1.65491453
H	-3.06782095	-2.55489263	0.00610696
H	-4.47507013	-2.34701941	-1.02290087
N	-4.75654975	-0.02244986	-0.11329167
C	1.67205061	2.76674394	0.17793311
H	1.04254905	3.53702966	0.58383967
C	2.89804705	3.11233891	-0.23015736
H	3.59340520	2.43061784	-0.67173182
H	3.22123511	4.12888239	-0.12104218
H	-5.59684250	-0.54333955	-0.23536379
Cl	3.24042967	0.07723495	0.82063527
Cl	2.19885756	0.07827128	-1.90936924
Cl	1.60703726	-2.59929081	-0.23184158
Cl	0.52389240	-1.10404517	1.97722175

2c-Z_{out}

C	-4.78329229	-1.05155981	-0.52199877
C	-3.60170418	0.85791014	0.13325234
C	-2.56873379	-0.12249340	-0.20755603
C	-3.29755089	-1.42627510	-0.51665527
C	-1.22080927	0.02796400	-0.23036882
C	-0.50019796	1.27096482	0.00123783
C	-0.36098217	-1.16028453	-0.58531616
C	0.84537394	1.40389118	0.02790347
C	0.96744583	-1.12581734	0.16057135
H	-0.84316038	-2.09141921	-0.34467814
H	-0.16050332	-1.15582636	-1.64874355
C	1.74551035	0.18647957	-0.15478101
H	-5.22448414	-1.05253275	-1.50728169
H	-1.05978235	2.17175085	0.11073009
H	-3.09771932	-2.16766129	0.24445442
H	-3.00207990	-1.84072412	-1.46795102
H	-5.38966903	-1.65580829	0.13365743
C	-3.48522737	2.26423057	0.62406326
H	-2.83032578	2.30618310	1.48172488
H	-3.07857524	2.89391955	-0.15527794
H	-4.45471045	2.64958944	0.90526100
N	-4.76456605	0.32952668	-0.02102982
C	1.38279540	2.77409033	0.14868196
H	0.66634290	3.47590709	0.53480979
C	2.57699660	3.24743449	-0.22337223
H	3.35393223	2.64346989	-0.64114052
H	2.78738001	4.29241004	-0.10698435
Cl	0.60614442	-1.20954772	1.91508015
Cl	1.89799669	-2.56766524	-0.27007494
Cl	3.20163866	0.26640270	0.85064252
Cl	2.24667702	0.17150285	-1.87979414
H	-5.60397117	0.83525187	0.16779890

2d- E_{out}

C	-5.44881101	1.33642802	-0.35563358
C	-4.16643145	-0.39120924	0.54732664
C	-3.18900303	0.60124317	0.11253160
C	-3.98585655	1.79369765	-0.40704842
C	-1.83334607	0.52757405	0.15571636
C	-1.04572680	1.67430735	-0.27005349
C	-1.04290079	-0.64896020	0.66950354
C	0.30529553	1.74242255	-0.30242779
C	0.29964755	-0.77832765	-0.05052569
H	-0.85118596	-0.51411719	1.72598301
H	-1.55906058	-1.57892765	0.54089511
C	1.13608668	0.52582189	0.07389095
H	-6.08355891	1.98510048	0.22736448
H	-1.57725541	2.56179096	-0.54242269
H	-3.69914985	2.05411935	-1.41407733
H	-3.83612948	2.66305320	0.21731897
H	-5.88898590	1.20558635	-1.33270370
C	-3.97500344	-1.71859657	1.20028558
H	-3.53557421	-2.40885449	0.49222139
H	-3.31448742	-1.63147271	2.04961034
H	-4.92263528	-2.11864319	1.52907550
N	-5.35211360	0.03113561	0.30397354
C	0.89004091	3.05671887	-0.64261351
H	0.21307411	3.68717729	-1.18903274
C	2.07282748	3.57241933	-0.29215916
H	2.81040046	3.04564453	0.27475355
H	2.31514666	4.57495420	-0.58558829
Br	2.77927147	0.37533313	-0.94396845
Br	1.64466965	0.80575047	2.01822697
Br	1.20700310	-2.33884459	0.66237504
Br	-0.09918484	-1.15163373	-1.94159423
H	-6.15984006	-0.50399126	0.53496549

2d-Z_{in}

C	-5.34697379	-0.97000600	0.85942055
C	-3.84290335	-1.26555050	0.85698493
C	-3.20000563	0.00737174	0.31712579
C	-4.29544161	0.86714412	-0.12156566
H	-5.93233971	-1.70220573	0.32614754
H	-5.75678927	-0.85201409	1.85144295
H	-3.49364754	-1.50475134	1.84959109
H	-3.62202583	-2.10803901	0.21632310
C	-1.86144945	0.22876914	0.25340159
C	-1.21961246	1.45301387	-0.19610807
C	-0.92888886	-0.84704672	0.75342204
C	0.11654736	1.65794659	-0.27190560
C	0.39355347	-0.84782185	-0.00879328
H	-0.72429828	-0.67679739	1.80287251
H	-1.36653652	-1.82505513	0.66159937
C	1.08744041	0.54002958	0.07717124
C	-4.27282780	2.18425292	-0.82003416
H	-3.86565611	2.93825828	-0.15980647
H	-3.65276256	2.12533331	-1.70251263
H	-5.27111178	2.47874939	-1.10764360
H	-1.83223561	2.28993305	-0.44107775
N	-5.41808761	0.31539684	0.15795578
C	0.54851865	3.02708233	-0.62978815
H	-0.20813810	3.58109767	-1.15461888
C	1.68086968	3.66729278	-0.32093124
H	2.48961558	3.22364713	0.21917072
H	1.80587575	4.68857115	-0.62321988
Br	1.63102233	0.89360335	2.00039261
Br	2.69855753	0.56257277	-0.99913283
Br	1.48581331	-2.29309204	0.68042767
Br	-0.02762548	-1.27885320	-1.88314760
H	-6.28756572	0.74331199	-0.07248667

2d- E_{in}

C	5.46564194	1.31123467	-0.36552388
C	4.17652134	-0.40630543	0.54703254
C	3.20263800	0.58359892	0.09918516
C	4.00350458	1.76971478	-0.42862146
C	1.84667777	0.51364312	0.13963642
C	1.06329120	1.65802112	-0.29952326
C	1.05268035	-0.65642508	0.66329757
C	-0.28738666	1.73241281	-0.32826300
C	-0.29511608	-0.78408406	-0.04686280
H	1.56437381	-1.58898603	0.53498210
H	0.86810850	-0.51668552	1.72028185
C	-1.12303805	0.52604397	0.07013838
H	5.91092321	1.17145733	-1.33903862
H	1.59781270	2.53886352	-0.58716211
H	3.85179488	2.64556715	0.18609653
H	3.72201452	2.02017339	-1.43968075
H	6.09801564	1.96423625	0.21525572
C	3.97992564	-1.72758110	1.21058313
H	3.31607205	-1.63192432	2.05640665
H	3.54210797	-2.42308012	0.50661416
H	4.92541879	-2.12666145	1.54672018
N	5.36395879	0.01187046	0.30492532
C	-0.86622789	3.04415701	-0.68907514
H	-0.19050040	3.65796421	-1.25561590
C	-2.04126059	3.57506999	-0.33594939
H	-2.77541497	3.06422146	0.24972551
H	-2.28124973	4.57305275	-0.64649065
H	6.16974620	-0.52275463	0.54384821
Br	-2.77624938	0.37365459	-0.92971544
Br	-1.61101539	0.83348031	2.01595121
Br	-1.20593364	-2.33171774	0.68839783
Br	0.08868687	-1.17874931	-1.93617902

2d-Z_{out}

C	5.34699408	-0.96896614	0.85995236
C	4.29463767	0.86734136	-0.12182384
C	3.19957585	0.00702254	0.31677089
C	3.84304255	-1.26526678	0.85741961
C	1.86091971	0.22785256	0.25286495
C	1.21966199	1.45210599	-0.19656354
C	0.92840915	-0.84807478	0.75275508
C	-0.11620195	1.65773392	-0.27168249
C	-0.39432151	-0.84846809	-0.00873274
H	1.36602647	-1.82582295	0.66001849
H	0.72421943	-0.67786483	1.80215080
C	-1.08710697	0.54004444	0.07737691
H	5.75674110	-0.85042342	1.85194987
H	1.83283734	2.28866311	-0.44121596
H	3.62274604	-2.10829357	0.21724925
H	3.49377874	-1.50407541	1.85014189
H	5.93280876	-1.70101051	0.32692896
C	4.27198688	2.18421952	-0.82081595
H	3.65193719	2.12526021	-1.70331892
H	3.86506751	2.93866293	-0.16087266
H	5.27040050	2.47835853	-1.10850042
N	5.41749647	0.31619819	0.15809634
C	-0.54707548	3.02721778	-0.62827627
H	0.21062494	3.58187030	-1.15089826
C	-1.67979916	3.66714171	-0.32090287
H	-2.48966390	3.22300225	0.21699920
H	-1.80371496	4.68888811	-0.62219017
Br	-2.69846731	0.56327333	-0.99969658
Br	-1.63001166	0.89415031	2.00068945
Br	-1.48752909	-2.29326690	0.68084508
Br	0.02630840	-1.27991743	-1.88367563
H	6.28678021	0.74458778	-0.07236584

3a- E_{out}

C	-1.54390616	0.92529689	-0.19295260
C	-0.63595298	-0.22500161	-0.24392833
C	-1.32327451	-1.58502911	-0.33312719
C	0.72358224	-0.10977798	-0.23249825
C	1.56823526	-1.28222935	-0.50167877
C	1.50281177	1.15811864	0.05503782
C	2.89835860	-1.28334240	-0.31908453
C	2.72640639	0.86420583	0.92659114
H	1.83265938	1.58981266	-0.88591155
H	0.89798822	1.89248208	0.55816758
C	3.66308004	-0.13065149	0.25674293
H	3.24328489	1.79166992	1.13491158
H	2.39477727	0.46535956	1.87966095
H	4.39811445	-0.49685570	0.96282520
H	4.22400877	0.35046277	-0.54047207
H	1.11512084	-2.15276743	-0.92823090
H	-0.68230861	-2.34219421	0.08496952
H	-1.50534735	-1.86791372	-1.36716724
C	-1.23411315	2.31474744	-0.68391687
H	-0.91968952	2.94535943	0.13627333
H	-0.45831989	2.30038392	-1.42881595
H	-2.12267486	2.75038376	-1.12129229
N	-2.75521263	0.73756250	0.22108678
C	-3.28914947	-0.50063279	0.68270198
H	-4.22293631	-0.42291876	1.19558059
C	-2.62422808	-1.61529529	0.41740564
H	-3.02898342	-2.55838551	0.72463233
H	-3.38178482	1.51349997	0.19579640
H	3.45473863	-2.15449305	-0.61109923

3a-Z_{in}

C	2.74171212	-1.55977267	-0.30706207
C	1.35042148	-1.57886511	0.25988197
C	0.64477078	-0.23533359	0.10316183
C	1.51745418	0.94036042	0.18985967
H	3.21152052	-2.48554560	-0.57146924
H	0.79227136	-2.34387515	-0.25278318
H	1.39915957	-1.87952964	1.30374374
C	-0.70274823	-0.15362728	-0.09038181
C	-1.41489584	1.06083132	-0.50929624
C	-1.58319512	-1.38322350	0.01220339
C	-2.75349749	1.12695214	-0.59032613
C	-2.94305995	-1.04227654	0.62317412
H	-1.72338983	-1.79061193	-0.98610425
H	-1.11485290	-2.14972131	0.60843409
C	-3.67487959	0.01435876	-0.19219856
H	-3.53697479	-1.94347334	0.69630628
H	-2.79459051	-0.68049924	1.63561204
H	-4.51235774	0.41578511	0.36522198
H	-4.09542066	-0.42340357	-1.09391162
C	1.10162702	2.31195188	0.65234391
H	0.91626096	2.95608331	-0.19679311
H	0.21191180	2.26774303	1.25525783
H	1.89792646	2.75115970	1.23876323
H	-0.85210521	1.89883276	-0.86016805
N	2.77872795	0.79230986	-0.05667513
C	3.40489153	-0.42312847	-0.46019096
H	4.39738789	-0.31174445	-0.83915454
H	3.37382219	1.58378816	0.06543052
H	-3.19734798	2.02072396	-0.98826172

3a- E_{in}

C	1.53214134	0.93821197	-0.19152789
C	0.63362191	-0.21941740	-0.24050345
C	1.33206718	-1.57436824	-0.31997581
C	-0.72689008	-0.11505824	-0.23515553
C	-1.56095710	-1.29549618	-0.50208943
C	-1.51746005	1.14801118	0.04225734
C	-2.89184894	-1.30634244	-0.32526006
C	-2.74257746	0.84892416	0.90990926
H	-0.92081925	1.88985671	0.54417851
H	-1.84648593	1.57208254	-0.90245451
C	-3.66825095	-0.15697516	0.24131977
H	-1.09907763	-2.16464233	-0.92201550
H	1.52083503	-1.86086972	-1.35185441
H	0.69530480	-2.33458158	0.09904996
C	1.21338218	2.32274731	-0.69053191
H	0.44115617	2.29858439	-1.43890451
H	0.89009938	2.95465956	0.12522201
H	2.10038153	2.76356810	-1.12590200
N	2.74317039	0.76221435	0.22853066
C	3.28496550	-0.46936710	0.69853006
H	4.21611234	-0.38175254	1.21462618
C	2.62994478	-1.59060104	0.43617006
H	3.04099407	-2.52892119	0.74966158
H	3.36380190	1.54284943	0.20152417
H	-3.43991091	-2.18345595	-0.61515262
H	-4.22970509	0.31542048	-0.56071613
H	-4.40326958	-0.52545750	0.94622375
H	-2.41203986	0.45788988	1.86659322
H	-3.26780365	1.77330854	1.11093222

3a-Z_{out}

C	-1.51699698	0.94013428	0.18796335
C	-0.64461263	-0.23570712	0.09921276
C	-1.34939229	-1.58002783	0.25480105
C	0.70282651	-0.15394948	-0.09447425
C	1.41564135	1.06057593	-0.51255008
C	1.58355239	-1.38330779	0.00771601
C	2.75440283	1.12740984	-0.58865726
C	2.94042380	-1.04212940	0.62529285
H	1.11371071	-2.15226287	0.59952014
H	1.72829308	-1.78719431	-0.99135333
C	3.67507514	0.01603231	-0.18562657
H	4.10135072	-0.42067239	-1.08513318
H	4.50880961	0.41856334	0.37659934
H	0.85330840	1.89734287	-0.86709875
H	-1.39118404	-1.88518295	1.29765404
H	-0.79424033	-2.34271619	-0.26475091
C	-1.09946486	2.31209569	0.64792687
H	-0.20840792	2.26830493	1.24887284
H	-0.91563699	2.95503133	-0.20249856
H	-1.89425131	2.75247227	1.23554487
H	3.53481414	-1.94285242	0.70034055
H	2.78689152	-0.68150959	1.63739921
C	-2.74431362	-1.56000982	-0.30287747
H	-3.21618758	-2.48576072	-0.56355002
C	-3.40826653	-0.42340274	-0.45207072
N	-2.77921511	0.79240617	-0.05384595
H	-3.37370004	1.58375145	0.07197583
H	-4.40302703	-0.31183350	-0.82503651
H	3.19925004	2.02063569	-0.98667914

3b- E_{out}

C	-2.47252182	0.90629652	-0.31630697
C	-1.65472052	-0.30821653	-0.31903378
C	-2.43537614	-1.61719939	-0.22306250
C	-0.29365129	-0.30016749	-0.42498838
C	0.44037546	-1.54888282	-0.63823881
C	0.60128182	0.91500949	-0.33429501
C	1.77575931	-1.62350179	-0.54605445
C	1.89588569	0.66516402	0.47792911
H	0.86281211	1.22373228	-1.34002662
H	0.09527179	1.74222188	0.13289826
C	2.71309321	-0.49686340	-0.17886739
H	-0.09857018	-2.42621051	-0.93013702
H	-1.81975774	-2.37026485	0.23891214
H	-2.69822449	-1.99317469	-1.20881307
C	-2.10124387	2.22219458	-0.94753664
H	-1.67983775	2.89074121	-0.20962872
H	-1.38783662	2.08654932	-1.74079757
H	-2.98698921	2.68897983	-1.35765873
N	-3.66381286	0.84978463	0.18711908
C	-4.25352463	-0.29799456	0.79069324
H	-5.14460688	-0.10426130	1.34699951
C	-3.68641185	-1.47923686	0.59629978
H	-4.13637839	-2.35687761	1.01462743
H	-4.23317973	1.66661720	0.12828752
C	3.78951358	-1.06756894	0.76214362
H	3.36436623	-1.54930498	1.63147207
H	4.37917164	-1.80796316	0.23549842
H	4.46855262	-0.29614486	1.10057494
C	3.42449377	-0.06317096	-1.47865329
H	4.23643152	0.62015948	-1.27155919
H	3.84930939	-0.93003371	-1.96947490
H	2.75414155	0.40879652	-2.18523610
C	2.67492109	1.98815494	0.49772288
H	2.85486731	2.37575902	-0.49588376
H	2.11721173	2.73895990	1.04610357
H	3.63126303	1.87858642	0.99119055
C	1.50469951	0.33628281	1.93041714
H	2.36681303	0.35374708	2.58154004
H	0.81020522	1.08091296	2.30414457
H	1.03625832	-0.63411711	2.03111061
H	2.24206401	-2.56483356	-0.77682156

3b-Z_{in}

C	3.63715887	-1.64460924	-0.45400548
C	2.22415634	-1.58424243	0.05174636
C	1.64681647	-0.17213972	0.00253828
C	2.61453038	0.90848526	0.20598342
H	4.03687731	-2.58520898	-0.77532649
H	1.62542762	-2.24103295	-0.55673630
H	2.19392840	-1.98711547	1.06116214
C	0.31511817	0.04442891	-0.20220673
C	-0.28909553	1.33912149	-0.51913297
C	-0.66943675	-1.10302272	-0.23250976
C	-1.61680094	1.50641254	-0.60220526
C	-2.03921558	-0.75985985	0.39771803
H	-0.80346432	-1.40079460	-1.26725933
H	-0.27753762	-1.96093226	0.29037340
C	-2.67472938	0.45539181	-0.35636428
C	2.30491120	2.27587537	0.75583437
H	2.18729787	2.98821190	-0.04965459
H	1.40448470	2.26537881	1.34415122
H	3.12417377	2.60782107	1.37985036
H	0.33632282	2.16559219	-0.77892940
N	3.86775294	0.66757177	-0.01006384
C	4.40342650	-0.56453224	-0.48495829
H	5.41842972	-0.51458551	-0.81416489
H	4.52290578	1.39192705	0.19258548
C	-3.81877781	1.11321536	0.43617914
H	-3.47558462	1.57258431	1.35269394
H	-4.28127014	1.88780293	-0.16348133
H	-4.58924556	0.39583632	0.68569491
C	-3.24048215	0.06505086	-1.73897155
H	-4.12317866	-0.55127546	-1.63979545
H	-3.52853731	0.95653457	-2.28251555
H	-2.52189517	-0.46597934	-2.34946159
C	-2.90793383	-2.02253297	0.30892147
H	-2.48198337	-2.80823473	0.92207633
H	-3.91087384	-1.84173023	0.67220591
H	-2.98151380	-2.40146373	-0.70131027
C	-1.82282390	-0.45154644	1.89110455
H	-2.76280087	-0.40050818	2.42165048
H	-1.24031925	-1.24186480	2.35097939
H	-1.30272284	0.48364808	2.05675836
H	-1.98010061	2.47086825	-0.91044920

3b- E_{in}

C	2.46437063	0.91740783	-0.29055647
C	1.65282412	-0.30207614	-0.30659820
C	2.44160588	-1.60455801	-0.19496512
C	0.29371043	-0.30089975	-0.43079287
C	-0.43347806	-1.55367242	-0.64658538
C	-0.60783155	0.91057782	-0.36006707
C	-1.76919471	-1.63317172	-0.56532848
C	-1.90729262	0.66127707	0.44459535
H	-0.11061936	1.74635379	0.10115292
H	-0.86301030	1.20601862	-1.37141781
C	-2.71436672	-0.50904161	-0.21021545
H	0.11147873	-2.42957093	-0.93154017
H	2.73818767	-1.97145913	-1.17466837
H	1.82014621	-2.36663749	0.24337560
C	2.10257924	2.22699209	-0.94005372
H	1.40657221	2.08216101	-1.74714276
H	1.66337079	2.90014933	-0.21682230
H	2.99539869	2.69350346	-1.33498213
N	3.64258042	0.86906915	0.24315241
C	4.22064123	-0.27282917	0.86950587
H	5.09451399	-0.07165655	1.44999035
C	3.66626921	-1.45803308	0.66241003
H	4.10856699	-2.33185119	1.09660281
H	4.20982053	1.68811545	0.19464225
C	-3.79358660	-1.07975660	0.72756977
H	-4.37954595	-1.82261542	0.20027055
H	-3.37098288	-1.55847473	1.59983846
H	-4.47563119	-0.30895172	1.06134710
C	-3.42001102	-0.08645632	-1.51676800
H	-3.83344020	-0.95880837	-2.00759758
H	-4.23949415	0.59038650	-1.31813758
H	-2.74883360	0.38900735	-2.22017770
C	-2.69250259	1.98074502	0.44903454
H	-2.14242207	2.73803356	0.99620517
H	-2.86663081	2.36038319	-0.54866999
H	-3.65211008	1.87031876	0.93594602
C	-1.52539782	0.34458220	1.90216418
H	-0.83962991	1.09690029	2.27667891
H	-2.39284675	0.35956299	2.54621490
H	-1.05044828	-0.62156898	2.01279930
H	-2.22991273	-2.57730819	-0.79589134

3b-Z_{out}

C	-2.61436154	0.90838767	0.20533128
C	-1.64662280	-0.17163300	-0.00005983
C	-2.22240142	-1.58461655	0.04714178
C	-0.31477023	0.04509105	-0.20447626
C	0.28999935	1.33985879	-0.52008375
C	0.66951839	-1.10251162	-0.23491502
C	1.61780964	1.50710340	-0.60175172
C	2.03858069	-0.75979744	0.39726381
C	2.67521425	0.45574168	-0.35549581
H	-0.33513215	2.16636890	-0.78021340
H	-2.18482898	-1.99179591	1.05459822
H	-1.62665740	-2.23794833	-0.56818541
C	-2.30432268	2.27707301	0.75183027
H	-1.40377550	2.26811227	1.33997910
H	-2.18685471	2.98728830	-0.05554222
H	-3.12340883	2.61077068	1.37516495
C	-3.63841025	-1.64576184	-0.44985219
H	-4.03952186	-2.58690453	-0.76793430
C	-4.40549323	-0.56619851	-0.47753793
N	-3.86821665	0.66669322	-0.00644759
H	-4.52287295	1.39112514	0.19751941
H	-5.42251391	-0.51730676	-0.80072802
C	1.82028229	-0.45186792	1.89046560
H	1.23601059	-1.24153056	2.34924506
H	2.75954533	-0.40233767	2.42242528
H	1.30128332	0.48399957	2.05572816
C	2.90717131	-2.02262557	0.30930508
H	2.98245860	-2.40102348	-0.70099731
H	3.90948881	-1.84234627	0.67455615
H	2.47979540	-2.80854824	0.92119215
H	1.98150365	2.47151502	-0.90962970
H	0.80468812	-1.39933234	-1.26979239
H	0.27699920	-1.96087357	0.28672917
C	3.81877725	1.11254046	0.43854865
H	4.58966564	0.39502270	0.68640813
H	4.28087546	1.88868970	-0.15941057
H	3.47544579	1.56969911	1.35608735
C	3.24219377	0.06599600	-1.73768714
H	3.53301479	0.95750510	-2.27970924
H	4.12339414	-0.55236519	-1.63801396
H	2.52336135	-0.46269345	-2.34993485

3c- E_{out}

C	-3.03579641	0.87487124	-0.43426218
C	-2.24820954	-0.37320744	-0.43307785
C	-3.08973176	-1.64131948	-0.36503421
C	-0.88900461	-0.39443419	-0.47534995
C	-0.15545588	-1.65747230	-0.61884167
C	-0.00569807	0.83276822	-0.37026334
C	1.17435469	-1.75567402	-0.50173852
C	1.26567640	0.55803948	0.44032109
H	0.29581323	1.16031017	-1.35562783
H	-0.50007742	1.64782359	0.12257969
C	2.07765926	-0.58965694	-0.21259009
H	-0.69204474	-2.54665449	-0.87116538
H	-2.49956392	-2.45718410	0.01256118
H	-3.43635899	-1.93518125	-1.35286407
C	-2.64909199	2.15528277	-1.12533148
H	-2.19209263	2.84232562	-0.42610232
H	-1.96052288	1.96830036	-1.93129641
H	-3.53206673	2.62923346	-1.53266922
N	-4.19842500	0.85718108	0.12586479
C	-4.78697237	-0.26850319	0.77655357
H	-5.63137011	-0.04141033	1.38992258
C	-4.27742371	-1.46887165	0.54090805
H	-4.72861720	-2.33297364	0.98487922
H	-4.75120136	1.68771386	0.08055811
Cl	3.43258223	-1.11056005	0.79722270
Cl	2.73755513	-0.05440511	-1.79268868
Cl	2.19803738	2.05743458	0.55597744
Cl	0.77132522	0.08910829	2.09565183
H	1.66955977	-2.68938054	-0.67310806

3c-Z_{in}

C	-4.16497146	1.65260998	-0.56273446
C	-2.79271808	1.56820586	0.04506924
C	-2.23436701	0.15204930	-0.01367171
C	-3.23564914	-0.91169263	0.18395037
H	-4.52304218	2.59751606	-0.91822540
H	-2.14708160	2.24154090	-0.49257434
H	-2.83448239	1.92984341	1.06973036
C	-0.91292579	-0.09750660	-0.21389009
C	-0.34464838	-1.41468368	-0.51535337
C	0.08783859	1.04120864	-0.23314752
C	0.97022011	-1.63711389	-0.63100094
C	1.44376804	0.62018668	0.34032760
H	0.23818034	1.38400815	-1.24855022
H	-0.24901136	1.87537956	0.35545516
C	2.01896700	-0.57283984	-0.46508350
C	-2.97154666	-2.25479700	0.81125693
H	-2.85499851	-3.01262448	0.04777359
H	-2.08413365	-2.23085777	1.41995721
H	-3.81132119	-2.53407441	1.43356747
H	-0.99529672	-2.23420334	-0.72689583
N	-4.46548964	-0.64952479	-0.10789157
C	-4.94515345	0.58434146	-0.64193582
H	-5.93533706	0.54537059	-1.04051051
H	-5.15065991	-1.34995967	0.08520388
Cl	3.46184205	-1.26267347	0.29045465
Cl	2.45956014	-0.04156798	-2.12018160
Cl	1.18388753	0.12699264	2.04440174
Cl	2.52814887	2.01556402	0.33782396
H	1.33663750	-2.59955470	-0.92429028

3c- E_{in}

C	3.05020442	0.88268395	-0.42326601
C	2.26711755	-0.36785358	-0.39738669
C	3.11206390	-1.63329422	-0.31928707
C	0.90763921	-0.39435331	-0.42819337
C	0.17857430	-1.66181456	-0.55482323
C	0.02050753	0.83035087	-0.32641187
C	-1.14995247	-1.76470677	-0.42750985
C	-1.24350056	0.55665217	0.49601930
H	0.51578304	1.65086412	0.15645219
H	-0.28996682	1.14919601	-1.31179366
C	-2.05566961	-0.59946950	-0.14205948
H	0.71762193	-2.55047357	-0.80391662
H	3.44429288	-1.94524417	-1.30649738
H	2.52831525	-2.44247122	0.08233105
C	2.65023017	2.15225834	-1.12657073
H	1.95984134	1.95007185	-1.92743065
H	2.19012929	2.84326027	-0.43343237
H	3.52726883	2.62926884	-1.54296826
N	4.21977211	0.87628245	0.12236724
C	4.82130360	-0.23921091	0.77887252
H	5.67396269	-0.00154440	1.37660342
C	4.31267368	-1.44416525	0.56593990
H	4.77365484	-2.30095540	1.01403772
H	4.76937273	1.70768851	0.05847253
H	-1.64250198	-2.70208081	-0.58602390
Cl	-3.40226045	-1.11570884	0.88136353
Cl	-2.72747140	-0.07960521	-1.72237335
Cl	-2.18160854	2.05295558	0.60718501
Cl	-0.73518147	0.10215673	2.15140410

3c-Z_{out}

C	3.23560226	-0.91170128	0.18449398
C	2.23431730	0.15224734	-0.01219120
C	2.79336141	1.56802656	0.04709127
C	0.91290112	-0.09719309	-0.21261321
C	0.34505753	-1.41439091	-0.51481131
C	-0.08793117	1.04142546	-0.23183275
C	-0.96966642	-1.63695562	-0.63188082
C	-1.44440427	0.61990808	0.33993070
H	0.24832402	1.87510090	0.35782638
H	-0.23731887	1.38509035	-1.24708369
C	-2.01864987	-0.57272117	-0.46680765
H	0.99605610	-2.23379416	-0.72582630
H	2.83837604	1.92802989	1.07217927
H	2.14664165	2.24258663	-0.48761899
C	2.97196895	-2.25421365	0.81328420
H	2.08443114	-2.22994050	1.42178034
H	2.85593517	-3.01301727	0.05068537
H	3.81175056	-2.53229682	1.43613073
C	4.16402563	1.65212192	-0.56442336
H	4.52140585	2.59683207	-0.92113740
C	4.94379424	0.58364352	-0.64513392
N	4.46498762	-0.64992151	-0.10955350
H	5.15042392	-1.35028442	0.08289449
H	5.93295478	0.54421897	-1.04620404
Cl	-3.46249606	-1.26280041	0.28662498
Cl	-2.45713930	-0.04051615	-2.12215423
Cl	-1.18640772	0.12573929	2.04397519
Cl	-2.52878619	2.01531994	0.33699752
H	-1.33573142	-2.59940096	-0.92558706

3d- E_{out}

C	3.79821424	0.48965066	0.84952809
C	3.00533539	-0.63138588	0.32819782
C	3.82029731	-1.78721050	-0.24676695
C	1.64179562	-0.65601612	0.34469461
C	0.91641047	-1.87283674	-0.03244567
C	0.75068755	0.51072019	0.72500764
C	-0.41490005	-1.92790568	-0.17527373
C	-0.52561416	0.56189433	-0.12368842
H	0.45626301	0.42219215	1.76217822
H	1.24258020	1.45392685	0.59244248
C	-1.32321824	-0.75045553	0.01228407
H	1.45870648	-2.78555226	-0.15407651
H	3.24561230	-2.29205137	-1.00444651
H	4.04790324	-2.52679593	0.51723853
C	3.36819441	1.43959172	1.93057185
H	2.94608590	2.33450783	1.49219183
H	2.63876999	0.99107145	2.58206501
H	4.22772744	1.72941192	2.51888802
N	4.99978178	0.64126608	0.41518903
C	5.63338131	-0.17155119	-0.56555392
H	6.54019800	0.23131501	-0.96184017
C	5.10055831	-1.32312685	-0.87703904
H	5.58511870	-1.95789154	-1.59140131
H	5.54823093	1.37472248	0.80784731
Br	-2.04015178	-0.95886843	1.89445709
Br	-2.83798424	-0.87215391	-1.18198252
Br	-1.56022744	2.16189583	0.43898882
Br	0.01190052	0.85546150	-1.98610865
H	-0.89457517	-2.86217908	-0.38299702

3d-Z_{in}

C	-4.93864330	1.07052836	-1.37310736
C	-3.56139281	1.26802248	-0.80879105
C	-3.01866051	-0.00650235	-0.17174618
C	-4.02606085	-0.85593841	0.47440667
H	-5.28982676	1.73990144	-2.13249735
H	-2.91238301	1.57903477	-1.61065796
H	-3.58320156	2.08724201	-0.09361998
C	-1.68990303	-0.30654737	-0.18776314
C	-1.11505917	-1.60752733	0.15993139
C	-0.68887234	0.71088011	-0.69989055
C	0.20391458	-1.84281075	0.18690771
C	0.65244910	0.60840365	0.03318031
H	-0.51704834	0.55031887	-1.75693174
H	-1.04843480	1.71523410	-0.57082327
C	1.24505380	-0.80746048	-0.11452001
C	-3.77507648	-1.77587318	1.63512237
H	-3.66205817	-2.79330489	1.28236745
H	-2.89176380	-1.49096607	2.17954841
H	-4.62506330	-1.74830421	2.30330603
H	-1.75885761	-2.44268594	0.32443674
N	-5.25010646	-0.74586124	0.09281331
C	-5.71418816	0.10897355	-0.94629371
H	-6.70609314	-0.09756810	-1.28581207
H	-5.94031492	-1.27896974	0.57517912
Br	2.82447748	-1.11271792	0.95930266
Br	1.76189824	-1.16239951	-2.03892246
Br	0.31798564	1.01911062	1.92496089
Br	1.84968875	2.02909564	-0.66409821
H	0.56831893	-2.83345407	0.36580103

3d- E_{in}

C	-3.82370085	0.44596186	0.86027556
C	-3.03136018	-0.62100417	0.23604888
C	-3.84329336	-1.72964685	-0.43040965
C	-1.66703488	-0.64583314	0.24354833
C	-0.94631183	-1.82797672	-0.23651366
C	-0.77462157	0.48524376	0.71704057
C	0.38571683	-1.87866051	-0.37277659
C	0.51803902	0.59803761	-0.10052296
H	-1.26251687	1.43724288	0.64698234
H	-0.49404524	0.32079007	1.74878988
C	1.29974237	-0.73005722	-0.07335911
H	-1.49270427	-2.72268112	-0.44289207
H	-4.03711821	-2.54554500	0.26166248
H	-3.27967540	-2.14568237	-1.24829608
C	-3.37957937	1.31598711	2.00122943
H	-2.64714224	0.81924831	2.61323492
H	-2.95563795	2.23687812	1.62289301
H	-4.23200306	1.56846927	2.61631490
N	-5.03694349	0.61717026	0.46658895
C	-5.68696946	-0.12198840	-0.56025604
H	-6.61067902	0.29715801	-0.89584250
C	-5.14745572	-1.23458983	-0.98179927
H	-5.64407172	-1.81558214	-1.73271173
H	-5.58195769	1.31257551	0.92716458
H	0.86131387	-2.79363929	-0.66027605
Br	2.82570061	-0.76257260	-1.25876815
Br	1.99309430	-1.10239643	1.79309908
Br	1.53168682	2.10946967	0.55610220
Br	-0.03017546	1.03733731	-1.99044931

3d-Z_{out}

C	4.02682213	-0.85993532	0.46492526
C	3.01948395	-0.02379827	-0.18576609
C	3.54502021	1.24822506	-0.84703607
C	1.68775024	-0.31724600	-0.18421872
C	1.10365487	-1.60755547	0.17816644
C	0.69298572	0.70397931	-0.70125819
C	-0.21807668	-1.82942652	0.20973154
C	-0.65254177	0.62780737	0.03035873
H	1.06357431	1.70584367	-0.58381285
H	0.52003113	0.53530718	-1.75706086
C	-1.25183516	-0.79017579	-0.09861286
H	1.73858393	-2.44774714	0.34744596
H	3.51160258	2.08892589	-0.15818937
H	2.91367673	1.51079405	-1.68048580
C	3.77653148	-1.81168225	1.60077482
H	2.89656446	-1.54034765	2.15727537
H	3.66093508	-2.81891340	1.22081065
H	4.62808469	-1.80411306	2.26711413
C	4.94607498	1.08844689	-1.35969909
H	5.30353633	1.76722305	-2.10766428
C	5.73388608	0.15106858	-0.90379283
N	5.26035938	-0.72017255	0.11515993
H	5.94704243	-1.25031034	0.60460723
H	6.74300718	-0.02437857	-1.20838106
Br	-2.82941743	-1.07703900	0.98087991
Br	-1.77359866	-1.16913221	-2.01876657
Br	-1.81180491	2.01531090	-0.65957852
Br	-0.30204146	1.04243158	1.92174807
H	-0.59066984	-2.81553697	0.39711714

4a- E_{out}

C	-2.35609388	0.68105313	-0.27667660
C	-1.19244606	-0.19565646	-0.16142884
C	-1.49710731	-1.69206467	-0.11822880
C	0.09654269	0.26269172	-0.12177542
C	1.20871672	-0.67715155	-0.24566268
C	0.51461932	1.70631545	0.06188786
C	2.51030024	-0.35246098	-0.06357263
C	1.74050581	1.79611100	0.96868724
H	0.75657073	2.13361220	-0.90720827
H	-0.27345016	2.29759910	0.49468937
C	2.91787220	1.02161148	0.39803355
H	2.00768898	2.83595728	1.10421212
H	1.48703249	1.40447476	1.94831205
H	3.69768047	0.94002716	1.14291475
H	3.35022384	1.55769339	-0.44229588
H	0.99078326	-1.67088508	-0.57813725
H	-0.73926396	-2.19507467	0.45917439
H	-1.46869611	-2.12864918	-1.11359881
C	-2.36287398	2.06836807	-0.86337437
H	-2.26296998	2.81084563	-0.08382219
H	-1.56298674	2.19686992	-1.57074767
H	-3.30149285	2.24097977	-1.37288625
N	-3.51848192	0.22179515	0.06450872
C	3.53769341	-1.35984375	-0.34753740
H	3.17413781	-2.32381635	-0.65520862
C	4.86209528	-1.17027299	-0.27388455
H	5.30263564	-0.23664286	0.01544632
H	5.53957806	-1.96577832	-0.51397292
C	-3.77397555	-1.07366433	0.59697735
H	-4.74882162	-1.20256814	1.01430516
C	-2.82695477	-1.99535882	0.50867517
H	-3.01640568	-2.98448921	0.87396018
H	-4.31056336	0.81079613	-0.07726707

4a-Z_{in}

C	-3.60436415	0.97768458	-0.63090031
C	-2.30815825	1.41910421	-0.01354353
C	-1.29724200	0.28061493	0.09522772
C	-1.86897996	-1.04915358	0.30664738
H	-4.25682705	1.71292776	-1.05685468
H	-1.90051991	2.20749402	-0.62420285
H	-2.51362939	1.85875581	0.95953932
C	0.04670533	0.51925900	0.01818534
C	1.06486306	-0.51202554	-0.16502100
C	0.57938346	1.93626075	0.01245591
C	2.39727042	-0.27382671	-0.16132782
C	1.91165006	2.01406586	0.75263247
H	0.71279845	2.25377371	-1.01884849
H	-0.11921273	2.61811633	0.47041488
C	2.95371135	1.09383048	0.13563269
H	2.26675932	3.03601775	0.74683437
H	1.75515658	1.74214765	1.79161561
H	3.80396377	1.00579247	0.79848669
H	3.32963869	1.51893493	-0.79077005
C	-1.18239465	-2.20563370	0.98479407
H	-0.76890418	-2.88274536	0.24940012
H	-0.39039886	-1.86693506	1.62904072
H	-1.90235746	-2.75434969	1.57762545
H	0.74845203	-1.49960693	-0.42400392
N	-3.10486818	-1.25297794	-0.02210619
C	3.31193706	-1.37171389	-0.49492446
H	2.84962734	-2.32244700	-0.69292935
C	4.64540137	-1.28094830	-0.58801354
H	5.18111524	-0.36849933	-0.41570869
H	5.23210914	-2.13910126	-0.85040147
C	-3.96570694	-0.29679949	-0.63376396
H	-4.87024367	-0.69961318	-1.03464061
H	-3.50175226	-2.14375027	0.18734416

4a- E_{in}

C	2.35028746	0.69804310	-0.27132639
C	1.19220122	-0.18629740	-0.15737368
C	1.50789307	-1.68006679	-0.10611292
C	-0.10005649	0.26321159	-0.12553449
C	-1.20538601	-0.68466179	-0.24951283
C	-0.52879680	1.70483161	0.04900504
C	-2.50974398	-0.36815463	-0.07288893
C	-1.75814177	1.79085599	0.95150405
H	0.25366837	2.30410059	0.48099884
H	-0.77068173	2.12507996	-0.92319139
C	-2.92835435	1.00502312	0.38153310
H	-3.36270792	1.53414549	-0.46216985
H	-3.70930001	0.92097724	1.12497940
H	-0.97957797	-1.67842898	-0.57659704
H	1.49144536	-2.12046330	-1.10011852
H	0.74926581	-2.18700469	0.46672858
C	2.35057342	2.08157623	-0.86680806
H	1.55379069	2.19972644	-1.57951295
H	2.24088090	2.82825786	-0.09261638
H	3.29084374	2.25775031	-1.37205156
H	-2.03306498	2.82952077	1.08046491
H	-1.50493603	1.40643847	1.93405099
N	3.51369366	0.24917875	0.08000780
C	-3.52929433	-1.38373854	-0.35585703
H	-3.15818316	-2.34667503	-0.65772256
C	-4.85521196	-1.20273803	-0.28785962
H	-5.30303966	-0.27070373	-0.00459996
H	-5.52647231	-2.00388476	-0.52667874
C	3.77454490	-1.04091249	0.62282655
H	4.74708930	-1.16008179	1.04836539
C	2.83493626	-1.97006888	0.53309786
H	3.02859177	-2.95538839	0.90641835
H	4.30255655	0.84277472	-0.06059896

4a-Z_{out}

C	1.86877052	-1.04895344	0.30650982
C	1.29731138	0.28075693	0.09470802
C	2.30814394	1.41925624	-0.01439955
C	-0.04667950	0.51938737	0.01742266
C	-1.06474998	-0.51190839	-0.16596118
C	-0.57956306	1.93624154	0.01148568
C	-2.39725791	-0.27385337	-0.16140351
C	-1.91113627	2.01383912	0.75296776
H	0.11927984	2.61858523	0.46831440
H	-0.71407420	2.25327873	-1.01983277
C	-2.95366971	1.09353369	0.13680907
H	-3.33085488	1.51892619	-0.78897104
H	-3.80313369	1.00495728	0.80061589
H	-0.74842979	-1.49925012	-0.42595766
H	2.51276669	1.85979171	0.95843487
H	1.90086498	2.20710537	-0.62594736
C	1.18166720	-2.20547947	0.98416007
H	0.38852100	-1.86713791	1.62710871
H	0.76969586	-2.88299658	0.24830601
H	1.90101474	-2.75357711	1.57837323
H	-2.26636429	3.03574383	0.74753569
H	-1.75359945	1.74183234	1.79176580
C	-3.31189430	-1.37161958	-0.49536934
H	-2.84962369	-2.32213184	-0.69460458
C	-4.64553568	-1.28101471	-0.58732303
H	-5.18123464	-0.36880573	-0.41367306
H	-5.23225089	-2.13905781	-0.85004798
C	3.60494622	0.97763513	-0.63025164
H	4.25795564	1.71281810	-1.05557194
C	3.96638128	-0.29687057	-0.63212631
N	3.10491936	-1.25288105	-0.02130569
H	3.50145504	-2.14381536	0.18818106
H	4.87137527	-0.69968276	-1.03203609

4b- E_{out}

C	-2.92617742	-0.71038235	0.44601497
C	-1.92215274	0.33066389	0.20551932
C	-2.47449872	1.71612850	-0.13416190
C	-0.56778442	0.10873711	0.30225214
C	0.36359336	1.23148525	0.28169420
C	0.10838480	-1.23508119	0.41748295
C	1.72105304	1.12501080	0.20945562
C	1.39590888	-1.31634452	-0.43508686
H	0.34897383	-1.41935851	1.46600870
H	-0.54191170	-2.03877704	0.08950060
C	2.43600706	-0.22843166	0.03885018
H	-0.04535472	2.22205838	0.40177596
H	-1.76702036	2.24192569	-0.76758247
H	-2.59973228	2.32689304	0.76640911
C	-2.73769425	-1.94125917	1.29674193
H	-2.44766360	-2.79203033	0.68183098
H	-1.97860813	-1.78054142	2.05359431
H	-3.67569439	-2.18639808	1.79492887
N	-4.12570933	-0.54231885	-0.03033980
C	2.43936394	2.42026162	0.32856914
H	1.78734990	3.27814874	0.20853821
C	3.72711451	2.69660307	0.61433722
H	4.48952016	1.95542671	0.79016648
H	4.03960768	3.72944870	0.69061963
C	-4.55715205	0.56674010	-0.81775188
H	-5.51212632	0.43586501	-1.29827469
C	-3.78614715	1.65273601	-0.86768252
H	-4.11738274	2.51310632	-1.43103695
H	-4.81893828	-1.23344223	0.19194829
C	3.56768673	-0.10449988	-1.00720537
H	3.24603360	0.42883882	-1.90090671
H	4.42808990	0.42218160	-0.60659517
H	3.91807109	-1.08991783	-1.31026929
C	3.06553293	-0.61689370	1.39763249
H	3.72244747	-1.47946072	1.29009925
H	3.66528975	0.19885710	1.79418570
H	2.31610036	-0.85302595	2.15385674
C	1.93280060	-2.75089459	-0.27008914
H	2.05713344	-3.03122291	0.77557817
H	1.23050477	-3.45842310	-0.71662066
H	2.88897231	-2.89321768	-0.77148826
C	1.01313330	-1.13342234	-1.91959856
H	1.83457093	-1.41109917	-2.57790681
H	0.17218732	-1.78511894	-2.17042318
H	0.72628993	-0.11034829	-2.16337089

4b-Z_{in}

C	4.14099194	-1.19626091	-0.80854689
C	2.76476146	-1.47600619	-0.26797333
C	1.97151027	-0.19656947	-0.00272717
C	2.76499553	0.96773568	0.40469140
H	4.67107480	-1.97669338	-1.33520115
H	2.23809546	-2.08672920	-0.99468926
H	2.85629647	-2.08399989	0.63867233
C	0.60207210	-0.17501713	-0.12281613
C	-0.21320900	1.03301661	-0.16590080
C	-0.17962306	-1.44641952	-0.34244657
C	-1.57523123	1.05297425	-0.22940930
C	-1.55194850	-1.42559847	0.36520155
H	-0.30909195	-1.58824916	-1.41802851
H	0.36929057	-2.31010178	0.02374763
C	-2.42842829	-0.22909155	-0.17335881
C	2.27289029	2.12137184	1.24243890
H	2.00173757	2.96480150	0.60792637
H	1.41090519	1.83565959	1.83454006
H	3.06712535	2.44567567	1.91511453
H	0.28897632	1.98127946	-0.25664047
N	4.03275115	0.98982673	0.11265574
C	-2.15387293	2.41245913	-0.39239207
H	-1.43979168	3.20361428	-0.19084534
C	-3.37511514	2.81666197	-0.79398123
H	-4.18397629	2.15571918	-1.05888260
H	-3.57842775	3.87601157	-0.87609351
C	4.72898685	-0.01390509	-0.62628832
H	5.71097156	0.27255686	-0.96350175
H	4.57949411	1.75999003	0.45303884
C	-3.64662137	-0.01903653	0.75493754
H	-3.37125569	0.45669966	1.69551335
H	-4.40608298	0.60003884	0.28780714
H	-4.11943697	-0.97231088	0.98551231
C	-2.94466567	-0.52190722	-1.60219762
H	-3.68804794	-1.31822083	-1.59053888
H	-3.41886241	0.35690885	-2.03269507
H	-2.14464823	-0.81461016	-2.28284598
C	-2.20163717	-2.79642499	0.09770509
H	-1.61650999	-3.57879024	0.58563034
H	-3.21311996	-2.85861550	0.49690604
H	-2.24327019	-3.03663790	-0.96420959
C	-1.31327863	-1.31695954	1.88719224
H	-2.22163551	-1.52955616	2.44848044
H	-0.56724084	-2.05129624	2.20039987
H	-0.96139260	-0.33123680	2.19414665

4b- E_{in}

C	-2.92499303	-0.71087951	-0.44747687
C	-1.92166479	0.33174399	-0.20964392
C	-2.47701376	1.71593307	0.12918481
C	-0.56748452	0.11035935	-0.30703198
C	0.36438367	1.23280920	-0.28774873
C	0.10823832	-1.23376810	-0.42060360
C	1.72161947	1.12560840	-0.21287476
C	1.39377886	-1.31488237	0.43498970
H	-0.54314650	-2.03719119	-0.09389496
H	0.35118973	-1.41839455	-1.46852437
C	2.43547864	-0.22791447	-0.03780460
H	-0.04399566	2.22325190	-0.41112198
H	-2.61570656	2.32164464	-0.77287919
H	-1.76585120	2.24868545	0.75237964
C	-2.73889687	-1.93767397	-1.30452625
H	-1.98052170	-1.77385255	-2.06144971
H	-2.44901121	-2.79188839	-0.69428496
H	-3.67783310	-2.17923748	-1.80276314
N	-4.12161878	-0.54651518	0.03714104
C	2.44102764	2.42015999	-0.33356447
H	1.78917248	3.27869091	-0.21732277
C	3.72958919	2.69522311	-0.61693885
H	4.49212927	1.95333367	-0.78914816
H	4.04266771	3.72775137	-0.69513617
C	-4.54870332	0.55898890	0.83209720
H	-5.49798547	0.42347110	1.32250722
C	-3.78048586	1.64726476	0.87705094
H	-4.10831984	2.50503910	1.44631739
H	-4.81546399	-1.23771618	-0.18315422
C	3.56403668	-0.10243031	1.01138345
H	4.42487866	0.42534351	0.61319602
H	3.23917000	0.43065133	1.90407132
H	3.91478466	-1.08739488	1.31556370
C	3.06886443	-0.61907099	-1.39401939
H	3.66974214	0.19583484	-1.79057327
H	3.72543660	-1.48145040	-1.28294747
H	2.32154014	-0.85668792	-2.15186923
C	1.93042603	-2.74982799	0.27271293
H	1.22724962	-3.45653728	0.71917247
H	2.05615650	-3.03157527	-0.77240629
H	2.88585470	-2.89177429	0.77564931
C	1.00772302	-1.13022108	1.91843325
H	0.16475400	-1.77994434	2.16761744
H	1.82696137	-1.40927869	2.57890219
H	0.72250663	-0.10637311	2.16087931

4b-Z_{out}

C	-2.76619512	0.96786627	0.40390325
C	-1.97151335	-0.19547506	-0.00374409
C	-2.76276552	-1.47537592	-0.27329504
C	-0.60175134	-0.17364325	-0.12132912
C	0.21407887	1.03396620	-0.16271197
C	0.17941090	-1.44553790	-0.34031649
C	1.57607088	1.05317947	-0.22746682
C	1.55201948	-1.42507579	0.36664652
C	2.42857492	-0.22934204	-0.17320688
H	-0.28735398	1.98273013	-0.25107405
H	-2.85044282	-2.08825465	0.63037118
H	-2.23626222	-2.08113563	-1.00436238
C	-2.27489981	2.12245151	1.24067305
H	-1.41680144	1.83564687	1.83808337
H	-1.99766563	2.96304655	0.60512523
H	-3.07143338	2.45154477	1.90825257
C	2.15556989	2.41250677	-0.38897882
H	1.44314929	3.20396712	-0.18309889
C	3.37576866	2.81585572	-0.79448797
H	4.18239240	2.15419179	-1.06417030
H	3.58042366	3.87502621	-0.87535841
C	-4.14095424	-1.19718006	-0.80917021
H	-4.67095876	-1.97788412	-1.33541554
C	-4.73021736	-0.01576447	-0.62520649
N	-4.03428249	0.98864795	0.11287848
H	-4.58144269	1.75835447	0.45362312
H	-5.71419317	0.26843014	-0.95843998
C	1.31434231	-1.31508673	1.88869248
H	0.56886338	-2.04944255	2.20319297
H	2.22318438	-1.52651083	2.44960434
H	0.96211035	-0.32923290	2.19480732
C	2.20070307	-2.79641769	0.09957629
H	2.24244591	-3.03674643	-0.96229899
H	3.21199146	-2.85945536	0.49909992
H	1.61483605	-3.57827791	0.58742828
C	3.64865429	-0.02053723	0.75284085
H	4.40771618	0.59812646	0.28445678
H	3.37569361	0.45491760	1.69425375
H	4.12111263	-0.97435739	0.98187015
C	2.94227135	-0.52235382	-1.60296946
H	3.68517371	-1.31914803	-1.59268006
H	2.14101108	-0.81436554	-2.28241652
H	3.41644592	0.35616883	-2.03403220
H	0.30827808	-1.58868933	-1.41581956
H	-0.37002338	-2.30849421	0.02688934

4c- E_{out}

C	3.33790456	-0.66352840	-0.58941033
C	2.41214187	0.44155090	-0.29768809
C	3.07990589	1.76795283	0.05111948
C	1.05539184	0.30825019	-0.33543437
C	0.18969231	1.47722159	-0.22123275
C	0.31921367	-1.00240129	-0.47959658
C	-1.15849050	1.46234427	-0.11345253
C	-0.94660696	-1.01194982	0.37526606
H	0.02836347	-1.16251353	-1.50840797
H	0.90541365	-1.84039594	-0.15561419
C	-1.90890096	0.13861839	-0.04217361
H	0.64379305	2.44128102	-0.30047902
H	2.42639904	2.34829930	0.67961146
H	3.26507598	2.36116564	-0.84101941
C	3.05275276	-1.83468784	-1.49204139
H	2.70392277	-2.68209480	-0.91793453
H	2.31134552	-1.58464547	-2.23112775
H	3.95916027	-2.12778802	-2.00431561
N	4.53596912	-0.60253049	-0.10926011
C	-1.85195957	2.76408538	-0.16147125
H	-1.19884178	3.59564410	0.02883793
C	-3.12431919	3.03219186	-0.47556327
H	-3.85269821	2.28466192	-0.70693012
H	-3.45302407	4.05234846	-0.50710478
C	5.04825668	0.44045313	0.71675863
H	5.97674427	0.21774520	1.19546877
C	4.37357750	1.57797729	0.79043503
H	4.76298780	2.38751480	1.37394492
H	5.17302488	-1.33058346	-0.35525056
Cl	-3.28254907	0.19650405	1.07438196
Cl	-2.53303060	-0.19016196	-1.69462692
Cl	-1.71049019	-2.60257946	0.22019383
Cl	-0.45426981	-0.80977085	2.08578909

4c-Z_{in}

C	4.48457362	-1.25121347	-0.99708048
C	3.12055851	-1.47238847	-0.40672182
C	2.42405398	-0.15954576	-0.06841517
C	3.31437920	0.91396590	0.39744870
H	4.93107861	-2.02639812	-1.58631306
H	2.53366186	-2.02511206	-1.12118255
H	3.21293047	-2.10445043	0.47336300
C	1.07220208	-0.02220937	-0.16616907
C	0.35578491	1.24563236	-0.10639996
C	0.20449205	-1.22522842	-0.45100317
C	-0.98733058	1.39750888	-0.15046889
C	-1.14250339	-1.09957347	0.25480946
H	0.03022389	-1.31882836	-1.51483110
H	0.65557791	-2.13703638	-0.10314574
C	-1.89940302	0.17830413	-0.21247557
C	2.93123440	2.01829241	1.34686407
H	2.71096677	2.92644299	0.80142119
H	2.07162246	1.74463059	1.93392576
H	3.75704239	2.22222732	2.01541097
H	0.92606875	2.14758435	-0.12797927
N	4.55963184	0.86602253	0.05617289
C	-1.50530388	2.77724479	-0.23575729
H	-0.78097197	3.51740761	0.05144225
C	-2.69150718	3.21060009	-0.67642415
H	-3.47660355	2.56589929	-1.00897940
H	-2.88553499	4.26465967	-0.71001602
C	5.15267244	-0.12816776	-0.77761809
H	6.12823104	0.11393772	-1.13901588
H	5.17235312	1.56022158	0.42950282
Cl	-3.37035316	0.38613891	0.75272416
Cl	-2.37111683	-0.01986332	-1.93393570
Cl	-0.82381391	-1.00567593	2.01830158
Cl	-2.07865687	-2.57033784	-0.04465150

4c- E_{in}

C	-3.34867773	-0.70633811	-0.55689441
C	-2.43580348	0.41074854	-0.27135244
C	-3.11746291	1.73452047	0.06083786
C	-1.07741605	0.29117391	-0.30118371
C	-0.22527463	1.47078406	-0.19590581
C	-0.32650112	-1.01305559	-0.42712845
C	1.12270041	1.47223611	-0.08485080
C	0.93727243	-0.99853501	0.43067655
H	-0.90452622	-1.85309425	-0.09381471
H	-0.03140771	-1.18312582	-1.45311599
C	1.88770997	0.15791287	0.00259353
H	-0.68986085	2.42882909	-0.28640811
H	-3.29730263	2.32004586	-0.83741417
H	-2.47477279	2.32406004	0.69204102
C	-3.04473958	-1.88643421	-1.44157116
H	-2.30015233	-1.63894796	-2.17825701
H	-2.69202255	-2.72253492	-0.85341591
H	-3.94412886	-2.19542073	-1.95685645
N	-4.55167287	-0.65075219	-0.08841929
C	1.80161357	2.78121357	-0.14404191
H	1.13943818	3.60708368	0.03961947
C	3.07086223	3.06036999	-0.46097864
H	3.80706042	2.31867133	-0.68637192
H	3.38865930	4.08366869	-0.50126858
C	-5.08168580	0.39726095	0.71970874
H	-6.01324739	0.17201998	1.19119866
C	-4.41746333	1.54121033	0.78785439
H	-4.81997778	2.35374488	1.35815833
H	-5.17921927	-1.38824943	-0.33060445
Cl	3.25792720	0.24378564	1.12143058
Cl	2.51920356	-0.18228325	-1.64458189
Cl	1.71918493	-2.58220690	0.29512035
Cl	0.43861966	-0.78275361	2.13745833

4c-Z_{out}

C	-3.31457268	0.91415581	0.39692408
C	-2.42411121	-0.15914477	-0.06913349
C	-3.12015259	-1.47222499	-0.40766019
C	-1.07221991	-0.02177711	-0.16676740
C	-0.35556445	1.24588711	-0.10654189
C	-0.20457851	-1.22485849	-0.45164337
C	0.98760502	1.39752981	-0.15009319
C	1.14223943	-1.09961975	0.25457029
H	-0.65588368	-2.13670754	-0.10418234
H	-0.03004079	-1.31820760	-1.51545226
C	1.89950295	0.17819884	-0.21216462
H	-0.92559369	2.14797907	-0.12808610
H	-3.21082996	-2.10507036	0.47202779
H	-2.53368354	-2.02388932	-1.12330342
C	-2.93130216	2.01934638	1.34527650
H	-2.07193844	1.74602591	1.93287380
H	-2.71054697	2.92681025	0.79889315
H	-3.75720374	2.22435405	2.01336887
C	1.50581257	2.77718624	-0.23509418
H	0.78152269	3.51744982	0.05194841
C	2.69222304	3.21039644	-0.67534347
H	3.47735775	2.56559965	-1.00761733
H	2.88645091	4.26442542	-0.70873388
C	-4.48509988	-1.25198982	-0.99604719
H	-4.93199580	-2.02766648	-1.58433117
C	-5.15365904	-0.12939669	-0.77578108
N	-4.56016512	0.86534962	0.05695523
H	-5.17283041	1.55940904	0.43061201
H	-6.13006390	0.11178587	-1.13549216
Cl	3.37027357	0.38542525	0.75343153
Cl	2.37158308	-0.01957507	-1.93356411
Cl	0.82307665	-1.00599183	2.01798977
Cl	2.07814781	-2.57050274	-0.04503558

4d- E_{out}

C	-3.93661520	-0.50903331	0.80500388
C	-3.07501667	0.57639040	0.31556864
C	-3.80539800	1.80691641	-0.21736822
C	-1.71087983	0.52027939	0.33185663
C	-0.92168400	1.70282043	0.01196346
C	-0.89659350	-0.70892121	0.65884676
C	0.42707279	1.76223275	-0.09298148
C	0.39093538	-0.76400250	-0.16623759
H	-0.62135319	-0.70803052	1.70448023
H	-1.43066263	-1.61449693	0.44988692
C	1.26123070	0.50182045	0.06122286
H	-1.43734094	2.63417668	-0.07707160
H	-3.22553690	2.25433708	-1.00805872
H	-3.91767028	2.56609305	0.55304163
C	-3.55129212	-1.55436867	1.81743102
H	-3.15798149	-2.43363045	1.32633682
H	-2.81171029	-1.17797537	2.50304087
H	-4.42258265	-1.85022995	2.38558555
N	-5.16528978	-0.54444249	0.40723819
C	1.01052459	3.10805241	-0.27681786
H	0.30483205	3.81913368	-0.66482220
C	2.22914759	3.55732750	0.04117075
H	3.00291062	2.94756997	0.45588696
H	2.46544660	4.59057750	-0.12174246
C	-5.77795162	0.37342532	-0.49716272
H	-6.73830691	0.07284438	-0.85584438
C	-5.15707329	1.48741252	-0.78015783
H	-5.62398242	2.20084029	-1.42969889
H	-5.75405128	-1.25703290	0.78304878
Br	1.91085765	0.52323122	1.98423324
Br	2.82726388	0.46861007	-1.08083986
Br	1.30714168	-2.41402882	0.28911580
Br	-0.13235358	-0.89790235	-2.05715714

4d-Z_{in}

C	-5.06177701	-1.09390592	1.32303246
C	-3.68849694	-1.31700987	0.76183537
C	-3.08540241	-0.04174041	0.18398124
C	-4.05176456	0.89054448	-0.41429441
H	-5.44978825	-1.79438806	2.03548820
H	-3.06353105	-1.69012824	1.55667922
H	-3.73838113	-2.10567709	0.01440045
C	-1.74043866	0.17681841	0.20595606
C	-1.09498486	1.44823308	-0.08673387
C	-0.80560881	-0.92119550	0.65648667
C	0.23907911	1.67891030	-0.09074918
C	0.53634916	-0.83691386	-0.07049656
H	-0.62802645	-0.84135915	1.72139822
H	-1.21446678	-1.89564176	0.46028517
C	1.21511809	0.54100891	0.16008549
C	-3.76150215	1.85945990	-1.52938725
H	-3.56851236	2.84693013	-1.13135600
H	-2.91079454	1.54175741	-2.10745597
H	-4.62045500	1.92557326	-2.18367579
H	-1.71301024	2.30869971	-0.21224831
N	-5.28331972	0.81874192	-0.03225923
C	0.65763469	3.08736887	-0.25681016
H	-0.10680837	3.70013391	-0.69841224
C	1.78746006	3.69344336	0.12278642
H	2.60714125	3.19301287	0.59157462
H	1.89817097	4.74687658	-0.04469883
C	-5.79539614	-0.07643454	0.95591493
H	-6.78051232	0.15349258	1.29917525
H	-5.94787002	1.40878619	-0.48674864
Br	2.84409736	0.68542657	-0.88114308
Br	1.72429839	0.70503685	2.11759078
Br	0.16687553	-1.09778456	-1.98830116
Br	1.62652013	-2.33387631	0.50457315

4d- E_{in}

C	3.93618366	-0.50961130	0.80437134
C	3.07451971	0.57656977	0.31510653
C	3.80592312	1.80721544	-0.21591712
C	1.71057593	0.52049638	0.33092629
C	0.92107217	1.70324102	0.01167651
C	0.89667070	-0.70924076	0.65786268
C	-0.42758115	1.76200577	-0.09311019
C	-0.39084882	-0.76415166	-0.16718809
H	1.43111685	-1.61494374	0.44946477
H	0.62084242	-0.70713446	1.70320430
C	-1.26139521	0.50139636	0.06102471
H	1.43653752	2.63467896	-0.07803679
H	3.91925100	2.56490899	0.55570942
H	3.22630464	2.25648695	-1.00563150
C	3.55160396	-1.55276032	1.81940285
H	2.81381268	-1.17394259	2.50566471
H	3.15609383	-2.43239257	1.33085884
H	4.42360777	-1.84874750	2.38640867
N	5.16389510	-0.54649106	0.40428734
C	-1.01099272	3.10739060	-0.27765681
H	-0.30479584	3.81899881	-0.66377467
C	-2.22938576	3.55681278	0.04120027
H	-3.00268536	2.94679399	0.45638953
H	-2.46535875	4.59048641	-0.11945936
C	5.77695807	0.37225889	-0.49957772
H	6.73670959	0.07091842	-0.85907665
C	5.15705759	1.48743905	-0.77989773
H	5.62411590	2.20177108	-1.42834416
H	5.75366309	-1.25701520	0.78251186
Br	-1.30753197	-2.41416961	0.28788325
Br	0.13525481	-0.89896969	-2.05794511
Br	-2.82608122	0.46805022	-1.08201948
Br	-1.91267531	0.52409953	1.98496554

4d-Z_{out}

C	4.05413874	0.89223812	-0.41113601
C	3.08626787	-0.03709361	0.18871123
C	3.68423487	-1.31315585	0.77117595
C	1.74082105	0.18109229	0.20692906
C	1.09323524	1.45064264	-0.08851346
C	0.80729211	-0.91764042	0.65766040
C	-0.24139735	1.67901842	-0.09338198
C	-0.53425768	-0.83701226	-0.06967770
H	1.21794237	-1.89147871	0.46261407
H	0.62886716	-0.83700587	1.72230709
C	-1.21546063	0.54002695	0.15832180
H	1.70944299	2.31209069	-0.21477922
H	3.71683065	-2.10907118	0.03045510
H	3.06430269	-1.67235794	1.57668984
C	3.76334434	1.86746450	-1.52051749
H	2.91602672	1.54967169	-2.10361314
H	3.56439852	2.85120656	-1.11651316
H	4.62401001	1.94216134	-2.17159648
C	-0.66237834	3.08671961	-0.25984723
H	0.10324653	3.70151625	-0.69655550
C	-1.79449874	3.69093517	0.11624555
H	-2.61552193	3.18891930	0.58091214
H	-1.90509881	4.74470662	-0.04918952
C	5.06571336	-1.10168027	1.31558521
H	5.45653440	-1.80732790	2.02139896
C	5.80285987	-0.08861107	0.94364538
N	5.28751263	0.81393435	-0.03592392
H	5.95188585	1.40196874	-0.49316548
H	6.79337957	0.13253282	1.27715708
Br	-2.84258392	0.67974480	-0.88604369
Br	-1.72841764	0.70645750	2.11570808
Br	-1.62197624	-2.33456818	0.50811270
Br	-0.16259320	-1.10184514	-1.98670263

Cartesian coordinates (in Å) for MP2 S_0 equilibrium geometries of motors 1a–4d

1a- E_{out}

C	-3.00735300	-1.23102300	0.27801400
C	-1.80515200	0.74820300	-0.07111000
C	-0.81119400	-0.28020400	-0.02853900
C	-1.54448100	-1.61229300	0.01286100
C	0.55236700	-0.14276200	-0.07965800
C	1.36225000	-1.33328600	-0.17408900
C	1.28738100	1.16928400	-0.09568800
C	2.71411400	-1.28663300	-0.21739000
C	2.64270400	1.05072400	0.59944000
H	1.44645400	1.45876100	-1.14103500
H	0.70541200	1.95490200	0.37380700
C	3.49169500	-0.02648200	-0.05686200
H	3.15089700	2.01293200	0.57234500
H	2.48386000	0.79333400	1.64830300
H	4.39375800	-0.22571200	0.52166000
H	3.83531500	0.30242900	-1.04440300
H	-3.71500400	-1.70756000	-0.39392000
H	3.25747100	-2.21101300	-0.37347000
H	0.87235600	-2.29227000	-0.26634500
H	-1.16119800	-2.26676600	0.79079600
H	-1.44803700	-2.12908100	-0.94203900
H	-3.31250100	-1.41740500	1.30619400
H	-3.84129200	0.77881000	0.02826700
C	-1.67492800	2.21793900	-0.25281300
H	-1.27382300	2.66995200	0.65357600
H	-0.99748400	2.44543500	-1.07101200
H	-2.64457500	2.66550100	-0.45812700
N	-2.99943200	0.21813600	0.04434300

1a-Z_{in}

C	3.00493700	-1.24265900	-0.17734300
C	1.51897100	-1.59670300	-0.02814200
C	0.80936600	-0.25206200	-0.03803600
C	1.81701500	0.75837400	0.08336700
H	3.64962000	-1.73373000	0.54551200
H	3.38555100	-1.43184900	-1.17949700
H	1.18384100	-2.24345300	-0.83437400
H	1.34006200	-2.11496800	0.91404400
C	-0.55110400	-0.09466800	-0.10517700
C	-1.22992400	1.17404100	-0.22187400
C	-1.42233800	-1.31905300	-0.13986100
C	-2.57996400	1.25916700	-0.25612400
C	-2.75490600	-1.07686200	0.56330400
H	-1.60672700	-1.56890500	-1.19175700
H	-0.90609300	-2.16972500	0.30095300
C	-3.48764500	0.09186500	-0.07655100
H	-3.36011900	-1.98063400	0.52535100
H	-2.56777100	-0.85289300	1.61519200
H	-4.35165500	0.39048800	0.51732100
H	-3.88373800	-0.19330700	-1.05800300
H	3.85422800	0.75037400	0.14736400
H	-3.02662100	2.23144400	-0.42768400
C	1.69668900	2.22887800	0.25781300
H	1.34831200	2.68381600	-0.66890100
H	0.97908700	2.46106800	1.04074400
H	2.65870200	2.66620500	0.51404300
H	-0.66362100	2.08089900	-0.35101300
N	3.00576600	0.20618100	0.06035000

1a- E_{in}

C	3.00740500	-1.23098900	0.27800300
C	1.80516400	0.74822600	-0.07105700
C	0.81123700	-0.28023800	-0.02861200
C	1.54457700	-1.61229000	0.01274900
C	-0.55230600	-0.14274800	-0.07940000
C	-1.36217300	-1.33326600	-0.17396000
C	-1.28731400	1.16930100	-0.09567100
C	-2.71402000	-1.28666100	-0.21757200
C	-2.64275300	1.05079100	0.59912000
H	-0.70552900	1.95487700	0.37413400
H	-1.44587100	1.45885800	-1.14105600
C	-3.49177400	-0.02667600	-0.05665000
H	-3.83646500	0.30184900	-1.04390700
H	-4.39324300	-0.22618000	0.52272700
H	3.31255500	-1.41748800	1.30613800
H	-3.25730400	-2.21100300	-0.37406000
H	-0.87222300	-2.29220300	-0.26632600
H	1.44821200	-2.12903400	-0.94216800
H	1.16127400	-2.26680400	0.79062500
H	3.71508800	-1.70730300	-0.39403100
H	3.84130900	0.77889200	0.02818800
C	1.67466700	2.21790900	-0.25293000
H	0.99670100	2.44515600	-1.07074000
H	1.27405100	2.67000300	0.65362200
H	2.64412800	2.66556500	-0.45885600
H	-3.15094500	2.01297700	0.57168200
H	-2.48399600	0.79382200	1.64809100
N	2.99942900	0.21826700	0.04454200

1a-Z_{out}

C	-3.00516500	-1.24227600	-0.17712300
C	-1.81674700	0.75845100	0.08356500
C	-0.80935600	-0.25218100	-0.03845200
C	-1.51920700	-1.59667800	-0.02847600
C	0.55108500	-0.09491400	-0.10603000
C	1.22991800	1.17377700	-0.22342700
C	1.42242300	-1.31917100	-0.14044100
C	2.57996800	1.25895300	-0.25653500
C	2.75424800	-1.07676700	0.56419200
H	0.90593800	-2.17017100	0.29944600
H	1.60814200	-1.56847400	-1.19223100
C	3.48754300	0.09180100	-0.07533200
H	3.88455200	-0.19387600	-1.05628800
H	4.35099400	0.39074300	0.51918200
H	-3.38621800	-1.43137000	-1.17913500
H	3.02675400	2.23109400	-0.42856000
H	0.66358000	2.08040400	-0.35413700
H	-1.34012200	-2.11522000	0.91352500
H	-1.18444300	-2.24330700	-0.83496800
H	-3.64968400	-1.73328700	0.54593900
H	-3.85394500	0.75082600	0.14829200
C	-1.69602000	2.22886200	0.25851400
H	-0.97697800	2.46067200	1.04022200
H	-1.34934900	2.68424000	-0.66864500
H	-2.65756700	2.66608400	0.51670300
H	3.35955100	-1.98052200	0.52708400
H	2.56598300	-0.85254900	1.61582800
N	-3.00561700	0.20650900	0.06071700

1b- E_{out}

C	-4.07030200	-1.06443500	0.41471800
C	-2.72409400	0.75517400	-0.18621400
C	-1.82600200	-0.35500900	-0.11170200
C	-2.67046600	-1.60375700	0.09060800
C	-0.46146800	-0.35413600	-0.24851800
C	0.23524700	-1.61343000	-0.27204000
C	0.39765900	0.86104100	-0.41469900
C	1.58646000	-1.67530900	-0.26858000
C	1.73863700	0.74226500	0.33485900
H	0.59120600	0.99832300	-1.48401500
H	-0.09870100	1.75948100	-0.05913800
C	2.51013500	-0.50336900	-0.18090200
H	-4.86507300	-1.52725500	-0.16275200
H	2.05600100	-2.65256700	-0.34037700
H	-0.33237400	-2.53294100	-0.31555100
H	-2.29146800	-2.22783800	0.89520700
H	-2.68926100	-2.20140900	-0.82095900
H	-4.31374100	-1.13302300	1.47359700
H	-4.73812700	0.98695000	0.03571500
C	-2.47725100	2.18566000	-0.50808100
H	-1.97745200	2.67339000	0.32796000
H	-1.83879900	2.27769200	-1.38228400
H	-3.41562100	2.70269700	-0.69545100
N	-3.95066000	0.35232500	0.04949600
C	2.51119100	2.03753100	0.09363400
H	1.98198800	2.87228100	0.55569300
H	3.50427300	1.99661000	0.53926800
H	2.62037900	2.25699300	-0.96733800
C	1.44216600	0.62897300	1.83354700
H	2.35187300	0.73615300	2.42109600
H	0.76502700	1.43031100	2.13557800
H	0.98022800	-0.32318700	2.09513100
C	3.08716700	-0.29119700	-1.59387600
H	3.90308200	0.42964400	-1.56554800
H	3.48857100	-1.23043800	-1.97425200
H	2.33531400	0.05684600	-2.30125400
C	3.67314200	-0.88986800	0.74224300
H	4.24134200	-1.70422800	0.29242300
H	4.35369400	-0.05067000	0.88099300
H	3.32892700	-1.22090300	1.71980700

1b-Z_{in}

C	3.91520600	-1.33264100	-0.27054900
C	2.39985000	-1.57710000	-0.24217400
C	1.79747900	-0.18305100	-0.17069900
C	2.86681300	0.72549400	0.10985400
H	4.47258600	-1.94033600	0.43606500
H	4.34419100	-1.45785600	-1.26325400
H	2.07016700	-2.12212900	-1.12237000
H	2.12044300	-2.15766400	0.63709100
C	0.46196300	0.09805600	-0.30025700
C	-0.10875300	1.42071700	-0.32959800
C	-0.51468800	-1.02113500	-0.48550400
C	-1.44887100	1.60110300	-0.29934400
C	-1.82136700	-0.79750200	0.29662900
H	-0.73654800	-1.10240300	-1.55528800
H	-0.08238300	-1.97406500	-0.17911900
C	-2.48012800	0.52443100	-0.18443700
H	4.88905800	0.54543800	0.30027900
H	-1.82776700	2.61657800	-0.37733500
C	2.84050900	2.17820000	0.41897600
H	2.61179600	2.74390400	-0.48384300
H	2.07271200	2.39511200	1.15735700
H	3.80512800	2.50948800	0.79620300
H	0.52217100	2.28995000	-0.41852500
N	4.01009800	0.08300000	0.10818200
C	-2.71782700	-2.01015100	0.05638800
H	-2.25972600	-2.89748900	0.49526600
H	-3.69297000	-1.88150800	0.52476700
H	-2.86914900	-2.20257200	-1.00451300
C	-1.48172600	-0.73574700	1.78943300
H	-2.38376600	-0.76720200	2.39746900
H	-0.87469300	-1.60049900	2.06378200
H	-0.92863400	0.16650200	2.05221600
C	-3.56900900	1.01562500	0.77852800
H	-4.06829900	1.88636500	0.35313600
H	-4.32414400	0.24580400	0.93333700
H	-3.16311100	1.30078400	1.74685100
C	-3.12147700	0.38431100	-1.57852000
H	-4.00408200	-0.25157500	-1.52678300
H	-3.43904700	1.36242300	-1.93981300
H	-2.43245600	-0.03171400	-2.31260800

1b- E_{in}

C	4.07025900	-1.06447600	0.41473600
C	2.72409600	0.75517300	-0.18615900
C	1.82600000	-0.35501400	-0.11175100
C	2.67045900	-1.60378600	0.09048100
C	0.46146800	-0.35417000	-0.24854600
C	-0.23522200	-1.61346400	-0.27194700
C	-0.39763900	0.86100700	-0.41482400
C	-1.58644900	-1.67534600	-0.26828300
C	-1.73863900	0.74235700	0.33468500
H	0.09874500	1.75945700	-0.05932300
H	-0.59110300	0.99822100	-1.48416300
C	-2.51013600	-0.50341700	-0.18077500
H	4.31358200	-1.13308000	1.47364100
H	-2.05595600	-2.65264500	-0.33976900
H	0.33237300	-2.53299400	-0.31539100
H	2.68930300	-2.20129900	-0.82117300
H	2.29140500	-2.22795700	0.89497900
H	4.86508900	-1.52729200	-0.16265200
H	4.73811600	0.98692200	0.03580100
C	2.47733000	2.18569600	-0.50794100
H	1.83898600	2.27781600	-1.38221500
H	1.97744700	2.67336600	0.32808100
H	3.41574100	2.70271300	-0.69515500
N	3.95065600	0.35228400	0.04953300
C	-3.67306500	-0.88969700	0.74250000
H	-4.35360100	-0.05046800	0.88114200
H	-4.24131400	-1.70413700	0.29287800
H	-3.32879200	-1.22055900	1.72010400
C	-3.08726100	-0.29161300	-1.59378200
H	-3.48874000	-1.23093800	-1.97387600
H	-3.90314900	0.42926400	-1.56559900
H	-2.33543400	0.05618400	-2.30130000
C	-1.44222200	0.62934900	1.83338600
H	-0.76514800	1.43078300	2.13532500
H	-2.35195200	0.73655500	2.42089500
H	-0.98022000	-0.32274000	2.09512500
C	-2.51119900	2.03755300	0.09319000
H	-1.98205800	2.87238800	0.55517700
H	-2.62027500	2.25686000	-0.96782300
H	-3.50432100	1.99668600	0.53873700

1b-Z_{out}

C	-3.91511200	-1.33273500	-0.27091900
C	-2.86697000	0.72543100	0.10989500
C	-1.79750600	-0.18302000	-0.17041900
C	-2.39977600	-1.57713900	-0.24184200
C	-0.46199500	0.09813300	-0.29995500
C	0.10877900	1.42075900	-0.32921400
C	0.51466200	-1.02107900	-0.48528000
C	1.44890000	1.60111900	-0.29920700
C	1.82144800	-0.79748000	0.29665000
H	0.08234500	-1.97397300	-0.17882000
H	0.73637600	-1.10235000	-1.55509300
C	2.48018800	0.52445200	-0.18462300
H	-4.34356500	-1.45779400	-1.26388000
H	1.82776800	2.61661000	-0.37713000
H	-0.52211600	2.29004600	-0.41779600
H	-2.12071600	-2.15741700	0.63772800
H	-2.06971300	-2.12241000	-1.12173700
H	-4.47285000	-1.94056900	0.43529000
H	-4.88927200	0.54523500	0.29975000
C	-2.84090000	2.17816000	0.41894500
H	-2.07348100	2.39519900	1.15768100
H	-2.61181400	2.74381500	-0.48381200
H	-3.80571300	2.50941600	0.79570800
N	-4.01021800	0.08286000	0.10794600
C	1.48206500	-0.73557400	1.78949600
H	0.87517100	-1.60036100	2.06404400
H	2.38422300	-0.76687000	2.39736300
H	0.92891700	0.16664100	2.05227400
C	2.71783900	-2.01018800	0.05637900
H	2.86896300	-2.20276200	-1.00452100
H	3.69307300	-1.88151400	0.52456400
H	2.25980200	-2.89746400	0.49544800
C	3.12126200	0.38430600	-1.57881300
H	3.43862400	1.36243500	-1.94024500
H	4.00396700	-0.25144800	-1.52720600
H	2.43217700	-0.03186600	-2.31275900
C	3.56926700	1.01560900	0.77815500
H	4.32443000	0.24577600	0.93276400
H	4.06846100	1.88637400	0.35270400
H	3.16356200	1.30071200	1.74657600

1c- E_{out}

C	-4.67166400	-1.02827100	0.38044900
C	-3.26803500	0.72389800	-0.29748600
C	-2.39746700	-0.40932200	-0.14071300
C	-3.27221300	-1.61644500	0.15343800
C	-1.03455100	-0.44808300	-0.25323400
C	-0.36073100	-1.71834300	-0.13961000
C	-0.16431900	0.74414800	-0.52530800
C	0.98462500	-1.83018300	-0.12705200
C	1.15995300	0.63468000	0.22789500
H	0.06233600	0.80246900	-1.59345800
H	-0.62063400	1.67621000	-0.21608300
C	1.90155900	-0.65273600	-0.19960100
H	-5.44903500	-1.49917800	-0.21429000
H	1.46289700	-2.79993500	-0.08543800
H	-0.94654100	-2.62461600	-0.07868500
H	-2.92778500	-2.16102600	1.02857700
H	-3.27479500	-2.30197200	-0.69366600
H	-4.97119500	-1.03471800	1.42662800
H	-5.27278000	1.01879200	-0.11088600
C	-2.97566800	2.12576900	-0.69313500
H	-2.44944600	2.63502600	0.11413700
H	-2.34604500	2.15239600	-1.57868900
H	-3.89671100	2.66704000	-0.89620100
N	-4.50143600	0.36532600	-0.04987900
Cl	2.12625200	2.07596700	-0.08435300
Cl	2.39081600	-0.51814500	-1.91797100
Cl	0.78290200	0.54494000	1.97070100
Cl	3.33125700	-0.94031700	0.79240800

1c-Z_{in}

C	-4.45128200	1.32337900	-0.43357800
C	-2.92998600	1.52389900	-0.43459600
C	-2.36535200	0.12720000	-0.24514100
C	-3.46429500	-0.73544400	0.09690900
H	-4.98301600	1.98704500	0.24194800
H	-4.89112300	1.39860900	-1.42627200
H	-2.59180100	1.98171700	-1.36048900
H	-2.62564100	2.16768100	0.39111500
C	-1.03752900	-0.19033700	-0.32698300
C	-0.48896200	-1.51965700	-0.21173800
C	-0.05259400	0.90800600	-0.60731000
C	0.84137000	-1.74412300	-0.16445500
C	1.23181900	0.69924200	0.18894200
H	0.20237500	0.91418900	-1.67099000
H	-0.44901400	1.88577000	-0.34565400
C	1.86502800	-0.65611000	-0.20151700
H	-5.47756000	-0.48493400	0.25585600
H	1.23141700	-2.75271500	-0.12525800
C	-3.47750600	-2.15927100	0.51675900
H	-3.21582500	-2.79651600	-0.32755500
H	-2.75011500	-2.32522200	1.30820900
H	-4.46372000	-2.44830400	0.87179600
H	-1.13633700	-2.38027900	-0.19522900
N	-4.58395500	-0.06307500	0.03358900
Cl	2.33431800	2.04222000	-0.09919400
Cl	0.78876500	0.66102200	1.92019400
Cl	3.22146500	-1.07039700	0.84783800
Cl	2.43273400	-0.58379900	-1.89921100

1c- E_{in}

C	4.67212400	-1.02829200	0.37968200
C	3.26814100	0.72396700	-0.29729500
C	2.39762100	-0.40929900	-0.14032800
C	3.27243800	-1.61636700	0.15388100
C	1.03468600	-0.44802800	-0.25248900
C	0.36090900	-1.71831600	-0.13845600
C	0.16442500	0.74412000	-0.52488900
C	-0.98443400	-1.83025100	-0.12620900
C	-1.16013200	0.63470600	0.22772800
H	0.62059000	1.67621800	-0.21551200
H	-0.06164500	0.80249800	-1.59316400
C	-1.90142300	-0.65288200	-0.19946200
H	4.97277200	-1.03510400	1.42553600
H	-1.46266900	-2.80001000	-0.08434900
H	0.94683700	-2.62447300	-0.07702300
H	3.27434600	-2.30239400	-0.69280800
H	2.92847800	-2.16037600	1.02956300
H	5.44888000	-1.49906700	-0.21597900
H	5.27292600	1.01888000	-0.11137900
C	2.97552500	2.12582700	-0.69270700
H	2.34584500	2.15245200	-1.57822300
H	2.44923400	2.63487800	0.11464800
H	3.89644100	2.66732100	-0.89574300
N	4.50160700	0.36540200	-0.05010700
Cl	-0.78384900	0.54584500	1.97075500
Cl	-2.12646800	2.07578700	-0.08557700
Cl	-3.33141200	-0.94025700	0.79218000
Cl	-2.39018600	-0.51900800	-1.91803800

1c-Z_{out}

C	4.45148400	1.32333100	-0.43424100
C	3.46454800	-0.73529300	0.09707500
C	2.36555000	0.12742900	-0.24455000
C	2.93020500	1.52405800	-0.43431000
C	1.03766400	-0.19001200	-0.32595000
C	0.48921400	-1.51938700	-0.21123500
C	0.05283300	0.90857100	-0.60571200
C	-0.84111500	-1.74404800	-0.16466000
C	-1.23214500	0.69914200	0.18938600
H	0.44913100	1.88602100	-0.34265800
H	-0.20128200	0.91599000	-1.66959700
C	-1.86485000	-0.65611800	-0.20184100
H	4.89070000	1.39835900	-1.42722400
H	-1.23108300	-2.75269000	-0.12598800
H	1.13671800	-2.37991700	-0.19482100
H	2.62647900	2.16792000	0.39156600
H	2.59146600	1.98189100	-1.35999900
H	4.98373600	1.98701900	0.24085400
H	5.47790800	-0.48492900	0.25514200
C	3.47774600	-2.15900700	0.51731600
H	2.74996200	-2.32489200	1.30840400
H	3.21665600	-2.79650600	-0.32700100
H	4.46382300	-2.44778000	0.87294600
N	4.58425500	-0.06306200	0.03308000
Cl	-3.22197800	-1.07090200	0.84619100
Cl	-2.43129500	-0.58316600	-1.90011700
Cl	-2.33463900	2.04198100	-0.09896000
Cl	-0.79037000	0.66026100	1.92107100

1d- E_{out}

C	5.38907600	-0.95557400	-0.69880300
C	3.97799100	0.29821900	0.69302200
C	3.10575800	-0.61168000	0.00597900
C	3.97795700	-1.54968900	-0.81109000
C	1.73931200	-0.67540800	0.05888600
C	1.06089100	-1.72539600	-0.65522500
C	0.86944300	0.25495300	0.85319200
C	-0.28699600	-1.79269500	-0.74318400
C	-0.43398200	0.54491700	0.11057900
H	0.61410800	-0.20947700	1.81102000
H	1.34395300	1.20826200	1.04749200
C	-1.19254100	-0.76717100	-0.15419300
H	6.14191400	-1.66850400	-0.37491100
H	-0.76694100	-2.62681800	-1.23828500
H	1.63956100	-2.50904600	-1.12374800
H	3.65353700	-1.60028700	-1.84724700
H	3.94874900	-2.55733500	-0.39714600
H	5.72376000	-0.47838300	-1.61775000
H	5.98921300	0.61256800	0.70582000
C	3.68425300	1.35778200	1.69240800
H	3.17334300	2.18995600	1.20810600
H	3.04012200	0.97594700	2.48031800
H	4.60377000	1.73196300	2.13636600
N	5.21622400	0.07686500	0.33062000
Br	-1.47055300	1.79887900	1.13065500
Br	0.06037200	1.36891200	-1.58457700
Br	-2.72454600	-0.51857500	-1.28704500
Br	-1.77857600	-1.55997300	1.53485900

1d-Z_{in}

C	-5.17288600	0.83080300	-1.06849500
C	-3.65311300	1.03577200	-1.12628800
C	-3.08427800	-0.15847000	-0.38157800
C	-4.18191000	-0.82192500	0.26473200
H	-5.72287800	1.70436000	-0.73096300
H	-5.59172400	0.48941000	-2.01333400
H	-3.29950400	1.08802900	-2.15270300
H	-3.36895100	1.96084200	-0.62335100
C	-1.75190900	-0.46003900	-0.30023000
C	-1.19640000	-1.62060700	0.34678200
C	-0.76778300	0.44886600	-0.97947100
C	0.13650100	-1.78004300	0.51000200
C	0.49181600	0.60570900	-0.13217800
H	-0.47961100	0.02193700	-1.94571200
H	-1.18429400	1.43730900	-1.15482800
C	1.14517300	-0.77058800	0.08248000
H	-6.20019500	-0.55381500	0.28335900
H	0.53079600	-2.68887000	0.94566000
C	-4.19012400	-1.95220300	1.22693500
H	-3.91350900	-2.87466700	0.71696800
H	-3.47048100	-1.77346600	2.02276900
H	-5.17835500	-2.08340900	1.66105100
H	-1.83436800	-2.42074000	0.68324300
N	-5.30588500	-0.24741000	-0.07969000
Br	-0.08236200	1.32966400	1.58602700
Br	1.67638000	1.86142600	-0.96879500
Br	2.59136600	-0.71537500	1.34716800
Br	1.82043800	-1.46767800	-1.61555600

1d- E_{in}

C	-5.38911500	-0.95582800	-0.69867700
C	-3.97809900	0.29831700	0.69289500
C	-3.10578000	-0.61162700	0.00594300
C	-3.97792800	-1.54974100	-0.81107200
C	-1.73933300	-0.67526000	0.05884100
C	-1.06093000	-1.72521600	-0.65539100
C	-0.86941800	0.25501600	0.85319900
C	0.28695200	-1.79257800	-0.74336800
C	0.43403000	0.54492900	0.11065000
H	-0.61418600	-0.20948100	1.81102600
H	-1.34385100	1.20835400	1.04755600
C	1.19254600	-0.76715600	-0.15424000
H	-6.14180400	-1.66882800	-0.37459100
H	0.76689200	-2.62665600	-1.23855200
H	-1.63968700	-2.50876300	-1.12398400
H	-3.65357300	-1.60029600	-1.84725100
H	-3.94854900	-2.55737300	-0.39711200
H	-5.72400100	-0.47879500	-1.61763300
H	-5.98936200	0.61237500	0.70582800
C	-3.68435500	1.35801600	1.69211600
H	-3.17331100	2.19003900	1.20770500
H	-3.04032400	0.97623600	2.48013500
H	-4.60386600	1.73238500	2.13592800
N	-5.21631000	0.07676500	0.33060400
Br	1.47060900	1.79879700	1.13083000
Br	-0.06027500	1.36910200	-1.58445800
Br	2.72453600	-0.51852900	-1.28705700
Br	1.77851200	-1.56022100	1.53472300

1d-Z_{out}

C	5.17294500	0.83070000	-1.06845800
C	4.18181400	-0.82193700	0.26474100
C	3.08428100	-0.15848000	-0.38164700
C	3.65318400	1.03577900	-1.12626400
C	1.75191000	-0.46000100	-0.30027000
C	1.19645500	-1.62049900	0.34686800
C	0.76775100	0.44881800	-0.97954500
C	-0.13642000	-1.77996600	0.51012300
C	-0.49182200	0.60573300	-0.13218400
H	1.18421400	1.43724200	-1.15504700
H	0.47949100	0.02175700	-1.94570000
C	-1.14511300	-0.77059700	0.08254100
H	5.59172600	0.48912800	-2.01326100
H	-0.53062900	-2.68878400	0.94586600
H	1.83442400	-2.42059400	0.68343300
H	3.36909800	1.96081900	-0.62322000
H	3.29959200	1.08820200	-2.15267500
H	5.72301100	1.70426600	-0.73107700
H	6.20010200	-0.55386900	0.28355800
C	4.19000600	-1.95228200	1.22688200
H	3.47053100	-1.77347800	2.02286400
H	3.91314600	-2.87467600	0.71692800
H	5.17828800	-2.08367200	1.66082600
N	5.30584500	-0.24740300	-0.07953000
Br	-1.67645600	1.86128800	-0.96891000
Br	0.08237100	1.32988600	1.58593200
Br	-2.59135400	-0.71538300	1.34721200
Br	-1.82038600	-1.46773800	-1.61544900

2a- E_{out}

C	-3.23368100	-1.78557000	0.27942200
C	-2.58656100	0.42477100	-0.13903200
C	-1.36200500	-0.28763300	0.01157300
C	-1.70835800	-1.76529800	0.10489100
C	-0.07979500	0.21414800	0.00443100
C	1.01400700	-0.70575200	0.01864400
C	0.25961200	1.67857900	-0.05425600
C	2.32885400	-0.32436600	-0.02396100
C	1.58853000	1.95716000	0.63991000
H	0.33487400	1.97742800	-1.10613200
H	-0.52241500	2.27957700	0.39863100
C	2.70298200	1.12503300	0.02620400
H	1.82353300	3.01795800	0.56909200
H	1.49717600	1.71185900	1.69965900
H	3.62444800	1.24628800	0.59416500
H	2.91721500	1.46803700	-0.99181300
H	-3.74249700	-2.47346000	-0.38944700
H	0.79994900	-1.76675100	0.00565800
H	-1.21039600	-2.25115200	0.93990800
H	-1.41661200	-2.28245300	-0.80966700
H	-3.53592500	-1.99747000	1.30370400
C	-2.84650500	1.86532800	-0.40362900
H	-2.65423400	2.45040100	0.49496300
H	-2.19831600	2.23619200	-1.19232500
H	-3.88303700	2.01860000	-0.69509000
N	-3.60376700	-0.40454400	-0.04805800
C	3.34622700	-1.34714100	-0.13844200
H	3.00088600	-2.37457200	-0.14794100
C	4.66385100	-1.10239000	-0.25606700
H	5.06401500	-0.09896200	-0.26456200
H	5.36686300	-1.91611900	-0.35548100
H	-4.56210200	-0.09479700	-0.13504500

2a-Z_{in}

C	3.84153300	-0.54100400	-0.35140000
C	2.52855000	-1.31035700	-0.15040300
C	1.47248100	-0.22316500	-0.03141800
C	2.16035100	1.01702300	0.12013200
H	4.65050100	-0.87663500	0.29063200
H	4.18064600	-0.55260500	-1.38603100
H	2.33381600	-1.98527700	-0.97960000
H	2.56718500	-1.90484700	0.76298600
C	0.11623100	-0.46184700	-0.02812800
C	-0.89033300	0.55405800	-0.02297800
C	-0.35801500	-1.88644900	-0.10501700
C	-2.23173500	0.28159200	-0.05083200
C	-1.69455000	-2.06379200	0.60337900
H	-0.46661200	-2.15234900	-1.16346500
H	0.39010400	-2.55860800	0.31227300
C	-2.73727400	-1.12673300	0.01562500
H	-2.02287100	-3.09848000	0.52067400
H	-1.56892900	-1.84471900	1.66539600
H	-3.65301600	-1.15879900	0.60469000
H	-3.00796500	-1.44665600	-0.99650300
C	1.64362300	2.38012000	0.40958500
H	1.12181000	2.77217800	-0.46302200
H	0.94326900	2.35259500	1.24095600
H	2.45883700	3.05715200	0.65382700
H	-0.60480300	1.59316600	-0.06770000
N	3.45626000	0.82945400	0.00421200
C	-3.15877600	1.38801900	-0.17430800
H	-2.72573700	2.38163000	-0.20307600
C	-4.49341900	1.25971300	-0.27780500
H	-4.98114500	0.29589700	-0.26676200
H	-5.12221500	2.13110300	-0.38507600
H	4.12129000	1.58600600	0.09173000

2a- E_{in}

C	3.23368100	-1.78557000	0.27942200
C	2.58656100	0.42477100	-0.13903200
C	1.36200500	-0.28763300	0.01157300
C	1.70835800	-1.76529800	0.10489100
C	0.07979500	0.21414800	0.00443100
C	-1.01400700	-0.70575200	0.01864400
C	-0.25961200	1.67857900	-0.05425600
C	-2.32885400	-0.32436600	-0.02396100
C	-1.58853000	1.95716000	0.63991000
H	0.52241500	2.27957700	0.39863100
H	-0.33487400	1.97742800	-1.10613200
C	-2.70298200	1.12503300	0.02620400
H	-2.91721500	1.46803700	-0.99181200
H	-3.62444800	1.24628800	0.59416500
H	3.53592500	-1.99747000	1.30370400
H	-0.79994900	-1.76675100	0.00565800
H	1.41661200	-2.28245300	-0.80966700
H	1.21039500	-2.25115200	0.93990800
H	3.74249700	-2.47346000	-0.38944700
C	2.84650500	1.86532800	-0.40363000
H	2.19831700	2.23619200	-1.19232500
H	2.65423400	2.45040100	0.49496300
H	3.88303700	2.01860000	-0.69509000
H	-1.82353300	3.01795800	0.56909200
H	-1.49717600	1.71185900	1.69965900
N	3.60376700	-0.40454400	-0.04805700
C	-3.34622700	-1.34714100	-0.13844200
H	-3.00088600	-2.37457200	-0.14794100
C	-4.66385100	-1.10239000	-0.25606700
H	-5.06401500	-0.09896200	-0.26456200
H	-5.36686300	-1.91611900	-0.35548100
H	4.56210200	-0.09479700	-0.13504500

2a-Z_{out}

C	-3.84153300	-0.54100400	-0.35140000
C	-2.16035100	1.01702300	0.12013200
C	-1.47248100	-0.22316500	-0.03141800
C	-2.52855000	-1.31035700	-0.15040300
C	-0.11623100	-0.46184700	-0.02812800
C	0.89033300	0.55405800	-0.02297800
C	0.35801500	-1.88644900	-0.10501700
C	2.23173500	0.28159200	-0.05083200
C	1.69455000	-2.06379200	0.60337900
H	-0.39010400	-2.55860800	0.31227300
H	0.46661200	-2.15234900	-1.16346500
C	2.73727400	-1.12673300	0.01562500
H	3.00796500	-1.44665600	-0.99650300
H	3.65301600	-1.15879900	0.60469000
H	-4.18064600	-0.55260500	-1.38603100
H	0.60480300	1.59316600	-0.06770000
H	-2.56718500	-1.90484700	0.76298600
H	-2.33381600	-1.98527700	-0.97960000
H	-4.65050100	-0.87663500	0.29063200
C	-1.64362300	2.38012000	0.40958500
H	-0.94326900	2.35259500	1.24095600
H	-1.12181000	2.77217800	-0.46302200
H	-2.45883700	3.05715200	0.65382700
H	2.02287100	-3.09848000	0.52067400
H	1.56892900	-1.84471900	1.66539600
N	-3.45626000	0.82945400	0.00421200
C	3.15877600	1.38801900	-0.17430800
H	2.72573700	2.38163000	-0.20307600
C	4.49341900	1.25971300	-0.27780500
H	4.98114500	0.29589700	-0.26676200
H	5.12221500	2.13110300	-0.38507600
H	-4.12129000	1.58600600	0.09173000

2b- E_{out}

C	4.15988800	1.50637100	0.47951100
C	3.16495400	-0.46865300	-0.28699600
C	2.07577700	0.41981500	-0.05660700
C	2.66591200	1.78454900	0.26045300
C	0.72863700	0.15605600	-0.15672300
C	-0.19494500	1.23300100	-0.03378200
C	0.12789900	-1.18563800	-0.42229300
C	-1.56001800	1.08999700	-0.06484800
C	-1.19637200	-1.37280200	0.33269200
H	-0.04418100	-1.28699300	-1.49908200
H	0.79359000	-1.99201700	-0.12600700
C	-2.22317900	-0.27371100	-0.09229700
H	4.81621500	2.18397000	-0.05855700
H	0.19694200	2.24020100	0.03544100
H	2.21396800	2.23216000	1.14169400
H	2.51864200	2.46606300	-0.57817300
H	4.43575100	1.50602600	1.53286500
C	3.18476600	-1.87802400	-0.76263500
H	2.85803800	-2.54500400	0.03439300
H	2.51484500	-2.00929900	-1.60757200
H	4.19095500	-2.16644200	-1.05852200
N	4.30414300	0.14536500	-0.04860500
C	-2.29795400	2.34694000	-0.08469700
H	-1.68736200	3.21869600	0.12755600
C	-3.58756300	2.58221400	-0.39086600
H	-4.29043500	1.81211900	-0.66043500
H	-3.95160900	3.59960400	-0.39564400
C	-3.41984800	-0.30343500	0.87604700
H	-3.18341300	0.16678300	1.82845200
H	-4.28540100	0.20217000	0.46192200
H	-3.71559600	-1.33322700	1.06719900
C	-2.73335300	-0.52498000	-1.52455300
H	-3.36277200	-1.41323500	-1.54940200
H	-3.32734200	0.31616600	-1.87314300
H	-1.91637500	-0.65899300	-2.23317600
C	-1.68976300	-2.78231600	0.00157000
H	-1.75237500	-2.95169900	-1.07219100
H	-0.99151100	-3.51250000	0.41335300
H	-2.66519200	-2.98912600	0.43817400
C	-0.90637500	-1.30808200	1.83709000
H	-1.76282800	-1.64578400	2.41687100
H	-0.07175800	-1.96941300	2.07772900
H	-0.64881900	-0.30253600	2.16946000
H	5.19824700	-0.31306100	-0.15936200

2b-Z_{in}

C	4.40472200	-0.83466800	-0.48408900
C	2.96656800	-1.36938200	-0.43133000
C	2.12012600	-0.13232100	-0.17927100
C	3.01018300	0.91988800	0.18614900
H	5.10955700	-1.40842900	0.11020400
H	4.78326000	-0.74995800	-1.50162300
H	2.69589500	-1.87355100	-1.35508200
H	2.85089400	-2.08155700	0.38642500
C	0.74575800	-0.10483300	-0.24233200
C	-0.05545600	1.06842600	-0.12352600
C	-0.00352600	-1.36696000	-0.51435900
C	-1.42790900	1.05767800	-0.11024000
C	-1.30876300	-1.43212100	0.28916400
H	-0.22139000	-1.41734200	-1.58668400
H	0.60096800	-2.24262800	-0.27498100
C	-2.23079900	-0.22973900	-0.09428400
C	2.72626400	2.29278100	0.67868100
H	2.37022000	2.91512400	-0.14225100
H	1.95533300	2.26944200	1.44506500
H	3.62473700	2.74853600	1.08843600
H	0.42007900	2.03709100	-0.11070600
N	4.25571500	0.51288200	0.07850600
C	-2.03751500	2.38344500	-0.13361100
H	-1.33291800	3.19323300	0.02860500
C	-3.30911800	2.74604200	-0.38379400
H	-4.10147000	2.04914000	-0.59827100
H	-3.56513700	3.79575800	-0.39684100
C	-3.37692500	-0.13032800	0.92875800
H	-3.04595500	0.30801800	1.86818300
H	-4.20049600	0.46821400	0.55502400
H	-3.77374100	-1.12256900	1.13556500
C	-2.83173700	-0.43020300	-1.49923700
H	-3.55501000	-1.24405900	-1.48553700
H	-3.34511400	0.46884500	-1.83025700
H	-2.06843300	-0.65867700	-2.24261100
C	-0.95564500	-1.40657200	1.78155300
H	-1.81745300	-1.66347200	2.39394200
H	-0.18020200	-2.14707700	1.98655300
H	-0.59002800	-0.43227300	2.10646600
C	-1.95583700	-2.78154200	-0.02563600
H	-2.07305200	-2.93848100	-1.09653900
H	-1.32209000	-3.58127000	0.35988400
H	-2.93159400	-2.88758800	0.44548100
H	5.04079400	1.10780500	0.30642600

2b- E_{in}

C	-4.15988500	1.50637100	0.47951700
C	-3.16495400	-0.46865200	-0.28699700
C	-2.07577600	0.41981600	-0.05660800
C	-2.66591000	1.78455000	0.26045100
C	-0.72863700	0.15605700	-0.15672600
C	0.19494600	1.23300100	-0.03378800
C	-0.12789900	-1.18563800	-0.42229500
C	1.56001800	1.08999700	-0.06485100
C	1.19637100	-1.37280300	0.33269100
H	-0.79359200	-1.99201700	-0.12600900
H	0.04418200	-1.28699400	-1.49908400
C	2.22317900	-0.27371200	-0.09229700
H	-4.43574200	1.50602200	1.53287200
H	-0.19694200	2.24020200	0.03543300
H	-2.51864500	2.46606100	-0.57817900
H	-2.21396300	2.23216400	1.14168800
H	-4.81621600	2.18397100	-0.05854500
C	-3.18476900	-1.87802200	-0.76263700
H	-2.51484700	-2.00930000	-1.60757300
H	-2.85804400	-2.54500300	0.03439200
H	-4.19095800	-2.16643800	-1.05852500
N	-4.30414300	0.14536700	-0.04860300
C	2.29795500	2.34693900	-0.08470000
H	1.68736200	3.21869600	0.12754700
C	3.58756600	2.58221100	-0.39086200
H	4.29043900	1.81211500	-0.66042600
H	3.95161300	3.59960000	-0.39564300
H	-5.19824700	-0.31305900	-0.15936000
C	3.41984500	-0.30343500	0.87605200
H	4.28540000	0.20216800	0.46192700
H	3.18340800	0.16678500	1.82845500
H	3.71559100	-1.33322600	1.06720600
C	2.73335800	-0.52498000	-1.52455000
H	3.32734700	0.31616600	-1.87313700
H	3.36277900	-1.41323400	-1.54939700
H	1.91638300	-0.65899400	-2.23317600
C	1.68976100	-2.78231600	0.00157100
H	0.99150900	-3.51250000	0.41335500
H	1.75237300	-2.95170100	-1.07219000
H	2.66519000	-2.98912600	0.43817600
C	0.90637200	-1.30808100	1.83708800
H	0.07175600	-1.96941400	2.07772800
H	1.76282500	-1.64578000	2.41687100
H	0.64881400	-0.30253600	2.16945700

2b-Z_{out}

C	-4.40472200	-0.83466800	-0.48408900
C	-3.01018300	0.91988800	0.18614900
C	-2.12012600	-0.13232100	-0.17927000
C	-2.96656800	-1.36938200	-0.43133000
C	-0.74575800	-0.10483300	-0.24233200
C	0.05545600	1.06842600	-0.12352600
C	0.00352600	-1.36696000	-0.51435900
C	1.42790900	1.05767800	-0.11024000
C	1.30876300	-1.43212100	0.28916400
H	-0.60096800	-2.24262800	-0.27498100
H	0.22139000	-1.41734200	-1.58668400
C	2.23079900	-0.22973900	-0.09428400
H	-4.78326000	-0.74995800	-1.50162300
H	-0.42007900	2.03709100	-0.11070600
H	-2.85089400	-2.08155700	0.38642500
H	-2.69589500	-1.87355100	-1.35508200
H	-5.10955700	-1.40842900	0.11020400
C	-2.72626400	2.29278100	0.67868100
H	-1.95533300	2.26944200	1.44506500
H	-2.37022000	2.91512400	-0.14225100
H	-3.62473700	2.74853600	1.08843600
N	-4.25571500	0.51288200	0.07850600
C	2.03751500	2.38344500	-0.13361100
H	1.33291800	3.19323300	0.02860500
C	3.30911800	2.74604200	-0.38379400
H	4.10147000	2.04914000	-0.59827100
H	3.56513700	3.79575800	-0.39684100
C	3.37692500	-0.13032800	0.92875800
H	4.20049600	0.46821400	0.55502400
H	3.04595500	0.30801800	1.86818300
H	3.77374100	-1.12256900	1.13556500
C	2.83173700	-0.43020300	-1.49923700
H	3.34511400	0.46884500	-1.83025700
H	3.55501000	-1.24405900	-1.48553700
H	2.06843300	-0.65867700	-2.24261100
C	0.95564500	-1.40657200	1.78155300
H	0.18020200	-2.14707700	1.98655300
H	1.81745300	-1.66347200	2.39394200
H	0.59002800	-0.43227300	2.10646600
C	1.95583700	-2.78154200	-0.02563600
H	1.32209000	-3.58127000	0.35988400
H	2.07305200	-2.93848100	-1.09653900
H	2.93159400	-2.88758800	0.44548100
H	-5.04079400	1.10780500	0.30642600

2c- E_{out}

C	4.72660700	1.35422600	0.43999000
C	3.55685600	-0.50681700	-0.37231200
C	2.54797600	0.46834100	-0.09529500
C	3.25322700	1.75828100	0.28570700
C	1.18453200	0.32376800	-0.18097300
C	0.35291800	1.46285100	0.03081000
C	0.49029000	-0.95805800	-0.52752200
C	-1.01737900	1.45493400	0.00920200
C	-0.83311200	-1.05249800	0.21808700
H	0.27845300	-0.99719300	-1.59947000
H	1.06627700	-1.83430300	-0.25503600
C	-1.75477400	0.14324800	-0.14500100
H	5.41560400	1.98643900	-0.11259500
H	0.82487400	2.42817600	0.16102100
H	2.86058100	2.17723300	1.20876400
H	3.13704400	2.50369500	-0.50141600
H	5.04448100	1.30614800	1.47988900
C	3.44764100	-1.89631200	-0.88961100
H	3.04613800	-2.54995700	-0.11536700
H	2.78251100	-1.93836800	-1.74791100
H	4.42497600	-2.27384400	-1.18113000
N	4.74145200	-0.00176800	-0.12080900
C	-1.70000100	2.73151200	0.06010700
H	-1.06705700	3.56402700	0.34540300
C	-2.97356000	2.99251600	-0.28621200
H	-3.65849500	2.22976000	-0.61893300
H	-3.33346700	4.01073700	-0.25445300
Cl	-3.21467100	0.06411900	0.85022200
Cl	-0.47335900	-1.00678700	1.96720900
Cl	-1.60131500	-2.59297300	-0.17315000
Cl	-2.19842200	0.02245200	-1.87886300
H	5.59263400	-0.53192500	-0.25707000

2c-Z_{in}

C	4.77427000	-0.97985200	-0.60203500
C	3.29290800	-1.38070900	-0.58149700
C	2.56229200	-0.09080300	-0.25379200
C	3.54637700	0.86285900	0.16005500
H	5.41677700	-1.63868900	-0.02545300
H	5.17267100	-0.88677800	-1.61090700
H	2.98229100	-1.80155600	-1.53429100
H	3.10650600	-2.12568400	0.19317500
C	1.19729300	0.05685000	-0.28748100
C	0.49619300	1.28180200	-0.07532900
C	0.35971300	-1.13729900	-0.63176000
C	-0.86798200	1.40285300	-0.04478000
C	-0.92961400	-1.11355900	0.17316200
H	0.10390200	-1.12533400	-1.69509100
H	0.87225200	-2.07130600	-0.41456800
C	-1.74095300	0.17148200	-0.14588300
C	3.38474900	2.22487900	0.72915800
H	3.05355600	2.91456000	-0.04721000
H	2.63801700	2.21672300	1.52008000
H	4.32695200	2.58988000	1.13109300
H	1.04820500	2.20573100	-0.00389200
N	4.74518100	0.35147900	0.01696800
C	-1.42155100	2.74252300	0.00536600
H	-0.69714100	3.51466200	0.23914900
C	-2.67927400	3.12309100	-0.28023200
H	-3.45385700	2.42692900	-0.55737200
H	-2.93420100	4.17265400	-0.25360400
Cl	-2.28940300	0.09382700	-1.85217500
Cl	-3.14458000	0.24718500	0.92794400
Cl	-1.86534100	-2.56672700	-0.17614400
Cl	-0.48191700	-1.10934500	1.90489700
H	5.58238400	0.85915900	0.27352200

2c- E_{in}

C	-4.72660600	1.35422600	0.43999100
C	-3.55685700	-0.50681700	-0.37231300
C	-2.54797600	0.46834100	-0.09529600
C	-3.25322700	1.75828200	0.28570500
C	-1.18453200	0.32376800	-0.18097600
C	-0.35291700	1.46285200	0.03080600
C	-0.49029000	-0.95805700	-0.52752400
C	1.01737900	1.45493400	0.00920100
C	0.83311200	-1.05249800	0.21808700
H	-1.06627700	-1.83430300	-0.25503900
H	-0.27845000	-0.99719300	-1.59947200
C	1.75477500	0.14324800	-0.14500100
H	-5.04447900	1.30614800	1.47989100
H	-0.82487300	2.42817700	0.16101600
H	-3.13704500	2.50369500	-0.50141800
H	-2.86058000	2.17723400	1.20876200
H	-5.41560400	1.98644000	-0.11259200
C	-3.44764200	-1.89631200	-0.88961100
H	-2.78251300	-1.93836800	-1.74791100
H	-3.04613900	-2.54995600	-0.11536700
H	-4.42497700	-2.27384400	-1.18113000
N	-4.74145200	-0.00176800	-0.12080800
C	1.70000200	2.73151200	0.06011000
H	1.06706200	3.56402700	0.34541400
C	2.97356000	2.99251300	-0.28621500
H	3.65849100	2.22975600	-0.61894300
H	3.33347100	4.01073300	-0.25445400
H	-5.59263500	-0.53192500	-0.25706800
Cl	3.21467000	0.06412000	0.85022400
Cl	2.19842500	0.02245100	-1.87886200
Cl	1.60131400	-2.59297300	-0.17314800
Cl	0.47335700	-1.00678600	1.96720900

2c-Z_{out}

C	-4.77427000	-0.97985200	-0.60203500
C	-3.54637700	0.86285900	0.16005500
C	-2.56229200	-0.09080300	-0.25379200
C	-3.29290800	-1.38070900	-0.58149700
C	-1.19729300	0.05685000	-0.28748100
C	-0.49619300	1.28180200	-0.07532900
C	-0.35971300	-1.13729900	-0.63176000
C	0.86798200	1.40285400	-0.04478000
C	0.92961400	-1.11355900	0.17316200
H	-0.87225200	-2.07130600	-0.41456800
H	-0.10390200	-1.12533400	-1.69509100
C	1.74095300	0.17148200	-0.14588300
H	-5.17267100	-0.88677800	-1.61090700
H	-1.04820500	2.20573100	-0.00389200
H	-3.10650600	-2.12568400	0.19317500
H	-2.98229100	-1.80155600	-1.53429100
H	-5.41677700	-1.63868900	-0.02545300
C	-3.38475000	2.22487900	0.72915800
H	-2.63801700	2.21672300	1.52008000
H	-3.05355600	2.91456000	-0.04721000
H	-4.32695200	2.58988000	1.13109300
N	-4.74518100	0.35147900	0.01696800
C	1.42155100	2.74252300	0.00536600
H	0.69714100	3.51466200	0.23914900
C	2.67927400	3.12309100	-0.28023200
H	3.45385700	2.42692900	-0.55737200
H	2.93420100	4.17265400	-0.25360400
Cl	0.48191700	-1.10934500	1.90489700
Cl	1.86534100	-2.56672700	-0.17614400
Cl	3.14458000	0.24718500	0.92794400
Cl	2.28940300	0.09382700	-1.85217500
H	-5.58238400	0.85915900	0.27352200

2d- E_{out}

C	-5.40637800	1.28958500	-0.43128100
C	-4.11171900	-0.37210500	0.59564300
C	-3.16771100	0.60287000	0.14805500
C	-3.95289900	1.78426000	-0.39391700
C	-1.79609700	0.54201600	0.20638500
C	-1.03509100	1.67610000	-0.19819400
C	-1.02254300	-0.63524700	0.71538900
C	0.33553000	1.74531300	-0.21365400
C	0.28867800	-0.76621700	-0.04780800
H	-0.78623200	-0.49979100	1.77546400
H	-1.55746600	-1.56955700	0.59683700
C	1.14568100	0.51252400	0.10047700
H	-6.11065000	1.96008300	0.05276500
H	-1.56273400	2.58533200	-0.45631600
H	-3.61059600	2.07718300	-1.38335400
H	-3.85355300	2.64505900	0.26777800
H	-5.75407600	1.07770400	-1.44069200
C	-3.90994300	-1.66578800	1.29984700
H	-3.48839300	-2.39976600	0.61306500
H	-3.22383700	-1.54890700	2.13448400
H	-4.85665000	-2.05081800	1.67169800
N	-5.32990100	0.02916600	0.31607100
C	0.92680200	3.04427100	-0.47109400
H	0.23403600	3.77368700	-0.87515700
C	2.17636600	3.45081000	-0.18428700
H	2.91584100	2.80410800	0.25890000
H	2.45896600	4.47495200	-0.38141000
Br	2.72886900	0.35480900	-0.99035700
Br	1.66720000	0.71606300	1.97716100
Br	1.20491400	-2.33510200	0.58319600
Br	-0.17737500	-1.02903400	-1.92300900
H	-6.14570200	-0.51954100	0.55536100

2d-Z_{in}

C	-5.31691800	-0.87862000	0.94249300
C	-3.81615300	-1.20017800	0.93548600
C	-3.16724300	0.06452600	0.40325000
C	-4.21093900	0.89318900	-0.11579600
H	-5.93425500	-1.64841900	0.48901100
H	-5.69646000	-0.65836100	1.93885600
H	-3.46118700	-1.46158200	1.92905100
H	-3.60451700	-2.03843700	0.26998800
C	-1.81137400	0.28303000	0.36784400
C	-1.18321400	1.49503400	-0.04263800
C	-0.90162100	-0.80434200	0.85178900
C	0.17309900	1.67993300	-0.13296900
C	0.36387600	-0.83003600	0.00828800
H	-0.61977100	-0.62120400	1.89377700
H	-1.37207600	-1.78270400	0.79376000
C	1.10928300	0.52166400	0.10616100
C	-4.13655400	2.16247900	-0.88286400
H	-3.82516200	2.97528700	-0.22674800
H	-3.40858000	2.07425200	-1.68644900
H	-5.10601800	2.41634900	-1.30507100
H	-1.78552000	2.37036700	-0.22869100
N	-5.37660900	0.34607300	0.13448000
C	0.63423700	3.03239900	-0.39157500
H	-0.14461000	3.70818000	-0.72695100
C	1.86140600	3.54103100	-0.18519600
H	2.68544800	2.95294600	0.18402600
H	2.03899100	4.58984800	-0.37494300
Br	1.74583700	0.76230300	1.94279800
Br	2.61665400	0.51479600	-1.09807300
Br	1.45512300	-2.31012600	0.56489200
Br	-0.20250700	-1.13340700	-1.83554300
H	-6.24611600	0.76548500	-0.16922300

2d- E_{in}

C	5.40653500	1.28927500	-0.43165500
C	4.11177000	-0.37198800	0.59580300
C	3.16780100	0.60272000	0.14758900
C	3.95301500	1.78391000	-0.39477200
C	1.79619400	0.54188700	0.20583400
C	1.03521800	1.67584000	-0.19916700
C	1.02261800	-0.63530400	0.71502500
C	-0.33536600	1.74520000	-0.21438200
C	-0.28869300	-0.76628500	-0.04799400
H	1.55753300	-1.56963000	0.59653900
H	0.78637500	-0.49979700	1.77511300
C	-1.14555100	0.51264300	0.10050800
H	5.75445700	1.07695900	-1.44090000
H	1.56293800	2.58489000	-0.45779400
H	3.85351600	2.64504300	0.26647000
H	3.61085900	2.07639800	-1.38439500
H	6.11068900	1.96004100	0.05220100
C	3.90994300	-1.66531600	1.30065200
H	3.22346000	-1.54812300	2.13493400
H	3.48884200	-2.39979200	0.61412300
H	4.85656700	-2.04994900	1.67313400
N	5.32998700	0.02921000	0.31628500
C	-0.92668300	3.04415400	-0.47180500
H	-0.23415900	3.77338800	-0.87661200
C	-2.17599400	3.45073600	-0.18407100
H	-2.91509200	2.80406300	0.25981000
H	-2.45886800	4.47479700	-0.38121300
H	6.14579500	-0.51927600	0.55603400
Br	-2.72916900	0.35493300	-0.98982800
Br	-1.66656300	0.71658900	1.97711800
Br	-1.20498400	-2.33498700	0.58359700
Br	0.17678200	-1.02963100	-1.92319600

2d-Z_{out}

C	5.31691800	-0.87862000	0.94249300
C	4.21093900	0.89318900	-0.11579600
C	3.16724300	0.06452600	0.40325000
C	3.81615300	-1.20017800	0.93548600
C	1.81137400	0.28303000	0.36784400
C	1.18321400	1.49503400	-0.04263800
C	0.90162100	-0.80434200	0.85178900
C	-0.17309900	1.67993300	-0.13296900
C	-0.36387600	-0.83003600	0.00828800
H	1.37207600	-1.78270400	0.79376000
H	0.61977100	-0.62120400	1.89377700
C	-1.10928300	0.52166400	0.10616100
H	5.69646000	-0.65836100	1.93885600
H	1.78552000	2.37036700	-0.22869100
H	3.60451700	-2.03843700	0.26998800
H	3.46118700	-1.46158200	1.92905100
H	5.93425500	-1.64841900	0.48901100
C	4.13655400	2.16247900	-0.88286400
H	3.40858000	2.07425200	-1.68644900
H	3.82516200	2.97528700	-0.22674800
H	5.10601800	2.41634900	-1.30507100
N	5.37660900	0.34607300	0.13448000
C	-0.63423700	3.03239900	-0.39157500
H	0.14461000	3.70818000	-0.72695100
C	-1.86140500	3.54103100	-0.18519600
H	-2.68544800	2.95294600	0.18402600
H	-2.03899100	4.58984800	-0.37494300
Br	-2.61665400	0.51479600	-1.09807300
Br	-1.74583700	0.76230300	1.94279800
Br	-1.45512300	-2.31012600	0.56489200
Br	0.20250600	-1.13340700	-1.83554300
H	6.24611600	0.76548500	-0.16922300

3a- E_{out}

C	-1.53165900	0.91111900	-0.17925800
C	-0.65060000	-0.21625100	-0.16916800
C	-1.28467100	-1.59975700	-0.20839600
C	0.72897600	-0.09883200	-0.17776700
C	1.52762400	-1.27093500	-0.44421000
C	1.50548400	1.16420000	0.07752900
C	2.88045900	-1.26672400	-0.36035300
C	2.76550200	0.86269900	0.89132600
H	1.80289500	1.60394500	-0.88123600
H	0.90920300	1.89639400	0.60933700
C	3.66492500	-0.11097200	0.14901400
H	3.29015600	1.79352400	1.09923800
H	2.47506100	0.42890900	1.85005700
H	4.47609900	-0.47054100	0.78267000
H	4.14809100	0.38197800	-0.70294900
H	1.04542500	-2.16761400	-0.80305700
H	-0.66453300	-2.29439000	0.35470700
H	-1.32217800	-1.98497700	-1.23461500
C	-1.17810800	2.31705700	-0.55202300
H	-0.88803100	2.88987900	0.32842000
H	-0.36618000	2.34843300	-1.26898000
H	-2.04643400	2.80480800	-0.99286900
N	-2.81116600	0.71830400	0.08762000
C	-3.37864500	-0.50550300	0.49526600
H	-4.38418100	-0.44519000	0.87776600
C	-2.66404400	-1.62216100	0.37155500
H	-3.10060100	-2.56441800	0.66744800
H	-3.42576300	1.51928900	0.02023000
H	3.41766500	-2.15179900	-0.68059500

3a-Z_{in}

C	2.74040900	-1.56919800	-0.30165300
C	1.30500500	-1.58320800	0.12291300
C	0.65615400	-0.20955000	0.04543700
C	1.50852000	0.93274100	0.17361600
H	3.22464600	-2.49640500	-0.56954400
H	0.76023000	-2.27672500	-0.51478200
H	1.23892700	-1.99132200	1.13884700
C	-0.71898300	-0.11573500	-0.07962700
C	-1.43178900	1.07915300	-0.46146600
C	-1.55794200	-1.35381400	0.06781300
C	-2.78241300	1.11033000	-0.56307000
C	-2.91891000	-1.02874100	0.68071400
H	-1.69889200	-1.79760800	-0.92590600
H	-1.04802700	-2.09566500	0.67780900
C	-3.66796300	-0.01812100	-0.17112500
H	-3.49531500	-1.94520900	0.79202900
H	-2.76697100	-0.61689800	1.68029000
H	-4.54680800	0.36772400	0.34639200
H	-4.04536500	-0.48837100	-1.08694400
C	1.08386100	2.32253700	0.53047000
H	0.90917600	2.91426900	-0.36840600
H	0.17803900	2.32146900	1.12683600
H	1.87604200	2.81017700	1.09709000
H	-0.88590400	1.94472000	-0.79702600
N	2.81320400	0.76640000	0.05358600
C	3.44451200	-0.43919000	-0.31578800
H	4.48546000	-0.35407700	-0.58085400
H	3.40219900	1.57384800	0.21220000
H	-3.24263900	2.00204400	-0.97253000

3a- E_{in}

C	1.53165700	0.91112000	-0.17925700
C	0.65060200	-0.21625200	-0.16915600
C	1.28468000	-1.59975500	-0.20839400
C	-0.72897600	-0.09884000	-0.17774600
C	-1.52762000	-1.27094600	-0.44418100
C	-1.50548500	1.16419400	0.07754100
C	-2.88045700	-1.26673000	-0.36035100
C	-2.76552200	0.86270300	0.89130900
H	-0.90921000	1.89638100	0.60936500
H	-1.80286900	1.60394600	-0.88122900
C	-3.66493200	-0.11097000	0.14898300
H	-1.04541900	-2.16763200	-0.80300600
H	1.32218700	-1.98496500	-1.23461700
H	0.66454800	-2.29439500	0.35470500
C	1.17810000	2.31706000	-0.55200900
H	0.36618000	2.34843800	-1.26897600
H	0.88800300	2.88986700	0.32843800
H	2.04642700	2.80482600	-0.99283600
N	2.81117000	0.71830700	0.08759900
C	3.37865600	-0.50549500	0.49525000
H	4.38419400	-0.44517700	0.87774400
C	2.66405500	-1.62215600	0.37155400
H	3.10061200	-2.56440900	0.66745600
H	3.42576300	1.51929400	0.02020300
H	-3.41765800	-2.15181000	-0.68059100
H	-4.14807500	0.38197300	-0.70299700
H	-4.47612300	-0.47053000	0.78262200
H	-2.47510600	0.42891600	1.85004900
H	-3.29017700	1.79353000	1.09920300

3a-Z_{out}

C	-1.50851300	0.93274300	0.17361300
C	-0.65615500	-0.20955200	0.04542100
C	-1.30501000	-1.58320800	0.12289400
C	0.71898200	-0.11574200	-0.07965000
C	1.43179300	1.07914500	-0.46148600
C	1.55794100	-1.35382100	0.06778200
C	2.78241900	1.11032500	-0.56306000
C	2.91889200	-1.02875000	0.68072400
H	1.04801900	-2.09569000	0.67774800
H	1.69892200	-1.79759000	-0.92594400
C	3.66796500	-0.01811700	-0.17108400
H	4.04540900	-0.48835900	-1.08688900
H	4.54678600	0.36773700	0.34646900
H	0.88591200	1.94470600	-0.79706500
H	-1.23891200	-1.99133500	1.13882100
H	-0.76025000	-2.27671900	-0.51482100
C	-1.08384300	2.32253800	0.53045600
H	-0.17801600	2.32146700	1.12681700
H	-0.90915700	2.91426300	-0.36842400
H	-1.87601600	2.81018800	1.09707800
H	3.49529800	-1.94521700	0.79204200
H	2.76692400	-0.61692000	1.68030100
C	-2.74042300	-1.56919000	-0.30164100
H	-3.22467100	-2.49639300	-0.56952200
C	-3.44452100	-0.43917800	-0.31575900
N	-2.81320000	0.76640800	0.05360300
H	-3.40218800	1.57386000	0.21222500
H	-4.48547400	-0.35406000	-0.58080200
H	3.24265100	2.00203700	-0.97252000

3b- E_{out}

C	-2.45772400	0.88876100	-0.31071000
C	-1.65014000	-0.29062700	-0.30462300
C	-2.36626700	-1.62875100	-0.19581700
C	-0.27259100	-0.26446300	-0.43973300
C	0.43281600	-1.49424900	-0.68637200
C	0.60373400	0.94445800	-0.32311200
C	1.78310700	-1.57162300	-0.60673800
C	1.87402800	0.65445300	0.50600500
H	0.89896200	1.27518000	-1.32424600
H	0.09163700	1.76984200	0.16180400
C	2.69406200	-0.46902000	-0.18220300
H	-0.11511500	-2.37341100	-0.99283600
H	-1.73093900	-2.33181700	0.33953500
H	-2.53785400	-2.06457100	-1.18766600
C	-2.05976800	2.23998800	-0.81796200
H	-1.67669900	2.86070900	-0.00825500
H	-1.30207400	2.16994500	-1.58953400
H	-2.93280000	2.74068700	-1.23501900
N	-3.71421400	0.79840200	0.09010400
C	-4.30464100	-0.35650400	0.64063600
H	-5.25804900	-0.20612200	1.11974000
C	-3.67365900	-1.52372000	0.52556200
H	-4.13027000	-2.41331500	0.93316100
H	-4.28529900	1.63093500	0.02437400
C	3.76136100	-1.06686600	0.74410000
H	3.32353900	-1.58630100	1.59386400
H	4.36927600	-1.78143300	0.18900700
H	4.42627500	-0.28956400	1.11900000
C	3.40674300	0.02246600	-1.45801900
H	4.21547800	0.70410800	-1.19853100
H	3.84417200	-0.82391400	-1.98731200
H	2.72876500	0.52749000	-2.14500000
C	2.65752700	1.96217200	0.60187500
H	2.85457600	2.39406000	-0.37807600
H	2.08816400	2.69011100	1.18153500
H	3.61001400	1.81598700	1.11001700
C	1.44627200	0.24509900	1.91887200
H	2.29945000	0.22978300	2.59435500
H	0.73324000	0.97223100	2.31209700
H	0.97704300	-0.73853500	1.94456600
H	2.25884700	-2.51033400	-0.87788300

3b-Z_{in}

C	3.63914600	-1.64176200	-0.40593700
C	2.18250600	-1.57416400	-0.06603900
C	1.64294600	-0.15203100	-0.08162700
C	2.56595800	0.90891900	0.17779500
H	4.07020500	-2.58201000	-0.71593400
H	1.62838300	-2.17838200	-0.78166700
H	2.02345800	-2.04216400	0.91296300
C	0.28947700	0.06234000	-0.27534900
C	-0.31248300	1.33157400	-0.58971000
C	-0.66137100	-1.09372700	-0.26376100
C	-1.65754400	1.48013800	-0.64206100
C	-1.99399000	-0.74594200	0.42905000
H	-0.85255000	-1.39995000	-1.29877000
H	-0.23299500	-1.95395100	0.24871100
C	-2.67038700	0.43176200	-0.32109000
C	2.21953500	2.30119300	0.60185100
H	2.14166400	2.95915700	-0.26394500
H	1.27979700	2.32969700	1.14291900
H	3.00755700	2.69238900	1.24415800
H	0.30140400	2.16747300	-0.88265700
N	3.86089300	0.65097000	0.12619300
C	4.42381700	-0.57186300	-0.29342100
H	5.48283300	-0.54993700	-0.49129200
H	4.49559600	1.39832500	0.37572300
C	-3.78988100	1.08539000	0.49964800
H	-3.41241900	1.57037200	1.39739600
H	-4.29450500	1.83979100	-0.10418900
H	-4.53446500	0.34625800	0.79321300
C	-3.27682900	-0.00606500	-1.66932200
H	-4.14665500	-0.63977200	-1.50263300
H	-3.60694600	0.86889200	-2.22915000
H	-2.56301600	-0.54670700	-2.28970600
C	-2.85597200	-2.00662300	0.42287300
H	-2.39032500	-2.77284200	1.04399300
H	-3.84563500	-1.81085900	0.83424500
H	-2.97516400	-2.41538500	-0.57914100
C	-1.69422000	-0.37512000	1.88552700
H	-2.61094600	-0.31434300	2.46895200
H	-1.06927000	-1.14565700	2.34050300
H	-1.17574600	0.58022300	1.97322600
H	-2.05076300	2.43848200	-0.97083500

3b- E_{in}

C	2.45772500	0.88876000	-0.31071100
C	1.65014000	-0.29062700	-0.30462200
C	2.36626900	-1.62875100	-0.19581900
C	0.27259200	-0.26446400	-0.43973200
C	-0.43281600	-1.49424900	-0.68637100
C	-0.60373400	0.94445700	-0.32311200
C	-1.78310700	-1.57162300	-0.60673700
C	-1.87402900	0.65445300	0.50600500
H	-0.09163600	1.76984200	0.16180400
H	-0.89896200	1.27517900	-1.32424500
C	-2.69406300	-0.46902000	-0.18220400
H	0.11511500	-2.37341100	-0.99283500
H	2.53785900	-2.06456600	-1.18766900
H	1.73094000	-2.33182000	0.33952700
C	2.05976900	2.23998800	-0.81796000
H	1.30207600	2.16994800	-1.58953300
H	1.67669700	2.86070700	-0.00825100
H	2.93280000	2.74069000	-1.23501400
N	3.71421700	0.79840000	0.09009900
C	4.30464100	-0.35650500	0.64063700
H	5.25804800	-0.20612100	1.11974300
C	3.67365700	-1.52372000	0.52556500
H	4.13026300	-2.41331400	0.93317100
H	4.28530100	1.63093300	0.02436800
C	-3.76136200	-1.06686600	0.74410000
H	-4.36927700	-1.78143300	0.18900500
H	-3.32354100	-1.58630100	1.59386400
H	-4.42627600	-0.28956400	1.11899900
C	-3.40674200	0.02246500	-1.45802000
H	-3.84417100	-0.82391500	-1.98731300
H	-4.21547800	0.70410600	-1.19853300
H	-2.72876400	0.52748900	-2.14500000
C	-2.65752700	1.96217200	0.60187400
H	-2.08816400	2.69011200	1.18153300
H	-2.85457700	2.39406000	-0.37807700
H	-3.61001400	1.81598800	1.11001700
C	-1.44627400	0.24510000	1.91887300
H	-0.73324300	0.97223200	2.31209800
H	-2.29945300	0.22978500	2.59435400
H	-0.97704400	-0.73853400	1.94456800
H	-2.25884700	-2.51033500	-0.87788100

3b-Z_{out}

C	-2.56571500	0.90895000	0.17771600
C	-1.64287300	-0.15218600	-0.08170000
C	-2.18268600	-1.57423200	-0.06596300
C	-0.28950700	0.06215300	-0.27586400
C	0.31251300	1.33139700	-0.59018800
C	0.66152100	-1.09383700	-0.26465500
C	1.65754700	1.47996000	-0.64250500
C	1.99370900	-0.74603100	0.42889600
C	2.67041100	0.43175300	-0.32096900
H	-0.30138400	2.16728800	-0.88320500
H	-2.02351200	-2.04230500	0.91298200
H	-1.62881100	-2.17855700	-0.78170200
C	-2.21886900	2.30105100	0.60199600
H	-1.27897600	2.32919600	1.14280900
H	-2.14106500	2.95923700	-0.26364600
H	-3.00665100	2.69230800	1.24456900
C	-3.63938100	-1.64157300	-0.40558400
H	-4.07074200	-2.58181000	-0.71520300
C	-4.42383300	-0.57149600	-0.29331400
N	-3.86068900	0.65135600	0.12598900
H	-4.49525000	1.39880900	0.37557800
H	-5.48287100	-0.54948300	-0.49106200
C	1.69325500	-0.37532900	1.88529700
H	1.06817800	-1.14599300	2.33987300
H	2.60975500	-0.31454400	2.46907400
H	1.17466700	0.57995800	1.97288400
C	2.85586700	-2.00662600	0.42311500
H	2.97560800	-2.41536500	-0.57884500
H	3.84530600	-1.81065500	0.83493400
H	2.39001800	-2.77287700	1.04402300
H	2.05081000	2.43818700	-0.97155500
H	0.85322200	-1.39927200	-1.29979500
H	0.23311300	-1.95443700	0.24713400
C	3.78920900	1.08573100	0.50054100
H	4.53381700	0.34678400	0.79454600
H	4.29399900	1.84026600	-0.10298700
H	3.41105200	1.57057900	1.39806700
C	3.27784600	-0.00615800	-1.66866900
H	3.60820900	0.86877800	-2.22839500
H	4.14765700	-0.63972800	-1.50137000
H	2.56458800	-0.54702500	-2.28952600

3c- E_{out}

C	-3.01175900	0.88616600	-0.37370000
C	-2.23569000	-0.32417300	-0.36352200
C	-2.99180200	-1.63861300	-0.25040800
C	-0.86032500	-0.33575300	-0.48011700
C	-0.17849900	-1.59009100	-0.68628200
C	0.02709000	0.87322000	-0.38611400
C	1.16702200	-1.71220400	-0.63939000
C	1.29926900	0.54720100	0.39923800
H	0.33255200	1.21127600	-1.37988400
H	-0.44407900	1.69515000	0.13827000
C	2.08055500	-0.57842800	-0.31307800
H	-0.74675200	-2.47162600	-0.94242800
H	-2.39077800	-2.34967000	0.31325700
H	-3.15229400	-2.08575200	-1.23904600
C	-2.57045100	2.22131400	-0.88464400
H	-2.14108800	2.82078000	-0.08170700
H	-1.83606500	2.12290300	-1.67612100
H	-3.42942900	2.76307700	-1.27813200
N	-4.26383500	0.83037700	0.03115400
C	-4.90450800	-0.30917800	0.56016300
H	-5.86205100	-0.12975100	1.02024700
C	-4.31289900	-1.49569800	0.43620500
H	-4.81011900	-2.37659100	0.81441300
H	-4.80780000	1.68296200	-0.02911500
Cl	3.43684800	-1.15282000	0.65576100
Cl	2.68784500	0.01704700	-1.89024500
Cl	2.26914600	2.01105800	0.55821300
Cl	0.80848400	-0.01077100	2.02218100
H	1.64722700	-2.65470200	-0.86842300

3c-Z_{in}

C	-4.18412800	1.66391900	-0.46812300
C	-2.73303700	1.56028300	-0.11801200
C	-2.22326800	0.13005900	-0.14260300
C	-3.17478000	-0.91577100	0.11970200
H	-4.59187600	2.61889500	-0.76466900
H	-2.16240600	2.16263600	-0.82240000
H	-2.57308900	2.01286800	0.86888000
C	-0.87948900	-0.11597300	-0.32882200
C	-0.30345500	-1.40369500	-0.62878400
C	0.08495600	1.03566500	-0.31346500
C	1.03140900	-1.60380900	-0.69101000
C	1.38870600	0.62592300	0.36947800
H	0.31764300	1.35632200	-1.33347900
H	-0.30545200	1.88810700	0.23519700
C	2.03880000	-0.54001400	-0.40681500
C	-2.85501800	-2.30108700	0.58257900
H	-2.76710300	-2.98074100	-0.26548900
H	-1.92728000	-2.32326700	1.14546200
H	-3.66001000	-2.66952100	1.21704900
H	-0.93677700	-2.23051300	-0.90397500
N	-4.45697800	-0.62735600	0.04150200
C	-4.99211100	0.60878400	-0.38036800
H	-6.04957100	0.60844900	-0.58680900
H	-5.11313800	-1.35748900	0.29253500
Cl	3.41444100	-1.22420300	0.45935800
Cl	2.57966700	0.04102100	-2.01311400
Cl	0.97567400	0.07179500	2.01975900
Cl	2.46212500	2.01726800	0.47893300
H	1.43397700	-2.55993100	-0.99929100

3c- E_{in}

C	3.01176100	0.88616900	-0.37369600
C	2.23569100	-0.32416900	-0.36353700
C	2.99180700	-1.63860800	-0.25043700
C	0.86032600	-0.33574600	-0.48013800
C	0.17849400	-1.59007700	-0.68632500
C	-0.02708800	0.87322500	-0.38610200
C	-1.16702500	-1.71218900	-0.63943000
C	-1.29926400	0.54719100	0.39925300
H	0.44408400	1.69514400	0.13829400
H	-0.33256000	1.21130200	-1.37986400
C	-2.08055800	-0.57842000	-0.31309400
H	0.74674300	-2.47160900	-0.94249500
H	3.15232700	-2.08572200	-1.23908200
H	2.39077300	-2.34968600	0.31319200
C	2.57046200	2.22132100	-0.88463800
H	1.83609000	2.12291700	-1.67612900
H	2.14108400	2.82078300	-0.08170600
H	3.42944600	2.76308900	-1.27810700
N	4.26383500	0.83037400	0.03116500
C	4.90449500	-0.30918500	0.56018100
H	5.86203000	-0.12976300	1.02028400
C	4.31288500	-1.49570200	0.43621300
H	4.81009500	-2.37659600	0.81443100
H	4.80780500	1.68295700	-0.02909400
H	-1.64723100	-2.65468200	-0.86848100
Cl	-3.43684600	-1.15283300	0.65574300
Cl	-2.68785200	0.01709800	-1.89023700
Cl	-2.26914100	2.01104600	0.55825900
Cl	-0.80848200	-0.01081700	2.02218300

3c-Z_{out}

C	3.17478000	-0.91577100	0.11970200
C	2.22326800	0.13005900	-0.14260300
C	2.73303700	1.56028300	-0.11801200
C	0.87948900	-0.11597300	-0.32882200
C	0.30345500	-1.40369500	-0.62878400
C	-0.08495600	1.03566500	-0.31346500
C	-1.03140900	-1.60380900	-0.69101000
C	-1.38870600	0.62592300	0.36947800
H	0.30545200	1.88810700	0.23519700
H	-0.31764300	1.35632200	-1.33347900
C	-2.03880000	-0.54001400	-0.40681500
H	0.93677700	-2.23051300	-0.90397500
H	2.57308900	2.01286800	0.86888000
H	2.16240600	2.16263600	-0.82240000
C	2.85501800	-2.30108700	0.58257900
H	1.92728000	-2.32326700	1.14546200
H	2.76710300	-2.98074100	-0.26548900
H	3.66001000	-2.66952100	1.21704900
C	4.18412800	1.66391900	-0.46812300
H	4.59187600	2.61889500	-0.76466900
C	4.99211100	0.60878400	-0.38036800
N	4.45697800	-0.62735600	0.04150200
H	5.11313800	-1.35748900	0.29253500
H	6.04957100	0.60844900	-0.58680900
Cl	-3.41444100	-1.22420300	0.45935800
Cl	-2.57966700	0.04102100	-2.01311400
Cl	-0.97567400	0.07179500	2.01975900
Cl	-2.46212500	2.01726800	0.47893400
H	-1.43397700	-2.55993100	-0.99929100

3d- E_{out}

C	3.74794500	0.81681400	0.55922000
C	2.97375100	-0.39083200	0.52157700
C	3.72441300	-1.70837500	0.40323500
C	1.59510000	-0.40602800	0.61403900
C	0.91643400	-1.66111500	0.80305300
C	0.70470700	0.80066800	0.51586700
C	-0.43098700	-1.78571100	0.74241700
C	-0.55603600	0.47330300	-0.28790800
H	0.38606900	1.12826600	1.51033200
H	1.18400400	1.62821700	0.00869500
C	-1.33791200	-0.65946500	0.39551100
H	1.48260700	-2.54232700	1.06545000
H	3.14073000	-2.39598900	-0.20710800
H	3.83492200	-2.18634900	1.38425200
C	3.28893300	2.15303900	1.05190300
H	2.87652500	2.74598800	0.23528000
H	2.53600900	2.05630900	1.82608900
H	4.13584200	2.70071300	1.46297200
N	5.01483500	0.76317900	0.19851400
C	5.67537500	-0.37524800	-0.30619000
H	6.65358100	-0.19640400	-0.72084800
C	5.07637400	-1.56127500	-0.21833000
H	5.58931900	-2.44012300	-0.57994200
H	5.55471100	1.61637200	0.27826400
Br	-2.02032200	-0.06238300	2.12874900
Br	-2.80616800	-1.29905100	-0.66447800
Br	-1.60249900	2.07198400	-0.48105900
Br	0.03357800	-0.10775800	-2.05164500
H	-0.90736100	-2.72927400	0.97576200

3d-Z_{in}

C	-4.92680400	1.50646800	-0.87820500
C	-3.47724200	1.44767800	-0.51142800
C	-2.97532300	0.02647300	-0.32824900
C	-3.93093400	-0.96953000	0.06612500
H	-5.32962700	2.41180800	-1.30742800
H	-2.90047600	1.94021400	-1.29232300
H	-3.31752800	2.03549900	0.40165700
C	-1.62786800	-0.24512100	-0.44821800
C	-1.05088600	-1.55903400	-0.56203500
C	-0.65847100	0.89671000	-0.56421000
C	0.28694900	-1.76535400	-0.55771400
C	0.61887200	0.58010200	0.21309700
H	-0.39083900	1.06656300	-1.61268800
H	-1.06558200	1.81883800	-0.15978000
C	1.28416700	-0.67847600	-0.36589900
C	-3.61641400	-2.27931800	0.71466800
H	-3.51859600	-3.06740800	-0.03242200
H	-2.69412100	-2.22241400	1.28472600
H	-4.42800900	-2.56004100	1.38465100
H	-1.67830200	-2.41380200	-0.75340700
N	-5.21299300	-0.69108500	-0.05618100
C	-5.73997700	0.47736500	-0.64630300
H	-6.79673000	0.45371100	-0.85516400
H	-5.87271000	-1.37801000	0.28877000
Br	2.74901800	-1.31117400	0.70437700
Br	1.93132500	-0.32279500	-2.17713300
Br	0.07325300	0.23862300	2.05711000
Br	1.78002300	2.10614500	0.18697500
H	0.69038300	-2.75311700	-0.73964400

3d- E_{in}

C	-3.74794500	0.81678700	0.55925500
C	-2.97375300	-0.39086000	0.52155400
C	-3.72442100	-1.70839400	0.40315800
C	-1.59510200	-0.40606300	0.61400700
C	-0.91643600	-1.66116000	0.80295600
C	-0.70471100	0.80063900	0.51589300
C	0.43098400	-1.78575200	0.74231600
C	0.55603800	0.47331600	-0.28788900
H	-1.18400800	1.62820900	0.00875600
H	-0.38608000	1.12819300	1.51037600
C	1.33791100	-0.65948600	0.39547600
H	-1.48260900	-2.54238700	1.06530400
H	-3.83493400	-2.18640800	1.38415500
H	-3.14074200	-2.39598600	-0.20721300
C	-3.28892900	2.15298600	1.05200400
H	-2.53600300	2.05621600	1.82618300
H	-2.87652400	2.74597500	0.23541000
H	-4.13583600	2.70064100	1.46310400
N	-5.01483400	0.76317300	0.19854400
C	-5.67537600	-0.37522900	-0.30621500
H	-6.65357800	-0.19636200	-0.72087200
C	-5.07638000	-1.56126200	-0.21840500
H	-5.58932700	-2.44009100	-0.58006000
H	-5.55470900	1.61636200	0.27833800
H	0.90735900	-2.72932700	0.97560900
Br	2.80617900	-1.29901100	-0.66453100
Br	2.02030200	-0.06249400	2.12875400
Br	1.60249900	2.07200900	-0.48095000
Br	-0.03356400	-0.10765800	-2.05166000

3d-Z_{out}

C	3.93093400	-0.96953000	0.06612600
C	2.97532300	0.02647300	-0.32824900
C	3.47724200	1.44767800	-0.51142800
C	1.62786800	-0.24512100	-0.44821800
C	1.05088600	-1.55903400	-0.56203500
C	0.65847100	0.89671000	-0.56421000
C	-0.28694900	-1.76535400	-0.55771400
C	-0.61887200	0.58010200	0.21309700
H	1.06558200	1.81883800	-0.15978000
H	0.39083900	1.06656300	-1.61268800
C	-1.28416700	-0.67847700	-0.36589900
H	1.67830200	-2.41380300	-0.75340600
H	3.31752800	2.03549900	0.40165700
H	2.90047600	1.94021400	-1.29232300
C	3.61641400	-2.27931800	0.71466800
H	2.69412100	-2.22241400	1.28472600
H	3.51859600	-3.06740800	-0.03242200
H	4.42800900	-2.56004100	1.38465100
C	4.92680400	1.50646700	-0.87820500
H	5.32962600	2.41180800	-1.30742800
C	5.73997700	0.47736500	-0.64630300
N	5.21299300	-0.69108500	-0.05618100
H	5.87271000	-1.37801000	0.28877000
H	6.79673000	0.45371100	-0.85516400
Br	-2.74901800	-1.31117400	0.70437700
Br	-1.93132500	-0.32279500	-2.17713300
Br	-1.78002300	2.10614500	0.18697500
Br	-0.07325300	0.23862300	2.05711000
H	-0.69038300	-2.75311700	-0.73964400

4a- E_{out}

C	-2.32515900	0.67223500	-0.27754900
C	-1.20469100	-0.18613800	-0.09124900
C	-1.46543000	-1.68358700	0.00666600
C	0.10878600	0.27265900	-0.05076800
C	1.17106700	-0.67732900	-0.14394900
C	0.52428400	1.71031200	0.10930700
C	2.50245000	-0.35276100	-0.05782400
C	1.79395400	1.80409900	0.95224000
H	0.72406500	2.14645200	-0.87582400
H	-0.25928500	2.29497500	0.57830200
C	2.92946800	1.03603100	0.29831600
H	2.06690700	2.85026100	1.08141500
H	1.59764300	1.39129800	1.94353800
H	3.79781000	0.99599900	0.95511700
H	3.25407400	1.54520500	-0.61599100
H	0.93616300	-1.70624500	-0.37718700
H	-0.76584500	-2.12130900	0.71789800
H	-1.27122000	-2.17689000	-0.95373300
C	-2.29611000	2.09333400	-0.74971500
H	-2.22562000	2.78222700	0.09153500
H	-1.46401800	2.27736700	-1.41890100
H	-3.21916900	2.31627500	-1.28306500
N	-3.54496800	0.18530600	-0.09432600
C	3.48280100	-1.37786100	-0.33587700
H	3.10135700	-2.36486400	-0.57032100
C	4.81338600	-1.17391200	-0.34309100
H	5.24782100	-0.20845900	-0.12763700
H	5.49192600	-1.98109500	-0.57634000
C	-3.83360200	-1.10545900	0.38349200
H	-4.86008600	-1.27826900	0.66242900
C	-2.85669800	-2.00796600	0.45105200
H	-3.08044900	-3.00240300	0.80728900
H	-4.32433400	0.80038400	-0.28456400

4a-Z_{in}

C	-3.58120000	1.00140200	-0.66749300
C	-2.24271200	1.42113600	-0.14308200
C	-1.29844700	0.24458600	0.05144700
C	-1.87582300	-1.03283800	0.30189800
H	-4.22658400	1.73420400	-1.12822000
H	-1.79892600	2.13046400	-0.83946000
H	-2.38355700	1.96941000	0.79670100
C	0.07315400	0.47608900	0.05067600
C	1.06731300	-0.53791900	-0.09556000
C	0.56935100	1.89362500	0.09813300
C	2.41387000	-0.27914900	-0.13396300
C	1.91726100	1.97516300	0.80581500
H	0.66769500	2.26736800	-0.92892800
H	-0.15311200	2.53475700	0.59911900
C	2.94574000	1.09703900	0.11433200
H	2.25576500	3.00954000	0.83216800
H	1.79534000	1.64639600	1.83967300
H	3.85951900	1.03699300	0.70490700
H	3.22934600	1.53188900	-0.85061500
C	-1.18526300	-2.21927400	0.89868100
H	-0.79806700	-2.87529200	0.11843300
H	-0.36384400	-1.92059200	1.54139800
H	-1.89826700	-2.79473800	1.48795400
H	0.76636000	-1.55034100	-0.31412700
N	-3.17025700	-1.20467100	0.07499000
C	3.31300600	-1.36309200	-0.46626900
H	2.86217300	-2.33463400	-0.63403500
C	4.64602300	-1.23423800	-0.59690200
H	5.14868300	-0.28900800	-0.45200000
H	5.25703400	-2.08441000	-0.86177700
C	-4.00957700	-0.25276200	-0.53480800
H	-4.97020300	-0.61996900	-0.85691600
H	-3.57371800	-2.09794900	0.32337100

4a- E_{in}

C	2.32515800	0.67223600	-0.27755200
C	1.20469200	-0.18613700	-0.09123800
C	1.46543600	-1.68358500	0.00666500
C	-0.10878600	0.27265700	-0.05075100
C	-1.17106600	-0.67733200	-0.14392900
C	-0.52428700	1.71031100	0.10931500
C	-2.50245000	-0.35276400	-0.05782000
C	-1.79396600	1.80410400	0.95223300
H	0.25927800	2.29497400	0.57831800
H	-0.72405200	2.14644800	-0.87582000
C	-2.92947200	1.03603200	0.29830300
H	-3.25406900	1.54519700	-0.61601300
H	-3.79782200	0.99600400	0.95509400
H	-0.93616100	-1.70625100	-0.37715600
H	1.27124000	-2.17687600	-0.95374200
H	0.76584800	-2.12131900	0.71788500
C	2.29610700	2.09334000	-0.74970200
H	1.46402800	2.27737300	-1.41890600
H	2.22558800	2.78222100	0.09155500
H	3.21917600	2.31629900	-1.28302500
H	-2.06691900	2.85026700	1.08139600
H	-1.59766700	1.39131000	1.94353500
N	3.54496900	0.18530100	-0.09435400
C	-3.48279900	-1.37786700	-0.33587300
H	-3.10135200	-2.36487200	-0.57030400
C	-4.81338300	-1.17391800	-0.34310500
H	-5.24782000	-0.20846300	-0.12766500
H	-5.49192000	-1.98110400	-0.57635200
C	3.83360800	-1.10545700	0.38348000
H	4.86009300	-1.27826100	0.66241600
C	2.85670200	-2.00796200	0.45106200
H	3.08045000	-3.00239000	0.80732100
H	4.32433400	0.80038000	-0.28459800

4a-Z_{out}

C	1.87582300	-1.03283800	0.30189800
C	1.29844700	0.24458600	0.05144700
C	2.24271200	1.42113600	-0.14308200
C	-0.07315400	0.47608900	0.05067600
C	-1.06731300	-0.53791900	-0.09556000
C	-0.56935100	1.89362500	0.09813300
C	-2.41387000	-0.27914900	-0.13396300
C	-1.91726100	1.97516300	0.80581500
H	0.15311200	2.53475700	0.59911900
H	-0.66769500	2.26736800	-0.92892800
C	-2.94574000	1.09703900	0.11433200
H	-3.22934600	1.53188900	-0.85061500
H	-3.85951900	1.03699300	0.70490700
H	-0.76636000	-1.55034100	-0.31412700
H	2.38355700	1.96941000	0.79670100
H	1.79892600	2.13046400	-0.83946000
C	1.18526300	-2.21927400	0.89868100
H	0.36384400	-1.92059200	1.54139800
H	0.79806700	-2.87529200	0.11843300
H	1.89826700	-2.79473800	1.48795400
H	-2.25576500	3.00954000	0.83216800
H	-1.79534000	1.64639600	1.83967300
C	-3.31300600	-1.36309200	-0.46626900
H	-2.86217300	-2.33463400	-0.63403500
C	-4.64602300	-1.23423800	-0.59690200
H	-5.14868300	-0.28900800	-0.45200000
H	-5.25703400	-2.08441000	-0.86177700
C	3.58120000	1.00140200	-0.66749300
H	4.22658400	1.73420400	-1.12822000
C	4.00957700	-0.25276200	-0.53480800
N	3.17025700	-1.20467100	0.07499000
H	3.57371800	-2.09794900	0.32337100
H	4.97020300	-0.61996900	-0.85691600

4b- E_{out}

C	2.90643700	-0.63080500	-0.49490800
C	1.91740200	0.34701400	-0.19485600
C	2.38941800	1.74132100	0.19254600
C	0.55209500	0.09869600	-0.28913700
C	-0.35391000	1.19468400	-0.24712800
C	-0.09370900	-1.24441200	-0.39880300
C	-1.72425400	1.07570000	-0.19343200
C	-1.35834100	-1.32101000	0.47462500
H	-0.36140000	-1.44386000	-1.44131800
H	0.57019900	-2.03916800	-0.07138500
C	-2.40527600	-0.26252300	0.00312800
H	0.04151000	2.19717900	-0.33858100
H	1.70599600	2.15537300	0.93324800
H	2.35182400	2.42005700	-0.66872700
C	2.69625200	-1.91520600	-1.23607500
H	2.48998500	-2.73353700	-0.54654900
H	1.87711100	-1.84182900	-1.94170300
H	3.60202100	-2.16642300	-1.78675100
N	4.16874200	-0.38841600	-0.16743600
C	-2.44204800	2.33213800	-0.35015800
H	-1.80503000	3.21018200	-0.32353800
C	-3.75092800	2.55217200	-0.58120000
H	-4.48525300	1.76941300	-0.66861800
H	-4.10001800	3.56652200	-0.71162300
C	4.60692000	0.72783600	0.56731200
H	5.62212300	0.67825800	0.92553600
C	3.77312200	1.74818300	0.76246400
H	4.11414400	2.60924100	1.31763000
H	4.86043800	-1.07387300	-0.43872100
C	-3.51849300	-0.14556300	1.06042800
H	-3.19653500	0.42816600	1.92723200
H	-4.40790000	0.32807400	0.65920800
H	-3.81207700	-1.13796200	1.39760100
C	-3.03450900	-0.67817800	-1.34170400
H	-3.67151200	-1.55019500	-1.20249800
H	-3.64741800	0.12407200	-1.74414000
H	-2.28091800	-0.91607800	-2.09193700
C	-1.88567900	-2.75117100	0.34499200
H	-2.02233800	-3.04454600	-0.69457700
H	-1.16895200	-3.43984400	0.79440900
H	-2.83191700	-2.88639400	0.86621200
C	-0.95485700	-1.09308400	1.93647600
H	-1.76391300	-1.36362500	2.61184100
H	-0.10077800	-1.72657000	2.18335600
H	-0.67843200	-0.05846900	2.13901300

4b-Z_{in}

C	4.13476500	-1.15631400	-0.84941900
C	2.71407000	-1.41787500	-0.45352700
C	1.96612500	-0.14217400	-0.09892600
C	2.72641700	0.96055200	0.38332600
H	4.68026500	-1.90495200	-1.40422100
H	2.20470000	-1.91929800	-1.27461900
H	2.70131400	-2.12396200	0.38599600
C	0.57868000	-0.12746800	-0.18289600
C	-0.22579600	1.04585300	-0.18524700
C	-0.16778500	-1.40498400	-0.37978100
C	-1.60082200	1.03921600	-0.22158000
C	-1.49562200	-1.40106100	0.39262500
H	-0.35505800	-1.55050000	-1.44987600
H	0.41755900	-2.26034900	-0.04322900
C	-2.40787200	-0.23833700	-0.11105400
C	2.19729700	2.13904000	1.13879500
H	1.97297600	2.96433900	0.46219100
H	1.29594500	1.88680600	1.68792600
H	2.95171400	2.48679700	1.84373200
H	0.25058200	2.00939200	-0.28032500
N	4.04411700	0.94048300	0.23978900
C	-2.19823400	2.35525500	-0.40652400
H	-1.49081000	3.17457900	-0.32573400
C	-3.46540400	2.69485100	-0.71105200
H	-4.26005400	1.98286100	-0.85589500
H	-3.71412900	3.73815400	-0.84294300
C	4.75362900	-0.03298000	-0.48950000
H	5.78053200	0.20933400	-0.70907500
H	4.57105900	1.70048300	0.64843800
C	-3.57861900	-0.05100500	0.87095100
H	-3.26988700	0.46585700	1.77749000
H	-4.39169700	0.51294800	0.42695000
H	-3.98239400	-1.02192300	1.15217800
C	-2.97331700	-0.55936300	-1.50917000
H	-3.69449500	-1.37238000	-1.44253000
H	-3.48027700	0.30548700	-1.92871400
H	-2.19113300	-0.84782000	-2.21091700
C	-2.13367300	-2.77412200	0.17606700
H	-1.51162000	-3.53657000	0.64656500
H	-3.12235200	-2.84062700	0.62725200
H	-2.22097600	-3.02240900	-0.88024700
C	-1.18226400	-1.25185900	1.88711700
H	-2.05873200	-1.46774900	2.49461000
H	-0.40626400	-1.96462600	2.17202200
H	-0.83505100	-0.25060300	2.14321800

4b- E_{in}

C	-2.90643800	-0.63080800	-0.49490300
C	-1.91740400	0.34701100	-0.19484900
C	-2.38942200	1.74131800	0.19255100
C	-0.55209600	0.09869400	-0.28912600
C	0.35390600	1.19468300	-0.24711300
C	0.09370900	-1.24441400	-0.39879100
C	1.72425100	1.07570200	-0.19342600
C	1.35835000	-1.32101100	0.47462400
H	-0.57019600	-2.03916900	-0.07136500
H	0.36138900	-1.44386700	-1.44130900
C	2.40527800	-0.26252100	0.00312000
H	-0.04151600	2.19717900	-0.33855600
H	-2.35182700	2.42005300	-0.66872400
H	-1.70600200	2.15537200	0.93325200
C	-2.69625400	-1.91520900	-1.23607100
H	-1.87711400	-1.84183200	-1.94170100
H	-2.48998400	-2.73354000	-0.54654500
H	-3.60202400	-2.16642800	-1.78674500
N	-4.16874500	-0.38841700	-0.16743700
C	2.44204000	2.33214300	-0.35014800
H	1.80502200	3.21018600	-0.32350900
C	3.75091700	2.55218200	-0.58120600
H	4.48524300	1.76942500	-0.66864300
H	4.10000400	3.56653400	-0.71162300
C	-4.60692500	0.72783400	0.56731100
H	-5.62212900	0.67825700	0.92553200
C	-3.77312700	1.74818100	0.76246500
H	-4.11415000	2.60923900	1.31763000
H	-4.86044000	-1.07387400	-0.43872300
C	3.51850700	-0.14556300	1.06040700
H	4.40790900	0.32807600	0.65917900
H	3.19655900	0.42816300	1.92721700
H	3.81209500	-1.13796300	1.39757400
C	3.03449500	-0.67817000	-1.34172100
H	3.64740000	0.12408200	-1.74416200
H	3.67150000	-1.55018700	-1.20252700
H	2.28089500	-0.91606700	-2.09194600
C	1.88569000	-2.75117100	0.34498300
H	1.16896700	-3.43984700	0.79440200
H	2.02234300	-3.04454200	-0.69458800
H	2.83193100	-2.88639400	0.86619600
C	0.95488000	-1.09309000	1.93648000
H	0.10080500	-1.72657900	2.18336700
H	1.76394300	-1.36363000	2.61183600
H	0.67845400	-0.05847600	2.13902200

4b-Z_{out}

C	-2.72609200	0.96034900	0.38363900
C	-1.96606000	-0.14234500	-0.09897300
C	-2.71424700	-1.41789100	-0.45351800
C	-0.57862700	-0.12771200	-0.18310100
C	0.22567800	1.04573000	-0.18538800
C	0.16785700	-1.40513800	-0.38015400
C	1.60069400	1.03921200	-0.22160400
C	1.49553800	-1.40114200	0.39258200
C	2.40779400	-0.23831100	-0.11094800
H	-0.25095700	2.00915300	-0.28055900
H	-2.70214500	-2.12372700	0.38622800
H	-2.20471900	-1.91970600	-1.27425900
C	-2.19675500	2.13851000	1.13948100
H	-1.29488600	1.88628900	1.68775600
H	-1.97327500	2.96432400	0.46321400
H	-2.95074800	2.48551500	1.84525000
C	2.19805700	2.35527200	-0.40665800
H	1.49059500	3.17455300	-0.32577100
C	3.46514300	2.69491100	-0.71143000
H	4.25984800	1.98300400	-0.85645300
H	3.71384200	3.73821500	-0.84340200
C	-4.13470600	-1.15578000	-0.85003800
H	-4.68009300	-1.90405700	-1.40542900
C	-4.75337700	-0.03242800	-0.48984900
N	-4.04382500	0.94051600	0.24011500
H	-4.57068500	1.70036800	0.64913800
H	-5.78011100	0.21034300	-0.70972300
C	1.18171900	-1.25195900	1.88696000
H	0.40565900	-1.96476300	2.17161300
H	2.05798900	-1.46779700	2.49475200
H	0.83436200	-0.25072300	2.14298000
C	2.13374000	-2.77416500	0.17623900
H	2.22142500	-3.02250700	-0.88002400
H	3.12225400	-2.84057700	0.62780400
H	1.51158300	-3.53665000	0.64654400
C	3.57831900	-0.05077000	0.87127500
H	4.39123400	0.51359900	0.42751700
H	3.26923100	0.46583600	1.77783900
H	3.98238900	-1.02159800	1.15239500
C	2.97354100	-0.55923900	-1.50896300
H	3.69499900	-1.37199200	-1.44217400
H	2.19153500	-0.84805600	-2.21076000
H	3.48022400	0.30575500	-1.92852900
H	0.35545000	-1.55044900	-1.45021500
H	-0.41751800	-2.26059100	-0.04386200

4c- E_{out}

C	3.31133300	-0.64562800	-0.57909100
C	2.40434600	0.40094000	-0.22693900
C	2.98835000	1.73022000	0.22798700
C	1.02540200	0.26935800	-0.31288300
C	0.20927400	1.43035500	-0.18463600
C	0.29126800	-1.02391200	-0.50982600
C	-1.16408900	1.44174100	-0.15384000
C	-0.98861200	-1.02314000	0.31834400
H	0.00828600	-1.16568700	-1.55607900
H	0.86431500	-1.88196300	-0.18012600
C	-1.92276200	0.13533400	-0.11861700
H	0.68222800	2.40232800	-0.19697100
H	2.36492600	2.13704300	1.02412700
H	2.96336400	2.46596200	-0.58547500
C	2.98823800	-1.87867900	-1.36408200
H	2.68207800	-2.69083300	-0.70466800
H	2.19864400	-1.69967900	-2.08511100
H	3.87427900	-2.20879800	-1.90443800
N	4.58654300	-0.51775000	-0.25428200
C	-1.82617200	2.72495000	-0.23246500
H	-1.16898300	3.57601800	-0.09557900
C	-3.11698800	2.96278900	-0.53327500
H	-3.82924300	2.17622700	-0.72214000
H	-3.46319600	3.98322000	-0.61278900
C	5.13460700	0.54107000	0.49349900
H	6.15476500	0.40368900	0.81198700
C	4.38967800	1.61792200	0.73667400
H	4.81567000	2.43992200	1.29251800
H	5.21614700	-1.25094800	-0.55475500
Cl	-3.32330300	0.18990700	0.95933800
Cl	-2.46493600	-0.16472300	-1.80199100
Cl	-1.78512000	-2.58780700	0.13450800
Cl	-0.53324700	-0.79985700	2.03075600

4c-Z_{in}

C	4.51066100	-1.23468100	-0.97612100
C	3.07255500	-1.40098500	-0.59538300
C	2.42562700	-0.09345900	-0.17322100
C	3.27169000	0.92151500	0.37311300
H	4.99850600	-2.00177700	-1.55884000
H	2.53103100	-1.81904200	-1.44248900
H	3.00141000	-2.14585100	0.20768900
C	1.04764800	0.03495600	-0.24135000
C	0.33510300	1.26627800	-0.16173100
C	0.21935200	-1.18535000	-0.50948200
C	-1.03165200	1.38692600	-0.18700000
C	-1.08756900	-1.09323900	0.26517900
H	-0.01334500	-1.27388700	-1.57505100
H	0.71939500	-2.09637700	-0.19117400
C	-1.89963200	0.14966300	-0.18427600
C	2.83069900	2.07357300	1.21892300
H	2.65137500	2.95822500	0.60687100
H	1.92243000	1.83604600	1.76437900
H	3.61428100	2.32220100	1.93368400
H	0.88190300	2.19525600	-0.20418000
N	4.57779700	0.80923700	0.20977700
C	-1.58316400	2.72052900	-0.30677000
H	-0.86145000	3.51599200	-0.15865500
C	-2.83930800	3.06402400	-0.64624100
H	-3.61159400	2.33936500	-0.84597200
H	-3.09425700	4.10930200	-0.74515200
C	5.21327000	-0.17817700	-0.57004700
H	6.25663500	-0.00497000	-0.77625700
H	5.16496500	1.49872400	0.66221300
Cl	-3.32276800	0.32148200	0.85186300
Cl	-2.41358000	-0.09099100	-1.88593500
Cl	-0.67379700	-0.92734600	1.99894800
Cl	-2.00853400	-2.57886800	0.03635500

4c- E_{in}

C	-3.31133100	-0.64562500	-0.57909500
C	-2.40434400	0.40094400	-0.22694700
C	-2.98834600	1.73022400	0.22798300
C	-1.02540000	0.26936100	-0.31289300
C	-0.20927100	1.43035700	-0.18464600
C	-0.29126800	-1.02391000	-0.50983400
C	1.16409300	1.44174000	-0.15384400
C	0.98860800	-1.02314000	0.31834300
H	-0.86431700	-1.88196100	-0.18013700
H	-0.00828000	-1.16568400	-1.55608500
C	1.92276300	0.13533200	-0.11861500
H	-0.68222300	2.40233000	-0.19698500
H	-2.96336500	2.46596700	-0.58547700
H	-2.36491800	2.13704500	1.02412200
C	-2.98823800	-1.87867400	-1.36409000
H	-2.19864300	-1.69967300	-2.08511800
H	-2.68208100	-2.69083100	-0.70467800
H	-3.87428000	-2.20878900	-1.90444800
N	-4.58654000	-0.51775000	-0.25427700
C	1.82617800	2.72494800	-0.23246800
H	1.16899000	3.57601800	-0.09558800
C	3.11699600	2.96278500	-0.53327200
H	3.82925000	2.17622100	-0.72213100
H	3.46320500	3.98321400	-0.61278700
C	-5.13460100	0.54106900	0.49350700
H	-6.15475600	0.40368700	0.81200100
C	-4.38967200	1.61792300	0.73667700
H	-4.81566400	2.43992300	1.29252200
H	-5.21614400	-1.25094900	-0.55474600
Cl	3.32329800	0.18990400	0.95934600
Cl	2.46494400	-0.16472900	-1.80198600
Cl	1.78511300	-2.58780800	0.13451400
Cl	0.53323300	-0.79985400	2.03075200

4c-Z_{out}

C	-3.27169000	0.92151500	0.37311300
C	-2.42562700	-0.09345900	-0.17322100
C	-3.07255500	-1.40098500	-0.59538300
C	-1.04764800	0.03495600	-0.24135000
C	-0.33510300	1.26627800	-0.16173100
C	-0.21935200	-1.18535000	-0.50948200
C	1.03165200	1.38692600	-0.18700000
C	1.08756900	-1.09323900	0.26517900
H	-0.71939500	-2.09637700	-0.19117400
H	0.01334500	-1.27388700	-1.57505100
C	1.89963200	0.14966300	-0.18427600
H	-0.88190300	2.19525600	-0.20418000
H	-3.00141000	-2.14585100	0.20768900
H	-2.53103100	-1.81904200	-1.44248900
C	-2.83069900	2.07357300	1.21892300
H	-1.92243000	1.83604600	1.76437900
H	-2.65137500	2.95822500	0.60687100
H	-3.61428000	2.32220100	1.93368400
C	1.58316400	2.72052900	-0.30677000
H	0.86145000	3.51599200	-0.15865500
C	2.83930800	3.06402400	-0.64624100
H	3.61159400	2.33936500	-0.84597200
H	3.09425700	4.10930200	-0.74515200
C	-4.51066100	-1.23468100	-0.97612100
H	-4.99850600	-2.00177700	-1.55884000
C	-5.21327000	-0.17817700	-0.57004700
N	-4.57779700	0.80923700	0.20977700
H	-5.16496500	1.49872400	0.66221300
H	-6.25663500	-0.00497000	-0.77625700
Cl	3.32276800	0.32148200	0.85186300
Cl	2.41358000	-0.09099100	-1.88593500
Cl	0.67379700	-0.92734600	1.99894800
Cl	2.00853400	-2.57886800	0.03635500

4d- E_{out}

C	-3.89207600	-0.48986800	0.81590800
C	-3.05074100	0.53971000	0.29637400
C	-3.71033500	1.75653700	-0.33553300
C	-1.66481700	0.49394900	0.36801800
C	-0.91766200	1.66474000	0.05775800
C	-0.85636700	-0.71619000	0.72903700
C	0.45452200	1.74906300	0.00501600
C	0.41436900	-0.75794700	-0.11339300
H	-0.55626600	-0.69139400	1.78101900
H	-1.38697800	-1.64045000	0.53678100
C	1.28167000	0.49653300	0.13313200
H	-1.44464800	2.60100900	-0.06215600
H	-3.12814000	2.06164600	-1.20546300
H	-3.69701900	2.60937600	0.35450700
C	-3.48538900	-1.58497600	1.75200400
H	-3.14646300	-2.46215300	1.20063000
H	-2.69312300	-1.26749900	2.42066700
H	-4.34092200	-1.88468500	2.35559300
N	-5.18026000	-0.47238000	0.51551300
C	1.02575300	3.07460800	-0.10837600
H	0.31042900	3.84500400	-0.37275000
C	2.29043700	3.45170100	0.15706600
H	3.05558500	2.75913500	0.46749500
H	2.55927500	4.49554300	0.08056300
C	-5.80101400	0.44418200	-0.35288500
H	-6.82177200	0.21728900	-0.61297500
C	-5.11845700	1.50839100	-0.77165300
H	-5.60146900	2.22233700	-1.42211700
H	-5.76236100	-1.18706300	0.93296600
Br	1.89483000	0.49289400	1.99329900
Br	2.80736700	0.47521300	-1.04622800
Br	1.35685300	-2.38407200	0.29540700
Br	-0.14201200	-0.81700700	-1.98128300

4d-Z_{in}

C	-5.07241100	-1.06952400	1.32838700
C	-3.62972600	-1.21351800	0.95577500
C	-3.06373000	0.04450200	0.32171700
C	-3.96930600	0.91268800	-0.36116200
H	-5.51142900	-1.76082100	2.03219100
H	-3.05782600	-1.46075400	1.84895000
H	-3.52057800	-2.07079100	0.27869800
C	-1.69341600	0.25199200	0.33396600
C	-1.05084200	1.49029600	0.05290500
C	-0.79474400	-0.86933400	0.75771900
C	0.30938800	1.68374700	0.02217100
C	0.48696200	-0.82492100	-0.06363200
H	-0.53297100	-0.77963500	1.81757700
H	-1.25571100	-1.84083700	0.60079200
C	1.23795000	0.50587300	0.16543500
C	-3.59836200	1.93866100	-1.38414800
H	-3.46068800	2.91687400	-0.92203700
H	-2.68318600	1.66379800	-1.90042100
H	-4.40029600	2.03102100	-2.11569000
H	-1.64639600	2.38645700	-0.02616700
N	-5.26654300	0.75537700	-0.16246800
C	0.77249400	3.05453300	-0.06990800
H	-0.00338300	3.76688100	-0.32739200
C	2.00127400	3.53346400	0.19597800
H	2.82349700	2.90491000	0.49614300
H	2.18138900	4.59678300	0.12822700
C	-5.83773100	-0.13148500	0.77208100
H	-6.88797600	0.01266600	0.96548200
H	-5.89523200	1.33133500	-0.70792800
Br	2.76422300	0.60460400	-1.01006600
Br	1.84171400	0.57373300	2.02755500
Br	-0.04893000	-0.95988500	-1.93873300
Br	1.56098700	-2.35637700	0.37282100

4d- E_{in}

C	3.89197700	-0.48992800	0.81587900
C	3.05073600	0.53962700	0.29620200
C	3.71039800	1.75637800	-0.33582000
C	1.66482200	0.49396100	0.36794600
C	0.91766000	1.66473000	0.05757600
C	0.85632800	-0.71610500	0.72907800
C	-0.45450100	1.74910100	0.00501200
C	-0.41432100	-0.75788300	-0.11348100
H	1.38693500	-1.64042100	0.53710900
H	0.55606800	-0.69113800	1.78101800
C	-1.28166500	0.49659100	0.13329600
H	1.44467700	2.60095000	-0.06259900
H	3.69685100	2.60936600	0.35405000
H	3.12835900	2.06132600	-1.20591400
C	3.48498800	-1.58515800	1.75169200
H	2.69287300	-1.26754400	2.42049500
H	3.14564100	-2.46205800	1.20014300
H	4.34043200	-1.88541600	2.35512900
N	5.18026800	-0.47234700	0.51589400
C	-1.02578100	3.07464700	-0.10838800
H	-0.31053500	3.84502400	-0.37303500
C	-2.29040100	3.45168500	0.15734400
H	-3.05544000	2.75906900	0.46793700
H	-2.55935800	4.49549400	0.08082600
C	5.80120200	0.44424800	-0.35234000
H	6.82209100	0.21748000	-0.61203000
C	5.11866700	1.50830700	-0.77148100
H	5.60181400	2.22222700	-1.42187300
H	5.76226000	-1.18708500	0.93338500
Br	-1.35685500	-2.38411000	0.29511700
Br	0.14206700	-0.81684100	-1.98130600
Br	-2.80742200	0.47535600	-1.04609000
Br	-1.89479600	0.49268000	1.99339300

4d-Z_{out}

C	3.96897600	0.91331200	-0.36048500
C	3.06367100	0.04497900	0.32257300
C	3.62977500	-1.21312800	0.95644500
C	1.69334300	0.25240800	0.33492100
C	1.05065600	1.49061900	0.05377200
C	0.79466000	-0.86893200	0.75865200
C	-0.30960500	1.68384900	0.02269600
C	-0.48669000	-0.82491000	-0.06338400
H	1.25579200	-1.84045800	0.60237100
H	0.53229100	-0.77881300	1.81831000
C	-1.23813600	0.50584300	0.16548100
H	1.64603300	2.38690200	-0.02528200
H	3.51962100	-2.07058000	0.27975900
H	3.05857000	-1.45989100	1.85021800
C	3.59738100	1.93979200	-1.38272800
H	2.68215400	1.66482600	-1.89888100
H	3.45933900	2.91763800	-0.91997100
H	4.39907200	2.03302600	-2.11441700
C	-0.77294500	3.05457600	-0.06932100
H	0.00274900	3.76718100	-0.32660400
C	-2.00190700	3.53312900	0.19648000
H	-2.82390800	2.90417400	0.49640600
H	-2.18227800	4.59640800	0.12893000
C	5.07286200	-1.06974400	1.32759500
H	5.51246100	-1.76150000	2.03059500
C	5.83799400	-0.13173900	0.77098200
N	5.26631500	0.75575700	-0.16265900
H	5.89476100	1.33192800	-0.70816800
H	6.88847500	0.01188200	0.96346800
Br	-2.76349100	0.60443400	-1.01123200
Br	-1.84315300	0.57334400	2.02712600
Br	-1.56073300	-2.35650400	0.37256800
Br	0.04996200	-0.95994100	-1.93818200