Electronic Supplementary Information

Understanding the mechanism of direct visible-light-activated [2+2] cycloadditions mediated by Rh and Ir photocatalysts: Combined computational and spectroscopic studies

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I. General Considerations

Reagent preparation. All reactions were carried out under an atmosphere of nitrogen with magnetic stirring in flame-dried glassware unless stated otherwise. Catalytic reactions were performed in Schlenk tubes (10 mL), placed 10 cm away from a 24 W blue LED lamp (Hongchangzhaoming from Chinese Taobao, https://hongchang-led.taobao.com, see Supplementary Figure 1 in our previous publication[1]). Prior to irradiation, the reactions mixtures were degassed thoroughly via freeze-pump-thaw for three cycles over the course of 45 min. CH_2Cl_2 was distilled under nitrogen from calcium hydride, DMF over 4 Å molecular sieves was bought commercially and acetone was dynamically dried with 3 Å molecular sieves. Commercially purchased compounds were used without further purification.

Product characterization. ^{1}H NMR, ^{13}C(1H) NMR and ^{19}F(1H, 13C) NMR spectra were recorded on a Bruker AV II 300 MHz, AV III HD 250 MHz, AV III 500 MHz, AV III HD 500 MHz, or AV II 600 MHz spectrometer at room temperature. The chemical shift δ is listed in ppm with the solvent resonance as internal standard. IR spectra were acquired on a Bruker Alpha FT-IR spectrophotometer. The resulting absorption bands are listed as wavenumbers (cm^{-1}) and the correlating intensities are specified as w (weak) or s (strong), m (medium). High-resolution mass spectrometry was measured via electrospray-ionization-technique (ESI) or atmospheric pressure chemical ionization-technique (APCI) on a Finnigan LTQ-FT Ultra mass spectrometer (Thermo Fischer Scientific). CD spectra were recorded on JASCO J-810 CD spectropolarimeter (parameters: 600-200 nm, bandwidth 1 nm, data pitch 0.5 nm, response 1 second, sensitivity standard, scanning speed 50 nm/min, accumulation of 3 scans).

II. Computational studies

1. Reaction energy profiles of the Rh/Ir–photocatalyzed [2+2] cycloadditions

We explored the reaction energy profile of the activated substrate **1** by means of density functional theory (DFT) calculations. Geometry optimizations and calculations of single point electronic energies, solvation energies and vibrational modes of the optimized geometries were conducted using the Jaguar 9.1 suite of programs.[2] Gas phase geometries were optimized using the B3LYP functional with Grimme's dispersion correction (D3).[3-6] We used LACVP[7-9] basis set that combines standard double zeta quality Pople basis set (6–31G(d,p)) for the main group elements and the double-zeta quality Los Alamos effective core potential basis set (LANL2DZ) for the heavy elements. We evaluated the single point energy with the cc-pVTZ(-f) basis set[10] for the main group elements and LACV3P** for the transition metals, both are triple-ζ quality basis sets. The frequency calculations were carried out at the same level of theory as the structure optimizations. The local minimum structures were confirmed not to have imaginary frequencies. Zero-point vibrational energies and entropy correction energies were derived from the calculated vibrational frequencies. The optimized gas phase geometries were used within the self-consistent reaction field (SCRF)[11-13] approximations with the dielectric constant ε = 20.9 (acetone) to obtain the solvation energy correction. Transition states were located by using the quadratic synchronous transit search method (QST).[14] For each transition state structure optimized, we checked that there is only one vibration mode with single imaginary frequency, whose vibrational motion corresponds to the formation and breakage of the reaction of interest. The final Gibbs free energy of each optimized intermediate and transition state was computed as follows:

$$(1)\quad G(sol) = G(gas) + G(Solv)$$

$$(2)\quad G(gas) = H(gas) - TS(gas)$$

$$(3)\quad H(gas) = E(SCF) + ZPE$$

$$(4)\quad \Delta G(sol) = \Sigma G(sol)\ for\ products - \Sigma G(sol)\ for\ reactants$$

To calculate the solvation corrected Gibbs energy (*G(sol)*), solvation correction energy (*G(Solv)*) was added to the gas phase Gibbs free energy (*G(gas)*). For the gas phase Gibbs free energy, enthalpy in the gas phase was added to the entropy correction term *S(gas)*, which was derived from the frequency calculations. *T* implies the temperature, which is 298.15 K. *E(SCF)* is the self-consistent field energy which is the computed electronic energy from the SCF convergence. Finally, *ZPE* is the vibrational zero-point energy, and *H(gas)* can be obtained by the summation of *E(SCF)* and *ZPE*. Note that the entropy to which we refer is specifically the vibrational/rotational/translational entropy of the solute(s). Entropies of the solvent are implicitly considered in the continuum model.

2. Identification of excited–state intermediates using DFT and TDDFT

Singlet and triplet excited state geometries were optimized using time-dependent DFT (TD–DFT) and triplet spin manifold density functional theory (DFT) in combination of a range separated density functional theory (CAM-B3LYP) augmented with the Grimme's dispersion correction (D3).[6],[15] The range separated DFT was chosen for our studies, as it has been shown to provide more reliable energetics of charge transfer states in the excited states than conventional global hybrid functionals.[16] We adopted the standard double-zeta quality Pople basis set (6-31G(d,p)) and the Los Alamos effective core potential (LANL2DZ) for the optimizations of the excited state species. Singlet MLCT states (**^{1}MLCT**) and triplet ligand-centered (**^{3}LC**) states were optimized using the time-dependent DFT (TDDFT) method namely at the TD-CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory. For the TD–DFT calculations, eigenstates of the time–dependent Hamiltonian were constructed based on configuration interaction singles (CIS), that is equivalent to the Tamm-Dancoff approximation.[17] Ground state geometries (S_0) and triplet metal-to-ligand charge transfer (**^{3}MLCT**) states were optimized at the (U)CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory. Adiabatic energies were computed by comparing the self-consistent electronic energies of the excited state of interest and the ground state. Of note, the TD-DFT methods have been reported to produce the energetics and the electronic properties of low-lying excited states, that agree with the experimental observations.[18] We compared the energetics of the excited state species using another range-separated hybrid functional (ωB97X-D3)[19] using the same double-ζ quality basis sets (6-31G(d,p)/LANL2DZ). The computed excited state energies from the two density functional theories agreed quantitatively (Table S2), confirming that the conclusions drawn from the (TD)CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory are robust regardless of the choice of the DFT. Q-Chem 5.0 software suite[20] was used for the calculations of the exited state species.

3. Calculations of the rates of ISC and IC between excited singlet and triplet states

We computed the rates of intersystem crossings (ISCs) and reverse-intersystem crossings (rISCs) between the first singlet metal-to-ligand charge transfer state (**M-1-^{1}MLCT**) and the triplet excited state species (**M-1-^{3}LC** and **M-1-^{3}MLCT**) based on the Marcus theory of electron transfer,[21]. The rate of intersystem crossing (k_{ISC}) is given as following:

$$(5)\quad k_{ISC} = \frac{2\pi}{\hbar}|V_{SOC}|^2\sqrt{\frac{\pi}{\lambda k_B T}}\exp\left(-\frac{(\Delta G+\lambda)^2}{4\lambda k_B T}\right)$$

, where V_{SOC} is the strength of spin-orbit coupling between the initial and the final excited states, ħ is the Planck constant, k_B is the Boltzmann constant, T is the temperature, ΔG is the adiabatic energy difference between the initial and the final excited states, and λ is the reorganization energy. We also calculated the rates of internal conversions (ICs) between the triplet ligand centered state (**M–1–^{3}LC**) and the triplet MLCT state (**M–1–^{3}MLCT**) based on the Marcus theory of electron transfer. In general, the computations of the rates of non-radiative intramolecular electronic transitions require the explicit considerations of vibronic Franck-Condon factors (FCFs), as the electronic couplings between the nuclear vibronic modes contribute significantly to the transitions. However, in the limit where the electronic coupling is weak, one expects that the Marcus equation becomes an effective

approximation to the realistic rates of internal conversions. In our situation, the strength of electronic coupling was below 31 cm-1 (Table 2), suggesting the use of Marcus equation is viable. Previously, Subotnik et. al. demonstrated that in the weak coupling limit, the Marcus equation reproduces the rates of intramolecular charge transfer reactions.[22] The rate of internal conversion (k_{IC}) is given as following:

$$(6)\quad k_{IC} = \frac{2\pi}{\hbar}|V_{EC}|^2\sqrt{\frac{\pi}{\lambda k_B T}}\exp\left(-\frac{(\Delta G+\lambda)^2}{4\lambda k_B T}\right)$$

, where V_{EC} is the strength of electronic coupling between the initial and the final excited states. We computed the Breit-Pauli spin-orbit Hamiltonian[23] and used the fragment charge difference (FCD)[24] method for the calculations of V_{SOC} and V_{EC}, respectively, that are implemented in Q-Chem 5.0 software suite.

We computed V_{SOC} and V_{EC} at the identified minimal energy crossing point (MECP) between the two diabatic states of interest, that were optimized based on the branching-plane method implemented in Q-Chem 5.0 software suite.[20] The reorganization energy (λ) is defined as following:

$$(7)\quad \lambda = (E^1_{MECP} - E^1_1) + (E^2_{MECP} - E^2_2)$$

, where E^1_1 (E^2_2) is the adiabatic energy of the initial (final) state and E^1_{MECP} (E^2_{MECP}) is the energy of the initial (final) state at the geometry of MECP. Detailed parameters used for the computations of the rates of ISC and IC are summarized in Table 2.

4. Computational analysis of the redox potential

We calculated the oxidation (E_{ox}) and the redox (E_{red}) potentials of the enone substrate **1** and 2,3-dimethyl-1,3-butadiene, following the protocol described in a previous publication.[25] In the beginning the geometries of the neutral, the reduced (–1e), and the oxidized (+1e) species were optimized at the B3LYP-D3/6-31G(d,p) level of the theory. The vibrational frequencies and the solvation corrections were computed using the optimized geometries. Of note, we consider the dielectric environment of dichloromethane (ε=9.08) in order to be consistent with the electrochemical measurements of the transition metal complexes. The Gibbs free energy of each species was computed using Eq. 1 in the main text. For the oxidation potential, the electron attachment energy of oxidized species ($\Delta\Delta G_{ox}$=*ΔG(neutral)–ΔG(oxidized)*) was computed. For the reduction potential, the electron attachment energy of neutral species ($\Delta\Delta G_{red}$ *ΔG(anion)–ΔG(neutral)*) was computed. The reference electrode potential was retrieved from the literature: the absolute redox potential of standard hydrogen electrode (SHE) is 4.18 V[26] and the relative potential of SCE to that of SHE is 0.24 V.[27] Finally, the relative potentials are given as following.

$$(8)\quad E_{ox} = -\Delta\Delta G_{ox} - 4.42\ V\ and$$

$$(9)\quad E_{red} = -\Delta\Delta G_{red} - 4.42\ V$$

5. Supplementary Figures and Tables

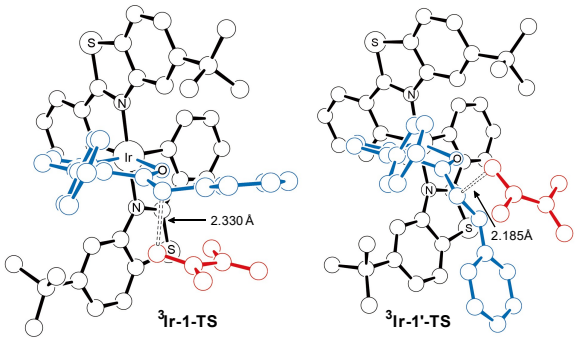


Figure S1. Optimized structures of ^{3}**Ir-1-TS** and ^{3}**Ir-1'-TS**.

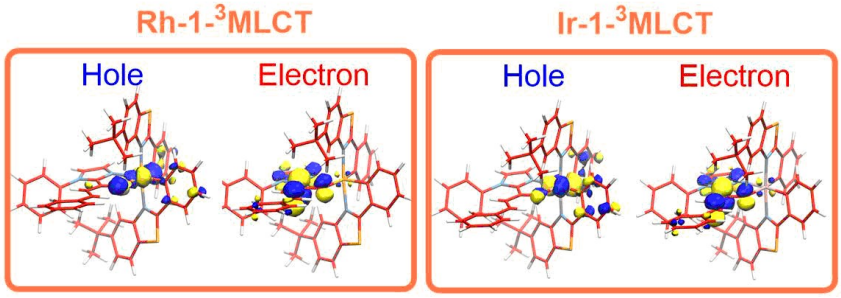


Figure S2. Natural transition orbitals (NTOs) of **M–1–^{3}MLCT** species computed at the unrestricted CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ. The multiplicity was set as 3 for for the calculations.

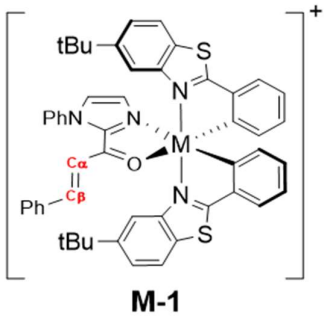


Figure S3. Definition of the α and β carbons (r(C_α–C_β)) of the substrate

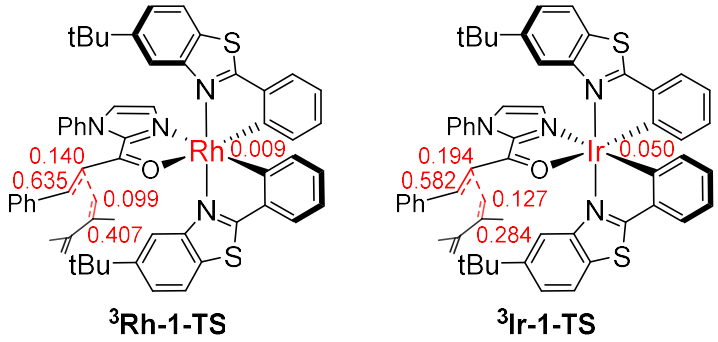


Figure S4. Selected Mulliken spin densities of **^{3}Rh–1–TS** and **^{3}Ir–1–TS**. (B3LYP-D3/cc-pVTZ(-f),LACV3P**(Rh, Ir) level)

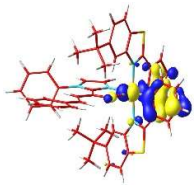
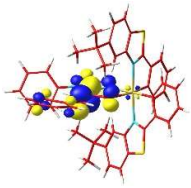
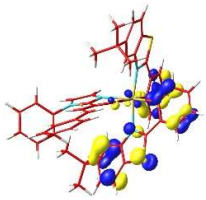
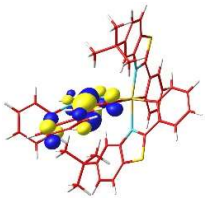
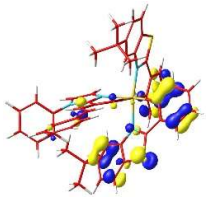
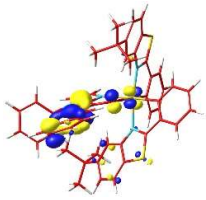
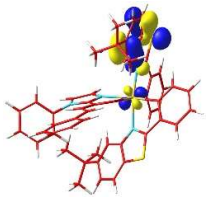
Table S1. Bond length of the α and β carbons (r(C_α–C_β)) of the substrate. Geometries were optimized at the (TD)CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory.

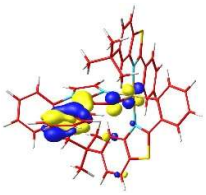
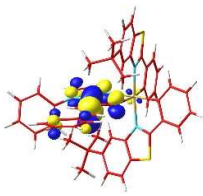
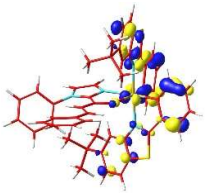
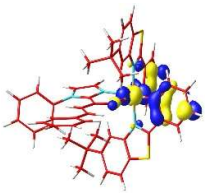
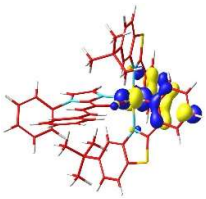
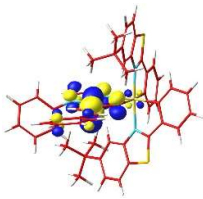
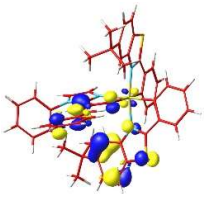
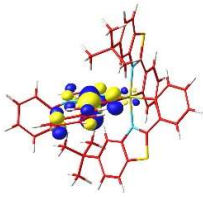
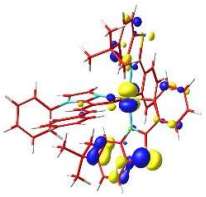
	Rh–1(Å)	**Ir–1**(Å)
M-1	1.349	1.351
^{1}MLCT	1.360	1.358
MECP(^{1}MLCT–^{3}LC)	1.347	1.383
^{3}LC	1.443	1.416
MECP(^{3}LC–^{3}MLCT)	1.400	1.390
^{3}MLCT	1.370	1.368
MECP(^{1}MLCT–^{3}MLCT)	1.408	1.398

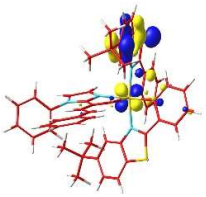
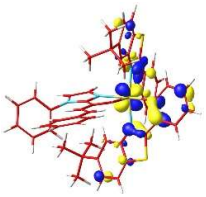
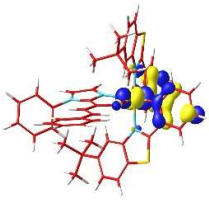
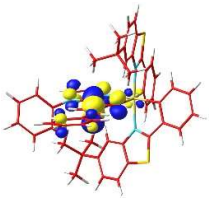
Table S2. Energetics of the singlet and triplet excited states using two different range-separated hybrid functionals: CAM-B3LYP-D3 and wB97X-D3. Energies are shown in eV.

	CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ		**wB97X-D3/6-31G(d,p)/LANL2DZ**	
State	**Rh–1**	**Ir–1**	**Rh–1**	**Ir–1**
^{1}MLCT	2.566	2.013	2.885	2.335
^{3}LC	2.149	2.001	2.027	2.143
^{3}MLCT	2.151	1.535	2.172	1.653

Table S3. Decomposition of excited state species computed at the TD-CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory. Canonical orbitals are shown at the isodensity of 0.05. A numbers in parentheses is the energies of each orbital in eV.

State	From	Amplitude	To
Rh-1-^{1}MLCT	HOMO (-8.942) 	0.928	LUMO (-4.577) 
Rh-1-^{3}LC	HOMO-6 (-10.022) 	0.216	LUMO (-4.462) 
	HOMO-5 (-10.002) 	0.359	
	HOMO-4 (-9.919) 	0.804	
	HOMO-2 (-9.734) 	0.231	

Rh-1-^{3}MLCT	HOMO-6 (-10.240) 	0.242	LUMO (-4.615) 
	HOMO-2 (-9.392) 	0.222	
	HOMO (-8.930) 	0.861	
Ir-1-^{1}MLCT	HOMO (-8.584) 	0.963	LUMO (-4.685) 
Ir-1-^{3}LC	HOMO-6 (-10.135) 	0.553	LUMO (-4.680) 
	HOMO-4 (-9.747) 	-0.395	

	HOMO-3 (-9.593)) 	-0.408	
	HOMO-1 (-9.190) 	0.461	
Ir-1-^{3}MLCT	HOMO (-8.565) 	0.953	LUMO (-4.719) 

6. Energy components of all DFT optimized geometries

Table S3. Computed energies of the optimized geometries.*

	E(SCF)	**ZPE**	**S(gas)**	**G(solv=acetone)**
Functional	B3LYP-D3	B3LYP-D3	B3LYP-D3	B3LYP-D3
Basis set	cc-pVTZ(-f)/LACV3P	6-31G(d,p)/LANL2DZ	6-31G(d,p)/LANL2DZ	6-31G(d,p)/LANL2DZ
^{1}RhS	-70652.898	419.920	264.716	-38.74
^{3}RhS	-70650.305	418.273	273.425	-39.02
^{1}IrS	-70522.867	420.666	261.208	-39.68
^{3}IrS	-70520.563	418.334	267.353	-39.63
^{1}1	-23928.369	173.583	136.673	-15.79
CH_3CN	-3613.765	28.481	57.933	-7.84
butadiene	-6387.035	89.439	80.077	-2.07
^{1}Rh-1	-87354.391	536.449	299.082	-38.02
^{3}Rh-1	-87352.563	534.030	301.066	-36.64
^{3}Rh-1-TS	-93740.125	625.280	331.204	-37.61
^{3}Rh–2	-93740.430	626.489	331.460	-37.17
^{1}Rh–3	-93741.781	629.441	319.022	-37.93

^{3}Rh–1'–TS	-93739.836	624.701	327.841	-36.66
^{3}Rh–2'	-93740.563	626.140	327.045	-37.61
^{1}Rh–3'	-93742.055	629.398	320.924	-36.62
^{1}Ir–1	-87224.320	536.699	298.571	-38.76
^{3}Ir–1	-87222.961	535.261	299.351	-37.31
^{3}Ir–1–TS	-93610.195	625.228	331.614	-37.93
^{3}Ir–2	-93610.414	626.265	334.290	-38.00
^{1}Ir–3	-93611.734	629.282	317.025	-37.41
^{3}Ir–1'–TS	-93609.781	625.290	332.663	-37.66
^{3}Ir–2'	-93610.539	626.926	332.530	-37.84
^{1}Ir–3'	-93611.969	630.003	320.176	-37.32
^{3}1	-23926.162	171.023	141.065	-16.15
^{3}1–TS	-30313.621	261.772	178.159	-16.64
^{3}2	-30314.355	263.328	176.350	-13.82
^{1}3	-30315.654	266.517	166.222	-14.16

* The unit of energy is kcal/mol, except for that of the SCF electronic energy (E(SCF)) which is in eV. The unit of entropy is cal/mol·K. The gas phase entropy (S(gas)) is computed at 298.15 K.

7. DFT optimized geometries and Computed Vibrational Frequencies

Table S4. Cartesian coordinates of all DFT optimized structures

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^{1}RhS

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N	-0.292206913	-2.163518906	-0.131973043
C	-0.308383733	-3.097877264	0.803988814
S	-1.299848199	-4.483157635	0.408675283
C	-1.618035793	-3.780995846	-1.175083280
C	-2.284692049	-4.325167179	-2.269757986
H	-2.785487652	-5.285507202	-2.201378107
C	-2.251345634	-3.628742218	-3.477451324
H	-2.744154215	-4.077181816	-4.331308365
C	-1.575405717	-2.398540497	-3.620320320
C	-0.967739403	-1.842150211	-2.493691444
H	-0.422828734	-0.911375761	-2.548543215
C	-0.981469512	-2.527616262	-1.280373931
C	0.578370273	-2.943646908	1.937116623
C	1.416241407	-1.801926374	1.853484511
C	2.387858152	-1.620833158	2.838154793
H	3.060149193	-0.772216260	2.803386688
C	2.501589298	-2.537338734	3.891014576
H	3.264793634	-2.382285595	4.649255276
C	1.655110836	-3.648089886	3.979489803
H	1.757898927	-4.350227833	4.800714970
C	0.693345428	-3.857773066	2.996401548
H	0.044844471	-4.729404449	3.042651892
C	-1.420916915	-1.678681254	-4.971384525
C	0.086766742	-1.592887640	-5.316389561
H	0.227797300	-1.089522481	-6.279384136
H	0.526772559	-2.593010902	-5.389765263
H	0.653074503	-1.039932370	-4.559562206
C	-2.136341333	-2.420085669	-6.115235329
H	-2.001240492	-1.872606039	-7.053162575
H	-3.212930918	-2.504598141	-5.934566021
H	-1.730343938	-3.426453829	-6.261844158
C	-2.009597778	-0.253326416	-4.866996288
H	-1.875029445	0.283715963	-5.812738419
H	-1.525572538	0.326111585	-4.073563099
H	-3.080930710	-0.285432041	-4.643930912
N	2.418638706	0.815002024	0.886903286
C	3.458190441	0.759516835	0.071052596
S	4.723875523	1.903938532	0.453286380
C	3.813321829	2.409998894	1.873348355
C	4.173305988	3.286746502	2.893324375
H	5.102555752	3.845772266	2.851346016
C	3.330044746	3.396409750	3.998610973
H	3.633801222	4.058590889	4.799914360
C	2.134889364	2.654762506	4.112440109
C	1.766558647	1.824642897	3.052430153
H	0.872914791	1.218795657	3.092693329
C	2.598022223	1.698931456	1.941211462
C	3.493896484	-0.293574989	-0.920793235
C	2.391971111	-1.183857799	-0.846614540
C	2.394911289	-2.307333946	-1.674631476
H	1.586312294	-3.026514292	-1.636557460
C	3.447387934	-2.517118931	-2.574720860
H	3.433660269	-3.397506237	-3.211984158
C	4.514616489	-1.616680384	-2.663862228
H	5.322499752	-1.792697668	-3.367079496
C	4.543761730	-0.504166603	-1.829128623
H	5.380810738	0.188012242	-1.872162700
C	1.262239099	2.663007498	5.379392147
C	1.773997307	3.656473637	6.437849522
H	1.117470980	3.636064529	7.313007832
H	1.788256645	4.683166504	6.057482243

H	2.782030821	3.400727510	6.780387878
C	-0.188664541	3.047415495	5.009556293
H	-0.822590172	3.038123846	5.902835846
H	-0.620627284	2.349801302	4.284174442
H	-0.229854614	4.050124645	4.571897507
C	1.280882716	1.241414309	5.994313240
H	0.661506832	1.208767176	6.897637844
H	2.299823284	0.951644063	6.271969795
H	0.902928352	0.487395793	5.295373440
C	0.440041155	1.726320982	-2.188100576
N	0.395307660	0.980998337	-1.303767323
C	-1.688349724	0.231602371	2.504802942
N	-0.837342381	0.146801114	1.724668980
C	0.508774757	2.643585682	-3.318549156
H	0.010524763	3.585194588	-3.071523190
H	1.555745602	2.844998360	-3.563991547
H	0.018330021	2.194862604	-4.187390804
C	-2.736524582	0.342529625	3.511479616
H	-3.581412315	-0.299337119	3.246191263
H	-2.341566563	0.032984007	4.483693600
H	-3.079437494	1.378725171	3.581169367
Rh	0.925386190	-0.547682285	0.368639529

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^{3}RhS

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N	-0.420030475	-2.368223190	-0.337891221
C	-0.054266330	-3.392483473	0.393289328
S	-0.496065527	-4.959660530	-0.279776901
C	-1.138904095	-4.142377853	-1.694499612
C	-1.662664533	-4.665408134	-2.874657869
H	-1.784275770	-5.735040665	-3.011812449
C	-1.999074817	-3.779146433	-3.896411657
H	-2.384066820	-4.198211193	-4.817957878
C	-1.833420873	-2.381632566	-3.775993109
C	-1.349356294	-1.876081347	-2.568144560
H	-1.196041465	-0.815693796	-2.413679361
C	-0.998384178	-2.745932341	-1.535343885
C	0.781987071	-3.206494331	1.574766159
C	1.396988750	-1.940758228	1.731993079
C	2.216336727	-1.721168518	2.843121767
H	2.697415590	-0.761474192	2.992370605
C	2.442234039	-2.745344400	3.767554283
H	3.099962950	-2.565891981	4.614062309
C	1.837185383	-3.996145725	3.608082533
H	2.014635563	-4.786546707	4.330480576
C	1.003745198	-4.223449230	2.517128468
H	0.520290852	-5.190045357	2.397482395
C	-2.091516495	-1.415984750	-4.944859028
C	-0.725716650	-0.858195662	-5.414743900
H	-0.863852859	-0.132064074	-6.224198341
H	-0.081810258	-1.661891580	-5.786491871
H	-0.192177057	-0.366075158	-4.594367981
C	-2.770430326	-2.110257387	-6.139395714
H	-2.955984354	-1.382224083	-6.934867382
H	-3.733102560	-2.548715830	-5.857006073
H	-2.142213821	-2.900706291	-6.562492847
C	-2.994708776	-0.249245435	-4.484131336
H	-3.179227114	0.437042952	-5.317749023
H	-2.542195559	0.329157263	-3.671284199
H	-3.962042570	-0.618080378	-4.128442287
N	2.597086668	0.955400229	1.110313177
C	3.720491171	0.559644639	0.555030406
S	5.165146351	1.252189517	1.284321308
C	4.149708748	2.088011742	2.452912569
C	4.496492863	2.886790037	3.540104866
H	5.531893730	3.135427237	3.749541998
C	3.477752924	3.337852001	4.379933834
H	3.761091709	3.939829350	5.234558105
C	2.119119406	3.019138575	4.164700985
C	1.790798068	2.254714727	3.043342829
H	0.769182384	1.973332405	2.822888851
C	2.794723511	1.788467765	2.195861101
C	3.714693308	-0.456032038	-0.492267936
C	2.499112129	-1.155875921	-0.696704447
C	2.461932659	-2.162184477	-1.664647341
H	1.551642060	-2.719083309	-1.848225951
C	3.602084637	-2.468338728	-2.415442467
H	3.556198835	-3.259019613	-3.159705877
C	4.795388699	-1.770930290	-2.214495420
H	5.676329136	-2.010671139	-2.801884413
C	4.851526737	-0.764676809	-1.255365729
H	5.777070999	-0.215504289	-1.102774024
C	1.004943490	3.411556482	5.151365280
C	1.501719117	4.368630886	6.250362873
H	0.674115539	4.629206657	6.917036533
H	1.894076943	5.299116135	5.827314377
H	2.283669710	3.912532568	6.865898132
C	-0.157099828	4.098054409	4.397753239
H	-0.952114820	4.372589111	5.099699974
H	-0.598059475	3.446509600	3.635373354
H	0.183125675	5.009956837	3.897108793
C	0.484957933	2.117817879	5.824401379
H	-0.328336418	2.347812653	6.522326946
H	1.282676697	1.619787455	6.385136127
H	0.110948943	1.403828502	5.082104683
C	0.341418922	1.637968898	-2.361801386
N	0.379675299	1.016475797	-1.385327697
C	-1.577719331	0.272889555	2.696115017
N	-0.832763016	0.181848645	1.814414740
C	0.280921638	2.409787655	-3.596624374
H	0.189959630	3.475629568	-3.368360043
H	1.190178633	2.241753578	-4.181330681
H	-0.583668053	2.090162516	-4.185871124
C	-2.498032808	0.390894711	3.819211960
H	-3.530067682	0.414320141	3.458581686
H	-2.369877815	-0.465149403	4.488292217
H	-2.286197662	1.309906602	4.373352528
Rh	0.894192159	-0.482773364	0.376677811

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^{1}IrS

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N	-0.313235790	-2.080615997	-0.024214048
C	-0.324622214	-2.900201559	1.020705104
S	-1.337356687	-4.306572914	0.804998696
C	-1.663347721	-3.799079180	-0.850145638
C	-2.350781918	-4.465729237	-1.860614300
H	-2.867539883	-5.399826527	-1.665625811
C	-2.317514181	-3.930425167	-3.147256136
H	-2.828596830	-4.473675251	-3.932257414
C	-1.612248182	-2.747298479	-3.453489542
C	-0.984050572	-2.061363459	-2.411737442
H	-0.402852029	-1.168710351	-2.592793703
C	-1.008662701	-2.580981970	-1.118474722
C	0.587791264	-2.624845028	2.105959415
C	1.419564247	-1.495338917	1.862648726
C	2.446345329	-1.247350216	2.780392885
H	3.127802372	-0.418943882	2.626201153
C	2.606824636	-2.056986809	3.909283400
H	3.411295652	-1.842188597	4.607876301
C	1.752783656	-3.140036106	4.153958321
H	1.889466882	-3.757608652	5.035838127
C	0.744417191	-3.432834864	3.243747473
H	0.093794458	-4.289032459	3.405115128
C	-1.427233934	-2.239061594	-4.893891811
C	0.064534850	-2.409600735	-5.275133133
H	0.242060125	-2.048830271	-6.294446468
H	0.355468363	-3.464501619	-5.233503342
H	0.724629819	-1.857180357	-4.597880840
C	-2.284809589	-3.020027876	-5.906003475
H	-2.136139631	-2.611245394	-6.909907341
H	-3.352278948	-2.950926065	-5.671855450
H	-2.007133961	-4.078251839	-5.942695618
C	-1.812749028	-0.745193183	-4.981883526
H	-1.682906389	-0.380738020	-6.006479740
H	-1.183990955	-0.130428866	-4.329626083
H	-2.857414484	-0.590178192	-4.692208290

N	2.268613338	1.087576509	0.648437560
C	3.280975103	1.078358769	-0.210610762
S	4.474646091	2.316704273	0.092588291
C	3.605222702	2.774516821	1.555456877
C	3.969897985	3.668757677	2.558240414
H	4.857996941	4.285216331	2.464171648
C	3.197596312	3.713031530	3.718248606
H	3.512357712	4.385890007	4.505628109
C	2.068576574	2.887527943	3.905660391
C	1.683685541	2.046943426	2.859411240
H	0.850277245	1.367614269	2.960734129
C	2.444685698	1.988167882	1.692651987
C	3.359393358	-0.018705539	-1.147634983
C	2.329289436	-0.983921111	-0.961461663
C	2.413558483	-2.161299467	-1.711743474
H	1.668754339	-2.939416647	-1.587515235
C	3.447276831	-2.350523949	-2.634211063
H	3.487635851	-3.274173737	-3.205661535
C	4.432014942	-1.374014854	-2.830723286
H	5.228088856	-1.535743475	-3.550310612
C	4.394456863	-0.206221908	-2.078032255
H	5.169603348	0.546792984	-2.198226690
C	1.309865594	2.800633907	5.241404533
C	1.795972347	3.844741106	6.262784958
H	1.215485930	3.757053137	7.186055660
H	1.674930096	4.866554260	5.888307571
H	2.848145008	3.695444107	6.525808334
C	-0.200835124	3.018946886	5.002448559
H	-0.747949421	2.950980902	5.948846340
H	-0.610957205	2.261973381	4.326111794
H	-0.392410249	4.004509926	4.565209389
C	1.538284302	1.388338089	5.834722042
H	1.002146721	1.282919168	6.784405708
H	2.602824450	1.216561675	6.025782108
H	1.193099618	0.598824441	5.159058571
C	-0.061140358	1.646267772	-2.256425142
N	0.135145113	0.911008298	-1.385133505
C	-1.778943896	0.606950223	2.136010885
N	-0.845796347	0.368139327	1.495951414
Ir	0.847974598	-0.380062491	0.275526285
C	-0.293706656	2.563743830	-3.364177942
H	0.576557755	2.562245369	-4.027658463
H	-1.174336672	2.249531031	-3.931613445
H	-0.451102048	3.577306032	-2.984193325
C	-2.945412397	0.905903280	2.955557585
H	-3.849726677	0.884003282	2.340719223
H	-3.034681082	0.160784930	3.751634836
H	-2.839296103	1.896656990	3.406388521

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^{3}IrS

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N	-0.380743921	-2.025059700	-0.047119804
C	-0.383346230	-2.960505247	1.033090830
S	-1.478371143	-4.323326588	0.732310057
C	-1.641114712	-3.775814056	-0.945013642
C	-2.262012720	-4.406264782	-2.006633043
H	-2.770584583	-5.355320930	-1.870839715
C	-2.197154999	-3.818473816	-3.281016827
H	-2.675558805	-4.339663982	-4.100884914
C	-1.507898569	-2.606107712	-3.522222757
C	-0.927096009	-1.955332518	-2.440583944
H	-0.351343155	-1.050557137	-2.570316792
C	-0.983853221	-2.518953562	-1.146882653
C	0.616672814	-2.809094667	1.980913997
C	1.443283558	-1.615255594	1.799268365
C	2.500584602	-1.407504678	2.676775217
H	3.142367363	-0.541654885	2.555562496
C	2.753164768	-2.301371336	3.727658033
H	3.581382036	-2.118258715	4.405733585
C	1.938835502	-3.447573662	3.911805391
H	2.154435158	-4.130246639	4.728723049
C	0.889994562	-3.709302187	3.060474634
H	0.279890507	-4.599049568	3.188138723
C	-1.296456695	-2.039877653	-4.937188625
C	0.202140287	-2.194044828	-5.295732975
H	0.398197591	-1.790068626	-6.294967175
H	0.494093657	-3.249514818	-5.293542862
H	0.847246230	-1.670603037	-4.582644939
C	-2.134205818	-2.779777050	-5.995559216
H	-1.976045728	-2.322813272	-6.976928711
H	-3.205349445	-2.730314970	-5.772926331
H	-1.846367359	-3.832681894	-6.079162121
C	-1.680786967	-0.542667568	-4.971341610
H	-1.539245129	-0.140752748	-5.980148792
H	-1.058594584	0.048672304	-4.291242599
H	-2.728988409	-0.398350507	-4.688570499
N	2.259686232	1.050863862	0.683408320
C	3.256675005	1.028566957	-0.191759482
S	4.465888023	2.257984400	0.076630734
C	3.598298073	2.775034428	1.518575072
C	3.946625710	3.734872341	2.464674711
H	4.836834431	4.343904018	2.344912767
C	3.141652822	3.871957779	3.594558954
H	3.434200764	4.606233120	4.334817410
C	1.997219205	3.074994802	3.806647301
C	1.645188451	2.145981073	2.825015068
H	0.792585313	1.494868040	2.945246220
C	2.436130047	1.995578647	1.687724471
C	3.302015781	-0.060030036	-1.140948415
C	2.251368284	-1.002367973	-0.966090977
C	2.315757990	-2.179424286	-1.718111634
H	1.567054510	-2.951644897	-1.589008451
C	3.343757868	-2.382988453	-2.645068884
H	3.367355347	-3.306354761	-3.217830181
C	4.342720985	-1.422561765	-2.840042114
H	5.133859634	-1.592094541	-3.563394547
C	4.329878330	-0.261201203	-2.074774265
H	5.121483326	0.474887282	-2.188274860
C	1.149969697	3.156772137	5.087419987
C	1.676976323	4.218199730	6.070399761
H	1.045033932	4.242077827	6.963546276
H	1.665273905	5.221374512	5.631330013
H	2.698062658	3.995866537	6.396972179
C	-0.305830896	3.518069029	4.713828564
H	-0.932229757	3.550917149	5.612127781
H	-0.737836003	2.785523176	4.023697853
H	-0.355155855	4.498303890	4.228597641
C	1.178409696	1.780279040	5.795001030
H	0.581060231	1.813126087	6.712823391
H	2.202238083	1.503745556	6.067160130
H	0.779313862	0.982061923	5.160305023
C	-0.226369590	1.796709895	-2.032409906
N	0.033876132	1.000332236	-1.234097004
C	-1.694574833	0.311091423	2.513867140
N	-0.847960532	0.221916139	1.730787516
Ir	0.806834459	-0.413979650	0.319567889
C	-0.549991667	2.783259153	-3.053847790
H	0.273578882	2.850263357	-3.771067381
H	-1.459291697	2.483528137	-3.582973242
H	-0.705515265	3.763398886	-2.594173431
C	-2.744782686	0.410840154	3.517700672
H	-3.704464674	0.636347175	3.043740273
H	-2.827722311	-0.539448321	4.054025650
H	-2.502464294	1.204567671	4.230669022

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C	-1.116748095	0.487937272	0.068502218
O	-0.808641255	-0.514546335	0.702414751
N	0.893651485	0.532315910	-1.387119412
C	1.219865441	1.064542770	-2.602018595
C	0.133570537	1.693319798	-3.165081501
H	-0.020805357	2.187739611	-4.112081051
C	-2.180159092	1.419181466	0.512035251
H	-2.281705379	2.363147974	-0.010317620
C	-2.994347572	1.104978681	1.536454439

H	-2.805808067	0.155755803	2.036163092
C	-0.379283130	0.829881847	-1.184846878
N	-0.896556497	1.548930287	-2.260558367
H	2.215151072	0.969559669	-3.013765097
C	-2.238486290	1.968031406	-2.501821280
C	-3.287421227	1.049340367	-2.406354427
C	-2.492743015	3.305934906	-2.816472292
C	-4.597925663	1.481168985	-2.604769468
H	-3.069760084	0.014323384	-2.166168213
C	-3.806233883	3.725179195	-3.030482054
H	-1.666329861	4.007470131	-2.869208574
C	-4.860981941	2.816731215	-2.918093681
H	-5.414343834	0.771235704	-2.516260624
H	-4.005184650	4.765209675	-3.271399498
H	-5.883450508	3.148148060	-3.072051048
C	-4.103319645	1.912120819	2.039998770
C	-4.661629677	1.598764420	3.292597055
C	-4.650641918	2.987887859	1.312307239
C	-5.710401058	2.349855900	3.818346262
H	-4.256659508	0.762739122	3.856880665
C	-5.700886726	3.733576775	1.836810827
H	-4.270150185	3.220735788	0.322993398
C	-6.231832981	3.422233105	3.093000174
H	-6.121905804	2.097351074	4.791257381
H	-6.115602016	4.557385921	1.262758374
H	-7.052014828	4.007706165	3.498505831

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C	1.253655553	0.047227357	-2.003616810
N	1.253512859	0.047232006	-3.163665056
C	1.253641725	0.047222812	-0.542453647
H	2.279430628	0.047229297	-0.162508652
H	0.740700126	-0.841138065	-0.162685499
H	0.740705132	0.935588062	-0.162701949

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C	-1.882208705	1.380021930	-0.108247057
C	-0.699654758	0.745020628	-0.029481621
C	0.585237324	1.542749286	0.008018168
C	-0.609314084	-0.733915269	0.022741122
C	-1.895012498	-1.531008363	-0.003180940
C	0.574348629	-1.369389653	0.081207030
H	-1.933127522	2.463990450	-0.146377295
H	-2.831426382	0.857278347	-0.138383731
H	0.382769644	2.616107225	-0.022485165
H	1.230442762	1.296241879	-0.843309462
H	1.158837557	1.330188751	0.917539299
H	-2.546590328	-1.263316154	0.836851954
H	-1.693646431	-2.603581667	0.052676957
H	-2.461141348	-1.340159059	-0.922523320
H	1.524010062	-0.846753001	0.097604886
H	0.625899673	-2.453491926	0.115928419

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^{1}Rh–1

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Rh	1.593413711	-1.095675588	0.094811670
N	0.817431688	-2.675305367	-1.043430924
C	0.635270536	-3.765655518	-0.312468022
S	-0.153587446	-5.073006630	-1.161557674
C	-0.247452796	-4.064329624	-2.595939159
C	-0.788355470	-4.361572266	-3.842589855
H	-1.240938783	-5.328026295	-4.040468693
C	-0.737864375	-3.386504412	-4.836000919
H	-1.165316224	-3.627145052	-5.801324368
C	-0.150354743	-2.123588800	-4.618727684
C	0.387446970	-1.846591115	-3.357525587
H	0.857915521	-0.897503793	-3.149052858
C	0.335808665	-2.804133654	-2.342032433
C	1.067792535	-3.769981146	1.066777945
C	1.624768734	-2.539120436	1.495685935
C	2.072190523	-2.451084375	2.817070961
H	2.512309551	-1.532312036	3.189345598
C	1.956076384	-3.546967268	3.679593086
H	2.310198545	-3.458441257	4.703692913
C	1.397182226	-4.755465031	3.245366096
H	1.315656781	-5.597218513	3.925620794
C	0.950822949	-4.869559765	1.933459997
H	0.515938163	-5.803503036	1.584933877
C	-0.083895124	-1.046697021	-5.717480183
C	1.394565701	-0.688074350	-5.995623112
H	1.459055066	0.071239047	-6.783188343
H	1.954855800	-1.568697691	-6.325763702
H	1.889350653	-0.288077742	-5.104444981
C	-0.732856214	-1.508968830	-7.035145283
H	-0.665324032	-0.709678531	-7.779918671
H	-1.793889523	-1.747087240	-6.903631210
H	-0.230451852	-2.388424873	-7.450425625
C	-0.830030441	0.215071142	-5.230658531
H	-0.808703184	0.999280334	-5.995898724
H	-0.369600415	0.622554958	-4.327428341
H	-1.878484011	-0.012796255	-5.008194923
C	-0.798014581	0.804719150	-0.331575930
O	-0.598127127	-0.265001118	0.286941767
N	1.400782466	0.576556861	-1.347594380
C	2.191062450	1.189720631	-2.272092342
C	1.481160641	2.224121332	-2.844789267
H	1.721969604	2.916648626	-3.636301994
C	-1.937993407	1.657456040	-0.058825005
H	-1.905559659	2.671214819	-0.431126922
C	-2.996798038	1.216762900	0.664014578
H	-2.968598127	0.182759151	1.004028559
N	2.455980539	0.271404862	1.376900434
C	3.756364346	0.407640100	1.185391784
S	4.493360996	1.611869216	2.216134548
C	2.927760601	1.904223561	2.969408512
C	2.586128473	2.767507553	4.009976864
H	3.321849346	3.427563906	4.458211899
C	1.276149511	2.747080564	4.476842403
H	1.018440247	3.417931557	5.288279057
C	0.290415972	1.878822803	3.950936794
C	0.643211544	1.044478416	2.890525341
H	-0.059740338	0.354537159	2.445812941
C	1.952165723	1.066472769	2.395289421
C	4.389266968	-0.466825217	0.221097142
C	3.499184370	-1.404998541	-0.368110240
C	4.006810665	-2.320941925	-1.290047884
H	3.350453854	-3.050075769	-1.753217936
C	5.365943909	-2.292581081	-1.626062036
H	5.751083851	-3.010076523	-2.345996618
C	6.236739635	-1.357723236	-1.050974607
H	7.287096024	-1.350144148	-1.323933840
C	5.750101089	-0.442638874	-0.122610316
H	6.418205261	0.283939123	0.333859265
C	-1.139534473	1.889673948	4.520777702
C	-1.123521447	2.062729836	6.056097507
H	-2.143790007	1.995285749	6.447557926
H	-0.726972222	3.033908606	6.365718365
H	-0.523889065	1.281805277	6.534331799
C	-1.908456445	3.071022034	3.883638144
H	-2.937391996	3.108947277	4.259030342
H	-1.950424790	2.965417147	2.795922995
H	-1.425550699	4.026461601	4.114716053
C	-1.882302284	0.575508893	4.205303669
H	-2.876813412	0.594906032	4.662508965
H	-1.342544436	-0.292002469	4.598848820
H	-2.021571875	0.427377760	3.131816387
C	0.230215907	1.215050697	-1.314829707
N	0.242239460	2.238118172	-2.240201950
H	3.195357561	0.847388446	-2.471862316
C	-0.821587920	3.121232510	-2.627480030
C	-2.046410561	2.593732834	-3.045260429
C	-0.603853345	4.498816490	-2.586768866
C	-3.069187641	3.464437723	-3.415226221
H	-2.194444418	1.520749927	-3.066867352

C	-1.631945729	5.360912323	-2.970927477
H	0.350391537	4.885612011	-2.242320299
C	-2.863121510	4.846299171	-3.381826162
H	-4.025145531	3.061514378	-3.735286713
H	-1.471529245	6.434123039	-2.939869642
H	-3.661798477	5.520586491	-3.675902605
C	-4.162857533	1.994950652	1.042004108
C	-5.076757908	1.431417823	1.954889774
C	-4.401898384	3.300400257	0.560243964
C	-6.182748318	2.153433084	2.393031836
H	-4.900830746	0.426426083	2.329551697
C	-5.510052204	4.015122414	0.995478272
H	-3.731134415	3.746453285	-0.167096555
C	-6.399958134	3.447641373	1.916052103
H	-6.874231339	1.710124016	3.103151321
H	-5.688690186	5.017977715	0.619005024
H	-7.263129234	4.013344765	2.254820585

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^{3}Rh–1

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Rh	1.528873801	-1.169805646	0.277152687
N	0.650143087	-2.658999681	-0.866000950
C	0.558440328	-3.816265583	-0.231241122
S	-0.258481801	-5.059305668	-1.143614292
C	-0.546230137	-3.900327921	-2.436052322
C	-1.247481585	-4.054275990	-3.629485369
H	-1.682335615	-5.008924961	-3.906671524
C	-1.403450966	-2.940012932	-4.452725410
H	-1.969046593	-3.065514326	-5.368023396
C	-0.868874907	-1.674669623	-4.124016762
C	-0.135162488	-1.553941488	-2.945234299
H	0.303691536	-0.615085661	-2.651657581
C	0.018234717	-2.650846004	-2.097677231
C	1.040292978	-3.877283573	1.131299973
C	1.517756939	-2.625953436	1.625112414
C	1.951772928	-2.550251007	2.957502842
H	2.320858002	-1.612702370	3.359080076
C	1.909926295	-3.683418512	3.768758059
H	2.244033098	-3.620063305	4.800601482
C	1.447053313	-4.909944057	3.267475128
H	1.428210735	-5.784087658	3.910828114
C	1.006727457	-5.011294365	1.949136138
H	0.638143122	-5.959704399	1.567134619
C	-1.096954346	-0.417102188	-4.981313229
C	0.265902340	0.207559019	-5.363732338
H	0.109058321	1.099551439	-5.981147289
H	0.875263095	-0.497246921	-5.939269066
H	0.843459427	0.511347830	-4.484552860
C	-1.875123143	-0.723214388	-6.273292065
H	-2.004695654	0.195939139	-6.853102684
H	-2.874386311	-1.118368506	-6.062448978
H	-1.344466209	-1.441882014	-6.906842232
C	-1.911017179	0.603244603	-4.147822380
H	-2.086663723	1.513693333	-4.732487679
H	-1.391565681	0.887021661	-3.227209330
H	-2.885066748	0.192447409	-3.862797737
C	-0.528176606	0.897276819	-0.320455015
O	-0.388968199	-0.257018149	0.322935671
N	1.673578382	0.481377840	-1.190673709
C	2.614443541	1.079326272	-1.990082502
C	2.142099142	2.303258896	-2.383040190
H	2.566649675	3.083051205	-2.995568037
C	-1.726270318	1.624397278	-0.241807565
H	-1.752698421	2.580606222	-0.744199693
C	-2.845040321	1.199971676	0.456113666
H	-2.829722643	0.194634095	0.870516956
N	2.519555569	0.166625023	1.503181458
C	3.826747179	0.160969839	1.311562896
S	4.666575432	1.404630661	2.199847460
C	3.129265308	1.956868887	2.854916334
C	2.863529682	3.002356529	3.737395287
H	3.660207987	3.628264427	4.126035213
C	1.542058229	3.224130869	4.110215187
H	1.343241453	4.043345451	4.790417671
C	0.467498720	2.428370714	3.645572186
C	0.752800465	1.384308457	2.764194965
H	-0.019507529	0.741799831	2.364642143
C	2.075835705	1.157383800	2.365756989
C	4.377102852	-0.811323404	0.386858523
C	3.411586761	-1.646612525	-0.237394243
C	3.826037884	-2.587718010	-1.178015471
H	3.098722458	-3.215410233	-1.682175159
C	5.187184334	-2.718580484	-1.473074913
H	5.509594917	-3.458338976	-2.200683355
C	6.138955116	-1.906690121	-0.843578219
H	7.191462517	-2.017974854	-1.084650040
C	5.738894463	-0.950512767	0.086730309
H	6.477024555	-0.315746188	0.570531487
C	-0.983023703	2.756682396	4.045081615
C	-1.055290818	3.355692148	5.466036797
H	-2.102106333	3.498119831	5.751826763
H	-0.571593344	4.334815979	5.535342216
H	-0.590705156	2.691706419	6.202829361
C	-1.528797984	3.787169456	3.025286198
H	-2.569919586	4.040555000	3.252377272
H	-1.498828292	3.381092072	2.010144949
H	-0.938243628	4.710227489	3.046890974
C	-1.874134541	1.498361707	4.012547970
H	-2.881971121	1.751560211	4.355369568
H	-1.478017449	0.713447273	4.665705681
H	-1.975994349	1.092865467	3.004108429
C	0.630814493	1.319154143	-1.072091103
N	0.888914585	2.455977917	-1.802605748
H	3.548341274	0.592673898	-2.226561546
C	0.121093512	3.663863659	-1.838951945
C	0.032152195	4.443013668	-0.682516336
C	-0.541356385	4.026757717	-3.010897398
C	-0.747005939	5.598520756	-0.700944960
H	0.545112669	4.123501301	0.219916970
C	-1.309862375	5.192571163	-3.022705317
H	-0.467501462	3.390810251	-3.887542963
C	-1.416610479	5.973694324	-1.870042443
H	-0.831723213	6.204748154	0.196135417
H	-1.833418250	5.483024597	-3.928609848
H	-2.023207188	6.874566555	-1.880970359
C	-4.018703938	2.000524998	0.691828072
C	-5.139590740	1.407756805	1.323059320
C	-4.100546360	3.377450228	0.354998231
C	-6.287160397	2.141564608	1.590065122
H	-5.090497494	0.356930882	1.597756028
C	-5.252370358	4.103747845	0.621419311
H	-3.252872705	3.879321814	-0.099554494
C	-6.353278160	3.494503498	1.237782598
H	-7.134316444	1.663375020	2.073549747
H	-5.296875477	5.156662941	0.356627047
H	-7.250240326	4.070205688	1.445910454

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^{3}Rh–1–TS

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Rh	1.211543679	-1.796411753	-0.185524628
N	0.217624217	-2.893134356	-1.652030945
C	-0.027322620	-4.138963223	-1.272145748
S	-0.951680243	-5.063119411	-2.434926510
C	-1.029146671	-3.650254965	-3.476063967
C	-1.684424400	-3.485358715	-4.696877956
H	-2.222817659	-4.306889057	-5.158571243
C	-1.648931742	-2.233837843	-5.299320698
H	-2.173399448	-2.103741169	-6.240259171
C	-0.962181151	-1.137245417	-4.727547646
C	-0.282498956	-1.332859278	-3.526296139
H	0.275177568	-0.542978764	-3.050536156
C	-0.330996275	-2.578385592	-2.887274027
C	0.441869706	-4.576517582	0.021324897
C	1.104680419	-3.562013626	0.759517610
C	1.573810697	-3.878585577	2.036951780
H	2.085330963	-3.130128145	2.633640766

C	1.385750055	-5.162457943	2.558621645
H	1.756648540	-5.394695282	3.553905725
C	0.731588840	-6.155712128	1.818567991
H	0.597383559	-7.148304939	2.237150908
C	0.254637539	-5.865541935	0.546321094
H	-0.258780748	-6.629978657	-0.032470465
C	-1.014817953	0.232300833	-5.425356388
C	-0.357274979	0.128842935	-6.820390701
H	-0.400255561	1.095456600	-7.334505558
H	-0.862708032	-0.606551528	-7.453138351
H	0.693572521	-0.166712508	-6.735656738
C	-2.492217302	0.668699622	-5.579867840
H	-2.548721790	1.652943969	-6.057932377
H	-2.986390591	0.733609378	-4.604300976
H	-3.065630913	-0.029256541	-6.196192265
C	-0.279807448	1.318658710	-4.618554592
H	-0.357766747	2.280050755	-5.137068272
H	0.784790516	1.095857620	-4.497546196
H	-0.714614928	1.440283895	-3.620197535
C	-1.024340510	0.277251631	-0.049184173
O	-0.838269353	-0.911098182	0.350528330
N	1.185465693	0.229264095	-1.063684106
C	2.089052200	1.077242494	-1.635218859
C	1.554969192	2.344717026	-1.649468064
H	1.940195203	3.290864706	-1.996670604
C	-2.304936409	0.922145665	0.085870117
H	-2.343151093	1.971016169	-0.166371241
C	-3.238012314	0.435727715	1.074864984
H	-3.134890795	-0.604515374	1.364853740
N	2.320390463	-0.912089169	1.329899549
C	3.622660637	-0.984543979	1.112386346
S	4.584986687	-0.137304813	2.300609589
C	3.109461784	0.341753900	3.132144451
C	2.951540947	1.104748964	4.286034584
H	3.809443474	1.511310577	4.811944008
C	1.660269141	1.332361698	4.755746841
H	1.548380971	1.927357435	5.653881073
C	0.516582966	0.809373975	4.113655567
C	0.695783079	0.043933209	2.957084894
H	-0.139417410	-0.395682186	2.430406809
C	1.984084606	-0.181380823	2.461855412
C	4.083426476	-1.712344766	-0.049844943
C	3.035541296	-2.271019459	-0.828948319
C	3.373862743	-2.988438606	-1.978268623
H	2.598005533	-3.431890726	-2.593853712
C	4.716512203	-3.136514664	-2.343464613
H	4.965752602	-3.697596312	-3.240595579
C	5.743998051	-2.577297688	-1.572602272
H	6.780116558	-2.702651501	-1.870144248
C	5.429180145	-1.863095284	-0.421719164
H	6.219016552	-1.425505877	0.184437081
C	-0.904950678	1.115494013	4.621181488
C	-0.909316897	1.595904350	6.086014748
H	-1.941055179	1.729924440	6.425707340
H	-0.404306442	2.559629202	6.208083630
H	-0.428422004	0.869518518	6.749573231
C	-1.496355653	2.234633207	3.731245518
H	-2.520407438	2.477181673	4.035065651
H	-1.528786778	1.925947666	2.682903528
H	-0.892035484	3.146649122	3.802855015
C	-1.801439404	-0.140114650	4.528271675
H	-2.804868937	0.090017147	4.902074814
H	-1.390923500	-0.959592104	5.127405643
H	-1.915127635	-0.494233042	3.500455856
C	0.109319948	0.939908266	-0.718692899
N	0.306482077	2.256324768	-1.070584655
H	3.046643019	0.726530552	-1.989381909
C	-0.522304177	3.389322996	-0.771580696
C	-1.275535822	3.982614756	-1.784293771
C	-0.562542558	3.862253904	0.541166544
C	-2.092779160	5.069737911	-1.468911409
H	-1.225747943	3.589872360	-2.794923067
C	-1.387265444	4.944033146	0.845924258
H	0.028583618	3.371113539	1.307619095
C	-2.150780916	5.547276497	-0.157609507
H	-2.685503960	5.540472984	-2.247233868
H	-1.435684443	5.311207294	1.866385937
H	-2.791217804	6.390575886	0.082999349
C	-4.264821053	1.204303980	1.677805066
C	-5.182367802	0.562978923	2.557911634
C	-4.423364639	2.605415821	1.469219089
C	-6.197701454	1.273171663	3.178393364
H	-5.075761318	-0.504049778	2.734450340
C	-5.443163872	3.304749250	2.095956087
H	-3.729566097	3.144041777	0.831371188
C	-6.339850426	2.648954630	2.951142073
H	-6.886014938	0.760163486	3.844008207
H	-5.543375969	4.373409271	1.926245928
H	-7.135001183	3.204510212	3.438994884
C	-3.118294001	0.249045506	-1.796646476
C	-4.060313702	-0.730120838	-1.405226111
H	-3.458175898	1.230592132	-2.108637094
H	-2.203482628	-0.089627340	-2.268679142
C	-5.436382294	-0.380120724	-1.142805338
C	-3.570666790	-2.140165806	-1.197685003
C	-5.918155670	1.025223017	-1.443175316
C	-6.314682961	-1.298325658	-0.645640075
H	-4.066580296	-2.833003044	-1.888127804
H	-2.494309902	-2.210329294	-1.346909642
H	-3.782476902	-2.488533020	-0.181187689
H	-5.770311356	1.280161023	-2.498957872
H	-6.982174873	1.128608942	-1.219171762
H	-5.385829449	1.769161701	-0.842465043
H	-6.028930664	-2.316813946	-0.408655375
H	-7.351250648	-1.034900308	-0.462135375

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^{3}Rh–2

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Rh	1.248246908	-1.788509727	-0.192045063
N	0.268993735	-2.858890533	-1.684386492
C	0.036798064	-4.117887020	-1.340619326
S	-0.903607547	-5.006532192	-2.513908863
C	-1.022829652	-3.556473494	-3.499057293
C	-1.716562271	-3.349086285	-4.692188263
H	-2.266748190	-4.154803276	-5.167430878
C	-1.707960486	-2.074756861	-5.245390415
H	-2.267973185	-1.910521150	-6.160068989
C	-1.007334232	-0.996135056	-4.655410767
C	-0.284710884	-1.235123634	-3.488471508
H	0.290117294	-0.461604685	-3.007569075
C	-0.312171847	-2.502763033	-2.893410921
C	0.511077046	-4.582219601	-0.056874748
C	1.158555627	-3.579506636	0.710478902
C	1.622176886	-3.919193268	1.983100414
H	2.124735594	-3.181315184	2.599867821
C	1.439294577	-5.215769291	2.475957870
H	1.804295778	-5.466315269	3.468823195
C	0.798263788	-6.196328163	1.709659696
H	0.666401267	-7.198264599	2.105875731
C	0.328889757	-5.882273674	0.439561278
H	-0.176309302	-6.636795998	-0.158962190
C	-1.094644547	0.401394516	-5.292205811
C	-0.505439878	0.358503550	-6.720655441
H	-0.577815831	1.344639421	-7.192671776
H	-1.038032889	-0.353609055	-7.357671738
H	0.549652040	0.066408269	-6.699345589
C	-2.579018116	0.837685943	-5.353678703
H	-2.662593603	1.836467147	-5.796336651
H	-3.018499136	0.871268809	-4.350769520
H	-3.183976412	0.157544896	-5.959516525
C	-0.326981574	1.460368633	-4.478269100
H	-0.421303749	2.436972141	-4.965240002
H	0.741085470	1.231864452	-4.403559208
H	-0.730178416	1.555730104	-3.463918924
C	-1.084580541	0.238248035	-0.264977068
O	-0.902000785	-0.883602738	0.234392643

N	1.221477509	0.262094200	-1.025035262
C	2.147830486	1.132882714	-1.511242747
C	1.604006052	2.400437355	-1.508664608
H	2.014563799	3.364277601	-1.767481565
C	-2.480233908	0.770482123	-0.482370317
H	-2.403218985	1.742200971	-0.972711980
C	-3.180213690	0.891395330	0.835801363
H	-3.061204672	0.046071645	1.506492257
N	2.334212542	-0.934877336	1.349997759
C	3.639802456	-1.003895283	1.153167129
S	4.582323074	-0.238303393	2.408854723
C	3.093157530	0.186255857	3.246662378
C	2.916727781	0.853123188	4.455937386
H	3.764972210	1.218605161	5.025820732
C	1.618707299	1.029332042	4.927188396
H	1.492976069	1.541510582	5.872957230
C	0.484162092	0.556860447	4.230469704
C	0.680104792	-0.095234022	3.008464575
H	-0.147316590	-0.485854983	2.430559158
C	1.978112936	-0.281802535	2.520884037
C	4.111996651	-1.687502980	-0.031087447
C	3.073391914	-2.232041121	-0.831461370
C	3.413518190	-2.924274445	-1.994277596
H	2.641210556	-3.356906891	-2.621001959
C	4.758675575	-3.058003187	-2.356162786
H	5.014871120	-3.598056078	-3.264012575
C	5.778833389	-2.511553764	-1.567548871
H	6.816735268	-2.626157284	-1.863677263
C	5.459148884	-1.825218797	-0.401249707
H	6.245457172	-1.400575757	0.218470275
C	-0.939357519	0.787772357	4.771144390
C	-0.939801395	1.115123391	6.278007507
H	-1.970804334	1.188837171	6.637393475
H	-0.457087010	2.073782444	6.493489265
H	-0.435636759	0.336970776	6.860535145
C	-1.559636712	1.980261922	4.007195473
H	-2.563529968	2.205587149	4.382411003
H	-1.654288530	1.758143187	2.940618038
H	-0.944165587	2.880038261	4.121915817
C	-1.814605236	-0.468280494	4.556704044
H	-2.814298153	-0.301820248	4.972680569
H	-1.380813003	-1.340538144	5.056556225
H	-1.940022469	-0.716092110	3.498487473
C	0.116185412	0.955308616	-0.737130344
N	0.323928416	2.283876657	-1.021653175
H	3.128244877	0.802199125	-1.819694519
C	-0.490484774	3.401910067	-0.636578023
C	-0.951445222	4.291321754	-1.605877042
C	-0.755222797	3.593123436	0.720542073
C	-1.690107822	5.403801441	-1.197592497
H	-0.738636613	4.108686924	-2.654764175
C	-1.505930901	4.698327065	1.112530947
H	-0.366915554	2.890591145	1.450457931
C	-1.965703964	5.606717110	0.156136468
H	-2.054168701	6.107621670	-1.939797521
H	-1.731954932	4.846636772	2.163647652
H	-2.547697783	6.469019890	0.466664046
C	-4.069480896	1.922792196	1.209008336
C	-4.762109756	1.820375800	2.451930285
C	-4.336266994	3.066144943	0.402622968
C	-5.654998302	2.797233105	2.858513355
H	-4.582151890	0.950150490	3.077352762
C	-5.232802868	4.037875652	0.821465433
H	-3.824975252	3.192734241	-0.546261668
C	-5.898393154	3.915626526	2.047838449
H	-6.172695160	2.693448067	3.808032751
H	-5.418701172	4.902283192	0.189883024
H	-6.600959301	4.679470062	2.367318153
C	-3.288826466	-0.193988621	-1.485957384
C	-4.040599346	-1.310853362	-0.816475451
H	-3.973341227	0.470995337	-2.017667532
H	-2.582042217	-0.586486459	-2.225037098
C	-5.407352448	-1.167875051	-0.455037117
C	-3.280829906	-2.563516617	-0.465914071
C	-6.208357334	0.029265016	-0.943474233
C	-6.051038742	-2.103954792	0.328370839
H	-3.873076916	-3.461459637	-0.672280133
H	-2.352011204	-2.629327774	-1.031931877
H	-2.998127222	-2.594782829	0.595704079
H	-6.206103802	0.092355974	-2.038305998
H	-7.250474930	-0.044232108	-0.622917235
H	-5.815677166	0.975257516	-0.559938014
H	-5.548421860	-2.976042032	0.730782270
H	-7.099350929	-1.990403175	0.584187627

^{1}Rh–3

Rh	1.212285995	-1.773177147	-0.181968451
N	0.137520447	-2.842390776	-1.626387358
C	-0.214574575	-4.044165134	-1.191791654
S	-1.350432158	-4.870561123	-2.230596781
C	-1.377141237	-3.471181393	-3.290208340
C	-2.134010792	-3.250046492	-4.441017628
H	-2.808269262	-4.009986401	-4.822919369
C	-2.020441294	-2.019247770	-5.075341225
H	-2.624230862	-1.842031717	-5.958948612
C	-1.155741215	-1.002429843	-4.607286930
C	-0.375298738	-1.260675550	-3.480576277
H	0.320928484	-0.535098612	-3.091179848
C	-0.501318693	-2.480729580	-2.805253267
C	0.281431884	-4.497467041	0.087307245
C	1.030881643	-3.521066427	0.791305304
C	1.517819643	-3.852688313	2.057727098
H	2.096508265	-3.135583401	2.630192041
C	1.262088060	-5.115095139	2.602922678
H	1.648397803	-5.358808994	3.589334965
C	0.520601928	-6.070403576	1.897881269
H	0.332585067	-7.046437740	2.334103823
C	0.024230842	-5.763478279	0.636885643
H	-0.557320952	-6.498129845	0.084725156
C	-1.107348680	0.345782042	-5.345823765
C	-0.493857861	0.130152375	-6.748295307
H	-0.457739830	1.075776339	-7.300595760
H	-1.083527327	-0.579183400	-7.337087154
H	0.525651455	-0.261976153	-6.672540665
C	-2.538006067	0.920076728	-5.493372917
H	-2.502451420	1.886709094	-6.007776737
H	-3.006541252	1.072620988	-4.515845299
H	-3.191002131	0.265499324	-6.077192783
C	-0.261893570	1.385619879	-4.587314606
H	-0.283959448	2.340488434	-5.123098850
H	0.787284374	1.086031795	-4.498639107
H	-0.657449603	1.554261923	-3.579762459
C	-0.996863663	0.365014672	-0.279009193
O	-0.858504355	-0.776913226	0.190875128
N	1.287274122	0.256389350	-1.094090104
C	2.234396458	1.067371249	-1.637455225
C	1.736567020	2.354655504	-1.689613581
H	2.173166752	3.286290407	-2.015590191
C	-2.347068310	0.985607266	-0.413162649
H	-2.267452002	2.067979097	-0.376301646
C	-3.453484297	0.362223506	0.476722240
H	-3.050407887	-0.431580961	1.111942768
N	2.282729387	-0.921653867	1.359549165
C	3.590852737	-1.050240636	1.220669508
S	4.507202148	-0.300823987	2.506652832
C	3.000106335	0.204187423	3.269657850
C	2.791247845	0.909487784	4.452513695
H	3.625151396	1.249523401	5.058160305
C	1.479229450	1.167094946	4.848069668
H	1.329789758	1.715446711	5.770178795
C	0.362109363	0.731983423	4.101906776
C	0.594058037	0.020173289	2.922044992
H	-0.222492129	-0.357468933	2.324873447
C	1.901976109	-0.234860823	2.502385378
C	4.074179649	-1.789436221	0.073692217

C	3.037434816	-2.316921234	-0.742601752
C	3.383387566	-3.065376282	-1.867491245
H	2.609405756	-3.489435196	-2.499130726
C	4.732533932	-3.268474579	-2.180726767
H	4.993041992	-3.852205276	-3.059874535
C	5.751463413	-2.737044811	-1.379370093
H	6.791881084	-2.906013727	-1.637515783
C	5.424973965	-1.996851683	-0.247680694
H	6.208783150	-1.583907843	0.382973045
C	-1.085222363	1.066699028	4.511293888
C	-1.175609708	1.609393597	5.949494362
H	-2.224485159	1.777796507	6.211820126
H	-0.656605661	2.566947937	6.062459469
H	-0.758019686	0.902716994	6.674269199
C	-1.618887663	2.147374153	3.541629076
H	-2.653909683	2.412806273	3.779584408
H	-1.605983496	1.791720033	2.506970406
H	-1.008614302	3.056989431	3.598257542
C	-1.983425140	-0.188633338	4.415685654
H	-3.010044813	0.066544928	4.697898388
H	-1.627026796	-0.978489578	5.085097790
H	-2.023180485	-0.597844601	3.401754856
C	0.216801539	1.006569743	-0.815469742
N	0.466034055	2.311025381	-1.172919750
H	3.196274996	0.686827838	-1.946991801
C	-0.330587029	3.472414017	-0.880317569
C	-0.921355605	4.189320564	-1.919325113
C	-0.488199592	3.849480152	0.454934567
C	-1.693783998	5.309519768	-1.606803775
H	-0.788692296	3.864848614	-2.946312189
C	-1.270091772	4.963411808	0.754118741
H	-0.016332990	3.267105341	1.240184784
C	-1.870206714	5.693638325	-0.275452793
H	-2.163694859	5.876614094	-2.404408932
H	-1.411933303	5.256191730	1.789728403
H	-2.477972746	6.561997414	-0.039688744
C	-4.272905827	1.286424518	1.343015313
C	-5.108872414	0.702787638	2.307216167
C	-4.248714924	2.683457136	1.247064233
C	-5.892224789	1.486730933	3.151031971
H	-5.139902115	-0.380220503	2.394754887
C	-5.028584957	3.473500252	2.094403744
H	-3.615289927	3.179348707	0.518498600
C	-5.852687836	2.879659891	3.049577475
H	-6.531033993	1.011698008	3.890488863
H	-4.989152431	4.555937767	2.005341768
H	-6.458910465	3.493925810	3.709121466
C	-3.105721712	0.488607079	-1.703252912
C	-4.129358292	-0.298803985	-0.820425212
H	-3.514448643	1.336318851	-2.253920317
H	-2.524476051	-0.129422367	-2.390070677
C	-5.605204105	0.013250835	-1.023206711
C	-3.821765900	-1.802899003	-0.866496444
C	-5.976140499	1.367812037	-1.581958652
C	-6.567558765	-0.855253994	-0.685579836
H	-4.136422157	-2.227433681	-1.824936509
H	-2.750758648	-1.981108785	-0.744030356
H	-4.333382130	-2.341871738	-0.063608952
H	-5.677555084	1.463708758	-2.633820057
H	-7.055293083	1.531674862	-1.530261278
H	-5.490658283	2.178669691	-1.029089689
H	-6.365081310	-1.844479918	-0.290875942
H	-7.616570473	-0.593897104	-0.792030990

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^{3}Rh–1'–TS

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Rh	1.804737449	-4.754946709	1.635438204
N	0.465489954	-6.325683594	1.282419562
C	0.185334817	-6.978895664	2.399753332
S	-1.205885172	-8.033529282	2.275478601
C	-1.418660879	-7.531899452	0.603805065
C	-2.400858641	-7.901822090	-0.308820099
H	-3.185924292	-8.600055695	-0.036964312
C	-2.364683867	-7.341094017	-1.583663702
H	-3.148062468	-7.618374348	-2.277602911
C	-1.357464075	-6.438606262	-1.979626298
C	-0.373617798	-6.086841583	-1.049539924
H	0.431090236	-5.411808968	-1.305444956
C	-0.410643667	-6.612389088	0.243949398
C	0.986858308	-6.726334095	3.576636076
C	1.926147699	-5.676531315	3.409547329
C	2.754668236	-5.356765747	4.487888336
H	3.489283562	-4.562879086	4.394371986
C	2.642706156	-6.055477619	5.694697380
H	3.296854734	-5.797472954	6.524012089
C	1.705080509	-7.085209846	5.851153374
H	1.632459998	-7.619096756	6.793436527
C	0.872099221	-7.423911572	4.790328503
H	0.144167423	-8.224623680	4.900586128
C	-1.297439694	-5.854593277	-3.402267218
C	-0.042432372	-6.406197548	-4.117688656
H	0.020602459	-6.012047768	-5.138346195
H	-0.078050733	-7.498752594	-4.177527905
H	0.875346839	-6.127668381	-3.589326620
C	-2.543841600	-6.214038372	-4.232850552
H	-2.474720716	-5.749126434	-5.221421719
H	-3.462405443	-5.855665684	-3.755212307
H	-2.633239985	-7.293956757	-4.388743401
C	-1.205361366	-4.314488411	-3.327509880
H	-1.190136909	-3.888906240	-4.337889671
H	-0.298372298	-3.981707096	-2.816045046
H	-2.069932938	-3.905797005	-2.795556307
C	-0.627990067	-3.111270189	0.832363784
O	-0.266663492	-3.657258034	1.918167233
N	1.527521849	-3.513185740	-0.171701252
C	2.265092611	-3.125146866	-1.255788684
C	1.608442307	-2.103742123	-1.897362471
H	1.859901428	-1.502733231	-2.757529259
C	-1.994859576	-3.071640491	0.396648616
H	-2.173966885	-2.584766150	-0.553595603
C	-2.890256643	-4.126013756	0.797075391
H	-2.604038477	-4.698279858	1.673353910
N	3.173147917	-3.292301893	2.105758190
C	4.382430077	-3.535631418	1.632145166
S	5.479066849	-2.181782722	1.795797825
C	4.186417103	-1.242585421	2.540688753
C	4.184742451	0.072580054	3.006142378
H	5.069704056	0.696862876	2.934571505
C	3.012598276	0.567749381	3.568725109
H	3.014021397	1.592545033	3.923460722
C	1.838677883	-0.211993173	3.701494217
C	1.851876020	-1.517458320	3.211711407
H	0.990614831	-2.169709444	3.261480808
C	3.019633770	-2.023973465	2.632679224
C	4.611275673	-4.827140331	1.023093343
C	3.452795744	-5.650514126	0.991141558
C	3.547912359	-6.919581413	0.419096351
H	2.678851366	-7.568614006	0.387586176
C	4.765788078	-7.352239132	-0.116139874
H	4.832356930	-8.342625618	-0.559411407
C	5.901434898	-6.531604290	-0.090251550
H	6.837207317	-6.884369373	-0.512688160
C	5.828933716	-5.265414238	0.479416937
H	6.705579281	-4.622016430	0.503726959
C	0.577412188	0.395802408	4.338482380
C	0.937553048	1.220689654	5.594604969
H	0.023419101	1.583014369	6.076563358
H	1.546551228	2.098239899	5.358996868
H	1.486682296	0.612169266	6.320106030
C	-0.104886077	1.319638014	3.300505161
H	-0.986411929	1.804979324	3.734903574
H	-0.433960319	0.745420396	2.427341700
H	0.578008235	2.102940321	2.954047203
C	-0.418414831	-0.701558411	4.759442806
H	-1.303037047	-0.247992173	5.218019485
H	0.026388263	-1.390871882	5.484261513

H	-0.751911223	-1.287628174	3.900428057
C	0.432289004	-2.754993916	-0.129852369
N	0.443284929	-1.875948906	-1.183440208
H	3.206259012	-3.597430944	-1.494765162
C	-0.443821341	-0.774900615	-1.407489538
C	-1.278231502	-0.765524387	-2.525458574
C	-0.424877912	0.292194873	-0.506690621
C	-2.118479013	0.329865277	-2.733087301
H	-1.268371820	-1.604119778	-3.212874889
C	-1.272348881	1.378993869	-0.719850481
H	0.255088359	0.262859106	0.339472234
C	-2.118486881	1.398095727	-1.832519412
H	-2.772112846	0.348385543	-3.600128412
H	-1.262646317	2.212715864	-0.024123978
H	-2.771938324	2.248795271	-2.002095699
C	-4.046241283	-4.513741493	0.081970237
C	-4.848087788	-5.581438065	0.582278728
C	-4.449731350	-3.916038990	-1.151208758
C	-5.964275360	-6.027214527	-0.104885936
H	-4.558498383	-6.051158905	1.517863750
C	-5.567898273	-4.373565674	-1.831708789
H	-3.872315407	-3.101339579	-1.574958801
C	-6.334666252	-5.430696011	-1.319382548
H	-6.555130959	-6.844706535	0.299020022
H	-5.850685596	-3.908872604	-2.772568703
H	-7.208702087	-5.783143520	-1.858697891
C	-2.713197470	-1.361741781	1.698291063
C	-4.098987579	-1.475924492	1.593352795
H	-2.206072330	-1.737850666	2.575819969
H	-2.188532352	-0.617860973	1.111297607
C	-4.848453999	-2.279696465	2.541936159
C	-4.793027401	-0.824722588	0.426453203
C	-4.155247688	-2.796877384	3.786615849
C	-6.160151958	-2.571589947	2.329209566
H	-5.598201275	-0.162618518	0.764169514
H	-4.093690395	-0.238484487	-0.175345287
H	-5.249403954	-1.579232216	-0.225479394
H	-3.729755402	-1.976347685	4.375570774
H	-4.854687214	-3.340799332	4.425487518
H	-3.332021713	-3.475069284	3.538683414
H	-6.699909687	-2.241842270	1.449478626
H	-6.719395638	-3.175367594	3.036685467

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^{3}Rh–2'

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Rh	1.772981167	-4.782521248	1.654557228
N	0.548501372	-6.445988178	1.382841229
C	0.454719096	-7.185852528	2.477829695
S	-0.690290451	-8.499573708	2.347790718
C	-1.063243389	-7.994523048	0.705460191
C	-1.965772271	-8.538549423	-0.206264839
H	-2.564976454	-9.406965256	0.048755132
C	-2.088083744	-7.935979843	-1.455405951
H	-2.804111481	-8.355564117	-2.150989771
C	-1.321821690	-6.811508656	-1.832754970
C	-0.404632330	-6.299270630	-0.913156152
H	0.228739530	-5.460583687	-1.155672908
C	-0.285362273	-6.871193409	0.357019842
C	1.256558895	-6.828895092	3.626723289
C	2.035145998	-5.658517838	3.438416004
C	2.843562126	-5.225256920	4.490911007
H	3.457809448	-4.337334156	4.380263805
C	2.867696762	-5.933779716	5.696929455
H	3.502277136	-5.586872101	6.508493900
C	2.092417240	-7.086067200	5.872605324
H	2.124904633	-7.626603127	6.813341618
C	1.281640410	-7.537992477	4.837659359
H	0.675984979	-8.431833267	4.967831135
C	-1.443400860	-6.194601536	-3.237418652
C	-0.339752913	-6.807919979	-4.131909370
H	-0.389560819	-6.390769958	-5.144233227
H	-0.454644918	-7.894646645	-4.206085205
H	0.656966746	-6.601955891	-3.724664688
C	-2.824517965	-6.472558498	-3.868350983
H	-2.901084185	-5.956329823	-4.830642223
H	-3.634513140	-6.115809917	-3.224991560
H	-2.982634783	-7.537575245	-4.067308426
C	-1.251610041	-4.662371635	-3.179651976
H	-1.423995852	-4.233783722	-4.173508167
H	-0.235954180	-4.382711411	-2.882058620
H	-1.959762573	-4.206829071	-2.480898142
C	-0.695444882	-3.034922600	0.930169404
O	-0.302983761	-3.620954990	1.952895164
N	1.371958256	-3.629975557	-0.190068781
C	2.082701445	-3.301815510	-1.301386118
C	1.419436812	-2.294656992	-1.970305443
H	1.657715201	-1.740751266	-2.865249157
C	-2.155837297	-2.680712700	0.760054827
H	-2.272391796	-2.009002447	-0.089921884
C	-2.815047026	-4.001846790	0.475304067
H	-2.507175684	-4.827388287	1.111193061
N	3.104941130	-3.261964560	2.048775673
C	4.315268040	-3.490820885	1.571085215
S	5.394970417	-2.123856068	1.725226998
C	4.095206738	-1.199605227	2.476767063
C	4.082279205	0.112718955	2.948060751
H	4.959987164	0.746526778	2.873149395
C	2.910292149	0.592291951	3.525443077
H	2.906040430	1.614979386	3.883907080
C	1.748276591	-0.202210963	3.671657801
C	1.776329398	-1.508089781	3.183608770
H	0.927552521	-2.171943665	3.269058466
C	2.939243555	-1.996297121	2.580081701
C	4.566089630	-4.788858891	0.984106243
C	3.431384563	-5.644524097	0.987572312
C	3.556540966	-6.928701878	0.456999540
H	2.708212614	-7.604690075	0.452722609
C	4.782349586	-7.344959736	-0.074393287
H	4.872520924	-8.347641945	-0.484220177
C	5.894526005	-6.493930340	-0.083817303
H	6.837207317	-6.835152149	-0.499803513
C	5.790872097	-5.212483883	0.445562065
H	6.650624752	-4.546595573	0.445628405
C	0.472248912	0.378949672	4.305279255
C	0.812736809	1.361273289	5.448449612
H	-0.107796103	1.695497990	5.937400818
H	1.328453064	2.257830620	5.092084885
H	1.444008350	0.883107066	6.204255104
C	-0.310705453	1.135327339	3.204904079
H	-1.226794243	1.576493979	3.613679409
H	-0.596263826	0.455495894	2.394647121
H	0.292693853	1.941603422	2.773503542
C	-0.422629744	-0.733620644	4.890803814
H	-1.298613548	-0.288661599	5.373240471
H	0.116316572	-1.320665479	5.641815662
H	-0.791164577	-1.422751307	4.126914501
C	0.285020381	-2.855149984	-0.153963491
N	0.284835160	-2.019470215	-1.246392369
H	3.009865761	-3.798318863	-1.546041846
C	-0.602706552	-0.929750979	-1.534902692
C	-1.427865148	-0.993845463	-2.657028437
C	-0.598437607	0.180593565	-0.689532995
C	-2.275840282	0.080688372	-2.929291964
H	-1.415059805	-1.876117229	-3.287962437
C	-1.454338312	1.244722843	-0.969264746
H	0.071794868	0.204323351	0.164357334
C	-2.292373180	1.194584966	-2.086785078
H	-2.927399158	0.042861320	-3.796932459
H	-1.462568402	2.112575531	-0.317173928
H	-2.958007574	2.024921179	-2.301448822
C	-3.873378277	-4.218620777	-0.433976680
C	-4.515553951	-5.491577625	-0.438766867
C	-4.371299267	-3.224753141	-1.325213313
C	-5.611142635	-5.736460686	-1.249987483
H	-4.134076595	-6.270355701	0.216214523
C	-5.461009979	-3.487521172	-2.140518427

H	-3.898562431	-2.248893738	-1.367559195
C	-6.096560001	-4.736494064	-2.104546309
H	-6.093842983	-6.709530830	-1.224939466
H	-5.829328537	-2.714902163	-2.809799433
H	-6.956343174	-4.930304050	-2.738610983
C	-2.765899420	-1.987401009	2.024139881
C	-4.210831642	-1.626868248	1.802592754
H	-2.619319201	-2.654570341	2.875921726
H	-2.180485249	-1.078327894	2.215813160
C	-5.276206017	-2.398112774	2.321894169
C	-4.474479198	-0.428087234	0.925482154
C	-4.983242989	-3.601124048	3.203756809
C	-6.595826626	-2.093572140	2.047452450
H	-5.041991234	0.346458793	1.458347797
H	-3.543425322	0.027919173	0.576550841
H	-5.063008308	-0.692543089	0.036867470
H	-4.415391922	-3.320752859	4.098497868
H	-5.908692360	-4.076835632	3.537313938
H	-4.396612644	-4.356380939	2.669742823
H	-6.885437489	-1.256592155	1.422625422
H	-7.402603626	-2.694711924	2.453024149

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^{1}Rh–3'

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Rh	1.822131872	-4.767979622	1.662280560
N	0.543539584	-6.399013996	1.397158027
C	0.391202509	-7.097145557	2.513271332
S	-0.791118205	-8.376794815	2.394415140
C	-1.089460850	-7.928534985	0.721779287
C	-1.957052231	-8.502754211	-0.202876061
H	-2.593780756	-9.338186264	0.070584655
C	-1.986419082	-7.982746124	-1.495253205
H	-2.669155359	-8.433323860	-2.204008341
C	-1.163175941	-6.910531998	-1.896138191
C	-0.297323525	-6.350265980	-0.951287985
H	0.369130462	-5.541961670	-1.214206100
C	-0.262976527	-6.844110966	0.355490357
C	1.185087919	-6.742938519	3.668078661
C	2.048371315	-5.637333870	3.454362392
C	2.872664452	-5.232002258	4.505790710
H	3.551377535	-4.394902706	4.376552582
C	2.826649189	-5.899795532	5.734847546
H	3.475194216	-5.573511600	6.543890476
C	1.962222338	-6.982789516	5.939173222
H	1.938787222	-7.489944458	6.898345470
C	1.137243390	-7.408291817	4.904026031
H	0.464142650	-8.249670029	5.052049637
C	-1.167871118	-6.362747669	-3.335680485
C	0.209536627	-6.645169258	-3.979869366
H	0.233904764	-6.266131878	-5.007841587
H	0.415813029	-7.720044136	-4.010045528
H	1.020503759	-6.162699223	-3.423869610
C	-2.260167122	-7.010921478	-4.205885887
H	-2.237352610	-6.574486256	-5.209503651
H	-3.257762909	-6.836612225	-3.790300608
H	-2.109199762	-8.089541435	-4.318069935
C	-1.419021249	-4.837943077	-3.313210964
H	-1.426527381	-4.447972775	-4.338262558
H	-0.633269608	-4.310832977	-2.764635324
H	-2.378160715	-4.602248669	-2.849082947
C	-0.591072083	-2.965576172	1.133420229
O	-0.099606588	-3.602221966	2.083110809
N	1.350653887	-3.603878021	-0.154347703
C	1.957425117	-3.340972662	-1.338216901
C	1.227243185	-2.376980782	-2.002180576
H	1.378331423	-1.878851771	-2.947391033
C	-2.023019791	-2.561733007	1.208991528
H	-2.261395454	-1.721757770	0.562976480
C	-2.915184498	-3.837432146	0.925352812
H	-2.305034876	-4.731919289	1.075343847
N	3.194878578	-3.273196459	2.036452532
C	4.397183418	-3.546484709	1.559612155
S	5.519507408	-2.211137295	1.683260441
C	4.250266552	-1.228998899	2.412501335
C	4.283348560	0.094165251	2.844479799
H	5.186812401	0.689611256	2.760985136
C	3.121479034	0.644475698	3.385095835
H	3.157786131	1.677173138	3.709657907
C	1.927861452	-0.095285259	3.524529219
C	1.919985652	-1.426357985	3.099693537
H	1.041887641	-2.047518015	3.205769539
C	3.066531658	-1.985570073	2.532335758
C	4.609353542	-4.853318691	0.975750506
C	3.450190783	-5.675796032	0.978069901
C	3.536139965	-6.955574989	0.427717745
H	2.668451548	-7.606990337	0.419755042
C	4.744673252	-7.399451256	-0.119545504
H	4.802583218	-8.397722244	-0.545901000
C	5.881312847	-6.581019402	-0.124923430
H	6.810315609	-6.942908764	-0.554159760
C	5.818140507	-5.304674149	0.422534466
H	6.696177959	-4.663014412	0.421191782
C	0.632327199	0.515213549	4.091447353
C	0.846598387	1.935561061	4.646366119
H	-0.093222491	2.317311287	5.056862831
H	1.170789361	2.635249138	3.868653297
H	1.588742375	1.946416140	5.450956345
C	-0.414553970	0.591308534	2.953970671
H	-1.361579418	0.998217046	3.326677799
H	-0.620036542	-0.398307025	2.533410072
H	-0.061116520	1.244364023	2.147432804
C	0.084619828	-0.377055734	5.229779243
H	-0.826089978	0.063939109	5.649431229
H	0.817846239	-0.474522263	6.036823273
H	-0.167569280	-1.383475900	4.881258488
C	0.260011941	-2.832849264	-0.063667066
N	0.160816103	-2.057304382	-1.198570251
H	2.863574743	-3.847516775	-1.635542750
C	-0.783041418	-1.031359673	-1.537252069
C	-1.504516006	-1.146521568	-2.725057125
C	-0.921658695	0.078459084	-0.703173161
C	-2.393750906	-0.130708352	-3.074918032
H	-1.389783025	-2.028036594	-3.345960140
C	-1.828963041	1.077113271	-1.053640604
H	-0.325391024	0.153016016	0.199955270
C	-2.563323021	0.974059880	-2.238381386
H	-2.964452505	-0.212944269	-3.994840145
H	-1.951413035	1.940853477	-0.407588094
H	-3.264096260	1.757240176	-2.510975838
C	-3.680446625	-3.991265774	-0.354007661
C	-4.132353306	-5.276797295	-0.690668643
C	-4.033679485	-2.918739319	-1.181676745
C	-4.925942421	-5.482084751	-1.817747951
H	-3.856503248	-6.118284702	-0.061206240
C	-4.812268257	-3.125356197	-2.321521521
H	-3.703304768	-1.911842108	-0.947767079
C	-5.266487598	-4.405717373	-2.640960932
H	-5.273093700	-6.483425140	-2.057656527
H	-5.067808151	-2.281569481	-2.956729412
H	-5.878315449	-4.565040588	-3.524276018
C	-2.633325338	-2.476766825	2.633793116
C	-3.723524094	-3.538793564	2.264860392
H	-1.927460790	-2.795982361	3.399304867
H	-3.025366068	-1.493146181	2.901409388
C	-3.827457190	-4.782015324	3.134479284
C	-5.065931797	-2.858744144	1.990716696
C	-2.567360401	-5.257303238	3.825207472
C	-4.965344429	-5.481008530	3.247665882
H	-5.538208485	-2.572734356	2.935424566
H	-4.929941177	-1.955831170	1.386908412
H	-5.750004768	-3.508081436	1.439136744
H	-2.315136671	-4.611621857	4.675866604
H	-2.686215162	-6.274138927	4.207474232
H	-1.694260955	-5.242149830	3.163867712
H	-5.897747993	-5.173470497	2.788267136
H	-4.999908924	-6.400961399	3.824829817

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Ir	1.584247112	-1.070814013	0.095691346
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S	-0.260642022	-5.000816822	-1.201638579
C	-0.296557039	-3.978198290	-2.628142357
C	-0.806345761	-4.261723995	-3.890235186
H	-1.273949385	-5.217987061	-4.102133751
C	-0.699877381	-3.289354801	-4.881517410
H	-1.100491524	-3.520333052	-5.860487461
C	-0.086163469	-2.043104649	-4.644520283
C	0.417010397	-1.778419256	-3.365679741
H	0.909730613	-0.843793154	-3.144793034
C	0.308530599	-2.733357191	-2.352923632
C	0.962780118	-3.755681276	1.051382303
C	1.557282329	-2.539244890	1.481194735
C	2.012430668	-2.484175682	2.804946184
H	2.480390310	-1.579351187	3.179972172
C	1.870147109	-3.579975843	3.657538891
H	2.231914043	-3.511817217	4.680636406
C	1.273369789	-4.768400669	3.215269566
H	1.171883821	-5.613120556	3.889312267
C	0.817612052	-4.859497547	1.907182813
H	0.356549412	-5.778419018	1.552536368
C	0.047963828	-0.971514165	-5.741934299
C	1.542979956	-0.636103272	-5.952662945
H	1.655469775	0.118636392	-6.739096642
H	2.104254246	-1.526558280	-6.253388405
H	2.003389359	-0.240324154	-5.041467190
C	-0.543628991	-1.432353735	-7.086862087
H	-0.428346217	-0.639274120	-7.832245827
H	-1.613213897	-1.653784633	-7.005562782
H	-0.035364028	-2.322272778	-7.471527100
C	-0.704388678	0.301997185	-5.296444893
H	-0.637204945	1.081662536	-6.063592434
H	-0.283421338	0.707861185	-4.373445988
H	-1.765075803	0.088404685	-5.123767376
C	-0.814491689	0.791824877	-0.299510717
O	-0.558233738	-0.257264197	0.347253501
N	1.378230572	0.589400291	-1.288352370
C	2.188509226	1.220573545	-2.182052374
C	1.480376601	2.250968695	-2.762196541
H	1.735235572	2.952184439	-3.541439295
C	-1.989874005	1.592329741	-0.050604001
H	-2.022226334	2.579507113	-0.490210146
C	-3.002262354	1.154854059	0.738796175
H	-2.910449505	0.154639453	1.159231305
N	2.509980917	0.277699739	1.357038736
C	3.812267780	0.407145262	1.140630245
S	4.569812775	1.626520038	2.134093285
C	3.022007942	1.927316189	2.921007395
C	2.706766605	2.806425810	3.955319881
H	3.455437899	3.469483852	4.376870155
C	1.405911446	2.800810099	4.449743271
H	1.169568658	3.483671188	5.257176876
C	0.406600922	1.931568742	3.954479694
C	0.733811915	1.081364512	2.897704363
H	0.017865194	0.390590131	2.475355148
C	2.031932116	1.086694121	2.378975868
C	4.418407917	-0.484330177	0.181819007
C	3.492613077	-1.409629703	-0.383013517
C	3.991685152	-2.358868361	-1.282652259
H	3.318886042	-3.086401224	-1.725764036
C	5.346077442	-2.369371176	-1.622528195
H	5.714071751	-3.113020420	-2.324718714
C	6.239878654	-1.438542366	-1.074170232
H	7.288804054	-1.460123062	-1.352171779
C	5.778073311	-0.493811309	-0.167067453
H	6.463376045	0.227234364	0.272289038
C	-1.018041730	1.957220793	4.536462784
C	-0.998994350	2.263822317	6.050601006
H	-2.011658430	2.180609226	6.458035946
H	-0.651808977	3.278241158	6.267853260
H	-0.356437862	1.560788512	6.590916157
C	-1.820587158	3.060440063	3.805133343
H	-2.849627733	3.102123976	4.180059433
H	-1.859901547	2.866557837	2.728903055
H	-1.362820506	4.043977261	3.956156015
C	-1.726223469	0.599732637	4.340749264
H	-2.711525917	0.625043988	4.817500591
H	-1.150891781	-0.217176482	4.788912773
H	-1.882582426	0.361424536	3.285406113
C	0.200056836	1.219903946	-1.275538325
N	0.225367904	2.245352030	-2.194888115
H	3.200625896	0.888315916	-2.356224537
C	-0.841770947	3.106533289	-2.617535830
C	-2.039801598	2.549254894	-3.072613478
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C	-3.066823483	3.395106554	-3.485300541
H	-2.161753893	1.472571969	-3.093648911
C	-1.683565140	5.324775696	-3.011902571
H	0.282959819	4.897387505	-2.213510752
C	-2.889750481	4.781175613	-3.458049059
H	-4.001988411	2.969426632	-3.835850716
H	-1.545737863	6.401229382	-2.987295389
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C	-4.189015388	1.908338070	1.096338272
C	-5.034467220	1.388911843	2.097322226
C	-4.512258053	3.152843714	0.511007071
C	-6.155480862	2.096355915	2.519943953
H	-4.792424679	0.431886524	2.552284241
C	-5.636343479	3.851240396	0.930708647
H	-3.895411491	3.563010216	-0.282960653
C	-6.457442760	3.329331875	1.938561082
H	-6.792954922	1.689063787	3.298839331
H	-5.881340027	4.805758953	0.474481642
H	-7.333400249	3.882803917	2.264414072

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Ir	1.535378218	-1.164521694	0.123939186
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C	0.485742629	-3.812455416	-0.284737676
S	-0.298526704	-5.090211868	-1.164627671
C	-0.309290707	-4.074469090	-2.596347094
C	-0.814150751	-4.354099274	-3.862426281
H	-1.284055829	-5.307472706	-4.081093311
C	-0.706133664	-3.374030113	-4.844762325
H	-1.107069135	-3.597706556	-5.825485229
C	-0.098867349	-2.123124838	-4.601612568
C	0.402909666	-1.863287687	-3.323882580
H	0.876542091	-0.923074603	-3.087426662
C	0.293588340	-2.827570915	-2.319436789
C	0.871189475	-3.809995413	1.106744647
C	1.455622196	-2.575568199	1.527186394
C	1.860158682	-2.468918085	2.871747255
H	2.301871777	-1.545216322	3.230103970
C	1.691004038	-3.535727024	3.750030279
H	2.006892443	-3.439100981	4.784939766
C	1.113757849	-4.738140106	3.313446283
H	0.986176193	-5.561754227	4.009160995
C	0.701152444	-4.879861355	1.989346027
H	0.251889467	-5.811444283	1.655476213
C	0.019970508	-1.041224480	-5.689548492
C	1.512851715	-0.699443281	-5.905249119
H	1.616418600	0.058657400	-6.689168930
H	2.077572823	-1.585767984	-6.212626934
H	1.972290158	-0.301166683	-4.994846821
C	-0.581954718	-1.493149400	-7.032486439
H	-0.479504049	-0.690766215	-7.769594669
H	-1.649674296	-1.720800519	-6.943253040
H	-0.071991488	-2.375439405	-7.433377743
C	-0.731986821	0.225290686	-5.220673561
H	-0.672882259	1.011142612	-5.981533527

H	-0.305012554	0.626848578	-4.298770428
H	-1.790251374	0.008019339	-5.040120602
C	-0.741207182	0.697506249	-0.332250595
O	-0.458454758	-0.467828006	0.250872135
N	1.431902170	0.484591573	-1.309104323
C	2.259819508	1.127612233	-2.194322586
C	1.592686892	2.201155424	-2.716736794
H	1.867132664	2.930611372	-3.461679935
C	-1.923509717	1.400137305	-0.020645441
H	-2.009494305	2.400250196	-0.423543394
C	-2.932150602	0.902290523	0.770619452
H	-2.829688549	-0.119485490	1.129243374
N	2.438556910	0.248849943	1.331223130
C	3.735033035	0.390645146	1.099740148
S	4.484749317	1.630650282	2.061680079
C	2.937871218	1.946814299	2.837845564
C	2.626908779	2.847836971	3.854062080
H	3.377274275	3.515412092	4.264899254
C	1.324883223	2.855981588	4.340814590
H	1.088557482	3.553915739	5.134821892
C	0.316028148	1.990776420	3.853420258
C	0.638273060	1.112346292	2.817793131
H	-0.088629641	0.439444035	2.382672548
C	1.944247246	1.094907284	2.314780951
C	4.349437714	-0.494201630	0.129228696
C	3.444106817	-1.435736299	-0.448158652
C	3.943689823	-2.337349892	-1.396300673
H	3.271090746	-3.046295643	-1.869148612
C	5.297085285	-2.324799776	-1.740329266
H	5.673162460	-3.035356998	-2.470963240
C	6.176446915	-1.403013349	-1.155552149
H	7.225514889	-1.400477767	-1.433872104
C	5.704891205	-0.485153288	-0.217276588
H	6.386863708	0.228525594	0.237823755
C	-1.111948371	2.054604053	4.423509598
C	-1.106465220	2.431583643	5.921225548
H	-2.125615358	2.376007557	6.316197872
H	-0.755406857	3.453042984	6.096046448
H	-0.479359001	1.748898029	6.504881859
C	-1.889805198	3.134929895	3.633394003
H	-2.925745487	3.196496248	3.984093189
H	-1.910586238	2.899125814	2.566776991
H	-1.426283836	4.119612217	3.759300232
C	-1.831536412	0.697869122	4.278994083
H	-2.828484297	0.760631323	4.725690842
H	-1.277024865	-0.098976880	4.786090374
H	-1.969287992	0.412043095	3.234128475
C	0.265595764	1.156632900	-1.250787616
N	0.328632563	2.217513084	-2.129756451
H	3.257566214	0.769836128	-2.396042109
C	-0.707586169	3.126936674	-2.512472391
C	-1.937156796	2.635935545	-2.961561680
C	-0.461194843	4.499509811	-2.459481239
C	-2.930782318	3.532596111	-3.346378565
H	-2.112725496	1.567205667	-2.985829353
C	-1.458505392	5.388969421	-2.861825466
H	0.494622380	4.861380577	-2.092826605
C	-2.693361998	4.909091473	-3.300875425
H	-3.889772415	3.153842688	-3.686851978
H	-1.272132158	6.457764626	-2.820049286
H	-3.469952106	5.604312897	-3.604999304
C	-4.114601612	1.628085732	1.191727519
C	-5.007483006	1.009166121	2.094346285
C	-4.407701969	2.948438883	0.775550663
C	-6.130333424	1.677024484	2.572422504
H	-4.800042152	-0.005347312	2.426198483
C	-5.531727314	3.611013651	1.253997803
H	-3.755898952	3.456048965	0.070446312
C	-6.398324013	2.984333277	2.158020973
H	-6.797891617	1.179608345	3.270528078
H	-5.738338947	4.625198364	0.923300624
H	-7.272885323	3.508803129	2.531364441

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Ir	1.380203485	-1.148406625	0.069532797
N	0.474709272	-2.585982323	-1.132657170
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S	-0.608655334	-4.914711952	-1.474339724
C	-0.566394031	-3.804274559	-2.837094784
C	-1.057211161	-3.975425243	-4.127777576
H	-1.548687220	-4.897687912	-4.420803070
C	-0.905162394	-2.933723450	-5.042285919
H	-1.294815779	-3.078671694	-6.042238712
C	-0.260334074	-1.727925181	-4.702445984
C	0.229746506	-1.578862429	-3.400423765
H	0.745715797	-0.681291342	-3.097438097
C	0.068248324	-2.600517035	-2.462794304
C	0.540075779	-3.816876650	0.903688610
C	1.174522519	-2.646634340	1.407693624
C	1.556200624	-2.662159443	2.755823374
H	2.048656464	-1.795205116	3.186443806
C	1.310987711	-3.777866840	3.557783842
H	1.617778659	-3.764409542	4.600755215
C	0.678792477	-4.918194294	3.041413784
H	0.496827930	-5.778062344	3.678360224
C	0.290300608	-4.940360069	1.709706783
H	-0.199930802	-5.819271564	1.297062874
C	-0.079705447	-0.570961535	-5.703269958
C	1.425488591	-0.241810292	-5.843582630
H	1.570394278	0.560773969	-6.575506687
H	1.987051725	-1.117434978	-6.184383392
H	1.860969901	0.090660453	-4.895751476
C	-0.638418734	-0.907125890	-7.097969532
H	-0.484521806	-0.058978602	-7.772747517
H	-1.713755131	-1.112802386	-7.067362309
H	-0.133931354	-1.773181558	-7.538264275
C	-0.825332820	0.676218569	-5.171877861
H	-0.676537395	1.524573565	-5.850500584
H	-0.462698251	0.967056751	-4.180931091
H	-1.901539326	0.485940009	-5.098698616
C	-0.876015306	0.806868911	-0.421221137
O	-0.649793804	-0.230608612	0.304077893
N	1.365974188	0.564835370	-1.267949343
C	2.277814150	1.233997583	-2.034471512
C	1.710443020	2.410238981	-2.461642742
H	2.092540979	3.222608328	-3.059936762
C	-2.168426752	1.400833011	-0.462131381
H	-2.275950193	2.302181482	-1.046703577
C	-3.122639179	1.146553993	0.578404725
H	-3.000844002	0.227131054	1.140276313
N	2.424299479	0.083633393	1.374451518
C	3.742374182	-0.041272603	1.280198574
S	4.631875038	1.034232497	2.328502417
C	3.111499071	1.690414667	2.923118353
C	2.892383575	2.685153008	3.871306658
H	3.722222090	3.183584452	4.362165451
C	1.577585816	3.026041508	4.181005955
H	1.418887615	3.802055597	4.919598103
C	0.471778929	2.393062830	3.575453997
C	0.713017583	1.389347792	2.631331682
H	-0.094339877	0.854142308	2.151809692
C	2.025129318	1.045856714	2.296803474
C	4.267856121	-1.010443687	0.351111263
C	3.253693819	-1.731138945	-0.342436403
C	3.671725035	-2.698599100	-1.265695572
H	2.932715893	-3.274258137	-1.814622402
C	5.029657841	-2.929200411	-1.492831111
H	5.329937458	-3.684619188	-2.214637995
C	6.013200760	-2.204925776	-0.804953218
H	7.064824104	-2.396896124	-0.993130803
C	5.633607388	-1.242557645	0.120810464
H	6.387595654	-0.675473869	0.661854863
C	-0.977637589	2.811650753	3.883988857
C	-1.075742841	3.700106382	5.138387203
H	-2.125749350	3.928094387	5.346178055

H	-0.557058036	4.655692577	5.009381294
H	-0.661108077	3.199575901	6.019641876
C	-1.509106517	3.613366365	2.671927929
H	-2.547928572	3.922627926	2.830630779
H	-1.479714632	3.012735128	1.759077668
H	-0.904527605	4.513628483	2.510390282
C	-1.865923166	1.566642404	4.108046532
H	-2.895622015	1.874656439	4.320119858
H	-1.502601504	0.975189030	4.954902649
H	-1.896576881	0.916052699	3.230036736
C	0.249666527	1.298586726	-1.210602999
N	0.432430774	2.451910257	-1.937664151
H	3.262131691	0.830950916	-2.218081236
C	-0.420346439	3.605244398	-1.987519383
C	-1.089989305	3.927366734	-3.166978121
C	-0.556743205	4.383014202	-0.835553885
C	-1.919672966	5.050533295	-3.186855078
H	-0.964452386	3.305452824	-4.047235489
C	-1.395760536	5.495227337	-0.863688648
H	-0.022033945	4.103862286	0.066666968
C	-2.075755835	5.829662800	-2.038468361
H	-2.445729971	5.313584328	-4.099461079
H	-1.516371250	6.098919868	0.030542780
H	-2.725010395	6.699848652	-2.059292793
C	-4.188064098	2.013615370	0.926727951
C	-5.101666927	1.607980251	1.942285776
C	-4.387333870	3.293927193	0.329852879
C	-6.145526409	2.429778337	2.335854053
H	-4.962898254	0.636563599	2.409296036
C	-5.435358047	4.105628967	0.733100593
H	-3.703289747	3.654292822	-0.430396855
C	-6.321593285	3.684680939	1.735455632
H	-6.827949524	2.100899458	3.114328861
H	-5.566895485	5.080635548	0.272056133
H	-7.137621880	4.329211235	2.047864676
C	-2.931390285	0.036158979	-2.189879179
C	-4.188398361	-0.272457927	-1.680901408
C	-5.339795113	0.652810514	-1.972342014
C	-4.378602028	-1.437527180	-0.825402617
C	-3.210702181	-2.372709274	-0.589339495
C	-5.577531338	-1.680135489	-0.238136292
H	-2.826040268	0.827122092	-2.924020290
H	-2.114888668	-0.673118591	-2.149235487
H	-5.031757832	1.480871081	-2.614932537
H	-5.750423908	1.080030918	-1.050819874
H	-6.152985573	0.116454147	-2.474655390
H	-2.855897427	-2.800344944	-1.533290148
H	-3.498222113	-3.200190783	0.062988341
H	-2.363788843	-1.855648398	-0.127006069
H	-6.439092636	-1.036014915	-0.368815541
H	-5.718209743	-2.544880867	0.402704656

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^{3}Ir–2

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Ir	1.734846830	-1.333852768	-0.047569402
N	0.180787489	-2.721954584	-0.121545896
C	-0.068342216	-3.284339190	1.057052255
S	-1.538294673	-4.223769665	1.097555041
C	-1.835793853	-3.807882547	-0.584346414
C	-2.908095837	-4.156747341	-1.398483038
H	-3.719954491	-4.770701408	-1.021635294
C	-2.922083855	-3.691309214	-2.712587118
H	-3.767740488	-3.958961487	-3.333432674
C	-1.878481507	-2.904480219	-3.241083860
C	-0.802444935	-2.578330517	-2.408012390
H	0.032243986	-1.999078512	-2.774001122
C	-0.787380338	-3.004759789	-1.078705072
C	0.835426092	-3.024367332	2.149139166
C	1.853780031	-2.085933447	1.822662830
C	2.778365374	-1.770622611	2.825453520
H	3.574070454	-1.059872031	2.623441935
C	2.690162659	-2.356484652	4.089652061
H	3.421166182	-2.097275019	4.851519108
C	1.676255465	-3.275599957	4.392968178
H	1.622314095	-3.723499775	5.380291939
C	0.742811084	-3.611753702	3.421763897
H	-0.047908723	-4.323780060	3.646968126
C	-1.892512321	-2.381283998	-4.688359737
C	-0.628258944	-2.873217821	-5.430085659
H	-0.635044396	-2.520153522	-6.467276573
H	-0.585845053	-3.966893911	-5.443850040
H	0.289874464	-2.506575823	-4.959813595
C	-3.132176161	-2.855259180	-5.469396114
H	-3.101943254	-2.457006454	-6.488493443
H	-4.062208176	-2.506394863	-5.007818222
H	-3.171887398	-3.946732044	-5.543409824
C	-1.903318882	-0.834888935	-4.660216808
H	-1.906528711	-0.436912924	-5.681965351
H	-1.024622440	-0.437915504	-4.145734310
H	-2.794966221	-0.456760794	-4.148171902
C	-0.456087559	0.668191850	-0.787915945
O	-0.067900740	0.088288173	0.248549953
N	1.429503441	-0.298996210	-1.931630731
C	2.095352888	-0.205574423	-3.114727497
C	1.534015775	0.816463947	-3.853993177
H	1.792948246	1.238229990	-4.813041687
C	-1.856232405	1.220391035	-0.846779227
H	-2.028881550	1.680115223	-1.820728302
C	-2.055341244	2.208270073	0.261534989
H	-1.679649949	1.900856137	1.233318686
N	3.337505102	-0.051404331	0.193674862
C	4.495321274	-0.549617589	-0.222209394
S	5.834657669	0.556908190	-0.058926258
C	4.740533829	1.760917306	0.617500186
C	5.012279510	3.051088572	1.063899040
H	6.015819073	3.461748123	1.017708659
C	3.961872101	3.806626797	1.579936028
H	4.185837269	4.807558537	1.927349687
C	2.642692804	3.311700344	1.670480609
C	2.387969255	2.015777826	1.208329558
H	1.399027824	1.579611301	1.257410049
C	3.430619001	1.245077610	0.684969366
C	4.498060703	-1.901755691	-0.724822402
C	3.216067314	-2.520191669	-0.668468952
C	3.112215281	-3.840191126	-1.120812774
H	2.153191328	-4.347684383	-1.080810905
C	4.230895996	-4.507563591	-1.624155521
H	4.127501011	-5.532134533	-1.972343087
C	5.485018730	-3.882699251	-1.685134411
H	6.343785286	-4.416627407	-2.078873396
C	5.620627403	-2.576307774	-1.232508183
H	6.587672234	-2.081397772	-1.269909859
C	1.488477230	4.180744648	2.201636553
C	1.994746566	5.446980000	2.920170784
H	1.145111203	5.997816086	3.335186958
H	2.515243292	6.128309727	2.238950253
H	2.671205044	5.201036930	3.745165348
C	0.614283741	4.609395504	0.999727070
H	-0.212503582	5.249841690	1.325079679
H	0.172568440	3.739415169	0.504941881
H	1.208813071	5.164526463	0.264555395
C	0.626532078	3.375932932	3.202192307
H	-0.187083960	4.003486156	3.582157135
H	1.224211812	3.040787458	4.056076050
H	0.171538025	2.492296457	2.744582415
C	0.460230738	0.625479817	-1.928895235
N	0.505762458	1.334923744	-3.104228735
H	2.923614264	-0.856880903	-3.349067450
C	-0.184891060	2.559308529	-3.401585340
C	-1.007045269	2.641413450	-4.523886681
C	0.023631953	3.654076815	-2.560941458
C	-1.635932326	3.855845690	-4.804619312
H	-1.155398726	1.771950126	-5.154857159
C	-0.617295623	4.856498718	-2.847465038
H	0.680678785	3.559139729	-1.702710986
C	-1.442682147	4.958474636	-3.969947100

H	-2.281231642	3.936303377	-5.674008846
H	-0.475095451	5.709200859	-2.191508770
H	-1.940233827	5.897758961	-4.191342354
C	-2.783957720	3.414717197	0.173993036
C	-2.997069359	4.178739071	1.359705806
C	-3.330688715	3.925569773	-1.038375616
C	-3.711868525	5.363725662	1.332890630
H	-2.589999199	3.809603453	2.296927691
C	-4.041481972	5.116029263	-1.053487062
H	-3.184701443	3.386936665	-1.967058778
C	-4.241687775	5.843857288	0.126748160
H	-3.864200830	5.922213078	2.252240658
H	-4.446220875	5.485177994	-1.992021441
H	-4.803650856	6.772730350	0.107896641
C	-4.276074409	0.436466187	-0.580619991
C	-4.956096649	0.474799693	0.661246359
C	-4.265081882	-0.024773380	1.921008468
H	-3.958554506	-1.073507309	1.828994870
H	-3.363743782	0.555853426	2.145224333
H	-4.927991867	0.049740277	2.786569118
C	-4.935130119	0.926330626	-1.843430877
H	-5.812996864	0.320433170	-2.103711367
H	-5.278317928	1.963216424	-1.744744778
H	-4.247469425	0.888315499	-2.694483280
C	-6.247778416	0.948456883	0.769157588
H	-6.805253029	1.326401472	-0.079622246
H	-6.758189201	0.963002205	1.726352811
C	-2.852309465	-0.016630469	-0.693066776
H	-2.710485935	-0.665079355	-1.566403270
H	-2.523376942	-0.576562345	0.183170646

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^{1}Ir–3

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Ir	1.812080264	-1.154984951	0.207295477
N	0.122448452	-2.363542318	0.027240064
C	-0.188658655	-3.007991552	1.150162935
S	-1.718969822	-3.841409445	1.084980011
C	-1.972699285	-3.224180698	-0.540492713
C	-3.083029032	-3.365909100	-1.373174071
H	-3.947147608	-3.943275690	-1.060350180
C	-3.066473722	-2.726513147	-2.606379509
H	-3.941672564	-2.816617727	-3.241341352
C	-1.957238317	-1.971505523	-3.054095745
C	-0.843981147	-1.870865345	-2.220485687
H	0.042009074	-1.334964395	-2.519144773
C	-0.859406888	-2.467963934	-0.952712715
C	0.686867118	-2.872098923	2.286654234
C	1.760923624	-1.968682766	2.056346893
C	2.642962694	-1.738510847	3.120473623
H	3.478676081	-1.057051539	2.993739128
C	2.458722115	-2.375207663	4.350404263
H	3.156533480	-2.181922197	5.161302090
C	1.392267227	-3.261639595	4.558338642
H	1.264783263	-3.748851776	5.519622326
C	0.499186844	-3.509958744	3.524075270
H	-0.335631490	-4.190835476	3.673911095
C	-2.035115004	-1.262770891	-4.417972088
C	-2.277659893	-2.305755615	-5.532921791
H	-2.339096546	-1.810894132	-6.508453369
H	-3.211239815	-2.855180740	-5.381581306
H	-1.461265206	-3.034235716	-5.570117950
C	-3.198627949	-0.241236880	-4.398007393
H	-3.282200813	0.258206725	-5.369675159
H	-3.027610302	0.527537465	-3.636260271
H	-4.161579132	-0.714084864	-4.185234547
C	-0.742954433	-0.493434727	-4.746139050
H	-0.837842464	-0.012485400	-5.725642204
H	0.130123898	-1.152552485	-4.784544468
H	-0.551176429	0.292770833	-4.009309769
C	-0.074486673	1.098712444	-0.749358714
O	0.104295067	0.488924980	0.322936207
N	1.832245946	-0.047612567	-1.671263337
C	2.667085171	0.016537540	-2.744930029
C	2.361607790	1.150504112	-3.471045494
H	2.813024044	1.587674618	-4.348237991
C	-1.375570536	1.750952601	-1.078400850
H	-1.365692616	2.085097313	-2.114979029
C	-1.844612718	2.848466396	-0.054838199
H	-1.081633091	3.065907478	0.693363428
N	3.529347658	-0.065262318	0.564136863
C	4.646584034	-0.668779969	0.180604309
S	6.080786705	0.296300620	0.411804408
C	5.085321903	1.591589451	1.070166945
C	5.465581417	2.838497639	1.557245255
H	6.505327225	3.149627209	1.556311011
C	4.475724697	3.677105665	2.061916590
H	4.783906937	4.641139507	2.446829796
C	3.111865759	3.310488939	2.100329876
C	2.745970726	2.061547279	1.588327289
H	1.718905926	1.718463421	1.594869137
C	3.729497433	1.207748055	1.079405665
C	4.530358791	-2.002674580	-0.353823364
C	3.189181805	-2.480731487	-0.367471606
C	2.965306520	-3.775447369	-0.847786605
H	1.956777573	-4.176920414	-0.862571836
C	4.029003620	-4.550493240	-1.315888882
H	3.833023310	-5.552256107	-1.689390063
C	5.343414307	-4.061769962	-1.311451197
H	6.156956673	-4.678252220	-1.679654837
C	5.597071648	-2.784811497	-0.826450706
H	6.612022400	-2.394722223	-0.810702324
C	2.044915915	4.265763283	2.663517237
C	2.668413401	5.362713337	3.551085711
H	1.875188351	5.963607788	4.006111622
H	3.303276062	6.048638821	2.980845213
H	3.267898321	4.931105137	4.359127998
C	1.324741960	4.947134972	1.475793958
H	0.595405281	5.681324482	1.836405039
H	0.787914038	4.213630676	0.866127908
H	2.037777662	5.472481251	0.829800487
C	1.012877107	3.489915133	3.512212276
H	0.284772933	4.186351299	3.941865683
H	1.502089739	2.961739540	4.337222099
H	0.448102236	2.756206512	2.930228710
C	1.010696054	1.005718112	-1.730572104
N	1.316923141	1.768213391	-2.827979088
H	3.425905466	-0.732090533	-2.914750814
C	0.815262079	3.079491854	-3.121398687
C	0.236697942	3.344953060	-4.361708641
C	0.937196910	4.066840172	-2.142167091
C	-0.234799087	4.633204937	-4.615980148
H	0.143491715	2.553786755	-5.099058628
C	0.447979420	5.343797207	-2.404054403
H	1.419531941	3.833040476	-1.198389530
C	-0.135849446	5.626807690	-3.639706135
H	-0.692406833	4.856280804	-5.574892521
H	0.512867570	6.111016750	-1.639905691
H	-0.522933722	6.620953083	-3.837826729
C	-2.322187662	4.137567997	-0.668341398
C	-2.134315014	5.334673405	0.036298402
C	-2.982641935	4.190103531	-1.905048013
C	-2.579957247	6.551503181	-0.479245305
H	-1.632290483	5.309422970	0.999736190
C	-3.429640293	5.404526711	-2.423807144
H	-3.153953552	3.280957937	-2.473712444
C	-3.226851463	6.590467453	-1.715333819
H	-2.422134161	7.467424870	0.083836615
H	-3.938468218	5.425508022	-3.383585453
H	-3.575868368	7.536248684	-2.120225906
C	-2.931865931	1.837758183	0.515279353
C	-2.578340054	1.318205714	1.911293507
C	-2.669864416	-0.167591691	2.152989626
H	-1.834088087	-0.686049759	1.669603825
H	-2.635349989	-0.400064677	3.220673800
H	-3.595582485	-0.588941693	1.740814090
C	-4.380367756	2.340490818	0.530698121

H	-5.052647591	1.537349701	0.851954341
H	-4.489947796	3.172842741	1.231959105
H	-4.702471256	2.682642221	-0.457096398
C	-2.265406132	2.173422575	2.892029762
H	-2.070634842	1.835764647	3.905786037
H	-2.204216003	3.246004343	2.723446608
C	-2.604950428	0.877092600	-0.668587148
H	-3.374334097	0.903864682	-1.444221020
H	-2.384451389	-0.164145321	-0.439493746

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^{3}Ir–1'–TS

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Ir	1.900879622	-0.832186759	0.775011063
N	0.961255908	-2.647558212	0.301633090
C	0.594978213	-3.321860552	1.387222171
S	-0.552107811	-4.602358341	1.080803514
C	-0.558486223	-4.169753075	-0.621613145
C	-1.296740532	-4.722242832	-1.661783576
H	-1.996510148	-5.532350063	-1.484567285
C	-1.131954670	-4.196956158	-2.940465450
H	-1.728743076	-4.618681431	-3.738209248
C	-0.227510899	-3.151184320	-3.210841894
C	0.512800574	-2.616130590	-2.150895357
H	1.235631347	-1.827632904	-2.306960583
C	0.333663881	-3.102810144	-0.854636133
C	1.082657218	-2.889730930	2.672337532
C	1.799495816	-1.663419366	2.610318661
C	2.303339958	-1.159969330	3.817002296
H	2.861480236	-0.228017628	3.819300890
C	2.096010685	-1.837951064	5.019790649
H	2.499418259	-1.425994635	5.941611767
C	1.379354000	-3.043041945	5.060063839
H	1.228762984	-3.559491396	6.002661228
C	0.868961096	-3.572197914	3.881978750
H	0.315112948	-4.508213043	3.897654533
C	-0.014740209	-2.608105183	-4.634395599
C	1.400065064	-3.004684925	-5.115417480
H	1.579700232	-2.630281925	-6.129604340
H	1.514923453	-4.093225479	-5.129014492
H	2.174695253	-2.593510628	-4.459695339
C	-1.054545999	-3.158710003	-5.628534317
H	-0.898123562	-2.708186626	-6.613757133
H	-2.076551676	-2.926058292	-5.309279919
H	-0.970172524	-4.243015766	-5.750862122
C	-0.139169127	-1.068870425	-4.626713753
H	-0.025883192	-0.675821662	-5.643852711
H	0.624773741	-0.595408320	-4.004490852
H	-1.122468472	-0.769365609	-4.249777794
C	-0.574914694	0.296622306	-0.595999420
O	-0.316279471	-0.178099260	0.558041215
N	1.764660835	0.250242412	-1.113294601
C	2.658386230	0.749249995	-2.020358562
C	2.001215219	1.628096700	-2.844571590
H	2.339158535	2.251398087	-3.657697201
C	-1.857032776	0.104808025	-1.219631314
H	-1.920813441	0.412223786	-2.256921291
C	-2.633092642	-1.037217498	-0.789592981
H	-2.409623384	-1.414838195	0.202767029
N	2.818002701	0.901331902	1.396388769
C	4.131994247	0.924373806	1.216574550
S	4.856023788	2.475296736	1.568014383
C	3.261766434	3.115600109	1.962347150
C	2.888389587	4.396685600	2.365203857
H	3.621366739	5.190433025	2.467757463
C	1.545399785	4.633826733	2.640480757
H	1.262647867	5.632941246	2.950559616
C	0.556418180	3.627043009	2.543281555
C	0.944910228	2.356646299	2.117204666
H	0.245492652	1.538565755	2.013239622
C	2.289618254	2.108072996	1.824380875
C	4.754221439	-0.291246712	0.756385922
C	3.819134474	-1.350109577	0.555886447
C	4.327729702	-2.586582899	0.140467316
H	3.648401022	-3.420691967	-0.008332737
C	5.695106983	-2.751231194	-0.091629602
H	6.067208290	-3.719054222	-0.418052435
C	6.598643303	-1.692317605	0.087107353
H	7.657237053	-1.838518143	-0.101938240
C	6.128524780	-0.458338380	0.516921520
H	6.816597939	0.370028913	0.669757247
C	-0.914617777	3.951482296	2.859087467
C	-1.026129723	4.902062893	4.072503090
H	-2.079344273	5.054760456	4.330257416
H	-0.599467278	5.888976574	3.871697903
H	-0.518891096	4.484441757	4.947889328
C	-1.540831208	4.635575771	1.620437741
H	-2.591796637	4.886373043	1.804831743
H	-1.499176383	3.975608110	0.747899652
H	-1.010087967	5.560802460	1.370357275
C	-1.714309931	2.675214052	3.190945864
H	-2.749670982	2.936878920	3.433525085
H	-1.287873983	2.152766466	4.053389072
H	-1.738331914	1.968214154	2.358101606
C	0.572192430	0.801183701	-1.360108972
N	0.679992437	1.653245807	-2.429520369
H	3.694632292	0.447395951	-2.011317730
C	-0.281065643	2.614950657	-2.888176203
C	-0.917380989	2.440670013	-4.116421700
C	-0.511871934	3.747890472	-2.103714466
C	-1.814751506	3.415899515	-4.557195187
H	-0.709233701	1.559430242	-4.712687969
C	-1.414497733	4.712611675	-2.550528049
H	0.015300000	3.861735344	-1.160902023
C	-2.064917088	4.546809196	-3.776543379
H	-2.314809322	3.292265654	-5.513117790
H	-1.603078604	5.594007015	-1.945288301
H	-2.762161970	5.302219868	-4.126243114
C	-3.584314346	-1.733613253	-1.570236683
C	-4.275432110	-2.837589979	-0.990319371
C	-3.874898672	-1.423605919	-2.931818247
C	-5.194853783	-3.572769880	-1.719204903
H	-4.065090179	-3.096171141	0.044282202
C	-4.796774387	-2.167373419	-3.652622223
H	-3.362189054	-0.601654947	-3.419063807
C	-5.464267731	-3.246433735	-3.056318760
H	-5.708898544	-4.408229351	-1.252243996
H	-4.998319149	-1.913955927	-4.689963818
H	-6.183753490	-3.825968981	-3.626556396
C	-4.308880806	1.530105233	-0.812504649
C	-5.184330463	0.817586303	0.093424223
C	-4.728231907	0.554227650	1.514644504
H	-3.837781429	-0.082403839	1.538502693
H	-4.475712299	1.485548258	2.033688545
H	-5.510962963	0.053015660	2.088591099
C	-4.778532982	1.907976985	-2.193395615
H	-5.049556255	1.017578125	-2.773285389
H	-5.670503139	2.543284655	-2.146063089
H	-4.004127502	2.448391676	-2.743830919
C	-6.410254002	0.384190559	-0.312257409
H	-6.781425476	0.531168997	-1.319361567
H	-7.066724300	-0.148727015	0.367841959
C	-2.981821060	1.816116095	-0.457543314
H	-2.658073187	1.698812127	0.567101359
H	-2.436012745	2.547038317	-1.040749907

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^{3}Ir–2'

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Ir	1.812064528	-0.786554158	0.819175959
N	0.881034195	-2.615275860	0.427670121
C	0.637985051	-3.320024014	1.528955579
S	-0.203926891	-4.821095467	1.243674874
C	-0.205784351	-4.477684021	-0.479186922
C	-0.718260705	-5.242218018	-1.522936702
H	-1.213607430	-6.188815117	-1.331269860
C	-0.573677897	-4.768239975	-2.825189114
H	-0.978021801	-5.369435787	-3.629863262

C	0.080843866	-3.553677559	-3.113134384
C	0.588827670	-2.801236153	-2.047935009
H	1.114664555	-1.874149203	-2.221253157
C	0.441375911	-3.249183893	-0.732987821
C	1.096895456	-2.808051109	2.794992685
C	1.779783130	-1.565820813	2.682402611
C	2.293369293	-1.011762381	3.861154079
H	2.831889391	-0.069321953	3.823755264
C	2.121931076	-1.654064894	5.089268208
H	2.531371832	-1.202478170	5.989436626
C	1.435219288	-2.872776985	5.181144714
H	1.310997963	-3.360169649	6.142694473
C	0.920516193	-3.454190016	4.030017376
H	0.389897078	-4.401766300	4.087291718
C	0.269453764	-3.043637753	-4.553778172
C	1.781922102	-2.986857653	-4.870244980
H	1.943017364	-2.637364149	-5.896187305
H	2.240147114	-3.976392984	-4.772866726
H	2.309761763	-2.304132223	-4.196123600
C	-0.418820679	-3.949709415	-5.590959072
H	-0.273503363	-3.537824869	-6.594697475
H	-1.497559428	-4.014104366	-5.412812710
H	-0.003068954	-4.962611198	-5.590211868
C	-0.334979087	-1.626241326	-4.681180477
H	-0.172480777	-1.238995194	-5.694272518
H	0.131267741	-0.931782544	-3.977413416
H	-1.409721255	-1.635527730	-4.484481335
C	-0.714907110	0.499297321	-0.312489063
O	-0.345524222	0.011347877	0.778544962
N	1.543865919	0.203311980	-1.091612339
C	2.345975399	0.527262211	-2.140921116
C	1.619492173	1.298579097	-3.022339821
H	1.887115955	1.778009892	-3.951170444
C	-2.184924841	0.612008572	-0.625352681
H	-2.335960627	1.356714129	-1.406330943
C	-2.491899967	-0.765475333	-1.148235083
H	-2.165088415	-1.587689042	-0.516137481
N	2.860012531	0.913302481	1.362561345
C	4.173653126	0.809954107	1.206360340
S	5.043144226	2.283354282	1.552298188
C	3.516838074	3.082097530	1.918580890
C	3.277110338	4.396092415	2.309392691
H	4.091746807	5.102778912	2.430887222
C	1.959674239	4.787756443	2.541190863
H	1.784506083	5.813309669	2.841870546
C	0.872752070	3.898879528	2.403831720
C	1.135160565	2.580649853	2.018427610
H	0.343317956	1.851077199	1.917737842
C	2.447525501	2.176187515	1.767977953
C	4.695950031	-0.455368817	0.756880045
C	3.682908058	-1.432258725	0.534240782
C	4.091761589	-2.695377350	0.089424536
H	3.352940321	-3.470776796	-0.086837061
C	5.442657471	-2.966743946	-0.134685934
H	5.737729549	-3.953798771	-0.481434971
C	6.425987720	-1.991255522	0.081612788
H	7.471679211	-2.220156670	-0.097731769
C	6.054061413	-0.731123626	0.529231131
H	6.807011604	0.034148507	0.702662051
C	-0.586542904	4.343426704	2.615943670
C	-0.688241303	5.732859612	3.271425724
H	-1.739842057	5.986552715	3.436478615
H	-0.260086864	6.518627644	2.640302658
H	-0.182931766	5.756610394	4.242174149
C	-1.274938107	4.406000137	1.231818557
H	-2.332829952	4.674371243	1.332198977
H	-1.220239043	3.437131882	0.726160407
H	-0.792626262	5.151805878	0.589424372
C	-1.328667521	3.327593803	3.515403509
H	-2.362144709	3.652577639	3.677299500
H	-0.842097104	3.245986462	4.492566586
H	-1.364983201	2.326634645	3.075232506
C	0.339207381	0.750956714	-1.300951123
N	0.359558403	1.439354420	-2.491452932
H	3.370941162	0.192641228	-2.192277431
C	-0.652888775	2.280808449	-3.064324856
C	-1.179988027	1.964399576	-4.314896107
C	-1.057455897	3.420424700	-2.367224216
C	-2.147861958	2.803498983	-4.868430614
H	-0.856826782	1.066847920	-4.829942226
C	-2.036823511	4.241350651	-2.923132420
H	-0.605298758	3.655901670	-1.410026431
C	-2.582450628	3.932943821	-4.172666073
H	-2.570557117	2.563527107	-5.839179039
H	-2.363796711	5.126042366	-2.385593653
H	-3.342180252	4.576624393	-4.605383873
C	-3.172032356	-1.076180458	-2.345848083
C	-3.369830847	-2.446938753	-2.683783054
C	-3.696594715	-0.093574636	-3.233437538
C	-4.051991940	-2.807565689	-3.833789825
H	-2.962522507	-3.211580276	-2.029244900
C	-4.370448589	-0.468297780	-4.384770393
H	-3.575104952	0.960277796	-3.010503292
C	-4.555441380	-1.822690010	-4.695456505
H	-4.192829132	-3.858722925	-4.069312572
H	-4.764118195	0.296709210	-5.048152924
H	-5.089424133	-2.107707024	-5.596852303
C	-4.494009495	1.171854973	0.211330056
C	-5.495125771	0.210958228	0.474855632
C	-5.145242691	-1.056369305	1.238815188
H	-4.388451576	-1.646970034	0.710459530
H	-4.746658802	-0.833319187	2.235242367
H	-6.025503635	-1.690095663	1.371380448
C	-4.803028107	2.431719542	-0.561206937
H	-5.178358555	2.212910652	-1.570395947
H	-5.574249744	3.035034180	-0.065000400
H	-3.915539026	3.063334942	-0.673474252
C	-6.800346851	0.384120315	0.053616818
H	-7.125804901	1.259924412	-0.496027291
H	-7.558530807	-0.362382889	0.264902860
C	-3.055300236	0.979079783	0.613601804
H	-2.921987295	0.203212947	1.369270682
H	-2.660376549	1.909185767	1.040571451

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^{1}Ir–3'

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Ir	1.774888873	-1.060772181	1.033058524
N	0.603417575	-2.792095423	0.979063392
C	0.498231590	-3.383221388	2.166602373
S	-0.631655395	-4.709825039	2.204407215
C	-0.990519047	-4.437479019	0.506853759
C	-1.870376229	-5.125400543	-0.323010713
H	-2.466179371	-5.950027466	0.055323735
C	-1.967982888	-4.733238697	-1.656096816
H	-2.662063122	-5.268818855	-2.291281223
C	-1.196541190	-3.680230618	-2.187313557
C	-0.314512968	-3.005436659	-1.335738540
H	0.314703256	-2.207787037	-1.702835679
C	-0.217334256	-3.366694212	0.010003113
C	1.272226214	-2.865899563	3.265291452
C	2.046306133	-1.723840356	2.919783592
C	2.840341806	-1.161433339	3.926410437
H	3.454109430	-0.292856067	3.707031012
C	2.849999905	-1.700071573	5.214900494
H	3.474259853	-1.245824456	5.980164051
C	2.069655180	-2.818538427	5.538418770
H	2.087617636	-3.225028276	6.544690132
C	1.276927948	-3.406080008	4.561953068
H	0.669808090	-4.276198864	4.801208496
C	-1.276973128	-3.268109560	-3.668413162
C	0.087306552	-3.547722340	-4.340202332
H	0.054209989	-3.269119263	-5.399591446
H	0.344105065	-4.609993935	-4.276887417
H	0.894772470	-2.977982998	-3.868267298
C	-2.369919777	-4.035592079	-4.435157776
H	-2.395862341	-3.697338820	-5.475985527

H	-3.360462666	-3.857300282	-4.004373074
H	-2.180543900	-5.113907337	-4.448550224
C	-1.595094919	-1.759746313	-3.767663002
H	-1.648176432	-1.458876133	-4.821099758
H	-0.818427444	-1.156773686	-3.288101673
H	-2.550047159	-1.524675965	-3.295012474
C	-0.740845025	0.512790084	0.366744727
O	-0.206809118	-0.040598683	1.354148865
N	1.220948458	-0.145027161	-0.854315519
C	1.816277623	0.020549105	-2.063022137
C	1.034066439	0.867757380	-2.821651697
H	1.160606861	1.268594503	-3.815539122
C	-2.181039095	0.876891613	0.452009946
H	-2.462548018	1.644649267	-0.264450699
C	-3.048882961	-0.441314280	0.326842040
H	-2.409866333	-1.300088763	0.547178328
N	3.043003798	0.560857117	1.237655878
C	4.275126934	0.340304494	0.796610296
S	5.301360607	1.752163529	0.848897040
C	3.959773779	2.689809561	1.502414703
C	3.904002905	4.035755157	1.853541970
H	4.769053459	4.681112766	1.739325404
C	2.705584288	4.541987896	2.355709791
H	2.673419952	5.592267990	2.618467569
C	1.561462760	3.736521006	2.534442663
C	1.642131209	2.384478092	2.187031984
H	0.806526184	1.714795709	2.331361532
C	2.826456547	1.867471218	1.658543348
C	4.590266228	-0.988522470	0.333192170
C	3.488886595	-1.889390349	0.423262417
C	3.697965145	-3.209932804	0.007233707
H	2.885581017	-3.927636385	0.069152460
C	4.939712524	-3.609637976	-0.490920037
H	5.080591679	-4.639104843	-0.810420930
C	6.009276390	-2.707310438	-0.585233808
H	6.967253685	-3.035515070	-0.976025879
C	5.837312222	-1.393165708	-0.171528161
H	6.660481930	-0.685395479	-0.236198813
C	0.226865396	4.298173904	3.061330318
C	0.357573628	5.750469685	3.554314852
H	-0.605138004	6.096221924	3.943229437
H	0.647900045	6.432910919	2.748435020
H	1.092334509	5.836824894	4.361026764
C	-0.806448042	4.270935535	1.909949660
H	-1.779072046	4.642312050	2.252810240
H	-0.952030778	3.254980087	1.530599594
H	-0.476653099	4.906371593	1.079598069
C	-0.287229657	3.431512594	4.234580040
H	-1.228446364	3.838548422	4.619946003
H	0.437364042	3.417059898	5.054955006
H	-0.475241631	2.396174431	3.934816837
C	0.089224711	0.577122092	-0.840329111
N	-0.047428828	1.216041684	-2.052255869
H	2.748372316	-0.467160374	-2.304995775
C	-1.038261890	2.166419268	-2.471809626
C	-1.784458637	1.907557845	-3.621009827
C	-1.197235823	3.348570347	-1.747750401
C	-2.720507622	2.852083206	-4.042526245
H	-1.651492596	0.974483192	-4.156736374
C	-2.148867369	4.275816917	-2.168995380
H	-0.580039859	3.534729958	-0.875574589
C	-2.909345150	4.028960705	-3.315318346
H	-3.310855150	2.659182072	-4.933000565
H	-2.285579920	5.195827961	-1.609087825
H	-3.645161390	4.756515980	-3.644022465
C	-3.848027229	-0.743414760	-0.904808640
C	-4.291701794	-2.063226700	-1.083053231
C	-4.240083218	0.226602823	-1.835218191
C	-5.112428188	-2.401121616	-2.157425880
H	-3.987302303	-2.825484514	-0.371451139
C	-5.048056602	-0.113397591	-2.921319246
H	-3.915199995	1.255800605	-1.725724220
C	-5.491304874	-1.426455617	-3.084182262
H	-5.451805115	-3.426607370	-2.274919033
H	-5.334061146	0.652057171	-3.637595892
H	-6.125585079	-1.689471602	-3.925778151
C	-3.826016665	-0.028444763	1.653653622
C	-3.881232977	-1.180132747	2.645467520
C	-2.592258692	-1.567972064	3.338236332
H	-1.739008427	-1.602014780	2.652646780
H	-2.327457190	-0.841050804	4.116517067
H	-2.680252075	-2.545840502	3.817901134
C	-5.188912392	0.599230111	1.353615761
H	-5.876306534	-0.114093252	0.892551541
H	-5.639025211	0.973107338	2.278258562
H	-5.087795258	1.437947035	0.657309473
C	-5.004529953	-1.875857830	2.869678259
H	-5.956390858	-1.626964808	2.414783955
H	-5.006253242	-2.731875420	3.538825512
C	-2.748566628	1.083935142	1.883783221
H	-2.012265921	0.849790931	2.651200771
H	-3.152398825	2.080649376	2.072877169

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C	-1.115658522	0.876566589	0.191233099
O	-0.846198678	-0.086180851	0.925636470
N	0.865707278	0.751071334	-1.302201271
C	1.153823853	1.130672216	-2.585821390
C	0.044321433	1.662108064	-3.197096825
H	-0.143723667	2.017584085	-4.198413849
C	-2.023331881	1.920817375	0.609564066
H	-2.103992939	2.813791990	-0.009692905
C	-2.811260223	1.845000386	1.839069486
H	-3.888221502	1.724918246	1.721619368
C	-0.407674819	1.043998361	-1.114464760
N	-0.965193033	1.610044360	-2.255120993
H	2.141587257	1.001396894	-3.006265879
C	-2.322982788	1.964628577	-2.493500948
C	-3.351173878	1.077920437	-2.154414892
C	-2.619660378	3.207716465	-3.060696125
C	-4.677585125	1.450544477	-2.367839575
H	-3.105212450	0.107362777	-1.737174869
C	-3.949150324	3.563195705	-3.285973310
H	-1.811491370	3.890855551	-3.302023888
C	-4.980434418	2.690370798	-2.934062481
H	-5.474801064	0.763756156	-2.100295067
H	-4.178151608	4.529695511	-3.724760532
H	-6.014769554	2.974874735	-3.101373434
C	-2.279727459	1.908824205	3.144832134
C	-3.146591902	1.871328950	4.277778625
C	-0.878327310	2.016099691	3.390833616
C	-2.642774343	1.935464621	5.565058708
H	-4.218182564	1.790043831	4.113668919
C	-0.389449328	2.082438707	4.685242653
H	-0.191779792	2.023005247	2.552313566
C	-1.260487914	2.043131113	5.782334805
H	-3.322091818	1.900213838	6.412165642
H	0.682200432	2.155627728	4.848204136
H	-0.868315339	2.088322163	6.793694496

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^{3}1–TS

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C	-1.190954804	12.178272247	-4.717985153
O	-1.013522029	11.201934814	-3.971983433
N	0.562471509	11.671601295	-6.399508953
C	1.311505198	12.394627571	-7.291903496
C	1.064074278	13.738133430	-7.158159256
H	1.478755713	14.614182472	-7.632659912
C	-2.442151546	12.902946472	-4.763879776
H	-2.512892008	13.791669846	-5.375445843
C	-3.467213154	12.635661125	-3.780010223
H	-3.354668617	11.709127426	-3.227183580
C	-0.142243624	12.554944038	-5.713556290
N	0.130769610	13.847600937	-6.143546581
H	1.990307093	11.913038254	-7.982339859

C	-0.389212370	15.071892738	-5.638123035
C	-0.946283400	15.999279976	-6.523681641
C	-0.378154635	15.324954987	-4.262671471
C	-1.499054790	17.180694580	-6.028063297
H	-0.964513898	15.777122498	-7.586003780
C	-0.947361290	16.500053406	-3.775701284
H	0.062225483	14.596375465	-3.590627909
C	-1.508831501	17.430158615	-4.654210091
H	-1.936216354	17.898303986	-6.716174126
H	-0.951481938	16.689420700	-2.706766844
H	-1.952429056	18.343595505	-4.269619942
C	-4.578647614	13.457715034	-3.509194851
C	-5.620803356	12.975633621	-2.658037663
C	-4.742057323	14.765277863	-4.066412926
C	-6.750281811	13.733922005	-2.404842377
H	-5.518185139	11.984925270	-2.224698782
C	-5.875443459	15.514686584	-3.797996283
H	-3.957941532	15.187024117	-4.687260151
C	-6.892312050	15.009388924	-2.972990990
H	-7.532274723	13.337361336	-1.763039708
H	-5.976027489	16.507152557	-4.229448795
H	-7.779262543	15.602558136	-2.771789551
C	-3.256937504	11.588367462	-6.618174553
C	-4.103444099	10.747200012	-5.916720867
H	-3.630795479	12.456170082	-7.148212910
H	-2.257883549	11.262535095	-6.882474422
C	-5.517040730	11.059833527	-5.741769791
C	-3.522304296	9.499417305	-5.299192429
C	-6.086088657	12.280523300	-6.432285786
C	-6.327760220	10.277389526	-4.986621380
H	-3.976117611	8.599740028	-5.733006477
H	-2.441467524	9.457679749	-5.438679218
H	-3.707823992	9.469404221	-4.220729351
H	-5.952579021	12.221569061	-7.518771172
H	-7.154128551	12.381527901	-6.227126598
H	-5.598240852	13.196870804	-6.086110115
H	-5.972388744	9.394065857	-4.468705177
H	-7.379716873	10.515497208	-4.868742466

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C	-1.532303929	12.223878860	-4.601299763
O	-1.457198739	11.409487724	-3.700574398
N	0.452255726	11.602617264	-5.958028316
C	1.345434070	12.265999794	-6.757516384
C	1.106412411	13.618576050	-6.730710030
H	1.615757227	14.462158203	-7.170224667
C	-2.858119965	12.863839149	-5.019885540
H	-2.649880648	13.837096214	-5.466919899
C	-3.774697065	13.002550125	-3.850106001
H	-3.817262650	12.148577690	-3.181339264
C	-0.336089075	12.531887054	-5.445786476
N	0.017059676	13.794019699	-5.899370193
H	2.112865448	11.739855766	-7.308134556
C	-0.508184671	15.051976204	-5.484147549
C	-0.818030059	16.019363403	-6.444880009
C	-0.730230391	15.303290367	-4.126676559
C	-1.353457212	17.242502213	-6.041090965
H	-0.659699678	15.800065041	-7.496050835
C	-1.288815141	16.519289017	-3.736993074
H	-0.475371182	14.547415733	-3.391275406
C	-1.597624183	17.492097855	-4.689295769
H	-1.597188115	17.992918015	-6.787300110
H	-1.483452797	16.704959869	-2.685683012
H	-2.034538507	18.436403275	-4.379834652
C	-4.566820145	14.135878563	-3.553927660
C	-5.407464504	14.119912148	-2.400026560
C	-4.578537464	15.323122978	-4.344981670
C	-6.195772648	15.208363533	-2.064859629
H	-5.418224335	13.227661133	-1.779537797
C	-5.370121002	16.407028198	-3.997114420
H	-3.951231003	15.392246246	-5.226493835
C	-6.185962200	16.364330292	-2.859065056
H	-6.825045586	15.164783478	-1.180022836
H	-5.353942394	17.299758911	-4.616892815
H	-6.804567814	17.216836929	-2.594710350
C	-3.473774433	11.998464584	-6.198574066
C	-3.805978298	10.573260307	-5.846252441
H	-4.353786469	12.550646782	-6.540005684
H	-2.744680405	12.016640663	-7.019786835
C	-5.113999844	10.176568031	-5.479718208
C	-2.678516626	9.570732117	-5.888178349
C	-6.252666950	11.183979988	-5.511855602
C	-5.401333809	8.880354881	-5.098424911
H	-2.921336174	8.730721474	-6.551946163
H	-1.743501782	10.015548706	-6.237055779
H	-2.473888874	9.153587341	-4.894960403
H	-6.409996510	11.581693649	-6.521687031
H	-7.190409660	10.723102570	-5.191600323
H	-6.058811665	12.038512230	-4.857041359
H	-4.642729759	8.108957291	-5.041380882
H	-6.410206318	8.590444565	-4.824138641

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C	-0.562797427	12.040766716	-5.575393200
O	-0.291954398	11.132640839	-4.807693958
N	1.366761804	11.989908218	-7.145217419
C	2.073900223	12.928937912	-7.852213383
C	1.647267103	14.196717262	-7.539459229
H	1.985028982	15.179403305	-7.830275536
C	-1.988229156	12.459773064	-5.869935513
H	-2.032901525	13.491579056	-6.218042374
C	-3.034957170	12.066086769	-4.799893856
H	-2.543620825	11.500109673	-4.001853943
C	0.505253077	12.670038223	-6.412033081
N	0.628089547	14.033754349	-6.619757175
H	2.853510141	12.645465851	-8.545619965
C	0.012636211	15.079530716	-5.873788357
C	-0.572067022	16.158834457	-6.541694164
C	0.008379630	15.022279739	-4.476198196
C	-1.155077100	17.188823700	-5.803226471
H	-0.576903403	16.176790237	-7.626883030
C	-0.590304732	16.049356461	-3.748444080
H	0.473501533	14.180884361	-3.973173857
C	-1.166010141	17.136997223	-4.407709122
H	-1.612703204	18.026315689	-6.321137905
H	-0.607768476	15.997100830	-2.664490938
H	-1.630558133	17.934928894	-3.836624384
C	-3.896641016	13.125525475	-4.157943249
C	-4.962162495	12.711592674	-3.341623306
C	-3.684071302	14.499145508	-4.318360806
C	-5.795464516	13.638855934	-2.721485615
H	-5.144089699	11.649292946	-3.209431410
C	-4.512462616	15.432424545	-3.690255404
H	-2.866791725	14.858220100	-4.930771351
C	-5.574978828	15.007952690	-2.894600868
H	-6.618758202	13.293417931	-2.101943731
H	-4.320654392	16.492877960	-3.830101252
H	-6.223777771	15.732652664	-2.410616398
C	-2.646385193	11.468471527	-6.891493320
C	-3.694134712	11.017980576	-5.816924572
H	-3.054005146	11.974742889	-7.766701698
H	-1.991369009	10.664097786	-7.235230446
C	-5.146316528	11.274407387	-6.184932232
C	-3.420167923	9.587504387	-5.343967438
C	-5.465176582	12.543508530	-6.946620941
C	-6.134547234	10.430895805	-5.858791828
H	-3.704424858	8.858995438	-6.109990597
H	-2.355164051	9.468974113	-5.125891209
H	-3.972457886	9.358320236	-4.426571369
H	-5.158277988	12.463957787	-7.996730804
H	-6.538303852	12.750106812	-6.932751656
H	-4.952361584	13.411991119	-6.523698807
H	-5.967301846	9.495887756	-5.336935043
H	-7.166340351	10.656020164	-6.114410400

Table S5. Vibrational frequencies of all DFT optimized structures

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^{1}RhS

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16.73 23.26 25.54 31.27 33.43 37.08
42.63 45.27 48.91 52.57 54.31 58.74
67.67 75.76 84.30 90.65 95.34 108.10
110.38 129.47 129.71 139.46 145.80 160.19
164.64 170.86 179.38 181.79 188.09 194.28
222.25 227.19 230.18 236.16 242.56 257.98
264.28 273.44 281.65 288.56 295.31 301.42
309.40 322.98 324.89 337.10 339.54 356.97
357.19 358.57 362.13 368.35 369.68 385.42
387.53 404.58 407.10 410.79 414.65 414.99
415.27 443.96 445.07 454.99 456.99 466.42
472.94 474.29 474.80 512.31 526.07 534.54
534.86 594.86 596.34 614.72 615.29 623.03
627.26 667.63 670.76 678.33 680.32 708.59
711.40 733.18 733.37 738.03 739.41 741.94
753.29 777.04 778.07 787.75 790.50 833.28
834.03 846.67 848.14 882.67 884.76 898.99
900.46 936.78 937.62 937.93 938.16 945.67
946.74 957.04 957.86 958.12 960.00 967.05
967.88 975.47 976.82 1003.51 1003.53 1004.86
1005.91 1043.06 1049.24 1056.04 1056.07 1056.19
1056.51 1057.66 1059.37 1064.59 1065.20 1073.91
1075.53 1089.56 1092.40 1133.32 1133.54 1159.06
1159.94 1204.78 1205.02 1205.26 1205.71 1233.15
1233.53 1239.12 1239.58 1271.51 1275.54 1290.63
1293.23 1304.69 1306.06 1315.40 1318.28 1327.20
1330.33 1344.70 1346.42 1362.00 1362.32 1415.62
1415.89 1416.80 1418.03 1420.16 1420.24 1451.93
1452.19 1460.65 1462.60 1469.31 1470.27 1470.96
1471.79 1472.05 1472.82 1484.35 1485.98 1497.87
1498.54 1498.82 1499.36 1499.97 1500.98 1507.97
1509.28 1521.75 1521.84 1526.38 1526.79 1529.51
1530.45 1538.82 1538.89 1606.50 1606.55 1609.79
1610.41 1631.45 1633.99 1658.65 1660.58 2384.92
2386.60 3035.71 3036.21 3038.63 3039.86 3045.61
3046.20 3061.01 3061.22 3106.92 3107.49 3111.43
3112.31 3113.66 3114.12 3116.61 3117.15 3118.62
3118.88 3121.13 3122.39 3143.12 3143.52 3146.37
3146.61 3177.59 3179.59 3185.87 3186.60 3205.61
3205.72 3211.02 3211.53 3230.25 3232.25 3233.06
3233.23 3265.21 3270.08

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^{3}RhS

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17.54 20.80 27.92 28.96 34.05 35.40
37.23 38.42 43.21 51.58 52.17 57.97
69.12 79.63 86.07 89.74 95.13 97.56
105.68 108.55 112.68 128.17 131.08 138.66
142.01 147.68 152.27 165.73 172.55 187.87
193.91 203.45 205.20 219.94 221.23 242.95
255.82 265.58 269.21 270.08 273.70 301.90
306.44 308.64 311.98 319.41 323.69 342.26
346.62 355.65 359.23 366.61 366.72 371.68
377.82 402.20 403.58 404.77 405.83 414.87
416.27 433.28 437.67 451.35 453.43 461.04
469.54 472.73 474.11 505.14 509.29 531.45
532.54 585.06 590.58 614.09 615.61 620.76
626.05 653.63 654.64 674.54 675.79 700.65
706.50 722.38 725.42 735.55 736.33 738.29
744.53 755.39 758.31 776.61 777.40 833.99
834.50 837.37 840.13 882.71 883.95 904.41
906.55 932.83 935.64 937.27 937.72 938.81
942.55 953.54 954.67 962.15 963.18 967.40
968.10 974.73 975.06 982.47 989.81 1004.39
1006.16 1027.20 1041.16 1055.64 1055.68 1055.90
1056.66 1059.38 1059.49 1063.28 1063.39 1073.20
1074.93 1083.66 1089.21 1129.37 1129.83 1155.79
1157.01 1202.83 1205.34 1206.06 1206.30 1233.35
1233.42 1238.29 1238.89 1265.33 1267.55 1279.69
1282.95 1295.24 1297.40 1301.31 1301.47 1322.87
1323.72 1335.82 1337.96 1355.91 1356.96 1415.06
1415.26 1415.81 1416.22 1419.86 1420.01 1451.25
1451.40 1461.51 1463.23 1467.57 1468.48 1469.19
1470.35 1471.11 1472.06 1479.95 1485.08 1495.45
1495.98 1499.27 1499.50 1502.48 1502.97 1508.85
1509.54 1521.69 1521.98 1527.52 1527.83 1536.22
1537.69 1539.89 1540.42 1599.99 1600.33 1602.73
1608.81 1620.82 1633.01 1657.47 1661.20 2379.60
2383.11 3033.41 3034.53 3038.89 3038.94 3046.78
3046.89 3060.74 3061.44 3102.78 3103.96 3107.68
3109.31 3114.23 3114.83 3118.48 3118.96 3119.48
3119.78 3123.46 3123.62 3143.89 3144.34 3146.33
3147.96 3176.77 3179.25 3185.77 3187.01 3205.16
3205.40 3209.55 3211.07 3223.62 3231.62 3231.95
3236.35 3240.05 3242.07

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^{1}IrS

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16.90 20.24 24.35 28.57 33.88 37.61
45.72 47.02 49.01 53.33 57.11 64.73
86.17 90.10 93.69 96.14 100.64 112.17
129.66 132.84 142.59 165.73 169.87 171.70
175.54 184.58 190.35 201.28 203.46 208.78
223.85 227.53 233.35 243.70 247.05 256.79
260.59 270.84 278.83 283.74 287.57 300.97
303.36 316.38 319.48 334.43 336.09 354.45
354.88 365.01 366.68 369.04 370.24 389.91
392.83 410.76 414.18 415.78 417.02 420.35
423.56 446.83 448.68 458.88 460.20 473.86
475.39 477.65 479.16 519.20 530.95 536.37
536.51 598.38 601.73 614.69 615.20 624.95
629.50 673.92 676.54 679.11 681.98 712.80

713.69	734.74	735.11	744.55	746.40	753.87
764.53	783.21	784.07	797.37	798.46	832.81
834.07	850.08	852.88	889.38	891.35	899.91
900.45	938.84	939.17	939.25	942.73	948.39
949.91	959.57	960.96	961.09	961.77	965.53
966.35	979.26	979.55	1005.80	1006.52	1010.71
1011.22	1050.40	1053.34	1053.93	1055.48	1055.90
1056.17	1057.14	1057.31	1065.94	1066.23	1075.65
1077.61	1091.62	1097.63	1134.41	1134.75	1161.51
1162.54	1204.82	1205.29	1206.07	1206.29	1233.65
1234.05	1241.29	1241.50	1272.63	1276.12	1292.86
1295.35	1304.67	1306.06	1319.44	1320.85	1330.01
1331.77	1347.36	1347.83	1363.03	1363.42	1413.59
1414.18	1418.49	1418.64	1420.76	1421.02	1452.16
1452.47	1455.51	1456.19	1469.21	1469.35	1470.21
1470.28	1470.67	1470.84	1484.82	1485.98	1497.49
1497.99	1498.92	1499.39	1499.98	1500.44	1506.43
1507.87	1519.49	1519.99	1524.53	1525.44	1528.55
1529.30	1538.71	1538.86	1606.06	1606.39	1607.78
1608.64	1637.83	1639.52	1657.77	1659.67	2385.73
2390.59	3036.50	3037.36	3040.24	3040.47	3046.94
3047.12	3059.87	3061.01	3110.23	3111.03	3113.61
3113.82	3114.86	3115.37	3117.45	3117.79	3119.22
3119.53	3123.06	3123.24	3141.68	3143.96	3145.90
3146.05	3176.89	3176.98	3185.51	3185.55	3206.24
3206.45	3211.25	3211.56	3218.31	3223.52	3234.12
3237.05	3263.46	3268.08			

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15.76	23.41	26.21	29.36	33.69	36.63
39.91	44.89	50.67	51.85	54.54	61.90
76.62	78.22	84.55	88.57	94.78	107.21
117.70	126.68	136.44	156.49	156.62	162.78
166.80	180.66	188.48	191.54	196.81	203.00
224.52	226.67	228.51	230.72	244.19	254.89
261.47	267.51	274.31	279.09	282.28	287.30
301.87	304.06	316.11	325.00	339.13	350.59
358.72	362.23	363.03	365.80	369.07	389.11
391.45	407.52	409.27	413.01	414.59	416.87
419.11	425.01	446.49	452.55	458.49	464.97
472.01	473.12	476.28	487.34	513.24	523.00
525.82	535.56	584.29	600.45	605.95	616.08
626.35	645.95	663.72	675.23	680.55	691.12
713.37	717.92	725.15	726.53	734.09	745.24
756.98	760.76	777.05	783.20	794.74	830.34
834.15	839.33	846.50	851.02	881.52	890.78
894.25	924.42	938.58	938.64	939.25	939.62
941.64	947.71	949.68	955.19	959.45	961.20
966.70	975.76	979.88	981.44	989.50	1001.19
1006.91	1010.99	1039.85	1052.62	1054.39	1054.54
1055.61	1056.11	1056.24	1058.46	1062.59	1064.36
1065.39	1078.50	1094.74	1111.64	1129.81	1133.62
1157.50	1161.91	1187.48	1195.20	1205.78	1206.45
1233.76	1234.23	1237.80	1239.28	1270.40	1275.26
1284.13	1294.83	1305.27	1311.02	1320.65	1322.38
1330.81	1338.78	1348.41	1349.79	1362.70	1413.56
1415.09	1416.24	1416.40	1419.26	1420.82	1421.21
1433.54	1446.32	1452.11	1453.76	1458.93	1470.02
1470.52	1470.88	1471.44	1472.13	1477.75	1487.90
1498.58	1498.70	1499.04	1499.88	1500.45	1505.72
1508.04	1518.97	1520.07	1522.78	1526.90	1527.03
1527.52	1538.99	1539.09	1548.31	1576.39	1585.30
1603.48	1607.46	1608.65	1636.27	1659.89	2382.37
2389.04	3036.88	3037.70	3039.17	3039.75	3045.84
3046.65	3059.21	3059.99	3107.71	3110.36	3112.04
3113.69	3114.86	3115.79	3117.04	3117.83	3118.96
3119.15	3121.84	3123.73	3141.52	3142.41	3143.40
3145.36	3180.82	3182.46	3187.36	3192.56	3205.09
3205.67	3205.70	3212.15	3215.96	3228.41	3233.56
3234.53	3264.38	3275.24			

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22.80	30.93	33.75	55.34	79.65	89.98
107.30	145.59	164.99	223.40	247.22	273.73
292.75	315.98	374.70	378.36	414.47	423.31
464.61	502.02	521.51	579.61	590.78	624.40
632.01	649.54	668.72	701.65	707.12	711.46
743.53	759.68	783.14	786.37	797.67	854.64
855.88	870.16	898.17	903.00	927.12	933.58
937.53	976.43	978.51	1000.30	1001.92	1003.34
1013.74	1018.42	1034.10	1055.46	1058.27	1092.51
1110.01	1117.67	1127.77	1167.78	1196.90	1197.90
1209.04	1218.72	1237.75	1243.93	1306.93	1331.07
1343.14	1353.11	1359.37	1362.20	1370.61	1372.50
1441.27	1487.17	1491.95	1497.37	1539.95	1541.96
1555.58	1630.24	1644.93	1657.86	1658.07	1677.31
1754.63	3166.97	3176.73	3182.59	3186.03	3192.76
3196.32	3202.47	3205.44	3208.95	3212.41	3218.14
3219.70	3253.89	3285.02			

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386.46	386.60	932.39	1061.24	1061.27	1420.15
1482.71	1483.05	2378.66	3058.52	3135.64	3136.10

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88.08	239.86	256.41	318.19	342.04	418.62
485.77	498.58	564.53	672.47	741.75	795.29
924.90	927.15	930.42	989.77	1024.92	1053.02
1072.62	1078.96	1213.15	1372.07	1425.03	1425.13
1455.63	1463.67	1497.34	1497.70	1510.43	1531.35
1680.17	1711.33	3036.38	3037.74	3092.11	3093.61
3128.90	3129.90	3167.18	3167.83	3251.21	3252.17

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^{1}Rh–1

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11.55	16.29	22.82	25.21	27.79	31.58

32.38	37.16	40.24	47.37	52.30	53.43
60.40	72.53	81.11	82.61	83.48	85.16
91.40	98.06	113.03	116.90	121.86	124.10
131.64	140.20	151.75	167.73	179.93	180.28
184.60	196.75	206.61	217.33	221.47	224.67
230.91	235.85	249.61	253.98	264.96	268.52
271.54	284.24	287.01	293.59	300.73	304.09
307.38	313.78	325.57	332.29	334.51	340.43
343.29	344.81	351.66	359.65	362.24	366.53
369.12	390.87	396.00	398.32	409.42	414.82
417.32	420.54	426.94	439.38	442.52	457.64
459.77	461.86	469.39	473.54	475.39	478.32
496.12	510.67	522.67	524.92	535.56	537.11
587.86	595.75	597.92	609.24	616.18	617.17
623.82	624.67	627.66	629.98	656.35	663.68
664.30	672.93	680.17	680.89	696.59	704.45
709.65	710.59	713.85	736.93	737.37	740.75
741.58	742.73	752.64	754.08	777.69	779.16
780.78	786.36	787.36	795.44	795.79	805.09
832.72	834.11	848.44	850.83	851.39	861.57
880.96	882.98	884.88	887.87	900.93	909.60
915.43	939.31	940.23	941.01	943.94	946.05
949.22	953.68	957.54	957.95	958.45	959.68
965.73	965.98	973.47	979.79	984.32	987.33
1003.41	1003.63	1004.51	1006.66	1008.85	1013.34
1015.02	1016.21	1020.61	1035.46	1043.01	1048.99
1055.50	1057.74	1058.07	1059.01	1059.52	1067.00
1069.21	1076.87	1088.85	1094.61	1113.47	1115.42
1122.46	1130.48	1135.88	1142.74	1157.88	1160.89
1183.17	1202.26	1202.80	1204.23	1204.93	1205.11
1207.11	1213.34	1220.77	1234.84	1237.29	1239.30
1243.81	1248.70	1258.69	1267.94	1271.18	1290.08
1291.52	1302.51	1307.56	1314.63	1319.79	1323.94
1328.31	1332.16	1339.92	1345.05	1347.25	1350.04
1354.96	1359.23	1364.03	1364.39	1374.66	1378.45
1394.81	1416.16	1417.77	1419.34	1420.29	1442.55
1450.89	1452.08	1459.58	1460.80	1468.62	1469.85
1481.59	1484.88	1486.39	1493.74	1494.77	1498.35
1498.70	1500.16	1500.76	1501.64	1503.05	1507.24
1508.95	1518.00	1521.00	1525.12	1526.80	1527.38
1534.05	1538.55	1539.37	1540.71	1541.28	1552.23
1599.63	1603.40	1606.80	1607.56	1608.91	1626.86
1632.59	1634.92	1646.99	1653.80	1654.82	1656.82
1657.74	1683.36	3037.40	3039.04	3039.58	3045.38
3046.19	3052.55	3105.70	3109.04	3110.58	3115.29
3115.74	3117.75	3121.32	3121.47	3125.31	3128.24
3136.44	3138.39	3173.76	3174.10	3176.52	3181.76
3184.74	3185.50	3189.95	3194.36	3199.17	3201.69
3203.20	3203.84	3208.04	3209.11	3209.19	3209.52
3214.86	3215.01	3215.23	3218.23	3222.62	3233.76
3233.80	3253.38	3259.25	3274.90	3279.89	3300.26

^{3}Rh-1

13.00	20.58	23.60	25.58	28.88	33.72
38.36	40.61	48.02	49.10	53.09	56.66
60.62	62.37	72.51	75.65	82.68	85.54
89.13	98.23	115.45	119.89	122.97	124.50
129.47	143.18	149.55	166.64	177.84	185.63
193.84	198.13	200.80	206.19	213.91	215.81
225.02	231.85	245.51	258.09	260.79	268.46
269.73	274.72	278.81	295.57	301.72	303.79
309.79	314.88	321.67	327.49	330.69	337.89
339.07	346.07	353.09	356.92	364.26	366.93
367.77	387.50	390.16	404.72	412.02	413.55
418.94	420.96	423.04	438.29	441.24	451.44
452.42	456.62	461.80	464.69	468.21	470.77
499.58	502.48	509.42	525.61	531.98	532.73
570.05	582.07	586.28	589.94	603.98	609.44
609.81	614.99	618.09	621.11	624.61	639.10
660.12	662.17	676.56	678.35	693.34	699.20
704.75	705.58	709.61	713.39	726.48	732.15
734.31	736.91	743.54	744.85	756.45	769.21
774.37	778.48	783.83	788.15	791.32	792.66
834.37	835.20	836.53	840.86	846.58	851.15
853.26	861.14	888.52	889.62	892.11	906.16
907.55	926.79	928.98	935.86	938.59	941.41
942.52	945.10	952.92	955.38	958.78	966.23
969.11	970.64	972.04	974.41	977.46	977.56
983.61	990.24	995.50	1000.88	1002.05	1004.81
1010.94	1012.56	1013.75	1015.57	1017.98	1036.13
1049.33	1053.78	1055.93	1056.17	1059.85	1063.21
1064.54	1068.57	1077.15	1079.27	1109.71	1111.37
1118.78	1129.20	1131.21	1132.32	1156.82	1159.49
1173.00	1190.89	1198.30	1200.47	1203.01	1203.90
1204.72	1205.51	1207.32	1232.86	1233.21	1236.00
1238.53	1241.30	1245.36	1261.98	1264.66	1267.82
1284.93	1288.41	1302.58	1304.14	1313.39	1316.05
1326.83	1328.98	1330.12	1341.54	1342.98	1344.86
1351.73	1359.40	1360.87	1362.20	1364.04	1368.30
1371.61	1393.47	1415.01	1419.13	1420.64	1420.88
1448.15	1451.55	1452.65	1456.20	1461.49	1464.24
1470.71	1475.38	1480.61	1484.80	1491.31	1493.00
1493.89	1494.77	1497.36	1498.65	1499.39	1500.47
1506.39	1507.19	1516.95	1518.99	1522.79	1524.35
1527.32	1529.58	1531.44	1532.62	1538.75	1541.23
1543.33	1564.61	1590.03	1597.56	1600.80	1602.74
1603.41	1612.97	1622.01	1633.40	1644.29	1648.20
1653.34	1654.55	3036.10	3037.56	3038.36	3044.61
3044.68	3052.43	3106.45	3109.39	3110.25	3115.14
3116.50	3118.14	3118.60	3119.41	3123.38	3123.49
3129.68	3144.98	3175.35	3179.36	3181.62	3182.88
3184.76	3188.87	3190.35	3191.96	3194.78	3196.61
3203.70	3204.13	3206.77	3207.83	3209.10	3210.35
3210.95	3211.19	3215.15	3216.53	3217.75	3231.07
3231.83	3253.32	3256.71	3278.41	3299.79	3301.23

^{3}Rh–1–TS

-231.40	16.00	22.92	26.23	29.43	30.98

34.52	37.15	37.76	45.18	48.70	50.07
55.73	57.60	63.79	65.93	69.01	71.55
74.25	80.37	82.37	86.02	88.46	90.80
96.73	110.65	121.02	122.46	124.62	126.11
144.77	149.99	154.78	164.40	168.40	175.31
181.85	188.52	199.99	204.96	206.16	214.62
221.80	223.53	227.01	233.63	239.93	245.77
257.30	262.10	267.61	271.18	284.11	288.82
296.95	303.09	316.91	322.64	327.69	332.52
337.31	340.89	342.15	346.16	346.87	354.36
357.49	361.16	361.44	367.62	374.48	386.04
392.07	399.14	406.91	414.61	420.17	420.99
423.09	424.23	427.24	439.40	442.32	457.37
460.91	462.89	470.43	472.54	473.38	477.08
482.75	497.34	504.44	511.23	523.28	524.01
533.61	537.52	562.37	582.07	591.78	598.49
608.53	612.89	618.76	619.70	625.71	626.40
627.78	653.11	657.33	661.64	671.80	674.24
680.85	681.74	687.43	705.40	706.55	711.26
713.82	729.94	739.40	739.87	741.22	742.81
746.66	750.23	753.57	758.14	778.55	779.33
780.23	788.04	789.11	791.61	793.64	802.19
834.05	836.99	837.01	844.47	848.50	851.05
864.92	874.02	883.46	884.93	887.15	904.18
907.35	915.56	916.43	927.69	938.92	940.12
940.49	945.45	947.07	951.13	952.79	955.29
957.16	957.73	963.40	967.53	968.73	970.73
977.76	978.28	988.47	996.79	997.58	1002.80
1002.92	1004.57	1004.69	1006.36	1010.17	1015.94
1019.20	1021.44	1027.17	1035.48	1046.87	1047.52
1053.72	1056.04	1056.43	1058.68	1060.34	1062.25
1062.92	1067.19	1071.39	1074.17	1083.75	1094.43
1109.48	1112.14	1118.76	1133.28	1134.46	1140.85
1159.63	1161.62	1177.58	1190.87	1199.29	1201.43
1203.46	1203.54	1205.10	1205.33	1208.65	1217.07
1217.87	1233.32	1234.14	1240.73	1241.29	1251.61
1261.86	1264.65	1268.41	1289.86	1292.38	1304.01
1304.03	1315.98	1318.19	1330.50	1331.19	1334.41
1340.19	1345.48	1345.55	1347.09	1349.17	1360.08
1362.24	1367.94	1369.16	1371.49	1388.97	1391.83
1408.54	1414.68	1417.93	1421.20	1422.00	1424.94
1444.26	1445.60	1451.48	1452.84	1459.39	1459.84
1467.37	1469.65	1478.24	1482.39	1483.06	1485.11
1486.07	1494.19	1495.88	1498.12	1499.71	1500.78
1501.41	1501.72	1502.28	1503.59	1507.60	1508.17
1514.28	1517.28	1518.47	1520.67	1524.77	1525.78
1527.77	1531.73	1534.46	1538.50	1540.09	1540.41
1547.88	1554.32	1566.18	1592.89	1596.10	1602.92
1603.78	1607.78	1609.49	1619.92	1634.70	1637.31
1645.58	1653.22	1654.53	1657.26	3034.81	3038.39
3041.20	3042.26	3043.34	3046.56	3046.79	3048.43
3096.86	3105.48	3106.91	3111.18	3112.00	3113.22
3115.43	3115.65	3119.17	3121.48	3124.56	3127.30
3129.37	3132.59	3139.94	3164.78	3172.79	3175.10
3175.51	3179.55	3180.89	3181.36	3182.99	3183.16
3193.01	3195.93	3198.44	3201.40	3202.07	3203.77
3204.38	3206.47	3207.62	3208.43	3210.55	3212.14
3213.45	3214.07	3215.44	3219.81	3231.35	3256.45
3258.63	3263.21	3265.15	3278.75	3297.48	3298.89

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^{3}Rh–2

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12.42	18.93	25.37	28.74	29.64	35.09
36.27	40.48	46.72	48.11	49.25	54.81
55.95	59.14	65.31	67.39	76.53	81.21
82.91	85.97	87.58	93.57	96.29	102.51
110.73	121.26	121.85	126.28	134.04	145.61
160.92	165.03	168.99	173.33	177.81	183.88
186.83	190.40	199.25	204.05	211.93	214.60
222.14	223.87	230.46	236.82	245.72	257.59
262.85	269.23	273.50	284.93	290.60	297.43
300.83	316.88	327.13	329.24	334.01	338.20
340.15	344.62	346.03	347.38	354.10	356.03
358.82	360.44	367.65	375.15	391.20	393.08
399.42	408.35	411.42	417.87	419.73	422.21
423.89	435.53	438.85	441.41	458.96	460.80
462.06	467.48	469.81	471.76	475.03	488.97
492.34	505.84	510.88	522.20	526.03	535.93
538.45	566.12	580.88	596.64	599.75	603.15
615.62	618.71	621.93	623.89	625.28	626.98
629.05	656.11	672.66	676.28	677.96	680.16
681.79	686.29	708.00	709.02	712.06	712.91
717.87	723.99	736.39	737.68	739.26	741.41
746.06	752.49	766.66	769.19	775.71	778.28
779.73	782.18	791.93	795.50	796.06	829.32
832.81	834.60	836.06	837.74	848.09	850.23
859.17	878.51	882.64	883.76	885.07	902.47
906.17	910.73	917.00	939.42	940.53	942.68
947.69	950.55	952.49	954.28	956.06	958.34
959.09	966.16	968.42	969.38	970.79	976.57
979.33	985.67	994.67	995.79	1002.16	1004.38
1004.67	1004.89	1006.34	1008.66	1014.64	1017.50
1021.02	1024.41	1046.59	1047.53	1054.30	1054.87
1055.91	1057.26	1059.93	1062.97	1063.04	1071.46
1076.09	1076.27	1089.57	1096.27	1096.48	1113.13
1129.81	1132.18	1133.77	1137.61	1157.17	1160.35
1161.72	1185.76	1194.36	1201.94	1203.93	1204.21
1204.40	1205.68	1207.78	1209.23	1218.34	1233.80
1234.64	1240.16	1240.79	1241.21	1253.84	1260.57
1266.33	1269.48	1279.35	1290.32	1293.56	1304.16
1305.64	1317.91	1320.07	1329.13	1330.58	1333.37
1337.27	1347.22	1348.76	1348.95	1351.52	1358.48
1359.81	1365.61	1367.53	1368.78	1375.45	1399.61
1411.19	1416.07	1417.40	1419.95	1422.18	1424.23
1437.12	1440.11	1451.09	1453.03	1460.55	1461.46
1464.73	1469.38	1470.54	1482.90	1486.01	1486.37
1488.78	1495.06	1495.65	1497.58	1498.34	1500.89
1501.60	1501.87	1502.72	1503.85	1504.09	1507.00
1507.87	1509.12	1519.18	1520.63	1522.01	1525.50
1525.65	1526.72	1527.88	1533.45	1538.79	1539.29
1541.39	1550.21	1558.58	1595.56	1603.79	1604.16

1609.52 1611.00 1618.91 1634.54 1637.09 1647.88
1651.10 1653.35 1656.12 1658.85 3020.58 3036.68
3036.83 3041.17 3041.63 3044.29 3046.46 3047.30
3062.53 3081.66 3105.48 3108.30 3111.05 3111.28
3111.46 3111.71 3114.49 3116.47 3117.03 3120.79
3122.71 3123.24 3124.77 3127.96 3128.33 3136.97
3171.14 3172.06 3174.80 3176.45 3179.05 3182.75
3183.40 3185.72 3194.13 3194.79 3198.23 3199.76
3201.56 3202.35 3205.39 3205.69 3208.97 3209.88
3210.97 3212.20 3215.11 3215.17 3216.14 3221.34
3234.21 3245.59 3261.35 3278.82 3298.29 3304.60

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^{1}Rh–3

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6.11 14.79 22.94 28.36 28.95 31.80
34.36 35.47 40.59 45.94 46.29 51.01
57.78 59.46 64.44 66.82 74.98 75.61
79.15 82.61 88.04 88.75 93.31 95.40
115.02 120.30 123.33 127.12 146.18 158.38
162.96 172.84 184.09 188.57 189.21 203.88
205.77 210.78 219.07 223.43 229.50 232.37
237.66 243.58 253.10 257.94 260.82 264.06
266.94 285.51 286.35 289.71 299.13 302.98
315.11 325.58 327.79 333.56 334.99 338.40
340.55 346.67 349.46 351.82 356.44 359.01
363.32 368.13 373.24 389.86 391.07 399.83
414.37 415.30 417.82 420.01 421.91 424.09
436.22 438.64 442.10 455.95 458.23 461.65
462.05 469.11 471.22 472.41 474.66 503.35
507.40 512.21 522.63 534.77 538.20 565.06
591.05 596.88 598.57 612.01 617.34 619.36
625.34 626.31 626.95 627.73 636.59 657.79
671.45 674.25 675.15 680.74 681.73 705.19
705.77 711.87 712.66 713.26 724.74 727.83
729.26 738.85 740.92 742.17 745.72 752.29
769.67 774.50 778.74 779.37 786.98 789.12
795.36 798.64 813.92 835.65 837.52 845.91
849.24 856.26 863.60 863.98 883.68 884.61
886.07 899.50 903.91 906.90 915.45 927.94
932.89 938.97 939.83 940.85 943.78 947.65
951.50 953.20 956.44 958.50 959.11 961.20
964.05 969.00 969.42 970.69 978.72 979.61
988.91 990.16 994.17 1002.28 1002.78 1004.68
1005.15 1007.37 1015.90 1016.77 1017.94 1029.56
1031.68 1044.91 1052.60 1055.99 1056.11 1059.13
1061.87 1063.29 1063.55 1065.48 1073.62 1075.96
1081.86 1082.53 1096.03 1113.66 1115.01 1124.42
1131.24 1131.70 1134.32 1146.01 1158.14 1162.35
1168.44 1186.49 1199.47 1202.29 1202.48 1203.91
1204.64 1204.77 1206.33 1210.46 1219.47 1225.80
1234.09 1234.53 1240.44 1241.08 1241.82 1253.26
1259.02 1265.69 1268.85 1288.31 1289.60 1293.55
1303.91 1304.29 1305.07 1316.99 1318.78 1330.33
1331.15 1337.79 1344.08 1346.19 1347.08 1349.11
1361.07 1363.32 1364.09 1367.13 1370.10 1401.57
1408.55 1416.04 1417.50 1421.69 1422.01 1424.55
1429.66 1451.14 1452.53 1452.94 1459.13 1460.60
1461.76 1468.64 1470.17 1481.49 1487.13 1489.02
1492.37 1494.67 1496.73 1497.89 1499.00 1499.71
1500.08 1501.11 1502.34 1503.22 1507.16 1507.78
1508.58 1517.06 1518.53 1522.01 1524.73 1525.53
1529.86 1531.39 1533.72 1538.03 1539.60 1540.03
1543.95 1550.89 1602.89 1603.94 1607.17 1611.33
1634.02 1637.23 1638.90 1646.37 1653.17 1653.41
1657.48 1662.68 1666.31 1712.38 3032.31 3032.89
3037.93 3041.61 3042.06 3047.71 3050.35 3053.31
3082.77 3096.04 3101.11 3106.51 3108.75 3113.32
3114.60 3115.93 3117.14 3119.62 3120.16 3123.14
3123.22 3124.97 3126.33 3132.05 3133.60 3141.62
3160.73 3166.03 3174.58 3175.02 3176.81 3177.62
3181.50 3183.59 3185.15 3192.37 3195.11 3199.53
3200.44 3203.30 3205.28 3206.38 3207.37 3208.23
3209.65 3213.35 3214.49 3215.80 3216.49 3221.48
3231.60 3248.81 3270.06 3278.55 3289.41 3297.56

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^{3}Rh–1'–TS

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-250.17 8.50 16.85 18.77 24.88 29.78
33.89 35.14 37.43 39.96 41.77 46.72
50.80 56.30 59.59 63.80 67.76 71.95
77.07 79.76 83.20 87.85 88.18 94.49
100.24 106.56 112.60 119.86 125.14 127.38
137.37 145.49 153.70 161.96 168.88 178.24
182.05 190.42 200.25 202.00 209.09 219.33
221.90 226.65 229.52 229.75 239.76 243.41
253.17 264.04 269.86 277.15 284.58 288.14
297.86 299.05 304.24 313.08 316.22 328.23
330.90 335.12 339.79 342.49 344.64 349.67
351.58 360.19 364.43 365.84 371.67 378.07
389.07 394.61 405.12 406.79 416.77 418.76
420.53 425.11 425.74 438.32 441.92 451.84
455.44 460.98 467.13 468.15 470.84 475.88
485.38 494.24 503.92 510.92 520.07 524.72
533.52 533.67 565.89 570.56 589.38 593.77
597.30 611.87 614.06 619.17 623.64 623.94
626.55 646.89 661.13 665.52 671.07 671.17
679.30 679.82 688.97 703.09 704.25 709.60
714.95 735.71 737.61 737.69 739.69 741.42
742.16 750.92 752.97 754.17 768.53 778.10
779.26 785.28 788.94 791.92 796.34 808.62
813.48 829.01 833.28 840.94 847.60 850.06
867.75 870.42 883.95 885.26 888.30 901.90
909.53 911.08 913.01 930.55 934.61 937.41
942.61 943.88 946.91 947.94 951.09 956.56
957.87 958.25 959.58 961.78 965.69 973.26
974.40 981.79 984.54 989.92 994.54 996.14
999.48 1003.26 1003.95 1004.65 1005.26 1010.35
1015.90 1018.57 1031.94 1038.32 1038.42 1044.50
1045.73 1052.00 1056.57 1057.31 1059.73 1060.81
1065.69 1068.23 1068.50 1069.79 1083.17 1086.96

1105.56	1111.20	1119.74	1131.32	1136.62	1139.12
1157.39	1159.12	1171.94	1189.64	1199.20	1200.50
1202.34	1202.64	1202.89	1207.17	1208.52	1215.95
1217.72	1232.57	1238.44	1240.05	1242.98	1247.56
1257.91	1268.94	1271.96	1287.94	1290.20	1303.53
1308.83	1313.40	1321.09	1328.29	1332.13	1336.50
1344.81	1346.81	1347.19	1348.66	1362.25	1363.12
1366.48	1367.84	1371.62	1375.84	1386.35	1392.40
1412.92	1416.90	1418.36	1418.87	1420.16	1425.05
1445.42	1449.54	1451.95	1457.41	1457.87	1458.79
1467.67	1471.47	1480.47	1481.33	1482.24	1483.59
1494.42	1495.54	1496.89	1498.65	1500.14	1500.36
1500.80	1501.43	1502.55	1506.81	1508.70	1510.13
1512.12	1518.71	1520.33	1522.86	1524.06	1525.27
1529.53	1532.74	1537.33	1540.53	1541.26	1542.02
1547.77	1553.07	1572.86	1588.56	1603.02	1606.63
1607.31	1607.52	1607.98	1616.19	1633.33	1636.13
1644.13	1654.60	1655.43	1658.02	3034.70	3037.03
3037.77	3038.59	3044.71	3045.93	3047.32	3052.84
3097.16	3106.51	3107.64	3109.44	3110.79	3112.75
3115.48	3116.00	3117.58	3120.32	3121.58	3126.27
3131.78	3137.57	3138.47	3139.61	3172.57	3174.18
3177.74	3179.57	3179.80	3183.42	3183.75	3189.50
3191.27	3196.20	3199.41	3200.70	3201.40	3202.14
3204.10	3204.93	3205.94	3206.79	3210.73	3211.28
3212.00	3214.58	3217.75	3229.01	3229.60	3235.53
3251.10	3253.76	3268.51	3275.66	3295.31	3296.69

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^{3}Rh–2'

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7.74	17.14	22.66	25.28	28.32	33.75
35.06	37.57	42.99	44.49	49.05	53.32
56.47	62.87	64.45	69.94	73.70	75.89
80.41	83.80	87.32	90.76	93.90	101.31
107.33	117.15	120.57	124.25	129.15	140.53
150.03	155.28	164.75	169.25	175.37	181.73
181.98	198.62	199.98	207.01	207.91	218.36
218.93	224.70	228.26	231.10	239.84	249.22
266.40	274.29	277.55	282.56	290.18	299.39
307.76	308.53	314.80	320.12	322.81	328.12
334.77	335.56	336.52	342.91	344.37	346.27
349.34	355.96	368.98	372.64	390.77	394.48
397.49	405.38	412.21	417.54	418.73	420.71
422.18	426.23	437.90	440.09	453.36	457.22
459.95	466.90	469.49	470.34	476.64	477.64
495.36	509.69	509.99	517.45	522.94	533.69
536.11	539.82	577.64	590.33	597.16	604.58
611.10	611.79	617.13	620.37	623.52	624.22
626.93	657.51	671.65	674.49	675.68	680.17
680.50	688.48	703.33	706.53	711.24	711.98
722.87	732.88	735.48	737.99	738.70	740.70
744.32	752.03	766.01	777.73	779.14	779.24
785.32	788.56	792.63	796.22	812.81	816.75
831.91	833.28	840.46	848.09	850.09	863.80
865.89	883.30	884.21	885.36	896.91	899.26
910.38	912.24	917.50	937.79	943.53	944.89
946.71	948.31	951.10	956.99	958.08	959.11
961.15	962.00	966.19	973.72	974.10	983.91
984.36	988.18	995.24	996.13	1002.81	1004.58
1004.61	1005.43	1007.53	1008.76	1017.04	1018.66
1020.43	1023.61	1045.47	1046.80	1053.43	1054.73
1055.31	1059.06	1059.65	1061.61	1066.78	1067.95
1070.45	1075.01	1084.77	1094.48	1094.91	1112.77
1118.69	1132.06	1133.56	1133.94	1157.54	1158.95
1161.03	1186.42	1195.91	1202.20	1203.24	1204.38
1204.56	1205.33	1208.79	1209.50	1228.99	1233.46
1236.34	1237.65	1240.92	1242.68	1258.02	1267.11
1267.93	1270.71	1289.73	1291.09	1303.23	1305.49
1307.26	1310.31	1315.87	1321.20	1328.18	1332.12
1338.95	1347.03	1349.15	1349.39	1351.85	1362.37
1363.91	1364.91	1365.32	1369.36	1374.24	1400.59
1411.81	1417.09	1418.10	1421.92	1422.21	1422.74
1443.63	1445.40	1451.58	1452.87	1457.96	1459.43
1460.82	1468.88	1472.18	1482.52	1486.02	1490.49
1494.11	1494.80	1496.66	1497.49	1497.89	1500.24
1501.48	1502.28	1502.58	1503.24	1504.66	1509.12
1511.53	1513.53	1519.40	1520.89	1521.87	1522.22
1525.05	1526.21	1532.53	1534.36	1541.02	1543.49
1544.10	1553.78	1558.51	1595.39	1603.03	1604.23
1608.90	1611.05	1618.97	1634.52	1636.78	1646.58
1650.54	1654.02	1655.14	1658.60	3017.46	3031.34
3031.89	3034.76	3039.96	3042.96	3046.75	3048.18
3053.09	3064.43	3101.34	3102.85	3106.71	3107.86
3108.95	3110.96	3115.09	3116.16	3116.98	3121.71
3125.71	3126.22	3131.59	3131.97	3134.87	3135.86
3143.27	3173.64	3174.93	3176.94	3179.36	3182.79
3184.27	3185.91	3186.86	3194.92	3195.84	3201.62
3202.50	3203.91	3204.18	3204.76	3209.20	3209.63
3211.83	3212.05	3215.72	3217.72	3224.91	3226.07
3232.62	3259.48	3263.28	3277.80	3285.16	3298.20

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^{1}Rh–3'

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17.03	20.98	25.65	30.88	33.74	37.05
41.30	44.91	46.53	51.25	52.82	56.16
60.67	65.09	67.11	71.73	79.95	83.25
84.82	89.17	91.03	95.96	99.60	107.54
119.98	123.68	125.07	128.35	141.19	154.05
162.82	169.69	178.63	180.92	198.19	203.54
208.65	212.82	221.40	223.78	228.82	232.88
238.26	250.69	254.27	256.32	260.03	268.50
269.89	282.42	287.20	293.95	296.90	308.01
311.59	318.06	323.64	330.49	334.03	338.84
341.63	344.31	351.97	354.27	358.96	361.49
363.05	368.78	370.06	383.83	388.00	395.98
406.95	415.33	416.56	419.68	420.46	424.06
440.03	442.12	446.36	452.40	455.24	459.03
463.43	466.40	466.69	470.93	477.12	502.74
508.45	513.93	524.00	531.96	534.93	564.66
582.98	588.31	595.33	606.92	614.95	616.47

616.70	622.93	624.29	627.02	630.44	656.89
669.62	673.62	676.46	678.96	681.02	701.65
702.56	706.56	709.25	712.69	719.65	722.15
734.30	736.84	739.22	741.25	743.02	752.79
765.39	777.12	778.67	779.51	785.53	787.51
791.17	800.19	810.32	833.67	834.95	847.02
848.28	850.58	860.05	862.38	865.14	883.56
884.79	885.53	902.54	911.97	924.69	932.52
934.13	938.73	940.46	942.20	942.88	946.12
946.44	955.12	956.19	958.18	959.09	959.48
962.07	963.06	966.53	976.51	978.79	980.47
980.95	981.76	987.08	1003.51	1004.39	1004.72
1005.51	1006.55	1010.91	1014.48	1017.01	1018.61
1035.23	1042.88	1050.18	1055.82	1058.38	1058.86
1059.33	1062.97	1068.14	1069.62	1069.77	1071.66
1084.45	1093.12	1101.58	1112.79	1115.56	1128.95
1130.89	1132.22	1132.50	1139.59	1158.49	1160.13
1183.85	1189.40	1189.96	1197.79	1202.11	1203.73
1204.09	1205.16	1206.08	1208.47	1212.84	1228.27
1234.28	1236.13	1237.25	1242.03	1242.70	1261.95
1267.58	1268.58	1271.47	1288.14	1289.70	1291.12
1302.44	1305.54	1314.05	1318.69	1322.55	1327.92
1330.82	1333.27	1346.60	1347.54	1348.52	1354.31
1359.71	1360.24	1364.96	1366.21	1369.62	1397.14
1401.36	1414.01	1419.32	1419.70	1421.20	1427.71
1432.65	1442.00	1451.47	1452.33	1457.42	1459.25
1461.33	1467.42	1469.51	1481.39	1483.50	1487.05
1490.75	1493.47	1497.64	1497.99	1498.58	1499.85
1500.32	1500.69	1501.30	1502.06	1506.57	1508.28
1508.64	1513.87	1520.88	1521.41	1525.82	1526.42
1528.45	1529.10	1531.01	1538.56	1539.48	1540.87
1542.22	1552.45	1605.00	1605.71	1608.02	1608.45
1633.48	1635.81	1636.60	1647.80	1649.83	1653.69
1655.00	1657.05	1661.12	1708.64	3031.58	3036.49
3036.70	3041.31	3042.10	3046.43	3047.46	3051.43
3089.21	3094.99	3096.38	3101.59	3107.86	3112.35
3112.37	3115.92	3116.23	3117.34	3118.73	3120.19
3121.80	3123.40	3124.23	3132.47	3138.00	3164.89
3167.73	3168.24	3174.49	3176.20	3177.89	3180.57
3183.13	3184.46	3184.96	3194.98	3195.68	3201.41
3203.56	3203.81	3204.91	3205.63	3207.62	3208.58
3213.34	3213.58	3214.88	3225.43	3228.50	3231.92
3237.62	3251.08	3259.23	3267.98	3278.08	3298.85

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^{1}Ir–1

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12.63	16.59	22.68	24.86	27.59	31.62
32.47	39.20	40.77	46.16	52.98	54.19
61.77	73.47	81.15	82.01	83.07	85.13
91.33	99.67	117.39	118.07	124.20	126.19
133.70	140.88	151.36	167.34	175.26	185.91
192.99	195.89	208.88	217.29	224.66	226.82
231.65	237.99	249.82	250.57	266.22	271.98
273.96	277.99	284.66	296.35	298.32	299.24
306.60	311.91	317.42	322.62	332.93	339.79

342.94	345.78	352.49	359.77	363.24	366.70
370.41	396.51	398.87	400.81	409.78	417.37
419.52	425.31	427.24	440.72	443.27	459.43
461.54	464.93	471.26	474.98	475.05	481.01
497.22	513.06	524.68	528.81	535.98	537.52
589.59	597.08	600.54	614.27	615.26	617.54
622.81	625.64	629.17	629.77	655.80	661.39
664.72	674.61	681.24	682.43	696.84	704.60
710.06	711.70	714.55	737.03	737.80	743.78
744.78	749.76	755.10	762.61	779.82	781.46
783.24	786.18	793.47	798.10	799.73	807.74
832.07	834.29	848.89	852.25	852.47	862.56
881.79	885.84	888.08	888.98	898.97	909.40
913.86	938.54	939.98	943.09	945.06	946.74
948.08	953.03	957.77	958.36	958.68	963.68
964.44	965.61	973.63	980.75	983.59	988.33
1005.33	1005.63	1007.90	1008.40	1009.82	1013.40
1015.51	1017.08	1020.43	1034.21	1047.38	1054.03
1055.52	1056.91	1057.67	1058.78	1059.59	1066.24
1072.02	1079.49	1089.95	1097.84	1115.34	1116.81
1123.23	1130.89	1136.41	1148.45	1161.48	1164.09
1187.37	1202.93	1203.32	1204.34	1204.42	1205.78
1207.26	1213.35	1221.07	1233.40	1237.06	1238.19
1243.58	1251.27	1263.62	1267.94	1271.51	1290.18
1291.87	1301.97	1307.63	1316.78	1321.82	1328.32
1331.15	1335.98	1342.26	1347.96	1350.82	1352.84
1356.71	1361.87	1365.03	1365.61	1376.09	1382.21
1400.16	1415.86	1416.76	1418.99	1420.13	1450.22
1451.49	1452.47	1453.10	1454.28	1468.79	1470.14
1482.80	1484.53	1488.06	1493.33	1495.12	1498.89
1499.29	1499.85	1501.23	1501.76	1503.39	1506.81
1508.51	1517.49	1517.81	1520.92	1525.31	1527.13
1532.44	1538.66	1538.88	1540.86	1541.16	1551.69
1584.88	1603.63	1606.46	1607.58	1609.76	1625.82
1640.20	1642.57	1647.36	1654.05	1655.89	1656.44
1658.32	1678.62	3037.80	3037.93	3039.60	3044.38
3045.99	3050.42	3106.25	3109.54	3109.54	3114.24
3116.22	3118.27	3120.27	3122.11	3122.17	3124.90
3129.74	3138.56	3173.60	3174.59	3175.97	3179.73
3183.79	3184.84	3188.52	3195.00	3197.31	3201.93
3202.23	3203.56	3204.07	3204.17	3206.73	3209.78
3210.45	3212.52	3215.13	3218.68	3226.09	3229.77
3235.11	3248.63	3258.32	3277.23	3283.71	3302.22

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^{3}Ir–1

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14.83	17.21	24.43	26.03	29.10	31.75
36.90	41.99	42.33	48.11	50.69	61.73
65.74	74.03	77.73	82.11	84.19	85.11
88.20	102.21	116.04	123.08	132.42	134.60
137.07	142.47	149.47	168.98	172.57	189.82
193.24	197.56	203.54	213.51	219.14	220.68
230.68	231.88	248.73	256.42	263.83	267.06
271.35	276.56	283.76	296.91	303.72	307.67
308.50	313.87	322.20	328.08	331.85	338.15

344.30 347.09 357.97 360.63 363.29 366.98
370.45 394.84 396.89 401.46 411.77 416.01
419.89 425.36 438.84 440.45 443.99 458.62
459.03 460.88 468.73 472.10 474.81 500.17
502.51 504.76 511.57 531.90 535.41 535.91
562.59 589.10 593.68 597.83 613.80 615.86
616.35 618.72 621.14 622.68 630.29 639.36
668.22 671.58 681.28 682.68 697.00 701.71
707.42 709.31 711.16 715.32 735.30 737.31
740.29 742.78 743.95 757.15 768.73 769.63
776.22 779.61 783.19 797.22 801.56 802.76
835.16 836.77 838.72 845.85 848.86 852.69
857.94 861.32 893.27 895.04 898.69 912.11
915.79 929.01 939.51 941.63 943.07 945.93
949.41 951.29 954.59 959.19 963.14 969.28
969.37 970.32 972.39 972.84 976.99 982.81
984.73 999.42 1000.82 1003.44 1007.62 1009.87
1011.31 1013.10 1014.54 1019.80 1025.99 1045.47
1054.09 1056.88 1057.29 1058.43 1060.60 1065.98
1067.15 1074.80 1080.42 1086.26 1110.71 1113.84
1117.10 1130.80 1130.98 1134.29 1157.48 1162.81
1175.22 1197.62 1201.00 1202.51 1204.43 1205.70
1208.62 1211.58 1212.62 1234.20 1236.52 1239.58
1240.54 1243.09 1251.10 1264.94 1270.14 1283.14
1287.55 1290.01 1301.67 1305.13 1316.14 1319.10
1323.37 1331.03 1334.65 1336.23 1346.58 1347.51
1354.95 1358.71 1362.29 1364.22 1365.95 1369.02
1369.94 1412.11 1417.97 1419.78 1420.24 1420.83
1448.08 1451.89 1453.26 1453.71 1462.81 1466.09
1475.93 1477.73 1480.05 1484.14 1489.06 1492.22
1495.44 1497.36 1499.76 1500.45 1501.49 1502.24
1506.44 1506.75 1516.86 1519.00 1520.90 1526.23
1527.98 1532.88 1535.79 1539.35 1542.12 1543.55
1555.40 1574.82 1590.56 1596.05 1600.68 1604.45
1615.47 1619.83 1622.29 1646.62 1646.84 1649.32
1653.17 1656.16 3038.73 3041.05 3041.69 3044.29
3047.24 3051.71 3110.93 3111.49 3112.77 3114.69
3116.31 3118.21 3118.48 3121.11 3122.83 3140.37
3141.22 3144.60 3171.85 3176.20 3179.30 3183.14
3185.16 3190.67 3191.06 3191.32 3192.70 3197.06
3198.50 3205.94 3206.88 3206.93 3207.14 3209.28
3210.70 3215.72 3216.01 3217.81 3230.71 3232.61
3235.20 3239.10 3246.45 3280.66 3282.53 3305.05

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^{3}Ir–1–TS

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-134.52 16.31 22.32 26.17 29.35 32.06
35.44 37.34 38.93 44.23 45.99 48.89
54.47 58.01 61.73 63.86 68.15 71.57
76.65 78.01 82.01 84.77 86.45 91.66
93.14 111.19 119.53 122.39 125.50 135.05
142.52 144.02 154.28 155.63 165.71 172.38
187.00 197.95 205.87 209.38 215.53 225.07
225.78 232.78 235.69 237.82 248.27 258.06
263.29 265.56 272.27 277.24 278.73 283.65
291.54 308.08 313.93 319.35 320.72 321.59
328.24 339.39 342.52 342.92 345.93 351.75
357.47 360.59 362.03 369.11 371.84 373.61
393.08 396.28 402.85 411.46 417.61 418.44
419.99 423.78 424.51 441.72 443.20 454.71
457.14 465.00 468.71 472.20 474.44 481.65
484.80 494.90 499.31 513.21 523.78 527.29
531.64 535.65 571.21 583.48 590.11 598.81
606.48 608.07 613.53 617.04 623.41 625.11
628.49 633.94 647.74 655.16 668.51 680.57
681.16 682.06 684.50 701.36 704.37 709.34
713.21 732.16 734.51 736.61 737.14 738.25
742.20 749.99 758.76 762.45 773.88 781.30
783.43 787.45 789.74 793.05 794.70 808.75
815.92 833.36 833.82 836.66 845.71 848.87
865.48 871.78 876.49 885.24 888.04 902.66
906.84 913.00 927.99 929.70 937.72 939.51
942.95 944.51 944.81 948.57 955.09 956.40
958.53 958.97 963.28 964.51 965.62 972.71
976.13 978.68 981.86 990.44 996.02 998.86
999.96 1001.29 1004.07 1004.56 1005.86 1006.74
1007.50 1017.38 1028.28 1043.83 1044.47 1045.91
1048.20 1050.61 1054.46 1056.77 1058.05 1063.71
1069.32 1070.52 1075.38 1084.88 1085.71 1092.98
1110.62 1111.59 1119.39 1132.02 1133.20 1140.95
1160.42 1162.63 1177.33 1192.56 1200.92 1201.17
1204.40 1204.77 1205.17 1205.35 1209.25 1213.34
1221.88 1234.11 1234.48 1241.54 1242.01 1251.23
1263.34 1264.22 1272.08 1287.92 1290.19 1301.69
1303.23 1314.93 1317.58 1331.01 1331.44 1337.49
1343.74 1346.33 1348.54 1352.45 1360.81 1362.21
1363.25 1369.50 1371.79 1378.38 1387.46 1391.67
1415.07 1417.26 1420.69 1421.35 1422.86 1431.56
1449.77 1450.96 1451.16 1452.22 1453.02 1455.29
1463.24 1465.09 1469.26 1482.29 1485.04 1485.26
1489.72 1492.68 1495.08 1498.53 1499.57 1499.82
1501.51 1501.79 1503.42 1506.96 1508.54 1509.53
1511.33 1516.93 1517.85 1518.68 1521.71 1525.72
1527.37 1528.75 1530.10 1538.75 1539.55 1542.16
1549.48 1552.21 1575.61 1592.80 1603.38 1604.37
1604.72 1607.86 1618.31 1623.58 1640.39 1642.32
1645.33 1653.53 1654.07 1656.59 3032.21 3034.90
3039.11 3041.81 3043.70 3044.70 3047.43 3052.07
3102.49 3104.14 3104.60 3110.09 3113.05 3115.43
3115.62 3117.52 3118.36 3120.18 3121.13 3123.09
3129.17 3132.83 3135.49 3141.03 3171.78 3173.96
3176.00 3178.87 3181.22 3181.86 3182.43 3186.81
3193.50 3197.53 3198.27 3200.77 3203.23 3203.73
3204.47 3209.26 3210.09 3210.47 3211.00 3213.50
3215.50 3218.26 3222.55 3232.10 3233.44 3257.29
3263.30 3265.95 3281.09 3281.59 3286.33 3300.85

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^{3}Ir–2

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14.25 17.94 20.84 24.83 28.40 29.65

33.05 36.25 38.02 39.93 45.90 50.27
58.15 61.52 65.46 67.79 77.82 81.48
83.96 85.87 86.97 90.33 96.13 99.75
110.18 121.34 122.11 125.78 133.46 142.09
151.90 163.61 164.55 167.49 171.60 177.62
192.09 201.28 204.68 205.45 212.27 225.36
226.76 233.15 237.36 237.83 247.61 262.78
268.58 269.41 276.30 279.53 283.54 290.81
304.45 308.39 321.44 321.70 323.24 330.15
336.98 342.63 344.17 348.01 349.92 359.38
359.64 363.61 372.23 372.54 393.22 397.28
400.61 407.59 414.50 417.25 417.76 421.96
423.40 432.79 441.23 443.12 459.49 460.14
465.71 467.27 473.55 474.49 477.05 482.19
496.30 511.09 513.06 520.95 527.54 535.13
535.74 541.79 573.22 595.25 597.50 606.93
611.12 613.69 614.02 615.59 621.37 625.89
628.83 654.96 667.46 672.98 676.70 682.30
683.09 686.88 695.04 702.20 705.83 710.92
727.13 731.83 738.80 741.58 743.61 744.13
749.32 761.66 762.36 774.32 780.28 782.35
783.62 792.26 793.88 798.89 799.30 827.07
835.03 835.97 836.15 840.01 847.41 852.32
859.23 861.49 883.25 886.05 888.61 908.33
911.37 912.04 915.38 939.05 941.55 944.77
946.54 947.97 949.82 954.62 957.68 959.60
960.43 964.89 966.23 966.98 972.44 978.64
979.61 982.89 991.38 993.90 995.67 1005.01
1006.18 1006.48 1006.90 1008.62 1010.66 1016.09
1020.71 1022.81 1041.50 1047.25 1052.25 1055.58
1056.70 1057.60 1060.69 1061.01 1069.41 1070.31
1070.81 1074.95 1087.23 1094.41 1098.19 1115.17
1117.89 1130.36 1133.09 1133.16 1159.43 1160.38
1163.79 1187.02 1194.77 1202.59 1203.03 1205.50
1206.44 1206.53 1207.96 1211.74 1229.48 1234.17
1235.21 1240.79 1241.93 1253.28 1255.38 1262.58
1267.34 1273.10 1289.56 1291.98 1303.60 1304.05
1308.85 1317.47 1320.33 1323.15 1331.74 1334.04
1335.60 1339.37 1348.09 1349.90 1352.77 1357.20
1359.90 1362.97 1367.58 1367.96 1372.77 1402.60
1411.71 1417.23 1417.64 1419.70 1421.02 1421.87
1439.58 1443.91 1451.40 1451.93 1452.29 1454.10
1464.70 1467.21 1468.65 1482.14 1485.69 1487.54
1492.95 1493.97 1495.64 1497.27 1498.53 1498.98
1501.05 1501.36 1503.02 1503.91 1505.15 1508.08
1509.19 1510.70 1517.84 1518.71 1521.02 1522.72
1525.20 1527.50 1528.18 1530.90 1537.40 1539.48
1540.90 1548.30 1559.50 1592.47 1603.45 1606.46
1606.80 1608.30 1616.67 1617.77 1639.19 1641.55
1648.59 1652.39 1653.47 1656.81 3022.13 3033.76
3037.17 3039.65 3041.23 3041.32 3045.57 3046.61
3052.16 3076.89 3099.38 3103.10 3106.81 3106.92
3110.73 3111.54 3115.09 3115.84 3119.10 3119.86
3123.35 3123.51 3123.77 3123.81 3130.75 3142.64
3145.11 3173.69 3175.05 3179.41 3179.75 3180.41
3183.94 3184.06 3191.38 3195.96 3196.70 3198.89
3201.68 3205.03 3205.17 3206.79 3209.38 3210.56
3213.42 3214.28 3219.77 3222.49 3228.53 3233.52
3235.77 3247.81 3265.72 3271.02 3282.72 3300.08

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^{1}Ir–3

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2.76 14.10 22.59 27.39 30.79 33.27
40.44 42.38 45.58 48.58 52.34 54.70
57.81 60.60 70.00 75.10 77.77 81.72
85.15 86.12 88.59 91.37 96.01 99.67
120.74 123.87 127.63 133.18 144.27 153.68
162.48 174.25 177.43 181.79 201.52 205.29
211.34 218.38 222.31 226.48 233.84 237.52
239.15 242.77 245.38 257.07 264.69 269.48
270.33 273.28 279.15 284.10 292.32 296.12
299.27 307.24 314.97 322.34 330.05 332.26
334.97 341.16 343.45 346.72 351.57 352.55
355.92 358.47 368.79 374.84 389.01 397.60
401.02 410.28 417.33 419.09 420.14 425.28
429.01 440.50 442.46 459.98 460.79 464.61
465.81 469.57 472.44 476.94 486.58 507.07
514.09 526.86 534.21 535.78 537.61 566.57
596.37 596.90 601.49 613.09 613.99 617.54
620.88 625.68 628.07 628.95 638.19 656.16
674.20 678.34 680.68 681.24 685.33 706.81
707.50 708.21 709.16 718.19 732.45 738.64
741.16 744.53 746.52 748.05 750.23 760.58
761.91 767.90 776.64 779.77 782.89 791.35
797.16 801.50 813.75 834.71 838.34 841.37
848.13 853.96 854.89 862.50 874.51 883.91
885.73 888.00 906.27 910.48 924.06 924.45
935.85 938.80 940.07 940.58 943.24 947.84
950.26 951.98 956.95 958.68 959.32 966.69
967.27 967.40 969.36 974.78 975.81 979.34
980.80 982.67 993.81 1004.37 1005.45 1005.81
1009.18 1009.57 1010.80 1012.10 1015.13 1018.99
1033.69 1049.46 1055.09 1055.43 1056.34 1057.72
1060.12 1061.04 1063.01 1070.60 1072.61 1075.26
1088.29 1095.99 1100.80 1113.56 1114.87 1127.09
1131.05 1132.83 1141.40 1151.38 1160.94 1162.81
1183.48 1189.01 1195.36 1200.70 1203.45 1203.68
1204.08 1204.85 1208.97 1210.59 1215.87 1224.89
1231.07 1233.91 1234.04 1239.38 1241.07 1259.10
1260.79 1265.29 1271.08 1290.03 1291.46 1292.54
1302.12 1305.77 1311.69 1315.96 1321.83 1329.98
1331.45 1336.95 1340.07 1348.25 1349.39 1351.19
1362.16 1367.49 1367.77 1368.16 1372.33 1396.79
1408.25 1409.88 1416.37 1417.12 1421.19 1422.90
1426.67 1449.57 1451.67 1451.72 1454.92 1456.32
1460.08 1466.43 1470.26 1482.50 1484.84 1485.64
1494.43 1495.74 1496.48 1497.67 1498.87 1499.08
1500.51 1501.48 1503.10 1504.03 1505.12 1505.57
1508.41 1509.79 1514.86 1517.15 1518.76 1523.52
1524.09 1526.74 1532.63 1538.67 1539.49 1541.18
1542.25 1552.52 1604.07 1604.49 1605.05 1607.23

1636.91 1638.20 1640.41 1647.12 1649.88 1653.79
1654.43 1656.65 1661.62 1712.44 3032.67 3033.25
3039.58 3041.79 3042.55 3045.71 3047.77 3047.90
3092.16 3094.69 3102.69 3107.95 3111.19 3112.39
3114.76 3116.10 3117.63 3118.10 3119.07 3123.16
3124.25 3125.63 3127.02 3127.64 3127.93 3132.08
3137.15 3147.64 3173.41 3173.80 3176.64 3176.78
3181.06 3181.57 3184.33 3190.87 3196.68 3197.37
3199.10 3200.58 3203.58 3205.28 3205.50 3207.43
3210.36 3213.03 3214.32 3214.74 3215.95 3225.35
3229.58 3234.17 3237.68 3283.19 3296.12 3300.88

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^{3}Ir–1'–TS

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-277.23 14.47 18.92 23.40 26.70 33.83
36.42 37.61 39.50 42.34 45.47 47.51
54.57 57.06 62.41 63.47 67.42 71.29
77.61 78.72 83.08 86.29 87.81 92.31
98.76 108.14 115.86 122.39 125.21 133.63
138.26 147.45 153.88 162.12 167.80 174.62
182.80 194.34 202.50 204.50 208.38 219.54
223.80 229.49 231.50 235.29 239.94 247.54
249.05 263.14 275.27 278.76 282.47 283.96
298.47 303.44 307.57 311.28 317.57 321.73
323.56 336.86 342.36 346.44 347.28 349.86
352.50 356.60 364.06 370.25 371.96 384.60
396.67 398.96 409.18 414.69 419.53 419.75
422.00 424.70 429.02 440.06 442.67 459.50
461.56 464.63 472.14 472.95 475.18 477.08
486.98 492.70 503.82 513.04 523.88 528.01
536.36 537.75 564.45 575.26 596.74 598.73
602.01 616.68 617.25 622.14 624.57 626.21
628.34 649.83 663.50 666.14 666.58 677.87
680.71 681.68 687.80 707.73 711.29 712.72
715.42 736.74 738.30 740.20 746.12 746.61
749.46 751.15 755.17 762.19 772.91 780.05
782.72 790.16 791.59 795.56 800.73 810.23
825.91 830.42 831.34 840.61 848.43 853.80
867.98 872.38 885.76 888.13 899.65 905.85
910.34 911.42 923.90 929.42 936.48 939.85
943.43 944.92 948.10 950.08 954.01 955.91
957.66 958.26 958.93 962.89 966.00 970.88
974.31 982.98 989.45 995.38 996.55 1002.75
1004.29 1004.83 1005.07 1009.43 1012.25 1016.77
1017.89 1020.27 1033.07 1040.03 1043.55 1045.74
1053.15 1053.44 1055.73 1058.21 1058.85 1060.73
1067.52 1067.94 1068.31 1074.11 1086.51 1093.96
1105.42 1111.88 1119.44 1132.67 1136.82 1141.24
1160.26 1161.89 1172.66 1186.61 1197.51 1201.45
1202.01 1203.20 1204.42 1207.54 1208.91 1211.86
1217.97 1232.28 1238.09 1238.39 1243.13 1246.41
1264.25 1268.54 1273.21 1288.74 1290.21 1301.88
1309.40 1316.18 1323.37 1329.68 1337.59 1338.35
1343.51 1346.71 1347.88 1351.03 1360.53 1362.94
1364.16 1367.62 1367.82 1371.88 1384.50 1394.17
1412.70 1413.32 1417.32 1419.04 1419.98 1424.67
1443.86 1449.74 1451.22 1451.87 1454.27 1462.26
1467.95 1471.54 1476.00 1481.23 1483.16 1484.35
1494.11 1494.60 1496.77 1498.28 1500.05 1500.65
1501.46 1502.04 1504.19 1506.89 1508.44 1509.61
1512.48 1516.14 1517.28 1519.95 1521.57 1523.58
1527.68 1529.42 1532.43 1540.19 1541.21 1541.44
1544.93 1554.29 1562.04 1591.85 1601.32 1601.59
1603.99 1607.20 1609.67 1617.29 1638.82 1641.07
1644.87 1653.99 1656.86 1658.79 3036.21 3037.05
3037.41 3037.85 3044.39 3045.58 3049.86 3051.50
3095.31 3106.69 3106.92 3110.57 3110.85 3114.53
3115.57 3117.78 3119.54 3120.51 3121.70 3127.10
3130.41 3133.21 3134.40 3138.99 3172.16 3173.76
3177.64 3177.75 3179.03 3181.71 3182.95 3192.49
3193.20 3194.92 3195.16 3199.27 3199.76 3201.77
3203.75 3205.75 3206.55 3207.14 3210.61 3212.10
3212.69 3216.18 3217.22 3223.90 3232.40 3242.51
3252.96 3254.81 3270.23 3281.43 3293.86 3300.57

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^{3}Ir–2'

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13.88 19.61 25.77 29.45 29.94 32.49
33.74 35.54 40.06 42.23 46.24 49.36
57.56 64.43 65.93 71.01 73.12 79.06
83.12 84.14 87.92 92.70 96.45 104.54
111.56 120.02 123.65 126.30 130.77 143.72
151.70 160.59 167.04 171.05 175.72 178.14
182.15 196.43 200.63 206.65 210.75 224.00
226.37 231.64 235.39 239.63 249.46 260.05
266.49 272.05 280.61 284.45 284.88 290.50
302.08 312.92 320.13 323.88 325.88 333.04
337.29 342.06 342.57 346.12 350.12 361.24
363.66 363.96 369.22 372.99 394.00 398.66
402.05 409.05 412.72 416.50 419.49 420.85
427.56 433.98 441.91 443.74 460.87 462.48
465.09 467.56 473.52 475.72 477.98 479.51
494.76 508.93 512.32 519.27 526.98 536.58
537.33 540.25 582.20 599.78 602.07 605.99
616.41 617.74 618.65 623.30 624.87 626.70
629.34 656.84 669.51 671.08 678.52 681.96
683.38 688.22 702.85 710.69 711.63 713.05
725.99 736.37 740.36 741.22 747.13 748.33
749.63 762.41 763.33 780.45 782.86 783.65
785.17 795.71 797.76 801.52 813.78 816.07
834.36 834.65 844.17 850.25 853.80 861.83
863.31 881.90 885.15 888.60 903.55 904.58
919.02 919.52 920.56 939.36 942.51 943.80
946.43 950.15 958.03 958.97 959.31 960.50
962.86 965.57 965.71 977.81 978.43 980.97
986.85 991.06 997.60 998.43 1004.65 1007.01
1008.82 1009.26 1009.94 1011.85 1016.63 1019.77
1020.84 1022.60 1046.94 1050.47 1055.76 1056.84
1057.47 1058.01 1061.50 1062.82 1067.32 1071.27
1073.68 1078.52 1091.60 1098.98 1104.42 1115.26

1118.97 1132.02 1134.79 1138.99 1158.17 1162.45
1164.25 1188.84 1195.17 1202.10 1204.60 1205.20
1206.17 1207.02 1209.04 1211.84 1228.69 1234.30
1236.05 1242.09 1242.38 1242.53 1258.05 1269.10
1269.78 1273.81 1290.00 1291.94 1301.33 1301.81
1306.67 1312.76 1316.82 1322.23 1330.68 1338.46
1340.09 1350.35 1350.63 1351.63 1354.14 1361.39
1362.85 1365.13 1365.73 1370.67 1378.96 1400.53
1411.98 1418.36 1419.30 1420.11 1421.88 1422.38
1446.36 1446.93 1451.65 1452.42 1453.07 1455.03
1456.68 1467.12 1471.36 1483.75 1486.66 1487.37
1492.93 1494.15 1495.62 1497.67 1498.70 1499.56
1500.16 1501.47 1502.86 1504.68 1506.97 1507.43
1509.54 1511.69 1517.96 1518.65 1522.58 1523.65
1526.02 1526.87 1528.62 1531.79 1539.07 1540.11
1541.35 1551.75 1557.05 1596.76 1605.24 1605.83
1607.47 1608.74 1611.16 1620.45 1639.98 1642.67
1648.55 1654.50 1654.82 1658.48 3014.26 3031.34
3037.54 3040.02 3041.24 3042.75 3045.84 3047.69
3054.08 3063.95 3098.51 3101.67 3103.24 3109.56
3112.74 3114.16 3115.17 3115.79 3117.27 3119.31
3120.35 3123.66 3125.77 3130.25 3133.97 3146.07
3150.92 3173.27 3174.37 3175.59 3178.60 3180.16
3183.38 3183.95 3189.65 3195.38 3197.67 3202.04
3203.27 3204.21 3204.77 3205.46 3210.96 3212.46
3212.66 3215.00 3220.42 3226.51 3232.33 3232.79
3233.92 3253.99 3262.88 3271.88 3282.29 3300.84

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^{1}Ir-3'

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16.17 22.51 27.74 30.70 35.36 38.33
41.72 42.98 46.19 49.24 51.86 59.38
61.23 65.61 68.07 71.80 79.13 83.40
84.17 86.82 90.01 92.55 95.54 110.38
121.12 124.46 125.01 137.11 142.24 154.20
163.96 170.89 174.99 185.30 200.81 208.34
209.76 215.62 223.36 233.80 234.72 235.51
240.93 246.55 254.21 258.53 265.10 268.96
274.73 281.61 282.20 288.43 299.37 304.60
311.27 320.25 322.93 326.24 326.77 340.07
342.78 344.23 352.54 358.45 360.15 362.00
363.73 370.33 370.93 388.23 395.26 399.11
410.21 416.97 419.08 419.63 421.07 425.55
441.34 442.69 456.78 458.93 459.79 461.82
466.13 469.36 471.70 473.37 478.34 505.16
509.77 516.47 527.51 535.63 536.56 571.78
585.82 597.33 599.51 611.77 617.96 620.13
621.60 626.02 627.75 628.35 632.22 658.39
674.10 677.23 677.99 681.27 683.35 704.17
709.42 710.19 711.22 713.39 721.40 724.94
736.70 740.68 743.62 746.17 749.52 762.38
768.37 779.41 781.08 783.17 786.34 790.41
798.94 802.69 813.10 833.95 834.68 849.65
853.09 857.79 861.69 863.64 864.25 885.14
886.41 888.66 902.07 912.92 920.84 932.48
935.35 939.29 941.81 943.73 945.31 946.51
948.23 957.05 957.43 957.96 959.00 960.43
963.31 966.07 966.48 976.87 978.05 979.69
982.22 982.29 986.70 1004.82 1006.43 1006.47
1009.17 1010.12 1012.39 1015.99 1017.28 1022.10
1034.68 1050.68 1056.68 1057.22 1058.49 1059.28
1060.79 1062.69 1068.68 1071.58 1071.82 1077.97
1089.60 1097.95 1103.54 1112.95 1116.20 1129.73
1132.01 1133.17 1133.73 1142.77 1162.09 1163.97
1185.49 1191.41 1192.47 1198.74 1202.62 1204.43
1205.52 1206.40 1206.66 1210.63 1213.09 1229.54
1234.83 1238.04 1238.88 1242.11 1242.62 1262.61
1268.80 1269.14 1272.57 1289.37 1291.05 1292.11
1301.76 1305.08 1317.29 1320.65 1325.05 1332.34
1335.16 1337.03 1347.78 1348.09 1351.79 1352.84
1360.61 1361.15 1364.89 1365.74 1370.02 1397.67
1403.94 1413.46 1420.04 1420.52 1421.50 1428.25
1432.37 1447.52 1451.67 1452.61 1453.20 1454.29
1461.81 1467.57 1469.42 1482.57 1486.35 1486.67
1490.98 1493.30 1497.71 1499.12 1499.57 1500.51
1500.78 1501.25 1501.69 1502.32 1506.80 1508.23
1508.98 1513.75 1517.69 1519.55 1524.67 1525.93
1528.75 1529.40 1529.86 1538.95 1539.63 1540.66
1542.92 1551.11 1603.68 1606.65 1607.48 1608.34
1619.52 1638.05 1640.13 1641.90 1648.77 1654.27
1654.69 1657.04 1661.90 1709.22 3032.33 3037.06
3037.30 3041.11 3042.04 3046.70 3047.24 3051.14
3091.29 3096.91 3098.53 3101.01 3107.78 3111.90
3113.45 3116.32 3116.36 3119.74 3119.77 3120.46
3122.61 3124.24 3125.49 3133.84 3137.89 3165.38
3166.23 3168.23 3173.36 3175.05 3175.14 3178.98
3181.08 3182.55 3185.56 3195.66 3196.68 3198.71
3201.21 3203.22 3203.88 3204.75 3205.10 3210.28
3211.15 3211.73 3215.19 3224.95 3231.37 3231.70
3235.39 3251.33 3262.67 3267.36 3282.68 3300.29

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17.69 27.16 42.20 58.57 65.69 76.33
113.28 133.79 163.96 184.68 257.26 280.68
308.32 317.12 364.07 383.69 407.41 423.49
480.82 491.82 520.64 557.12 565.20 606.69
620.71 625.79 628.42 647.21 683.00 695.47
711.31 724.47 749.23 763.16 765.78 780.88
827.38 828.99 851.78 855.96 868.24 896.48
924.46 933.01 966.56 979.00 987.07 988.23
996.99 1003.90 1017.51 1043.45 1052.52 1063.92
1111.84 1118.95 1125.61 1147.34 1165.01 1189.91
1196.86 1197.52 1211.42 1231.89 1236.40 1315.89
1342.42 1342.93 1356.06 1364.47 1365.90 1389.74
1428.50 1442.76 1490.31 1493.42 1499.88 1516.40
1543.28 1558.20 1586.43 1591.74 1617.15 1644.79
1658.49 3137.77 3146.92 3172.53 3182.83 3186.39
3191.84 3195.42 3204.90 3206.83 3212.44 3218.54
3223.56 3254.28 3288.10

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-250.01	12.39	19.00	26.59	38.86	47.56
56.96	68.04	77.13	84.58	104.75	112.31
120.08	145.04	167.50	171.36	188.37	206.42
235.29	246.13	282.47	311.72	321.83	339.04
367.40	371.57	386.88	416.73	421.49	422.49
467.55	485.17	492.81	498.85	522.66	563.75
568.94	584.89	622.94	624.66	646.76	664.26
679.74	681.31	703.70	710.93	735.77	744.85
748.04	759.71	776.64	782.51	792.94	809.35
822.46	830.29	854.92	863.87	884.00	898.30
899.61	928.07	929.99	932.42	957.60	964.66
977.96	983.98	992.11	995.48	1002.12	1006.01
1017.58	1025.59	1036.61	1041.89	1056.49	1057.13
1073.57	1095.78	1110.22	1116.50	1127.55	1159.84
1178.17	1191.09	1196.98	1208.80	1209.70	1215.42
1233.72	1256.12	1314.40	1341.67	1343.23	1354.83
1362.64	1365.46	1374.31	1382.12	1384.40	1421.80
1427.11	1440.64	1446.83	1475.80	1486.18	1493.16
1498.66	1499.61	1505.60	1507.20	1517.34	1537.32
1543.36	1559.70	1582.99	1587.40	1609.15	1618.92
1632.42	1643.98	1658.18	3037.83	3043.77	3098.27
3108.55	3136.56	3157.01	3172.25	3173.81	3178.29
3179.69	3184.46	3193.53	3194.99	3199.10	3204.26
3206.77	3210.40	3210.97	3219.56	3244.35	3251.94
3259.68	3272.27	3286.14			

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12.03	27.20	30.87	39.86	43.27	53.07
70.13	80.92	93.53	115.47	118.55	132.12
164.46	172.13	177.33	186.83	193.63	212.50
269.90	290.69	312.30	327.48	334.14	367.12
370.10	409.71	422.00	425.12	440.12	476.82
480.88	486.55	503.81	522.15	553.66	567.46
582.36	610.75	623.74	625.54	647.15	677.30
685.92	707.46	708.61	710.23	721.53	748.70
758.97	772.26	779.93	785.74	796.35	829.88
854.11	869.43	880.36	886.61	895.02	920.22
927.53	931.14	951.88	964.83	979.05	985.90
990.13	996.16	1002.84	1008.84	1017.99	1019.98
1025.63	1042.46	1050.70	1061.00	1063.71	1096.45
1112.86	1126.37	1130.20	1162.73	1169.46	1190.02
1198.70	1201.10	1210.71	1213.12	1227.22	1243.54
1260.58	1269.42	1318.22	1336.59	1342.29	1354.21
1357.58	1363.36	1365.13	1367.06	1378.84	1417.37
1425.63	1440.21	1445.49	1465.56	1489.12	1499.39
1499.64	1501.10	1501.96	1503.69	1514.54	1523.08
1526.76	1542.93	1556.65	1557.05	1592.90	1618.82
1646.33	1658.90	1784.39	3022.47	3026.80	3040.99
3077.70	3101.99	3104.98	3115.78	3131.52	3132.05
3171.07	3172.21	3177.74	3186.97	3190.05	3197.93
3201.40	3203.15	3205.63	3211.28	3212.07	3219.46
3256.23	3262.49	3289.52			

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13.34	27.98	31.09	50.42	59.42	76.17
90.07	95.09	102.97	111.62	116.91	165.68
170.81	177.82	204.71	221.93	264.65	283.42
310.71	320.33	338.28	349.43	369.22	370.12
408.66	421.34	423.06	423.22	461.02	469.40
493.21	510.82	561.02	580.22	611.34	624.80
627.99	635.17	646.43	683.53	708.45	711.32
712.87	716.71	731.27	750.45	759.85	774.32
783.25	811.65	853.57	856.21	857.90	868.11
903.37	911.33	922.09	927.29	929.07	933.18
939.45	972.48	975.49	981.60	989.34	994.42
996.73	1005.31	1015.63	1017.98	1028.16	1031.81
1057.80	1061.29	1073.09	1082.87	1103.03	1111.51
1122.75	1127.36	1140.86	1162.90	1173.35	1194.14
1198.18	1204.19	1212.11	1216.67	1222.20	1231.95
1253.14	1255.10	1284.21	1295.85	1326.95	1341.55
1345.20	1358.98	1362.97	1366.05	1368.62	1403.89
1424.14	1428.41	1443.26	1461.09	1488.42	1492.28
1493.51	1500.07	1504.70	1512.48	1519.23	1532.63
1541.77	1543.50	1558.55	1638.39	1645.36	1659.04
1663.24	1711.88	1777.97	3038.72	3042.07	3068.62
3087.67	3103.79	3114.15	3127.83	3129.10	3135.19
3151.70	3161.50	3172.15	3181.53	3187.45	3194.47
3197.55	3203.48	3205.46	3211.91	3218.55	3233.08
3247.77	3255.92	3289.05			

8. (TD)DFT optimized geometries

Table S6. Cartesian coordinates of optimized structures of ground excited state geometries.

(A) Optimized geometries at the (TD)CAM-B3LYP-D3/6-31G(d,p)/LANL2DZ level of the theory

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Rh–1

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Rh	1.6949	-0.7367	0.2869
N	0.5594	-2.0623	-0.8687
C	0.0848	-3.0229	-0.1061
S	-1.1779	-3.9631	-0.8331
C	-1.0227	-3.0106	-2.2844
C	-1.6954	-3.1606	-3.4920
H	-2.4708	-3.9091	-3.6117
C	-1.3262	-2.3520	-4.5473
H	-1.8281	-2.4897	-5.4976
C	-0.2948	-1.3959	-4.4437
C	0.3370	-1.2304	-3.2141
H	1.1439	-0.5229	-3.0860
C	-0.0272	-2.0384	-2.1275
C	0.6378	-3.2237	1.2135
C	1.5818	-2.2506	1.5869

C	2.2178	-2.4128	2.8153
H	2.9599	-1.6977	3.1513
C	1.9108	-3.4979	3.6322
H	2.4233	-3.6111	4.5826
C	0.9605	-4.4445	3.2502
H	0.7338	-5.2851	3.8965
C	0.3182	-4.3096	2.0324
H	-0.4122	-5.0485	1.7129
C	0.1508	-0.6669	-5.7194
C	0.8088	-1.7007	-6.6531
H	1.1628	-1.2126	-7.5660
H	0.1061	-2.4855	-6.9454
H	1.6636	-2.1799	-6.1679
C	-1.0476	-0.0315	-6.4456
H	-0.7039	0.4614	-7.3592
H	-1.5379	0.7229	-5.8256
H	-1.7967	-0.7690	-6.7403
C	1.1665	0.4405	-5.4303
H	1.4568	0.9278	-6.3646
H	2.0776	0.0551	-4.9648
H	0.7409	1.2042	-4.7754
C	-0.7785	0.9696	-0.1952
O	-0.3988	0.1173	0.6267
N	1.4891	1.0077	-1.0442
C	2.2438	1.6899	-1.9406
C	1.4307	2.5481	-2.6372
H	1.6292	3.2268	-3.4515
C	-2.1266	1.5005	-0.1810
H	-2.3648	2.3250	-0.8353
C	-3.0541	0.9637	0.6380
H	-2.7305	0.1486	1.2822
N	2.8224	0.3337	1.5949
C	4.1180	0.2023	1.4500
S	5.0416	1.0270	2.6700
C	3.5476	1.5418	3.4397
C	3.3263	2.2663	4.6057
H	4.1523	2.6503	5.1937
C	2.0149	2.4759	5.0171
H	1.8567	3.0330	5.9316
C	0.9092	1.9815	4.3002
C	1.1513	1.2724	3.1326
H	0.3445	0.8540	2.5466
C	2.4568	1.0609	2.7105
C	4.5616	-0.6641	0.3722
C	3.4922	-1.3042	-0.2931
C	3.7848	-2.1819	-1.3321
H	2.9840	-2.6947	-1.8553
C	5.1085	-2.4059	-1.7021
H	5.3269	-3.0935	-2.5136
C	6.1575	-1.7652	-1.0430
H	7.1825	-1.9533	-1.3420
C	5.8871	-0.8921	-0.0006
H	6.6985	-0.3917	0.5197
C	-0.5484	2.1703	4.7408
C	-0.6619	2.9533	6.0519
H	-1.7146	3.0597	6.3264
H	-0.2422	3.9591	5.9609
H	-0.1579	2.4396	6.8753
C	-1.3176	2.9335	3.6462
H	-2.3578	3.0820	3.9519
H	-1.3271	2.3865	2.6993
H	-0.8738	3.9165	3.4650
C	-1.2034	0.7894	4.9361
H	-2.2431	0.9098	5.2563
H	-0.6792	0.2080	5.6992
H	-1.2031	0.2056	4.0115
C	0.2409	1.4406	-1.1577
N	0.1618	2.3733	-2.1529
H	3.3022	1.5102	-2.0469
C	-1.0231	2.9041	-2.7662
C	-1.8909	2.0250	-3.4087
C	-1.2815	4.2663	-2.7069
C	-3.0486	2.5271	-3.9885
H	-1.6592	0.9653	-3.4426
C	-2.4399	4.7587	-3.2992
H	-0.5921	4.9254	-2.1909
C	-3.3233	3.8914	-3.9338
H	-3.7336	1.8512	-4.4890
H	-2.6538	5.8209	-3.2573
H	-4.2269	4.2798	-4.3912
C	-4.4486	1.3576	0.7466
C	-5.2205	0.8020	1.7753
C	-5.0523	2.2619	-0.1417
C	-6.5543	1.1519	1.9283
H	-4.7635	0.0936	2.4600
C	-6.3845	2.6055	0.0093
H	-4.4836	2.6809	-0.9655
C	-7.1371	2.0547	1.0460
H	-7.1404	0.7182	2.7312
H	-6.8453	3.3015	-0.6835
H	-8.1813	2.3266	1.1595

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Rh–1–^{1}MLCT

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Rh	-0.7878	-1.4418	0.3233
N	-1.9758	-0.5483	1.7905
C	-1.6987	-0.9984	2.9907
S	-2.4629	-0.1385	4.2812
C	-3.2335	0.8999	3.1075
C	-4.1433	1.9329	3.2994
H	-4.4511	2.2309	4.2952
C	-4.6669	2.5635	2.1815
H	-5.3857	3.3574	2.3379
C	-4.3090	2.1944	0.8705
C	-3.3823	1.1747	0.7016
H	-3.0723	0.8562	-0.2827
C	-2.8471	0.5296	1.8126
C	-0.8324	-2.1586	3.0896
C	-0.3176	-2.5927	1.8386
C	0.5115	-3.7228	1.8182
H	0.9318	-4.0739	0.8837
C	0.7899	-4.4067	2.9913
H	1.4181	-5.2908	2.9642
C	0.2677	-3.9683	4.2106
H	0.4928	-4.5127	5.1208
C	-0.5432	-2.8392	4.2644
H	-0.9506	-2.5072	5.2140
C	-4.9011	2.8656	-0.3744
C	-5.5171	1.7959	-1.2958
H	-5.9601	2.2728	-2.1747
H	-6.3046	1.2377	-0.7818
H	-4.7714	1.0806	-1.6539
C	-5.9925	3.8826	-0.0254
H	-6.3969	4.3159	-0.9437
H	-5.6048	4.7070	0.5795
H	-6.8236	3.4182	0.5133
C	-3.7757	3.5923	-1.1301
H	-4.1743	4.0849	-2.0219
H	-2.9976	2.8975	-1.4547
H	-3.3130	4.3574	-0.5002
C	0.6339	1.1160	-0.0876
O	0.5388	0.1169	0.7627
N	-1.0892	-0.0109	-1.2987
C	-1.8098	0.1209	-2.4535
C	-1.4605	1.2863	-3.0598
H	-1.8045	1.7623	-3.9635
C	1.6291	2.1066	0.1117
H	1.7503	2.8636	-0.6506
C	2.4376	2.0874	1.2056
H	2.2551	1.3069	1.9378
N	0.4145	-2.4638	-1.0013
C	-0.2481	-3.3013	-1.7591
S	0.7293	-4.1815	-2.8812
C	2.1425	-3.3502	-2.2710
C	3.4734	-3.4848	-2.6436

H	3.7728	-4.1798	-3.4199
C	4.4140	-2.7050	-1.9906
H	5.4503	-2.8165	-2.2810
C	4.0701	-1.7853	-0.9806
C	2.7329	-1.6632	-0.6214
H	2.3967	-0.9630	0.1316
C	1.7789	-2.4491	-1.2608
C	-1.6856	-3.3854	-1.5741
C	-2.1852	-2.5540	-0.5447
C	-3.5613	-2.4977	-0.3330
H	-3.9733	-1.8353	0.4194
C	-4.4128	-3.2927	-1.0941
H	-5.4827	-3.2564	-0.9162
C	-3.9082	-4.1325	-2.0873
H	-4.5843	-4.7411	-2.6778
C	-2.5419	-4.1805	-2.3324
H	-2.1521	-4.8230	-3.1162
C	5.1138	-0.8817	-0.3195
C	6.5440	-1.3815	-0.5550
H	7.2450	-0.7461	-0.0082
H	6.8285	-1.3382	-1.6098
H	6.6765	-2.4084	-0.2010
C	4.9694	0.5264	-0.9249
H	5.6787	1.2164	-0.4591
H	3.9643	0.9197	-0.7648
H	5.1643	0.5064	-2.0014
C	4.8752	-0.8146	1.1982
H	5.6276	-0.1721	1.6631
H	4.9427	-1.8082	1.6507
H	3.8994	-0.3920	1.4425
C	-0.2843	1.0549	-1.1895
N	-0.5033	1.8835	-2.2601
H	-2.5307	-0.6203	-2.7638
C	0.0659	3.1638	-2.5342
C	-0.1982	4.2294	-1.6809
C	0.8531	3.3275	-3.6673
C	0.3550	5.4723	-1.9576
H	-0.8190	4.0698	-0.8069
C	1.3915	4.5790	-3.9441
H	1.0461	2.4780	-4.3140
C	1.1488	5.6479	-3.0881
H	0.1600	6.3067	-1.2928
H	2.0089	4.7153	-4.8253
H	1.5761	6.6213	-3.3029
C	3.5487	2.9794	1.4808
C	4.3510	2.7228	2.6025
C	3.8777	4.0778	0.6698
C	5.4433	3.5231	2.9026
H	4.1073	1.8772	3.2394
C	4.9677	4.8775	0.9719
H	3.2725	4.3137	-0.2002
C	5.7575	4.6051	2.0874
H	6.0494	3.3040	3.7757
H	5.2057	5.7234	0.3351
H	6.6096	5.2349	2.3195

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Rh–1–MECP(^{1}MLCT–^{3}LC)

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Rh	1.5582	-0.9169	0.1906
N	0.4873	-2.2607	-0.9711
C	-0.0352	-3.2023	-0.2240
S	-1.1988	-4.1970	-1.0229
C	-0.9377	-3.2867	-2.4861
C	-1.4949	-3.4843	-3.7427
H	-2.2354	-4.2575	-3.9135
C	-1.0587	-2.6831	-4.7827
H	-1.4803	-2.8546	-5.7639
C	-0.0815	-1.6841	-4.6099
C	0.4315	-1.4710	-3.3335
H	1.1713	-0.7052	-3.1490
C	0.0105	-2.2746	-2.2719
C	0.4202	-3.3285	1.1459
C	1.3339	-2.3201	1.5420
C	1.8538	-2.3736	2.8425
H	2.5450	-1.6149	3.1873
C	1.4909	-3.4050	3.6958
H	1.9099	-3.4499	4.6953
C	0.5858	-4.3876	3.2849
H	0.3047	-5.1835	3.9655
C	0.0448	-4.3521	2.0051
H	-0.6534	-5.1199	1.6852
C	0.4289	-0.8472	-5.7913
C	1.9677	-0.8606	-5.8058
H	2.3365	-0.2840	-6.6585
H	2.3488	-1.8817	-5.8966
H	2.3924	-0.4156	-4.9025
C	-0.0622	-1.3838	-7.1420
H	0.3724	-0.7874	-7.9481
H	-1.1489	-1.3143	-7.2416
H	0.2361	-2.4239	-7.3014
C	-0.0654	0.5991	-5.6348
H	0.3013	1.2165	-6.4604
H	0.2908	1.0369	-4.7013
H	-1.1576	0.6478	-5.6372
C	-0.7432	0.8844	-0.2274
O	-0.3630	-0.1211	0.5284
N	1.4504	0.7819	-1.1802
C	2.1977	1.4256	-2.1312
C	1.4179	2.3496	-2.7543
H	1.6172	3.0340	-3.5627
C	-2.0154	1.4879	-0.0189
H	-2.2481	2.3760	-0.5909
C	-2.9053	1.0065	0.8818
H	-2.6177	0.1224	1.4432
N	2.6401	0.2572	1.4572
C	3.9323	0.2262	1.2502
S	4.8455	1.1446	2.4002
C	3.3558	1.5737	3.2230
C	3.1408	2.3157	4.3797
H	3.9650	2.7632	4.9233
C	1.8363	2.4604	4.8333
H	1.6802	3.0310	5.7399
C	0.7282	1.8983	4.1666
C	0.9603	1.1721	3.0082
H	0.1579	0.7267	2.4335
C	2.2648	1.0077	2.5544
C	4.3919	-0.5906	0.1356
C	3.3508	-1.2893	-0.5273
C	3.6488	-2.0702	-1.6439
H	2.8573	-2.5775	-2.1842
C	4.9689	-2.1971	-2.0595
H	5.2057	-2.8175	-2.9176
C	5.9930	-1.5312	-1.3842
H	7.0177	-1.6353	-1.7228
C	5.7098	-0.7259	-0.2856
H	6.5108	-0.2053	0.2295
C	-0.7199	2.0765	4.6399
C	-0.7982	2.6677	6.0508
H	-1.8438	2.7323	6.3615
H	-0.3861	3.6796	6.0964
H	-0.2723	2.0445	6.7805
C	-1.4439	3.0174	3.6594
H	-2.4893	3.1399	3.9575
H	-1.4355	2.6183	2.6426
H	-0.9754	4.0057	3.6448
C	-1.4419	0.7157	4.6476
H	-2.4679	0.8461	5.0035
H	-0.9405	0.0032	5.3091
H	-1.4983	0.2734	3.6502
C	0.2210	1.3168	-1.1941
N	0.1588	2.2700	-2.1791
H	3.2303	1.1719	-2.3122
C	-1.0105	2.9034	-2.7042
C	-2.0475	2.1180	-3.2036
C	-1.0946	4.2893	-2.7191

C	-3.1854	2.7333	-3.7053
H	-1.9624	1.0374	-3.1773
C	-2.2336	4.8978	-3.2366
H	-0.2806	4.8804	-2.3140
C	-3.2796	4.1229	-3.7237
H	-4.0001	2.1266	-4.0859
H	-2.3055	5.9799	-3.2472
H	-4.1699	4.6004	-4.1184
C	-4.2148	1.5683	1.1888
C	-4.9125	1.0854	2.3036
C	-4.8176	2.5729	0.4168
C	-6.1570	1.5949	2.6483
H	-4.4647	0.2999	2.9059
C	-6.0604	3.0810	0.7613
H	-4.3191	2.9465	-0.4721
C	-6.7359	2.5976	1.8794
H	-6.6775	1.2060	3.5174
H	-6.5115	3.8563	0.1501
H	-7.7096	2.9965	2.1433

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Rh–1–^{3}LC

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Rh	1.6358	-0.7099	0.2443
N	0.4390	-1.9873	-0.8891
C	-0.1017	-2.8997	-0.1138
S	-1.4155	-3.7725	-0.8391
C	-1.1722	-2.8721	-2.3148
C	-1.8172	-3.0128	-3.5350
H	-2.6433	-3.7048	-3.6556
C	-1.3505	-2.2799	-4.6141
H	-1.8381	-2.4198	-5.5694
C	-0.2490	-1.4122	-4.5133
C	0.3410	-1.2328	-3.2613
H	1.1917	-0.5771	-3.1327
C	-0.1152	-1.9630	-2.1613
C	0.4460	-3.1177	1.2055
C	1.4702	-2.2153	1.5505
C	2.1187	-2.4196	2.7656
H	2.9223	-1.7641	3.0806
C	1.7457	-3.4713	3.5989
H	2.2695	-3.6177	4.5385
C	0.7148	-4.3423	3.2476
H	0.4365	-5.1569	3.9069
C	0.0597	-4.1679	2.0415
H	-0.7312	-4.8509	1.7425
C	0.3369	-0.7165	-5.7527
C	1.8527	-0.9770	-5.8139
H	2.2765	-0.5150	-6.7102
H	2.0646	-2.0489	-5.8528
H	2.3785	-0.5611	-4.9509
C	-0.2816	-1.2312	-7.0593
H	0.2029	-0.7391	-7.9067
H	-1.3504	-1.0094	-7.1265
H	-0.1434	-2.3093	-7.1794
C	0.0882	0.7965	-5.6733
H	0.5564	1.3026	-6.5230
H	0.5068	1.2165	-4.7577
H	-0.9806	1.0255	-5.6950
N	2.8540	0.2916	1.5393
C	4.1367	0.0798	1.3745
S	5.1273	0.7844	2.6180
C	3.6796	1.3588	3.4314
C	3.5160	2.0315	4.6374
H	4.3703	2.3282	5.2353
C	2.2247	2.3006	5.0774
H	2.1120	2.8128	6.0245
C	1.0831	1.9201	4.3478
C	1.2689	1.2648	3.1397
H	0.4333	0.9300	2.5394
C	2.5529	0.9903	2.6920
C	4.5123	-0.7751	0.2632
C	3.3970	-1.3349	-0.3989
C	3.6227	-2.1798	-1.4818
H	2.7862	-2.6253	-2.0109
C	4.9249	-2.4563	-1.8906
H	5.0901	-3.1180	-2.7356
C	6.0193	-1.9007	-1.2284
H	7.0269	-2.1298	-1.5568
C	5.8161	-1.0572	-0.1471
H	6.6630	-0.6192	0.3729
C	-0.3558	2.1690	4.8164
C	-0.4111	2.9031	6.1588
H	-1.4527	3.0597	6.4515
H	0.0680	3.8845	6.1029
H	0.0703	2.3273	6.9541
C	-1.0951	3.0147	3.7625
H	-2.1188	3.2161	4.0925
H	-1.1550	2.4979	2.8001
H	-0.5934	3.9730	3.6028
C	-1.0808	0.8173	4.9638
H	-2.1106	0.9780	5.2986
H	-0.5815	0.1796	5.6981
H	-1.1156	0.2706	4.0172
C	-0.8197	1.0253	-0.1692
O	-0.4281	0.1548	0.6747
N	1.4111	1.0204	-1.1078
C	2.1241	1.6655	-2.0725
C	1.2916	2.5145	-2.7471
H	1.4551	3.1756	-3.5830
C	-2.1250	1.5488	-0.0753
H	-2.4047	2.3570	-0.7354
C	-3.0805	1.0703	0.8946
H	-2.7133	0.3960	1.6593
C	0.1661	1.4696	-1.1677
N	0.0439	2.3738	-2.1833
H	3.1728	1.4672	-2.2300
C	-1.1658	2.9181	-2.7264
C	-2.0934	2.0531	-3.3037
C	-1.3963	4.2855	-2.6615
C	-3.2780	2.5743	-3.8078
H	-1.8807	0.9901	-3.3536
C	-2.5813	4.7982	-3.1800
H	-0.6599	4.9342	-2.2000
C	-3.5220	3.9447	-3.7464
H	-4.0078	1.9099	-4.2579
H	-2.7698	5.8651	-3.1340
H	-4.4456	4.3482	-4.1475
C	-4.4291	1.4107	0.8653
C	-5.3017	0.9086	1.8902
C	-5.0205	2.2380	-0.1512
C	-6.6371	1.2197	1.9019
H	-4.8764	0.2772	2.6637
C	-6.3620	2.5364	-0.1220
H	-4.4135	2.6235	-0.9622
C	-7.1840	2.0385	0.8986
H	-7.2765	0.8334	2.6883
H	-6.7898	3.1629	-0.8976
H	-8.2403	2.2834	0.9131

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Rh–1–MECP(^{3}LC–^{3}MLCT)

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Rh	1.5933	-0.9014	0.2197
N	0.4774	-2.1946	-0.9630
C	-0.1177	-3.0853	-0.2059
S	-1.4405	-3.8993	-0.9588
C	-1.1510	-2.9814	-2.4113
C	-1.8177	-3.0493	-3.6319
H	-2.6777	-3.6954	-3.7672
C	-1.3361	-2.2846	-4.6735
H	-1.8451	-2.3412	-5.6286
C	-0.1919	-1.4642	-4.5533
C	0.4245	-1.3651	-3.3135
H	1.2909	-0.7385	-3.1598
C	-0.0616	-2.1195	-2.2368

C	0.3720	-3.2813	1.1445
C	1.3562	-2.3432	1.5366
C	1.9178	-2.4690	2.8117
H	2.6685	-1.7660	3.1517
C	1.5201	-3.5023	3.6492
H	1.9715	-3.6039	4.6304
C	0.5411	-4.4134	3.2457
H	0.2353	-5.2115	3.9130
C	-0.0406	-4.3046	1.9888
H	-0.7958	-5.0176	1.6712
C	0.3353	-0.7574	-5.8087
C	1.6584	-0.0327	-5.5482
H	2.0080	0.4329	-6.4729
H	2.4377	-0.7227	-5.2100
H	1.5497	0.7550	-4.8005
C	0.5771	-1.8034	-6.9141
H	0.9876	-1.3146	-7.8024
H	-0.3424	-2.3093	-7.2175
H	1.2894	-2.5660	-6.5868
C	-0.6984	0.2695	-6.3018
H	-0.3465	0.7396	-7.2245
H	-0.8586	1.0556	-5.5605
H	-1.6643	-0.1955	-6.5167
N	2.7047	0.2107	1.5084
C	3.9960	0.1513	1.3050
S	4.9255	1.0180	2.4833
C	3.4417	1.4659	3.3095
C	3.2347	2.1871	4.4810
H	4.0649	2.6017	5.0412
C	1.9301	2.3561	4.9275
H	1.7811	2.9109	5.8451
C	0.8144	1.8375	4.2394
C	1.0399	1.1293	3.0689
H	0.2302	0.7154	2.4815
C	2.3423	0.9425	2.6216
C	4.4358	-0.6535	0.1732
C	3.3786	-1.3087	-0.5055
C	3.6565	-2.0863	-1.6266
H	2.8516	-2.5681	-2.1708
C	4.9749	-2.2460	-2.0402
H	5.1961	-2.8644	-2.9040
C	6.0155	-1.6187	-1.3550
H	7.0380	-1.7492	-1.6911
C	5.7514	-0.8215	-0.2463
H	6.5650	-0.3333	0.2807
C	-0.6354	2.0356	4.6995
C	-0.7192	2.6510	6.0991
H	-1.7666	2.7391	6.3976
H	-0.2884	3.6557	6.1314
H	-0.2124	2.0311	6.8448
C	-1.3481	2.9640	3.6987
H	-2.3950	3.0964	3.9877
H	-1.3358	2.5492	2.6879
H	-0.8747	3.9495	3.6704
C	-1.3661	0.6791	4.7223
H	-2.3935	0.8196	5.0707
H	-0.8726	-0.0276	5.3956
H	-1.4182	0.2235	3.7301
C	-0.7078	0.9071	-0.2291
O	-0.3240	-0.0793	0.5482
N	1.5103	0.8261	-1.1257
C	2.2690	1.4794	-2.0607
C	1.4867	2.3811	-2.7140
H	1.6938	3.0628	-3.5228
C	-1.9877	1.4965	-0.0445
H	-2.2177	2.3767	-0.6302
C	-2.8868	1.0209	0.8575
H	-2.6018	0.1450	1.4327
C	0.2747	1.3384	-1.1789
N	0.2151	2.2777	-2.1736
H	3.3102	1.2435	-2.2141
C	-0.9625	2.8528	-2.7451
C	-1.9396	2.0121	-3.2749
C	-1.1164	4.2324	-2.7693
C	-3.0893	2.5669	-3.8200
H	-1.7979	0.9368	-3.2447
C	-2.2671	4.7793	-3.3282
H	-0.3477	4.8658	-2.3403
C	-3.2545	3.9495	-3.8473
H	-3.8564	1.9178	-4.2284
H	-2.3941	5.8561	-3.3475
H	-4.1537	4.3793	-4.2753
C	-4.1984	1.5792	1.1408
C	-4.9286	1.0706	2.2254
C	-4.7785	2.6064	0.3776
C	-6.1809	1.5734	2.5467
H	-4.4981	0.2708	2.8214
C	-6.0297	3.1062	0.6987
H	-4.2543	3.0046	-0.4853
C	-6.7372	2.5956	1.7854
H	-6.7261	1.1655	3.3916
H	-6.4627	3.8979	0.0956
H	-7.7173	2.9899	2.0319

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Rh–1–^{3}MLCT

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Rh	1.5564	-0.9363	0.1880
N	0.5341	-2.3235	-0.9671
C	0.0616	-3.2948	-0.2240
S	-1.0601	-4.3357	-1.0245
C	-0.8518	-3.4018	-2.4831
C	-1.4060	-3.6168	-3.7376
H	-2.1108	-4.4225	-3.9093
C	-1.0131	-2.7903	-4.7760
H	-1.4323	-2.9755	-5.7559
C	-0.0813	-1.7511	-4.6013
C	0.4287	-1.5227	-3.3255
H	1.1398	-0.7296	-3.1426
C	0.0502	-2.3493	-2.2668
C	0.5291	-3.4091	1.1433
C	1.3924	-2.3650	1.5426
C	1.9277	-2.4040	2.8318
H	2.5882	-1.6183	3.1777
C	1.6154	-3.4582	3.6838
H	2.0437	-3.4880	4.6802
C	0.7552	-4.4766	3.2744
H	0.5161	-5.2901	3.9504
C	0.2050	-4.4555	1.9985
H	-0.4604	-5.2512	1.6760
C	0.3995	-0.8922	-5.7791
C	1.9377	-0.9141	-5.8302
H	2.2920	-0.3178	-6.6757
H	2.3095	-1.9349	-5.9558
H	2.3855	-0.4981	-4.9241
C	-0.1275	-1.3986	-7.1274
H	0.2744	-0.7756	-7.9303
H	-1.2178	-1.3415	-7.1895
H	0.1782	-2.4299	-7.3251
C	-0.0832	0.5532	-5.5847
H	0.2746	1.1864	-6.4022
H	0.2879	0.9721	-4.6479
H	-1.1752	0.6068	-5.5721
C	-0.7277	0.8878	-0.2828
O	-0.3446	-0.1455	0.4543
N	1.4698	0.7543	-1.2139
C	2.2433	1.3910	-2.1476
C	1.4899	2.3409	-2.7672
H	1.7110	3.0286	-3.5673
C	-1.9812	1.4866	-0.0531
H	-2.2214	2.3807	-0.6121
C	-2.8659	0.9891	0.8673
H	-2.5706	0.0910	1.4026
N	2.6149	0.2670	1.4499
C	3.9082	0.2547	1.2454
S	4.8036	1.1986	2.3881

C	3.3048	1.6194	3.1989
C	3.0763	2.3835	4.3384
H	3.8936	2.8493	4.8770
C	1.7680	2.5295	4.7793
H	1.6012	3.1192	5.6715
C	0.6691	1.9460	4.1166
C	0.9157	1.1927	2.9777
H	0.1194	0.7290	2.4094
C	2.2243	1.0282	2.5359
C	4.3874	-0.5548	0.1328
C	3.3688	-1.2654	-0.5425
C	3.6809	-2.0359	-1.6570
H	2.9013	-2.5545	-2.2039
C	5.0080	-2.1380	-2.0660
H	5.2586	-2.7498	-2.9265
C	6.0158	-1.4599	-1.3820
H	7.0445	-1.5457	-1.7138
C	5.7112	-0.6659	-0.2817
H	6.4993	-0.1341	0.2422
C	-0.7833	2.1384	4.5712
C	-0.8741	2.7371	5.9784
H	-1.9227	2.8076	6.2774
H	-0.4586	3.7475	6.0240
H	-0.3584	2.1152	6.7164
C	-1.4843	3.0833	3.5776
H	-2.5326	3.2174	3.8601
H	-1.4650	2.6793	2.5627
H	-1.0048	4.0662	3.5659
C	-1.5210	0.7865	4.5771
H	-2.5497	0.9304	4.9196
H	-1.0352	0.0714	5.2473
H	-1.5724	0.3403	3.5814
C	0.2577	1.3180	-1.2354
N	0.2251	2.2826	-2.2038
H	3.2706	1.1115	-2.3217
C	-0.9224	2.9764	-2.7029
C	-1.9930	2.2456	-3.2126
C	-0.9494	4.3643	-2.6800
C	-3.1091	2.9191	-3.6880
H	-1.9507	1.1624	-3.2147
C	-2.0669	5.0311	-3.1714
H	-0.1086	4.9114	-2.2676
C	-3.1470	4.3113	-3.6692
H	-3.9502	2.3558	-4.0774
H	-2.0954	6.1150	-3.1539
H	-4.0201	4.8343	-4.0441
C	-4.1570	1.5498	1.2144
C	-4.8639	0.9957	2.2941
C	-4.7421	2.6273	0.5268
C	-6.0962	1.5003	2.6809
H	-4.4289	0.1588	2.8333
C	-5.9742	3.1290	0.9140
H	-4.2368	3.0659	-0.3280
C	-6.6575	2.5717	1.9934
H	-6.6226	1.0556	3.5194
H	-6.4108	3.9598	0.3688
H	-7.6224	2.9679	2.2915

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Rh–1–MECP(^{1}MLCT–^{3}MLCT)

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Rh	1.6030	-0.5896	0.3593
N	0.1317	-1.6615	-0.6494
C	-0.5333	-2.4350	0.1879
S	-2.0543	-3.0306	-0.4043
C	-1.7427	-2.1876	-1.8914
C	-2.4986	-2.1585	-3.0518
H	-3.4716	-2.6312	-3.0931
C	-1.9590	-1.5489	-4.1708
H	-2.5468	-1.5676	-5.0796
C	-0.6616	-0.9715	-4.1942
C	0.0457	-0.9319	-3.0056
H	1.0350	-0.4958	-2.9522
C	-0.4898	-1.5333	-1.8545
C	0.0457	-2.7223	1.4601
C	1.2446	-1.9827	1.7262
C	1.8896	-2.2455	2.9479
H	2.7957	-1.7149	3.2125
C	1.3754	-3.1874	3.8107
H	1.8962	-3.3898	4.7452
C	0.1813	-3.9025	3.5228
H	-0.2000	-4.6356	4.2244
C	-0.4850	-3.6724	2.3477
H	-1.3923	-4.2202	2.1069
C	-0.0126	-0.4592	-5.4941
C	1.3393	-1.1677	-5.6887
H	1.8044	-0.8286	-6.6181
H	1.2043	-2.2501	-5.7515
H	2.0347	-0.9559	-4.8734
C	-0.8687	-0.7343	-6.7387
H	-0.3359	-0.3815	-7.6258
H	-1.8244	-0.2032	-6.7094
H	-1.0626	-1.8019	-6.8724
C	0.2221	1.0567	-5.4039
H	0.7452	1.4101	-6.2980
H	0.8307	1.3083	-4.5331
H	-0.7212	1.6055	-5.3347
C	-0.7336	1.2507	0.0002
O	-0.3012	0.4178	0.9124
N	1.4796	1.1282	-0.9558
C	2.1961	1.7167	-1.9629
C	1.4075	2.6127	-2.6119
H	1.5809	3.2583	-3.4583
C	-2.0872	1.5535	-0.0743
H	-2.4264	2.1986	-0.8688
C	-3.0336	0.8836	0.7253
H	-2.6449	0.3522	1.5859
N	2.9904	0.2819	1.5296
C	4.2328	-0.0487	1.2993
S	5.3459	0.6329	2.4485
C	3.9998	1.3733	3.3092
C	3.9510	2.1179	4.4857
H	4.8588	2.3827	5.0186
C	2.7064	2.4886	4.9903
H	2.6817	3.0434	5.9207
C	1.5002	2.1286	4.3573
C	1.5809	1.4148	3.1724
H	0.6920	1.0871	2.6513
C	2.8116	1.0542	2.6612
C	4.4567	-0.9958	0.2119
C	3.2584	-1.4660	-0.3474
C	3.3153	-2.4013	-1.3693
H	2.4041	-2.7897	-1.8158
C	4.5577	-2.8493	-1.8308
H	4.5966	-3.5795	-2.6338
C	5.7411	-2.3687	-1.2849
H	6.6951	-2.7234	-1.6578
C	5.6949	-1.4389	-0.2538
H	6.6132	-1.0624	0.1877
C	0.0931	2.4390	4.8859
C	0.1215	3.2314	6.1943
H	-0.8987	3.4279	6.5356
H	0.6213	4.1968	6.0763
H	0.6319	2.6724	6.9833
C	-0.6727	3.2432	3.8174
H	-1.6713	3.5042	4.1828
H	-0.7890	2.6519	2.9019
H	-0.1477	4.1688	3.5646
C	-0.6707	1.1198	5.1323
H	-1.6758	1.3322	5.5110
H	-0.1545	0.4992	5.8698
H	-0.7788	0.5278	4.2195
C	0.2600	1.6727	-0.9704
N	0.1698	2.5793	-1.9923
H	3.2187	1.4409	-2.1547
C	-0.9846	3.2333	-2.5374

C	-1.9555	2.4788	-3.1939
C	-1.1034	4.6113	-2.4264
C	-3.0651	3.1189	-3.7288
H	-1.8416	1.4031	-3.2723
C	-2.2129	5.2465	-2.9784
H	-0.3361	5.1769	-1.9086
C	-3.1933	4.5026	-3.6237
H	-3.8259	2.5353	-4.2373
H	-2.3094	6.3241	-2.8955
H	-4.0574	5.0018	-4.0494
C	-4.3314	0.5280	0.2531
C	-5.1103	-0.3834	1.0094
C	-4.8737	0.9934	-0.9740
C	-6.2950	-0.8877	0.5122
H	-4.7244	-0.7337	1.9604
C	-6.0685	0.4968	-1.4539
H	-4.3175	1.7006	-1.5772
C	-6.7912	-0.4437	-0.7160
H	-6.8564	-1.6152	1.0895
H	-6.4504	0.8476	-2.4070
H	-7.7278	-0.8325	-1.0960

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Ir–1

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Ir	1.6057	-0.7834	0.1573
N	0.4837	-2.1335	-0.9488
C	0.0026	-3.1063	-0.1985
S	-1.1669	-4.1100	-0.9906
C	-0.9469	-3.1828	-2.4536
C	-1.5156	-3.3868	-3.7019
H	-2.2516	-4.1672	-3.8606
C	-1.0923	-2.5940	-4.7562
H	-1.5216	-2.7772	-5.7320
C	-0.1072	-1.6048	-4.6002
C	0.4123	-1.3791	-3.3249
H	1.1833	-0.6394	-3.1606
C	-0.0045	-2.1650	-2.2498
C	0.5087	-3.2656	1.1414
C	1.4457	-2.2727	1.4996
C	2.0557	-2.4117	2.7482
H	2.7934	-1.6884	3.0777
C	1.7305	-3.4706	3.5889
H	2.2236	-3.5576	4.5523
C	0.7850	-4.4285	3.2168
H	0.5440	-5.2491	3.8833
C	0.1703	-4.3288	1.9830
H	-0.5534	-5.0762	1.6679
C	0.4361	-0.8151	-5.8007
C	1.9678	-0.9588	-5.8501
H	2.3689	-0.4170	-6.7116
H	2.2576	-2.0088	-5.9439
H	2.4495	-0.5587	-4.9543
C	-0.1288	-1.3154	-7.1363
H	0.3157	-0.7440	-7.9552
H	-1.2127	-1.1835	-7.2000
H	0.1017	-2.3705	-7.3067
C	0.0673	0.6686	-5.6565
H	0.4932	1.2486	-6.4807
H	0.4477	1.0834	-4.7213
H	-1.0170	0.8073	-5.6738
C	-0.8296	0.9635	-0.2456
O	-0.4375	0.0703	0.5351
N	1.3856	0.9006	-1.1899
C	2.1450	1.5645	-2.0977
C	1.3486	2.4748	-2.7477
H	1.5525	3.1590	-3.5560
C	-2.1358	1.5659	-0.1117
H	-2.3914	2.3969	-0.7516
C	-2.9933	1.1003	0.8220
H	-2.6468	0.2710	1.4347
N	2.7524	0.3189	1.4357
C	4.0528	0.1916	1.2859
S	4.9787	1.0181	2.5012
C	3.4886	1.5210	3.2842
C	3.2774	2.2290	4.4620
H	4.1093	2.6082	5.0447
C	1.9708	2.4240	4.8952
H	1.8214	2.9639	5.8216
C	0.8606	1.9325	4.1845
C	1.0938	1.2434	3.0028
H	0.2814	0.8267	2.4252
C	2.3940	1.0417	2.5610
C	4.4971	-0.6775	0.2163
C	3.4212	-1.3321	-0.4327
C	3.7363	-2.2197	-1.4646
H	2.9426	-2.7492	-1.9828
C	5.0585	-2.4327	-1.8360
H	5.2819	-3.1264	-2.6412
C	6.1054	-1.7735	-1.1878
H	7.1314	-1.9536	-1.4882
C	5.8260	-0.8944	-0.1559
H	6.6321	-0.3788	0.3580
C	-0.5939	2.1149	4.6387
C	-0.6930	2.7584	6.0245
H	-1.7428	2.8457	6.3159
H	-0.2661	3.7651	6.0381
H	-0.1867	2.1570	6.7849
C	-1.3277	3.0102	3.6234
H	-2.3778	3.1267	3.9096
H	-1.3030	2.5800	2.6187
H	-0.8755	4.0047	3.5758
C	-1.2978	0.7449	4.6903
H	-2.3313	0.8703	5.0286
H	-0.7942	0.0660	5.3834
H	-1.3249	0.2580	3.7113
C	0.1550	1.4003	-1.2487
N	0.0911	2.3564	-2.2198
H	3.1880	1.3310	-2.2429
C	-1.0883	2.9771	-2.7541
C	-2.0626	2.1719	-3.3380
C	-1.2370	4.3545	-2.6733
C	-3.2157	2.7649	-3.8344
H	-1.9142	1.0989	-3.3941
C	-2.3917	4.9383	-3.1838
H	-0.4662	4.9554	-2.2033
C	-3.3803	4.1458	-3.7575
H	-3.9837	2.1478	-4.2877
H	-2.5201	6.0133	-3.1244
H	-4.2807	4.6054	-4.1504
C	-4.3286	1.5908	1.1066
C	-5.0022	1.0687	2.2193
C	-4.9691	2.5604	0.3184
C	-6.2753	1.5104	2.5481
H	-4.5154	0.3128	2.8287
C	-6.2408	2.9968	0.6461
H	-4.4777	2.9610	-0.5623
C	-6.8951	2.4753	1.7620
H	-6.7856	1.1007	3.4130
H	-6.7317	3.7435	0.0311
H	-7.8927	2.8202	2.0132

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Ir–1–^{1}MLCT

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Ir	1.5832	-0.9203	0.1664
N	0.4815	-2.2526	-0.9644
C	-0.0447	-3.2067	-0.2279
S	-1.1831	-4.2071	-1.0520
C	-0.9078	-3.2863	-2.5074
C	-1.4458	-3.4819	-3.7721
H	-2.1767	-4.2610	-3.9567
C	-1.0043	-2.6706	-4.8025
H	-1.4124	-2.8396	-5.7899
C	-0.0378	-1.6659	-4.6111
C	0.4594	-1.4586	-3.3272

H	1.1953	-0.6926	-3.1302
C	0.0285	-2.2686	-2.2758
C	0.4016	-3.3352	1.1426
C	1.3303	-2.3312	1.5248
C	1.8537	-2.3994	2.8261
H	2.5583	-1.6489	3.1642
C	1.4756	-3.4181	3.6865
H	1.8950	-3.4646	4.6858
C	0.5536	-4.3889	3.2836
H	0.2620	-5.1770	3.9689
C	0.0108	-4.3503	2.0058
H	-0.6999	-5.1086	1.6904
C	0.4786	-0.8142	-5.7791
C	2.0173	-0.8213	-5.7820
H	2.3908	-0.2319	-6.6239
H	2.4030	-1.8395	-5.8833
H	2.4336	-0.3881	-4.8692
C	-0.0001	-1.3369	-7.1396
H	0.4356	-0.7278	-7.9355
H	-1.0867	-1.2740	-7.2452
H	0.3064	-2.3728	-7.3095
C	-0.0233	0.6284	-5.6104
H	0.3491	1.2578	-6.4243
H	0.3210	1.0568	-4.6678
H	-1.1157	0.6721	-5.6243
C	-0.7543	0.8643	-0.2260
O	-0.3593	-0.1385	0.5260
N	1.4372	0.7805	-1.1739
C	2.1992	1.4394	-2.1020
C	1.4263	2.3799	-2.7097
H	1.6350	3.0805	-3.5016
C	-2.0353	1.4423	-0.0193
H	-2.2884	2.3227	-0.5939
C	-2.9127	0.9429	0.8900
H	-2.6016	0.0649	1.4480
N	2.6903	0.2696	1.4043
C	3.9867	0.2254	1.2045
S	4.8997	1.1595	2.3396
C	3.4107	1.6170	3.1474
C	3.1997	2.3850	4.2876
H	4.0273	2.8369	4.8224
C	1.8963	2.5499	4.7371
H	1.7434	3.1405	5.6313
C	0.7865	1.9801	4.0815
C	1.0159	1.2272	2.9391
H	0.2094	0.7701	2.3805
C	2.3183	1.0450	2.4889
C	4.4455	-0.6269	0.1178
C	3.3910	-1.3458	-0.5121
C	3.7149	-2.1885	-1.5828
H	2.9291	-2.7311	-2.0981
C	5.0337	-2.3282	-1.9934
H	5.2746	-2.9880	-2.8205
C	6.0557	-1.6278	-1.3502
H	7.0818	-1.7461	-1.6797
C	5.7654	-0.7745	-0.2908
H	6.5637	-0.2307	0.2045
C	-0.6616	2.1737	4.5487
C	-0.7405	2.8105	5.9393
H	-1.7863	2.8879	6.2464
H	-0.3251	3.8219	5.9516
H	-0.2171	2.2103	6.6896
C	-1.3854	3.0830	3.5385
H	-2.4319	3.2120	3.8302
H	-1.3733	2.6529	2.5345
H	-0.9186	4.0711	3.4950
C	-1.3833	0.8135	4.5985
H	-2.4105	0.9539	4.9473
H	-0.8827	0.1229	5.2833
H	-1.4358	0.3391	3.6158
C	0.2102	1.3210	-1.1831
N	0.1630	2.2940	-2.1458
H	3.2313	1.1813	-2.2773
C	-1.0007	2.9501	-2.6568
C	-2.0324	2.1843	-3.1955
C	-1.0847	4.3352	-2.6144
C	-3.1673	2.8191	-3.6797
H	-1.9453	1.1036	-3.2136
C	-2.2207	4.9634	-3.1145
H	-0.2741	4.9094	-2.1791
C	-3.2624	4.2081	-3.6405
H	-3.9782	2.2283	-4.0917
H	-2.2938	6.0449	-3.0813
H	-4.1501	4.7011	-4.0218
C	-4.2264	1.4770	1.2072
C	-4.9293	0.9337	2.2927
C	-4.8324	2.5152	0.4807
C	-6.1812	1.4130	2.6497
H	-4.4782	0.1249	2.8604
C	-6.0828	2.9925	0.8380
H	-4.3288	2.9418	-0.3809
C	-6.7635	2.4468	1.9247
H	-6.7054	0.9777	3.4942
H	-6.5360	3.7940	0.2633
H	-7.7432	2.8231	2.1992

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Ir–1–MECP(^{1}MLCT–^{3}LC)

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Ir	1.5447	-0.8839	0.1542
N	0.4769	-2.2377	-0.9747
C	-0.0144	-3.2217	-0.2476
S	-1.1055	-4.2595	-1.0925
C	-0.8530	-3.3179	-2.5407
C	-1.3686	-3.5282	-3.8115
H	-2.0657	-4.3351	-4.0074
C	-0.9475	-2.6962	-4.8353
H	-1.3365	-2.8783	-5.8281
C	-0.0226	-1.6580	-4.6283
C	0.4512	-1.4373	-3.3366
H	1.1611	-0.6497	-3.1305
C	0.0401	-2.2663	-2.2932
C	0.4264	-3.3505	1.1203
C	1.3224	-2.3280	1.5132
C	1.8503	-2.4073	2.8068
H	2.5417	-1.6503	3.1585
C	1.4955	-3.4480	3.6545
H	1.9203	-3.4959	4.6520
C	0.5993	-4.4386	3.2442
H	0.3312	-5.2444	3.9182
C	0.0602	-4.3930	1.9690
H	-0.6278	-5.1652	1.6364
C	0.4830	-0.7871	-5.7869
C	2.0215	-0.7555	-5.7739
H	2.3892	-0.1555	-6.6110
H	2.4335	-1.7634	-5.8724
H	2.4165	-0.3143	-4.8556
C	0.0315	-1.3146	-7.1547
H	0.4538	-0.6865	-7.9432
H	-1.0558	-1.2866	-7.2682
H	0.3730	-2.3388	-7.3288
C	-0.0555	0.6421	-5.6174
H	0.3142	1.2864	-6.4207
H	0.2644	1.0719	-4.6666
H	-1.1486	0.6594	-5.6496
C	-0.7896	0.8829	-0.2347
O	-0.3764	-0.0955	0.5413
N	1.4037	0.8095	-1.1850
C	2.1667	1.4736	-2.1075
C	1.3911	2.4145	-2.7139
H	1.5972	3.1184	-3.5038
C	-2.0744	1.4204	-0.0404
H	-2.3690	2.2670	-0.6445
C	-2.9409	0.9143	0.9110
H	-2.5903	0.0694	1.4943
N	2.6911	0.2555	1.4038

C	3.9895	0.1491	1.2270
S	4.9250	1.0371	2.3826
C	3.4451	1.5604	3.1682
C	3.2526	2.3373	4.3047
H	4.0926	2.7516	4.8506
C	1.9517	2.5632	4.7370
H	1.8135	3.1618	5.6282
C	0.8294	2.0404	4.0672
C	1.0424	1.2739	2.9298
H	0.2228	0.8405	2.3724
C	2.3392	1.0373	2.4923
C	4.4311	-0.7280	0.1585
C	3.3593	-1.4024	-0.4824
C	3.6726	-2.2726	-1.5313
H	2.8805	-2.7998	-2.0530
C	4.9932	-2.4678	-1.9159
H	5.2199	-3.1500	-2.7292
C	6.0340	-1.8011	-1.2671
H	7.0600	-1.9652	-1.5766
C	5.7553	-0.9283	-0.2252
H	6.5624	-0.4081	0.2817
C	-0.6170	2.2863	4.5150
C	-0.6924	3.0223	5.8557
H	-1.7387	3.1535	6.1429
H	-0.2428	4.0174	5.7992
H	-0.1976	2.4618	6.6542
C	-1.3297	3.1323	3.4438
H	-2.3715	3.3041	3.7308
H	-1.3341	2.6303	2.4733
H	-0.8434	4.1046	3.3237
C	-1.3522	0.9397	4.6556
H	-2.3841	1.1112	4.9764
H	-0.8672	0.2992	5.3974
H	-1.3880	0.3932	3.7101
C	0.1805	1.3472	-1.1967
N	0.1296	2.3229	-2.1511
H	3.1992	1.2153	-2.2810
C	-1.0358	3.0002	-2.6327
C	-2.0574	2.2570	-3.2198
C	-1.1341	4.3790	-2.5044
C	-3.1986	2.9083	-3.6671
H	-1.9564	1.1809	-3.3072
C	-2.2760	5.0243	-2.9678
H	-0.3297	4.9336	-2.0338
C	-3.3084	4.2911	-3.5422
H	-4.0013	2.3357	-4.1188
H	-2.3609	6.1010	-2.8695
H	-4.2000	4.7975	-3.8960
C	-4.2541	1.4135	1.2061
C	-4.9725	0.8350	2.2735
C	-4.8716	2.4586	0.4842
C	-6.2384	1.2797	2.6089
H	-4.5139	0.0276	2.8366
C	-6.1373	2.8985	0.8232
H	-4.3594	2.9178	-0.3548
C	-6.8284	2.3154	1.8864
H	-6.7721	0.8202	3.4341
H	-6.5973	3.7013	0.2564
H	-7.8217	2.6651	2.1466

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Ir–1–^{3}LC

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Ir	1.5275	-0.8067	0.1531
N	0.4543	-2.1675	-0.9681
C	-0.0163	-3.1641	-0.2413
S	-1.1032	-4.2107	-1.0865
C	-0.8650	-3.2647	-2.5355
C	-1.3753	-3.4842	-3.8063
H	-2.0650	-4.2981	-3.9999
C	-0.9547	-2.6575	-4.8355
H	-1.3370	-2.8505	-5.8289
C	-0.0332	-1.6172	-4.6313
C	0.4307	-1.3837	-3.3369
H	1.1458	-0.5998	-3.1354
C	0.0189	-2.2058	-2.2886
C	0.4401	-3.3072	1.1178
C	1.3298	-2.2866	1.5123
C	1.8828	-2.3969	2.7880
H	2.5802	-1.6491	3.1479
C	1.5504	-3.4611	3.6207
H	1.9992	-3.5259	4.6071
C	0.6553	-4.4502	3.2113
H	0.4084	-5.2743	3.8711
C	0.0964	-4.3764	1.9488
H	-0.5886	-5.1471	1.6054
C	0.4865	-0.7625	-5.7964
C	2.0245	-0.7230	-5.7610
H	2.4025	-0.1386	-6.6047
H	2.4423	-1.7308	-5.8314
H	2.4038	-0.2619	-4.8459
C	0.0592	-1.3151	-7.1623
H	0.4924	-0.6998	-7.9551
H	-1.0262	-1.2934	-7.2942
H	0.4067	-2.3410	-7.3117
C	-0.0600	0.6671	-5.6616
H	0.3209	1.2997	-6.4690
H	0.2429	1.1130	-4.7126
H	-1.1525	0.6788	-5.7130
C	-0.8147	0.9402	-0.2323
O	-0.3864	0.0162	0.5856
N	1.3763	0.8697	-1.1943
C	2.1330	1.5307	-2.1210
C	1.3440	2.4521	-2.7461
H	1.5416	3.1451	-3.5480
C	-2.1051	1.4460	-0.0619
H	-2.4398	2.2365	-0.7184
C	-2.9688	0.9578	0.9493
H	-2.5748	0.1823	1.5956
N	2.7184	0.2604	1.4214
C	4.0144	0.0922	1.2629
S	4.9746	0.9123	2.4519
C	3.5090	1.4826	3.2328
C	3.3366	2.2399	4.3851
H	4.1880	2.6064	4.9474
C	2.0421	2.5083	4.8150
H	1.9210	3.0907	5.7194
C	0.9084	2.0411	4.1265
C	1.1031	1.2934	2.9731
H	0.2709	0.8915	2.4120
C	2.3908	1.0220	2.5328
C	4.4300	-0.7948	0.1985
C	3.3360	-1.4082	-0.4580
C	3.6263	-2.2858	-1.5056
H	2.8210	-2.7806	-2.0391
C	4.9422	-2.5372	-1.8752
H	5.1455	-3.2264	-2.6893
C	6.0076	-1.9213	-1.2151
H	7.0282	-2.1296	-1.5155
C	5.7528	-1.0463	-0.1739
H	6.5731	-0.5602	0.3461
C	-0.5332	2.3108	4.5760
C	-0.5957	3.0901	5.8927
H	-1.6392	3.2515	6.1758
H	-0.1234	4.0725	5.8054
H	-0.1134	2.5444	6.7086
C	-1.2540	3.1264	3.4866
H	-2.2873	3.3266	3.7864
H	-1.2855	2.5883	2.5354
H	-0.7552	4.0850	3.3183
C	-1.2704	0.9713	4.7646
H	-2.3015	1.1531	5.0835
H	-0.7828	0.3560	5.5255
H	-1.3041	0.3921	3.8383
C	0.1515	1.3902	-1.2221
N	0.0854	2.3504	-2.1868

H	3.1690	1.2817	-2.2872
C	-1.0922	3.0110	-2.6658
C	-2.0911	2.2528	-3.2725
C	-1.2257	4.3838	-2.5080
C	-3.2476	2.8841	-3.7106
H	-1.9585	1.1826	-3.3885
C	-2.3825	5.0087	-2.9626
H	-0.4369	4.9490	-2.0239
C	-3.3933	4.2609	-3.5567
H	-4.0321	2.3013	-4.1809
H	-2.4951	6.0807	-2.8436
H	-4.2954	4.7518	-3.9058
C	-4.2879	1.4115	1.1726
C	-5.0214	0.8691	2.2650
C	-4.9367	2.3843	0.3592
C	-6.3102	1.2746	2.5286
H	-4.5428	0.1242	2.8930
C	-6.2273	2.7820	0.6338
H	-4.4224	2.8119	-0.4941
C	-6.9238	2.2351	1.7162
H	-6.8521	0.8489	3.3662
H	-6.7081	3.5229	0.0040
H	-7.9396	2.5534	1.9241

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Ir–1–MECP(^{3}LC–^{3}MLCT)

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Ir	1.5355	-0.8604	0.1535
N	0.4683	-2.2163	-0.9740
C	-0.0192	-3.2032	-0.2473
S	-1.1102	-4.2410	-1.0934
C	-0.8589	-3.2984	-2.5417
C	-1.3714	-3.5106	-3.8133
H	-2.0681	-4.3179	-4.0094
C	-0.9465	-2.6819	-4.8383
H	-1.3320	-2.8668	-5.8319
C	-0.0198	-1.6454	-4.6313
C	0.4488	-1.4212	-3.3381
H	1.1614	-0.6362	-3.1324
C	0.0332	-2.2466	-2.2936
C	0.4257	-3.3368	1.1184
C	1.3204	-2.3160	1.5126
C	1.8567	-2.4059	2.8002
H	2.5504	-1.6522	3.1546
C	1.5080	-3.4540	3.6432
H	1.9403	-3.5080	4.6373
C	0.6114	-4.4430	3.2326
H	0.3493	-5.2547	3.9019
C	0.0661	-4.3878	1.9611
H	-0.6213	-5.1591	1.6249
C	0.4921	-0.7805	-5.7918
C	2.0296	-0.7258	-5.7573
H	2.4004	-0.1360	-6.6003
H	2.4585	-1.7289	-5.8302
H	2.4042	-0.2603	-4.8424
C	0.0684	-1.3304	-7.1599
H	0.4980	-0.7091	-7.9499
H	-1.0170	-1.3142	-7.2926
H	0.4220	-2.3537	-7.3135
C	-0.0678	0.6431	-5.6465
H	0.3029	1.2830	-6.4530
H	0.2359	1.0873	-4.6970
H	-1.1606	0.6453	-5.6913
N	2.6952	0.2565	1.4091
C	3.9934	0.1318	1.2380
S	4.9361	0.9968	2.4058
C	3.4600	1.5330	3.1903
C	3.2735	2.3018	4.3332
H	4.1171	2.7002	4.8854
C	1.9742	2.5405	4.7642
H	1.8411	3.1325	5.6606
C	0.8482	2.0372	4.0864
C	1.0557	1.2788	2.9426
H	0.2322	0.8583	2.3814
C	2.3501	1.0309	2.5055
C	4.4274	-0.7459	0.1686
C	3.3491	-1.4012	-0.4787
C	3.6550	-2.2701	-1.5299
H	2.8588	-2.7861	-2.0566
C	4.9745	-2.4806	-1.9108
H	5.1944	-3.1625	-2.7263
C	6.0227	-1.8305	-1.2569
H	7.0473	-2.0066	-1.5645
C	5.7513	-0.9600	-0.2127
H	6.5624	-0.4511	0.2993
C	-0.5970	2.2914	4.5337
C	-0.6692	3.0353	5.8702
H	-1.7149	3.1763	6.1553
H	-0.2111	4.0263	5.8090
H	-0.1802	2.4752	6.6725
C	-1.3087	3.1339	3.4589
H	-2.3488	3.3132	3.7481
H	-1.3192	2.6256	2.4916
H	-0.8178	4.1027	3.3302
C	-1.3358	0.9477	4.6821
H	-2.3677	1.1232	5.0013
H	-0.8527	0.3105	5.4280
H	-1.3708	0.3951	3.7400
C	-0.7980	0.9000	-0.2382
O	-0.3779	-0.0638	0.5525
N	1.3946	0.8244	-1.1896
C	2.1564	1.4864	-2.1148
C	1.3762	2.4176	-2.7311
H	1.5799	3.1158	-3.5266
C	-2.0832	1.4297	-0.0474
H	-2.3895	2.2615	-0.6661
C	-2.9456	0.9298	0.9211
H	-2.5845	0.0985	1.5167
C	0.1696	1.3559	-1.2091
N	0.1143	2.3230	-2.1707
H	3.1906	1.2320	-2.2839
C	-1.0553	2.9932	-2.6531
C	-2.0705	2.2433	-3.2427
C	-1.1647	4.3707	-2.5198
C	-3.2170	2.8869	-3.6877
H	-1.9599	1.1686	-3.3356
C	-2.3119	5.0082	-2.9810
H	-0.3647	4.9303	-2.0475
C	-3.3383	4.2684	-3.5579
H	-4.0148	2.3095	-4.1421
H	-2.4055	6.0838	-2.8794
H	-4.2338	4.7686	-3.9104
C	-4.2582	1.4223	1.2069
C	-4.9779	0.8474	2.2786
C	-4.8819	2.4583	0.4730
C	-6.2472	1.2853	2.6044
H	-4.5150	0.0484	2.8501
C	-6.1514	2.8909	0.8038
H	-4.3701	2.9151	-0.3675
C	-6.8421	2.3111	1.8697
H	-6.7814	0.8296	3.4314
H	-6.6156	3.6856	0.2291
H	-7.8390	2.6555	2.1231

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Ir–1–^{3}MLCT

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Ir	1.5800	-0.9243	0.1725
N	0.4800	-2.2627	-0.9555
C	-0.0433	-3.2170	-0.2175
S	-1.1915	-4.2094	-1.0360
C	-0.9233	-3.2863	-2.4918
C	-1.4695	-3.4785	-3.7534
H	-2.2055	-4.2538	-3.9339
C	-1.0292	-2.6697	-4.7866
H	-1.4434	-2.8367	-5.7717

C	-0.0556	-1.6716	-4.6004
C	0.4483	-1.4657	-3.3183
H	1.1914	-0.7052	-3.1263
C	0.0186	-2.2731	-2.2647
C	0.4098	-3.3487	1.1519
C	1.3271	-2.3403	1.5392
C	1.8552	-2.4089	2.8346
H	2.5509	-1.6518	3.1771
C	1.4911	-3.4396	3.6918
H	1.9143	-3.4862	4.6896
C	0.5813	-4.4169	3.2856
H	0.3009	-5.2140	3.9655
C	0.0338	-4.3748	2.0088
H	-0.6683	-5.1395	1.6894
C	0.4667	-0.8284	-5.7720
C	2.0051	-0.8664	-5.7867
H	2.3845	-0.2821	-6.6295
H	2.3692	-1.8921	-5.8938
H	2.4374	-0.4457	-4.8754
C	-0.0327	-1.3405	-7.1290
H	0.4059	-0.7371	-7.9278
H	-1.1191	-1.2597	-7.2245
H	0.2549	-2.3810	-7.3040
C	-0.0059	0.6235	-5.6000
H	0.3749	1.2461	-6.4152
H	0.3500	1.0454	-4.6587
H	-1.0973	0.6875	-5.6097
C	-0.7599	0.8587	-0.2414
O	-0.3418	-0.1380	0.5251
N	1.4336	0.7632	-1.1737
C	2.2121	1.4220	-2.0897
C	1.4490	2.3649	-2.7057
H	1.6684	3.0650	-3.4953
C	-2.0372	1.4210	-0.0363
H	-2.3078	2.2846	-0.6280
C	-2.9060	0.9271	0.8979
H	-2.5805	0.0608	1.4666
N	2.6845	0.2627	1.4135
C	3.9819	0.2211	1.2160
S	4.8903	1.1502	2.3580
C	3.3983	1.6059	3.1621
C	3.1834	2.3761	4.2999
H	4.0094	2.8257	4.8391
C	1.8775	2.5485	4.7400
H	1.7214	3.1418	5.6319
C	0.7696	1.9844	4.0768
C	1.0032	1.2264	2.9385
H	0.1984	0.7740	2.3727
C	2.3077	1.0364	2.4983
C	4.4435	-0.6159	0.1186
C	3.3925	-1.3189	-0.5310
C	3.7126	-2.1322	-1.6228
H	2.9250	-2.6568	-2.1543
C	5.0333	-2.2673	-2.0328
H	5.2743	-2.9067	-2.8758
C	6.0549	-1.5874	-1.3684
H	7.0819	-1.7013	-1.6973
C	5.7646	-0.7584	-0.2899
H	6.5631	-0.2283	0.2197
C	-0.6814	2.1900	4.5297
C	-0.7694	2.8436	5.9119
H	-1.8175	2.9310	6.2081
H	-0.3477	3.8526	5.9157
H	-0.2568	2.2494	6.6744
C	-1.3925	3.0911	3.5030
H	-2.4402	3.2300	3.7859
H	-1.3770	2.6485	2.5044
H	-0.9191	4.0757	3.4507
C	-1.4095	0.8336	4.5883
H	-2.4404	0.9824	4.9226
H	-0.9198	0.1497	5.2875
H	-1.4521	0.3475	3.6109
C	0.2106	1.3101	-1.1966
N	0.1784	2.2819	-2.1566
H	3.2447	1.1576	-2.2532
C	-0.9760	2.9586	-2.6632
C	-2.0152	2.2111	-3.2126
C	-1.0424	4.3439	-2.6051
C	-3.1409	2.8653	-3.6925
H	-1.9413	1.1297	-3.2418
C	-2.1691	4.9916	-3.1012
H	-0.2258	4.9031	-2.1617
C	-3.2186	4.2549	-3.6382
H	-3.9581	2.2893	-4.1128
H	-2.2291	6.0734	-3.0562
H	-4.0991	4.7630	-4.0163
C	-4.2182	1.4554	1.2196
C	-4.9196	0.9037	2.3036
C	-4.8283	2.4989	0.5020
C	-6.1721	1.3773	2.6650
H	-4.4658	0.0922	2.8657
C	-6.0798	2.9702	0.8641
H	-4.3260	2.9361	-0.3552
C	-6.7583	2.4150	1.9476
H	-6.6942	0.9349	3.5073
H	-6.5350	3.7755	0.2964
H	-7.7387	2.7871	2.2260

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Ir–1–MECP(^{1}MLCT–^{3}MLCT)

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Ir	1.7431	-1.0277	0.1737
N	0.4871	-2.3023	-0.8124
C	-0.0176	-3.2624	-0.0056
S	-1.2872	-4.2036	-0.7101
C	-1.0665	-3.3366	-2.2029
C	-1.7261	-3.5154	-3.4126
H	-2.5199	-4.2464	-3.5176
C	-1.3334	-2.7375	-4.4888
H	-1.8434	-2.8882	-5.4300
C	-0.2975	-1.7842	-4.4095
C	0.3376	-1.6004	-3.1899
H	1.1383	-0.8823	-3.0715
C	-0.0485	-2.3671	-2.0784
C	0.5217	-3.3639	1.2829
C	1.5440	-2.3480	1.5390
C	2.1644	-2.4058	2.8297
H	2.9366	-1.6872	3.0683
C	1.7925	-3.3430	3.7344
H	2.2703	-3.3787	4.7059
C	0.7669	-4.3145	3.4534
H	0.5081	-5.0398	4.2123
C	0.1373	-4.3229	2.2501
H	-0.6322	-5.0527	2.0275
C	0.1390	-0.9684	-5.6301
C	1.6557	-1.1333	-5.8292
H	1.9828	-0.5605	-6.7016
H	1.9150	-2.1831	-5.9960
H	2.2227	-0.7750	-4.9660
C	-0.5666	-1.4129	-6.9180
H	-0.1985	-0.8170	-7.7564
H	-1.6492	-1.2626	-6.8657
H	-0.3700	-2.4625	-7.1546
C	-0.1954	0.5133	-5.3855
H	0.1283	1.1190	-6.2371
H	0.3016	0.8967	-4.4927
H	-1.2753	0.6484	-5.2652
C	-0.7069	0.7423	-0.1178
O	-0.3360	-0.1766	0.7408
N	1.5150	0.7353	-1.2134
C	2.1888	1.4053	-2.1831
C	1.4431	2.4807	-2.5667
H	1.6312	3.2953	-3.2452
C	-2.0131	1.1638	-0.2039
H	-2.2764	1.9388	-0.9037
C	-3.0149	0.6114	0.5998

H	-2.7048	-0.1251	1.3317
N	2.8585	0.2518	1.2956
C	4.1546	0.2388	1.0736
S	5.0418	1.3363	2.0885
C	3.5391	1.8094	2.8777
C	3.2869	2.7081	3.9107
H	4.0906	3.2609	4.3862
C	1.9676	2.8846	4.3263
H	1.7834	3.5827	5.1349
C	0.8854	2.1926	3.7441
C	1.1597	1.2879	2.7280
H	0.3807	0.7224	2.2212
C	2.4730	1.1129	2.3027
C	4.6178	-0.7262	0.0990
C	3.5664	-1.5598	-0.3803
C	3.9009	-2.5436	-1.3230
H	3.1264	-3.1974	-1.7138
C	5.2029	-2.6585	-1.7945
H	5.4412	-3.4105	-2.5420
C	6.2159	-1.8158	-1.3184
H	7.2279	-1.9205	-1.6923
C	5.9251	-0.8492	-0.3708
H	6.7059	-0.1887	-0.0072
C	-0.5831	2.4143	4.1308
C	-0.7220	3.1909	5.4434
H	-1.7797	3.2959	5.6977
H	-0.3063	4.2000	5.3725
H	-0.2289	2.6717	6.2709
C	-1.2670	3.2069	2.9981
H	-2.3222	3.3704	3.2363
H	-1.2220	2.6630	2.0509
H	-0.7926	4.1833	2.8606
C	-1.3125	1.0632	4.2866
H	-2.3501	1.2405	4.5838
H	-0.8401	0.4445	5.0555
H	-1.3356	0.4982	3.3513
C	0.3445	1.3242	-1.0239
N	0.2774	2.4147	-1.8262
H	3.1754	1.1016	-2.5002
C	-0.7884	3.3656	-1.9396
C	-1.6807	3.2701	-3.0013
C	-0.9275	4.3444	-0.9658
C	-2.7384	4.1695	-3.0778
H	-1.5513	2.4897	-3.7426
C	-1.9927	5.2312	-1.0448
H	-0.2255	4.3838	-0.1402
C	-2.8977	5.1449	-2.0977
H	-3.4432	4.1018	-3.8997
H	-2.1188	5.9886	-0.2791

(B) Optimized geometries at the (TD)wB97X-D3/6-31G(d,p)/LANL2DZ level of the theory

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Rh–1

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Rh	1.70489	-0.77386	0.24910
N	0.61326	-2.11822	-0.93897
C	0.12018	-3.07611	-0.18502
S	-1.13851	-4.00371	-0.92582
C	-0.96024	-3.05430	-2.37469
C	-1.62298	-3.19596	-3.59229
H	-2.40618	-3.93542	-3.72326
C	-1.23123	-2.39059	-4.64367
H	-1.72839	-2.51877	-5.60004
C	-0.18344	-1.45023	-4.52913
C	0.43503	-1.29158	-3.29183
H	1.25446	-0.59597	-3.15397
C	0.04294	-2.09191	-2.20684
C	0.65685	-3.27504	1.14673
C	1.59485	-2.29905	1.53271
C	2.21628	-2.46230	2.77092
H	2.95791	-1.74888	3.11644
C	1.89657	-3.54682	3.58591
H	2.39629	-3.65696	4.54422
C	0.94962	-4.49368	3.19234
H	0.71185	-5.33248	3.83815
C	0.32549	-4.36084	1.96279
H	-0.40157	-5.10069	1.63511
C	0.28678	-0.72431	-5.79969
C	0.89338	-1.77484	-6.75176
H	1.25736	-1.29428	-7.66577
H	0.15797	-2.53092	-7.04187
H	1.73528	-2.29048	-6.27946
C	-0.89255	-0.02606	-6.50215
H	-0.54558	0.44707	-7.42619
H	-1.32688	0.75595	-5.87149
H	-1.68877	-0.72412	-6.77428
C	1.35355	0.33336	-5.50076
H	1.66025	0.82194	-6.43025
H	2.25078	-0.10054	-5.04744
H	0.96782	1.10625	-4.82897
C	-0.80846	0.90927	-0.22193
O	-0.43064	0.03136	0.56907
N	1.46194	0.99072	-1.07885
C	2.19651	1.68945	-1.98196
C	1.36173	2.53275	-2.67430
H	1.54232	3.22365	-3.48388
C	-2.14383	1.47919	-0.15215
H	-2.39299	2.30833	-0.80017
C	-3.02972	0.99841	0.74422
H	-2.69586	0.18575	1.38848
N	2.78198	0.31722	1.58609
C	4.08357	0.21969	1.46599
S	4.96565	1.06711	2.69588
C	3.45171	1.55517	3.43439
C	3.19954	2.28727	4.59231
H	4.00969	2.69008	5.19087
C	1.87759	2.48014	4.97833
H	1.69421	3.04339	5.88637
C	0.79049	1.96306	4.24537
C	1.06389	1.24364	3.08933
H	0.27256	0.80636	2.49165
C	2.38183	1.04745	2.69140
C	4.56966	-0.63704	0.39363
C	3.52629	-1.29659	-0.29449
C	3.85748	-2.16399	-1.33384
H	3.07700	-2.69278	-1.87411
C	5.19368	-2.35910	-1.67840
H	5.44192	-3.04080	-2.48728
C	6.21717	-1.70002	-0.99489
H	7.25246	-1.86750	-1.27276
C	5.90839	-0.83614	0.04658
H	6.70171	-0.32245	0.58388
C	-0.67864	2.15975	4.65102
C	-0.81693	2.86934	6.00333
H	-1.87588	2.97566	6.25728
H	-0.38446	3.87480	5.98251
H	-0.33910	2.30371	6.80987
C	-1.38370	3.00623	3.57335
H	-2.43961	3.14862	3.82861
H	-1.34325	2.52272	2.59185
H	-0.91945	3.99325	3.48191
C	-1.37525	0.78785	4.74729
H	-2.42027	0.91994	5.04864
H	-0.88688	0.14568	5.48641
H	-1.36972	0.25610	3.79017
C	0.20430	1.39774	-1.18913
N	0.10060	2.33235	-2.17883
H	3.25871	1.53300	-2.09570
C	-1.10427	2.84695	-2.76781
C	-1.95363	1.96032	-3.42654
C	-1.40551	4.19895	-2.65670
C	-3.13747	2.44337	-3.97320

H	-1.68927	0.90794	-3.49727
C	-2.59121	4.67163	-3.21322
H	-0.73173	4.86261	-2.12411
C	-3.45620	3.79644	-3.86591
H	-3.80768	1.76227	-4.48778
H	-2.84006	5.72452	-3.12974
H	-4.38024	4.17093	-4.29488
C	-4.39186	1.47535	0.95052
C	-5.07141	1.07436	2.10882
C	-5.04040	2.32188	0.03746
C	-6.36102	1.52406	2.36378
H	-4.57534	0.41237	2.81437
C	-6.33068	2.76242	0.28957
H	-4.54383	2.61872	-0.88276
C	-6.99098	2.36854	1.45404
H	-6.87601	1.21147	3.26648
H	-6.83062	3.41088	-0.42308
H	-8.00193	2.71481	1.64635

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Rh–1–^{1}MLCT

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Rh	-1.01711	-1.24562	0.25285
N	-2.16757	-0.19185	1.64967
C	-2.08654	-0.70647	2.85227
S	-2.81857	0.23815	4.09715
C	-3.30025	1.41293	2.89974
C	-4.06002	2.57035	3.04664
H	-4.40980	2.89400	4.02113
C	-4.38429	3.29165	1.90693
H	-4.99206	4.18101	2.02583
C	-3.97146	2.89607	0.61857
C	-3.18558	1.75594	0.49864
H	-2.83899	1.40628	-0.46592
C	-2.85590	1.01586	1.63224
C	-1.43576	-2.00298	2.98446
C	-0.90255	-2.49967	1.76964
C	-0.28237	-3.75237	1.77428
H	0.14090	-4.15879	0.86174
C	-0.20976	-4.49111	2.95104
H	0.26382	-5.46799	2.94395
C	-0.73984	-3.98822	4.13968
H	-0.67901	-4.57421	5.05077
C	-1.35320	-2.73876	4.16245
H	-1.76742	-2.35310	5.09000
C	-4.36246	3.66384	-0.65295
C	-5.00722	2.69099	-1.65989
H	-5.31714	3.23312	-2.55903
H	-5.89313	2.21109	-1.23218
H	-4.31246	1.90579	-1.97399
C	-5.36182	4.79142	-0.36556
H	-5.63063	5.29007	-1.30125
H	-4.94343	5.55367	0.29947
H	-6.28605	4.40989	0.08078
C	-3.09287	4.27053	-1.27668
H	-3.34110	4.82995	-2.18463
H	-2.37533	3.49127	-1.55221
H	-2.60141	4.95760	-0.58020
C	0.85076	1.01990	-0.04279
O	0.46551	0.10166	0.81277
N	-0.95555	0.23037	-1.39228
C	-1.56508	0.52886	-2.58382
C	-0.98396	1.64055	-3.11425
H	-1.18663	2.20305	-4.01235
C	2.05444	1.74703	0.21014
H	2.41818	2.40162	-0.57413
C	2.74202	1.59286	1.36843
H	2.31184	0.93424	2.11980
N	0.07459	-2.44495	-1.03041
C	-0.67714	-3.11189	-1.87024
S	0.19120	-4.08233	-3.00079
C	1.68960	-3.54504	-2.28368
C	2.99632	-3.89047	-2.61471
H	3.20984	-4.58106	-3.42355
C	4.02299	-3.32876	-1.87370
H	5.03984	-3.60048	-2.13171
C	3.79341	-2.42967	-0.81125
C	2.47994	-2.09380	-0.49768
H	2.23657	-1.39511	0.29485
C	1.43577	-2.65483	-1.23183
C	-2.12063	-2.95249	-1.76185
C	-2.53350	-2.07267	-0.73740
C	-3.89075	-1.80640	-0.57751
H	-4.23098	-1.11059	0.18207
C	-4.82117	-2.43902	-1.40138
H	-5.87967	-2.23925	-1.26457
C	-4.40847	-3.32344	-2.39766
H	-5.14268	-3.80638	-3.03420
C	-3.05528	-3.58339	-2.58243
H	-2.73479	-4.26826	-3.36320
C	4.95437	-1.77563	-0.05152
C	6.25610	-2.57934	-0.18797
H	7.03125	-2.12413	0.43503
H	6.63771	-2.58455	-1.21367
H	6.12899	-3.61658	0.13991
C	5.16738	-0.36875	-0.64237
H	5.95608	0.16236	-0.09928
H	4.25284	0.22621	-0.57377
H	5.45545	-0.42996	-1.69725
C	4.62100	-1.66520	1.44597
H	5.46222	-1.21250	1.97917
H	4.42695	-2.65129	1.88076
H	3.75066	-1.03091	1.63054
C	0.00717	1.14156	-1.19409
N	0.00739	2.03291	-2.23379
H	-2.37824	-0.06568	-2.97536
C	0.76348	3.24063	-2.34335
C	0.59643	4.23313	-1.38073
C	1.64744	3.40582	-3.40403
C	1.34157	5.40165	-1.47424
H	-0.10047	4.07251	-0.56406
C	2.38052	4.58610	-3.49593
H	1.76750	2.61277	-4.13612
C	2.23290	5.57881	-2.53098
H	1.22183	6.17588	-0.72335
H	3.07534	4.72491	-4.31789
H	2.81166	6.49422	-2.60180
C	4.03622	2.18324	1.69729
C	4.66962	1.78513	2.88272
C	4.69578	3.10194	0.86605
C	5.92561	2.27182	3.22406
H	4.16657	1.07728	3.53724
C	5.94883	3.59029	1.20848
H	4.22589	3.44267	-0.05290
C	6.57175	3.17504	2.38543
H	6.39875	1.94519	4.14517
H	6.44654	4.30031	0.55475
H	7.55312	3.55764	2.64794

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Rh–1–^{3}LC

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Rh	0.79581	1.54502	0.54221
N	2.19882	1.27487	2.04125
C	2.01664	2.04429	3.08991
S	3.20557	1.85503	4.33514
C	4.00047	0.62913	3.37403
C	5.12678	-0.13971	3.65372
H	5.67272	-0.01902	4.58345
C	5.53371	-1.08263	2.71766
H	6.40615	-1.68333	2.94838
C	4.84878	-1.27919	1.50340
C	3.73727	-0.48871	1.23851
H	3.17400	-0.59286	0.32019
C	3.31210	0.45418	2.16810
C	0.86520	2.92758	3.08029

C	0.11045	2.84724	1.88984
C	-1.03401	3.63663	1.79322
H	-1.64107	3.61265	0.89299
C	-1.41203	4.46489	2.84942
H	-2.30962	5.07039	2.75799
C	-0.65660	4.52952	4.02021
H	-0.96291	5.17937	4.83312
C	0.48933	3.75708	4.13921
H	1.08101	3.79296	5.05074
C	5.25318	-2.33590	0.46448
C	5.53973	-1.64513	-0.88244
H	5.85163	-2.38434	-1.62796
H	6.33843	-0.90406	-0.78197
H	4.65314	-1.13526	-1.27398
C	6.50193	-3.11972	0.88650
H	6.74822	-3.86071	0.12011
H	6.34766	-3.65974	1.82628
H	7.37206	-2.46556	1.00198
C	4.08968	-3.33145	0.28382
H	4.35990	-4.10116	-0.44721
H	3.18322	-2.83260	-0.07769
H	3.84522	-3.82824	1.22791
C	-0.23512	-1.31260	0.14118
O	-0.32874	-0.43916	1.05201
N	1.42105	0.03285	-1.01325
C	2.00809	0.11671	-2.24341
C	1.48534	-0.85574	-3.05063
H	1.65865	-1.10749	-4.08567
C	-0.82575	-2.59245	0.26080
H	-0.59115	-3.32167	-0.50683
C	-1.71573	-2.96953	1.33400
H	-1.66129	-2.40997	2.26233
N	-0.58144	2.08420	-0.93889
C	-0.04091	2.88075	-1.83056
S	-0.97961	3.09506	-3.27040
C	-2.20524	2.04703	-2.60521
C	-3.42104	1.65060	-3.16119
H	-3.71364	1.96714	-4.15692
C	-4.25498	0.85086	-2.40014
H	-5.20220	0.54232	-2.83167
C	-3.93218	0.45250	-1.08364
C	-2.70460	0.83697	-0.55642
H	-2.40281	0.56448	0.44736
C	-1.83287	1.61844	-1.32567
C	1.26626	3.43926	-1.54798
C	1.83566	2.97656	-0.34238
C	3.10255	3.44474	-0.00182
H	3.58421	3.10692	0.90925
C	3.77028	4.33892	-0.83650
H	4.75779	4.69201	-0.55346
C	3.19496	4.78722	-2.02652
H	3.72894	5.48359	-2.66422
C	1.93571	4.33489	-2.38717
H	1.47493	4.67593	-3.31157
C	-4.93720	-0.39529	-0.29156
C	-6.31821	0.28612	-0.29374
H	-7.02421	-0.30401	0.29928
H	-6.73778	0.37943	-1.29946
H	-6.26310	1.28768	0.14349
C	-5.04489	-1.78175	-0.95317
H	-5.71779	-2.42926	-0.38092
H	-4.06725	-2.27252	-0.99579
H	-5.43720	-1.71239	-1.97363
C	-4.50097	-0.57789	1.16653
H	-5.23304	-1.19590	1.69519
H	-4.43049	0.38069	1.69036
H	-3.53433	-1.08364	1.24044
C	0.56384	-0.97197	-1.05523
N	0.56112	-1.54181	-2.29552
H	2.74724	0.86989	-2.47215
C	-0.37625	-2.49095	-2.82865
C	0.05562	-3.77104	-3.16265
C	-1.70020	-2.09853	-3.01867
C	-0.86024	-4.67844	-3.68992
H	1.09348	-4.04882	-3.00493
C	-2.60553	-3.01506	-3.54321
H	-2.01518	-1.09053	-2.76182
C	-2.18845	-4.30199	-3.87746
H	-0.53403	-5.67880	-3.95545
H	-3.63834	-2.71820	-3.69429
H	-2.89887	-5.01140	-4.29049
C	-2.72823	-3.92756	1.15314
C	-3.68335	-4.15338	2.19336
C	-2.89409	-4.66046	-0.06530
C	-4.72655	-5.03339	2.01884
H	-3.57669	-3.60681	3.12598
C	-3.94692	-5.53718	-0.22407
H	-2.19610	-4.52643	-0.88533
C	-4.87059	-5.73079	0.80826
H	-5.44324	-5.19023	2.81862
H	-4.05543	-6.08028	-1.15773
H	-5.69414	-6.42521	0.67665

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Rh–1–^{3}MLCT

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Rh	0.67712	1.69271	0.55251
N	2.11089	1.29395	1.99298
C	2.04542	2.06764	3.05045
S	3.23924	1.74039	4.25410
C	3.85316	0.43120	3.27119
C	4.87952	-0.47665	3.52302
H	5.46577	-0.42482	4.43423
C	5.12310	-1.47131	2.58495
H	5.91351	-2.18281	2.79485
C	4.37636	-1.58856	1.39524
C	3.37683	-0.65699	1.15314
H	2.77432	-0.69393	0.25641
C	3.11361	0.34002	2.08625
C	0.95974	3.03511	3.08958
C	0.13498	3.00149	1.93832
C	-0.97898	3.84218	1.88832
H	-1.63100	3.83830	1.02106
C	-1.26567	4.68326	2.96106
H	-2.14021	5.32538	2.92011
C	-0.44291	4.70738	4.08684
H	-0.67673	5.36929	4.91408
C	0.67440	3.87973	4.15741
H	1.30342	3.88771	5.04337
C	4.58237	-2.71785	0.37416
C	4.83105	-2.11553	-1.02162
H	4.98890	-2.91586	-1.75250
H	5.72090	-1.47828	-1.02430
H	3.98466	-1.51392	-1.36975
C	5.77233	-3.61494	0.73627
H	5.89363	-4.39241	-0.02383
H	5.62831	-4.11982	1.69688
H	6.70913	-3.04951	0.77787
C	3.30569	-3.58202	0.33331
H	3.42997	-4.40146	-0.38359
H	2.42724	-2.99936	0.03349
H	3.09163	-4.02033	1.31275
C	-0.17068	-1.08837	-0.02553
O	-0.13617	-0.17600	0.94175
N	1.33096	0.39797	-1.14018
C	1.98040	0.52134	-2.33975
C	1.65029	-0.54016	-3.12808
H	1.93714	-0.81295	-4.13171
C	-0.91577	-2.27035	0.10758
H	-0.91078	-2.94538	-0.73939
C	-1.65492	-2.58621	1.22280
H	-1.59793	-1.91527	2.07755
N	-0.71126	2.36395	-0.84767
C	-0.21697	3.29472	-1.62964
S	-1.26478	3.79915	-2.90236
C	-2.45518	2.65056	-2.35301

C	-3.70972	2.37230	-2.88788
H	-4.08349	2.90370	-3.75662
C	-4.46779	1.38641	-2.28164
H	-5.44128	1.16499	-2.70346
C	-4.02569	0.66967	-1.14884
C	-2.77259	0.97131	-0.62061
H	-2.37430	0.45250	0.24383
C	-1.98845	1.95800	-1.22812
C	1.15086	3.73226	-1.40579
C	1.81408	3.06851	-0.35777
C	3.16077	3.31981	-0.13372
H	3.70246	2.78773	0.64069
C	3.82534	4.25740	-0.92452
H	4.87709	4.45723	-0.74365
C	3.15843	4.93637	-1.94373
H	3.68894	5.66126	-2.55187
C	1.81797	4.67204	-2.19231
H	1.30086	5.18201	-3.00122
C	-4.87795	-0.47336	-0.57474
C	-6.37895	-0.24573	-0.82096
H	-6.95091	-1.02774	-0.31318
H	-6.64566	-0.29950	-1.88084
H	-6.71230	0.72085	-0.42944
C	-4.44629	-1.77388	-1.28119
H	-5.00808	-2.62961	-0.89273
H	-3.38286	-1.97250	-1.11788
H	-4.62334	-1.70780	-2.36101
C	-4.66674	-0.62078	0.93970
H	-5.28734	-1.43755	1.32008
H	-4.94354	0.29628	1.46986
H	-3.63373	-0.87129	1.19054
C	0.60348	-0.72185	-1.18581
N	0.77352	-1.32415	-2.39898
H	2.63768	1.35076	-2.55375
C	0.08038	-2.47104	-2.90771
C	0.73016	-3.69922	-2.95756
C	-1.24117	-2.33287	-3.32610
C	0.03774	-4.81314	-3.42402
H	1.75809	-3.77632	-2.61644
C	-1.92685	-3.45320	-3.78247
H	-1.72781	-1.36324	-3.27027
C	-1.28868	-4.69144	-3.83083
H	0.53363	-5.77760	-3.46214
H	-2.96065	-3.35896	-4.09934
H	-1.82628	-5.56392	-4.18863
C	-2.55657	-3.72026	1.34062
C	-3.28111	-3.88545	2.53339
C	-2.78116	-4.64039	0.29865
C	-4.19366	-4.92116	2.68350
H	-3.12275	-3.18135	3.34668
C	-3.69193	-5.67568	0.45167
H	-2.25039	-4.54362	-0.64514
C	-4.40417	-5.82196	1.64230
H	-4.74261	-5.02546	3.61455
H	-3.85249	-6.37514	-0.36375
H	-5.11812	-6.63190	1.75622

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Ir–1

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Ir	1.60419	-0.77730	0.16191
N	0.45234	-2.09695	-0.95426
C	-0.06437	-3.05496	-0.20947
S	-1.26827	-4.01008	-1.00413
C	-1.01253	-3.09139	-2.46511
C	-1.58040	-3.27511	-3.72039
H	-2.34654	-4.02557	-3.88561
C	-1.11246	-2.50479	-4.77432
H	-1.53921	-2.67436	-5.75567
C	-0.08262	-1.55902	-4.61413
C	0.42971	-1.34736	-3.33323
H	1.23545	-0.64338	-3.16069
C	-0.03247	-2.11084	-2.25812
C	0.44399	-3.23545	1.13189
C	1.42106	-2.27777	1.48489
C	2.03837	-2.44812	2.72904
H	2.81066	-1.75808	3.05610
C	1.67798	-3.49682	3.57002
H	2.17615	-3.60450	4.52958
C	0.69094	-4.41607	3.20391
H	0.42299	-5.22822	3.87149
C	0.07107	-4.28902	1.97319
H	-0.68435	-5.00799	1.66340
C	0.51799	-0.80818	-5.81540
C	2.04991	-0.97208	-5.79910
H	2.49147	-0.47457	-6.66846
H	2.33000	-2.02936	-5.83503
H	2.50381	-0.53589	-4.90383
C	-0.00345	-1.34616	-7.15577
H	0.48749	-0.81612	-7.97732
H	-1.08117	-1.19156	-7.27183
H	0.20910	-2.41284	-7.27858
C	0.16301	0.68502	-5.72783
H	0.62391	1.23601	-6.55439
H	0.52259	1.12117	-4.79132
H	-0.91944	0.83934	-5.78449
C	-0.84610	0.97059	-0.23632
O	-0.45300	0.08652	0.54895
N	1.38092	0.93389	-1.17235
C	2.13113	1.60081	-2.08800
C	1.32259	2.49609	-2.74642
H	1.51837	3.18346	-3.55544
C	-2.16378	1.56176	-0.11348
H	-2.42965	2.38659	-0.76059
C	-3.01164	1.09303	0.82744
H	-2.65094	0.27762	1.45343
N	2.76564	0.30403	1.43879
C	4.06493	0.17926	1.27864
S	5.00061	1.00673	2.48102
C	3.52174	1.51473	3.27480
C	3.32542	2.23240	4.45200
H	4.16472	2.61445	5.02348
C	2.02291	2.43390	4.89626
H	1.88383	2.98165	5.82147
C	0.90246	1.93925	4.20047
C	1.12079	1.23913	3.02087
H	0.29993	0.81738	2.45382
C	2.41808	1.03278	2.56636
C	4.49832	-0.69088	0.20044
C	3.41189	-1.33640	-0.44162
C	3.71406	-2.22076	-1.48374
H	2.91342	-2.74473	-1.99981
C	5.03317	-2.43928	-1.86741
H	5.24583	-3.13210	-2.67716
C	6.09045	-1.78991	-1.22326
H	7.11388	-1.97596	-1.53155
C	5.82470	-0.91332	-0.18348
H	6.64078	-0.40663	0.32597
C	-0.54678	2.13025	4.67431
C	-0.62369	2.81789	6.04262
H	-1.67003	2.92083	6.34572
H	-0.19037	3.82291	6.01911
H	-0.11119	2.23802	6.81707
C	-1.29995	2.99330	3.64363
H	-2.34506	3.12529	3.94492
H	-1.29721	2.52891	2.65207
H	-0.84424	3.98422	3.55162
C	-1.23718	0.75568	4.78050
H	-2.26586	0.87938	5.13662
H	-0.71086	0.10129	5.48182
H	-1.27769	0.23993	3.81536
C	0.14398	1.41618	-1.23829
N	0.06727	2.36375	-2.21515
H	3.17874	1.38312	-2.23212
C	-1.12715	2.95601	-2.75142
C	-2.06000	2.12600	-3.37038

C	-1.33516	4.32426	-2.62848
C	-3.23263	2.68487	-3.86513
H	-1.86563	1.05997	-3.45444
C	-2.51059	4.87303	-3.13477
H	-0.59705	4.94279	-2.12780
C	-3.45752	4.05582	-3.74705
H	-3.96837	2.04967	-4.34756
H	-2.68747	5.93960	-3.04236
H	-4.37288	4.48853	-4.13813
C	-4.35785	1.57082	1.10767
C	-4.98707	1.12268	2.27752
C	-5.04265	2.45603	0.25962
C	-6.26397	1.55957	2.60604
H	-4.46118	0.43268	2.93272
C	-6.32035	2.88445	0.58539
H	-4.58427	2.79435	-0.66597
C	-6.93094	2.44022	1.75925
H	-6.73992	1.20911	3.51613
H	-6.85001	3.56245	-0.07638
H	-7.93256	2.77716	2.00842

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Ir–1–^{1}MLCT

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Ir	1.56117	-0.99178	0.15372
N	0.51635	-2.35867	-0.99838
C	0.01839	-3.34035	-0.27917
S	-1.07783	-4.36647	-1.12189
C	-0.83060	-3.41835	-2.56308
C	-1.35856	-3.61449	-3.83510
H	-2.06459	-4.41369	-4.03410
C	-0.94172	-2.77225	-4.85253
H	-1.34400	-2.93905	-5.84464
C	-0.00675	-1.73882	-4.64311
C	0.48073	-1.53599	-3.35434
H	1.19860	-0.75371	-3.14205
C	0.06970	-2.37333	-2.31467
C	0.45631	-3.46387	1.09979
C	1.34102	-2.43019	1.49946
C	1.85732	-2.49049	2.80312
H	2.53824	-1.72164	3.15404
C	1.50516	-3.52966	3.65504
H	1.91868	-3.56798	4.65796
C	0.62090	-4.52832	3.23738
H	0.35024	-5.33095	3.91541
C	0.09041	-4.49990	1.95286
H	-0.59292	-5.27981	1.62714
C	0.48143	-0.84441	-5.79411
C	2.02006	-0.77875	-5.78071
H	2.37553	-0.16922	-6.61742
H	2.45815	-1.77708	-5.87893
H	2.40585	-0.32732	-4.86145
C	0.03713	-1.36974	-7.16677
H	0.45288	-0.73170	-7.95197
H	-1.05126	-1.35209	-7.28310
H	0.38969	-2.39018	-7.34880
C	-0.09255	0.56997	-5.60313
H	0.24186	1.23235	-6.40845
H	0.23635	1.00262	-4.65405
H	-1.18724	0.55684	-5.61155
C	-0.75527	0.80057	-0.25722
O	-0.39055	-0.24668	0.44440
N	1.43741	0.70522	-1.19797
C	2.21015	1.37803	-2.11178
C	1.45092	2.34649	-2.69490
H	1.67168	3.06495	-3.46889
C	-2.02395	1.41159	0.00342
H	-2.23746	2.35634	-0.48352
C	-2.91207	0.86359	0.86572
H	-2.64162	-0.08592	1.32252
N	2.62754	0.23040	1.39866
C	3.92659	0.21910	1.20707
S	4.80706	1.21438	2.30787
C	3.30652	1.66923	3.08583
C	3.07712	2.49792	4.18196
H	3.89479	2.99261	4.69518
C	1.76757	2.67225	4.60801
H	1.59706	3.31601	5.46327
C	0.66908	2.04933	3.97748
C	0.91875	1.22571	2.88687
H	0.12187	0.71980	2.35300
C	2.22946	1.04190	2.45208
C	4.42051	-0.63837	0.13490
C	3.39236	-1.37408	-0.51138
C	3.74602	-2.21586	-1.57165
H	2.97925	-2.77734	-2.09777
C	5.07706	-2.33782	-1.95744
H	5.34204	-2.99998	-2.77609
C	6.07675	-1.62062	-1.29775
H	7.11169	-1.72678	-1.60565
C	5.75312	-0.76773	-0.24662
H	6.53562	-0.21237	0.26315
C	-0.78438	2.29109	4.41358
C	-0.87083	2.92832	5.80696
H	-1.92076	3.03025	6.09644
H	-0.43377	3.93150	5.83029
H	-0.37376	2.31498	6.56609
C	-1.43984	3.23650	3.38758
H	-2.48788	3.41618	3.64973
H	-1.41974	2.80465	2.38285
H	-0.92278	4.20105	3.35742
C	-1.56282	0.96242	4.44506
H	-2.59586	1.14881	4.75544
H	-1.11493	0.25460	5.15001
H	-1.60604	0.48456	3.46258
C	0.21755	1.26748	-1.19549
N	0.18788	2.26823	-2.13033
H	3.24021	1.11208	-2.29481
C	-0.96480	2.97916	-2.59097
C	-2.03479	2.26562	-3.12984
C	-1.00403	4.36524	-2.49015
C	-3.16324	2.95430	-3.55671
H	-1.98209	1.18251	-3.19238
C	-2.13352	5.04752	-2.93470
H	-0.16491	4.89637	-2.05173
C	-3.21304	4.34435	-3.46121
H	-4.00446	2.40592	-3.96825
H	-2.17267	6.12930	-2.85680
H	-4.09530	4.87862	-3.79914
C	-4.19011	1.43894	1.27959
C	-4.88178	0.83676	2.33988
C	-4.75111	2.57768	0.68042
C	-6.08376	1.35950	2.80147
H	-4.46211	-0.05097	2.80700
C	-5.95278	3.09816	1.14013
H	-4.25292	3.05331	-0.16050
C	-6.62253	2.49522	2.20458
H	-6.60062	0.87906	3.62675
H	-6.37426	3.97933	0.66550
H	-7.56156	2.90672	2.56173

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Ir–1–^{3}LC

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Ir	1.57211	-0.77159	0.17509
N	0.42380	-2.09362	-0.93796
C	-0.09107	-3.05526	-0.19718
S	-1.27725	-4.02178	-1.00354
C	-1.01757	-3.09977	-2.46198
C	-1.57346	-3.28750	-3.72206
H	-2.33028	-4.04573	-3.89455
C	-1.10624	-2.50926	-4.77039
H	-1.52352	-2.68122	-5.75542
C	-0.08961	-1.55098	-4.59985
C	0.41134	-1.33696	-3.31498
H	1.20446	-0.62142	-3.13302

C	-0.04984	-2.10929	-2.24606
C	0.40523	-3.22891	1.14947
C	1.37117	-2.26336	1.50940
C	1.97428	-2.42288	2.76156
H	2.73710	-1.72521	3.09462
C	1.61225	-3.47090	3.60283
H	2.10018	-3.57077	4.56850
C	0.63744	-4.39972	3.22870
H	0.36851	-5.21169	3.89613
C	0.03097	-4.28225	1.99032
H	-0.71507	-5.00834	1.67445
C	0.50667	-0.78564	-5.79401
C	2.04136	-0.91793	-5.76517
H	2.47946	-0.40948	-6.62996
H	2.34367	-1.96913	-5.80099
H	2.47860	-0.47398	-4.86558
C	0.00733	-1.33078	-7.13993
H	0.49706	-0.79141	-7.95613
H	-1.07169	-1.19389	-7.26611
H	0.23871	-2.39366	-7.26190
C	0.12044	0.69980	-5.70511
H	0.57277	1.26158	-6.52919
H	0.46762	1.14190	-4.76676
H	-0.96497	0.83102	-5.76659
C	-0.82018	0.97284	-0.21321
O	-0.41278	0.06876	0.60633
N	1.39115	0.93251	-1.16087
C	2.13853	1.59637	-2.09164
C	1.33547	2.50145	-2.73081
H	1.52616	3.19507	-3.53527
C	-2.11991	1.48799	-0.07384
H	-2.43643	2.28336	-0.73611
C	-3.01347	1.00862	0.93736
H	-2.62540	0.26970	1.63054
N	2.77219	0.29294	1.42953
C	4.06683	0.15080	1.24668
S	5.03381	0.98191	2.42110
C	3.57602	1.51929	3.23435
C	3.41011	2.25931	4.40222
H	4.26436	2.63995	4.95207
C	2.11804	2.48743	4.86447
H	2.00212	3.05306	5.78215
C	0.97989	1.99816	4.19472
C	1.16759	1.27446	3.02422
H	0.33214	0.85601	2.47549
C	2.45371	1.04188	2.55258
C	4.47225	-0.73106	0.16761
C	3.36832	-1.36346	-0.45672
C	3.64643	-2.25130	-1.50261
H	2.83380	-2.76570	-2.00927
C	4.95716	-2.48609	-1.90504
H	5.14989	-3.18184	-2.71727
C	6.03136	-1.84874	-1.27735
H	7.04796	-2.04614	-1.60079
C	5.79052	-0.96815	-0.23506
H	6.61940	-0.46951	0.26150
C	-0.45918	2.21333	4.68724
C	-0.50999	2.95930	6.02559
H	-1.55067	3.08427	6.33972
H	-0.06784	3.95828	5.95352
H	0.00846	2.40789	6.81665
C	-1.23023	3.03285	3.63435
H	-2.26853	3.18171	3.95076
H	-1.25005	2.52319	2.66500
H	-0.77307	4.01669	3.48888
C	-1.14649	0.84438	4.86241
H	-2.17296	0.98136	5.21998
H	-0.61273	0.22461	5.58911
H	-1.19116	0.28563	3.92183
C	0.16080	1.43111	-1.20272
N	0.08016	2.38230	-2.17415
H	3.18117	1.36631	-2.25065
C	-1.11994	2.98665	-2.67642
C	-2.05729	2.17496	-3.31469
C	-1.34100	4.34700	-2.49692
C	-3.24199	2.74145	-3.77099
H	-1.85574	1.11440	-3.44064
C	-2.52790	4.90544	-2.96570
H	-0.59999	4.95200	-1.98419
C	-3.47682	4.10510	-3.59671
H	-3.97845	2.11914	-4.26914
H	-2.71160	5.96633	-2.83036
H	-4.40013	4.54498	-3.96040
C	-4.34209	1.44629	1.07810
C	-5.11643	0.96223	2.17910
C	-4.97583	2.35268	0.16961
C	-6.42022	1.36119	2.36020
H	-4.64922	0.27299	2.87694
C	-6.28422	2.74018	0.36390
H	-4.43670	2.73075	-0.69363
C	-7.01554	2.25427	1.45517
H	-6.99050	0.98606	3.20382
H	-6.75313	3.42546	-0.33513
H	-8.04494	2.56603	1.60010

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Ir–1–^{3}MLCT

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Ir	1.56227	-1.00506	0.14949
N	0.52113	-2.38003	-0.99272
C	0.02646	-3.36179	-0.27133
S	-1.06919	-4.39005	-1.11134
C	-0.82607	-3.44304	-2.55446
C	-1.35541	-3.64082	-3.82559
H	-2.05998	-4.44166	-4.02316
C	-0.94233	-2.79796	-4.84440
H	-1.34581	-2.96632	-5.83574
C	-0.01008	-1.76217	-4.63664
C	0.47857	-1.55753	-3.34849
H	1.19515	-0.77346	-3.13812
C	0.07209	-2.39590	-2.30821
C	0.46545	-3.47875	1.10834
C	1.33402	-2.43203	1.50857
C	1.84591	-2.47909	2.81330
H	2.51033	-1.69684	3.16634
C	1.50910	-3.52412	3.66698
H	1.92009	-3.55271	4.67131
C	0.64492	-4.53804	3.24825
H	0.38588	-5.34468	3.92625
C	0.11615	-4.51954	1.96148
H	-0.55276	-5.31165	1.63490
C	0.47685	-0.86729	-5.78773
C	2.01593	-0.81013	-5.78080
H	2.37161	-0.19998	-6.61699
H	2.44773	-1.81072	-5.88391
H	2.40801	-0.36424	-4.86141
C	0.02341	-1.38665	-7.15956
H	0.43619	-0.74709	-7.94510
H	-1.06564	-1.36605	-7.26915
H	0.37232	-2.40734	-7.34704
C	-0.08873	0.54971	-5.59110
H	0.24778	1.21299	-6.39478
H	0.24407	0.97822	-4.64121
H	-1.18352	0.54171	-5.59871
C	-0.77416	0.78630	-0.26293
O	-0.38191	-0.26071	0.44496
N	1.42139	0.69344	-1.20139
C	2.20400	1.36646	-2.10550
C	1.45277	2.34377	-2.68560
H	1.67852	3.06757	-3.45309
C	-2.03504	1.37455	-0.01785
H	-2.27397	2.29389	-0.53932
C	-2.91880	0.83780	0.87976
H	-2.63181	-0.09543	1.35950
N	2.62729	0.22382	1.38867
C	3.92706	0.21172	1.19957

S	4.80467	1.20915	2.30038
C	3.30205	1.66843	3.07231
C	3.06947	2.50360	4.16265
H	3.88584	2.99871	4.67755
C	1.75779	2.68481	4.58017
H	1.58451	3.33384	5.43091
C	0.66065	2.06370	3.94590
C	0.91316	1.23234	2.86145
H	0.11880	0.72695	2.32199
C	2.22595	1.04062	2.43686
C	4.42224	-0.64474	0.12681
C	3.39474	-1.37452	-0.52793
C	3.74876	-2.20890	-1.59389
H	2.98178	-2.76280	-2.12796
C	5.08141	-2.33417	-1.97449
H	5.34742	-2.99161	-2.79667
C	6.08068	-1.62598	-1.30460
H	7.11679	-1.73462	-1.60806
C	5.75593	-0.77759	-0.24976
H	6.53866	-0.22853	0.26657
C	-0.79479	2.31352	4.37017
C	-0.88894	2.97802	5.75006
H	-1.94062	3.08845	6.02996
H	-0.44883	3.98021	5.75672
H	-0.39926	2.37836	6.52481
C	-1.44534	3.23883	3.32276
H	-2.49541	3.42106	3.57485
H	-1.41851	2.78909	2.32597
H	-0.92954	4.20362	3.27906
C	-1.57156	0.98463	4.42316
H	-2.60879	1.17569	4.71637
H	-1.13045	0.29410	5.14935
H	-1.60153	0.48460	3.45141
C	0.20857	1.26228	-1.19967
N	0.18785	2.26628	-2.12391
H	3.23271	1.09266	-2.28641
C	-0.95325	3.01410	-2.55896
C	-2.02180	2.34146	-3.14972
C	-0.97951	4.39224	-2.38006
C	-3.13761	3.06466	-3.55259
H	-1.97972	1.26270	-3.26736
C	-2.09711	5.10943	-2.79885
H	-0.14037	4.88945	-1.90364
C	-3.17522	4.44740	-3.37911
H	-3.97889	2.54890	-4.00415
H	-2.12778	6.18540	-2.66072
H	-4.04785	5.00907	-3.69723
C	-4.19282	1.40980	1.28626
C	-4.90660	0.78859	2.32456
C	-4.73936	2.56963	0.70867
C	-6.11184	1.30738	2.77918
H	-4.49904	-0.11219	2.77754
C	-5.94487	3.08554	1.16264
H	-4.22377	3.06790	-0.10823
C	-6.63569	2.46091	2.20124
H	-6.64397	0.81102	3.58533
H	-6.35263	3.98211	0.70482
H	-7.57734	2.87003	2.55443

III. Procedures for the Photochemical Measurements

Photophysical experiments have been performed in dichloromethane air-equilibrated solution in quartz cuvette (optical pathlength 1 cm). All absorption spectra were recorded with a UV/VIS spectrophotometer Perkin Elmer Lambda 650. All emission spectra and emission intensity decay of rhodium complexes were recorded with Perkin Elmer LS 50 spectrofluorometers equipped with Hamamatsu R928 photomultiplier.

Emission intensity decay of **IrS** at RT was performed using an Edinburgh FLS920 spectrofluorimeter equipped with a TCC900 card for data acquisition in time-correlated single-photon counting experiments (0.5 ns time resolution) with a D2 lamp and an LDH-P-C-405 pulsed diode laser.

Emission intensity decay of **IrS** at 77K was performed on a homemade time-resolved phosphorimeter equipped with an Avalanche PhotoDiode C12703 with a peak sensitivity wavelength of 800 nm of the emitted light and a 400 nm pulsed LED as the excitation source. The estimated experimental errors is 5%.

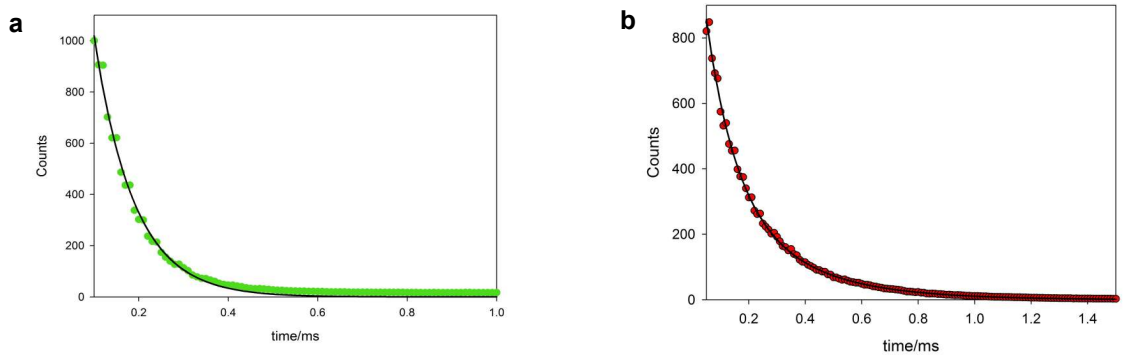


Figure S4. (a) Emission intensity decay at 77K of **RhS** (green dots) in CH_2Cl_2:CH_3Cl 1:1 (v/v) (setup parameters: λ_{exc} 350 nm, λ_{em} 515 nm, integration time 0.1 s, cycle time 20 ms, first delay time 0.05 ms, gate time 0.5 ms, delay time interval 0.01 ms). The black curve represents the mathematical fit of the experimental data; (b) emission intensity decay at 77K of **Rh-1** (red dots) in CH_2Cl_2:CH_3Cl 1:1 (v/v) (setup parameters: λ_{exc} 350 nm, λ_{em} 590 nm, integration time 0.1 s, cycle time 20 ms, first delay time 0.05 ms, gate time 0.5 ms, delay time interval 0.01 ms). The black curve represents the mathematical fit of the experimental data.

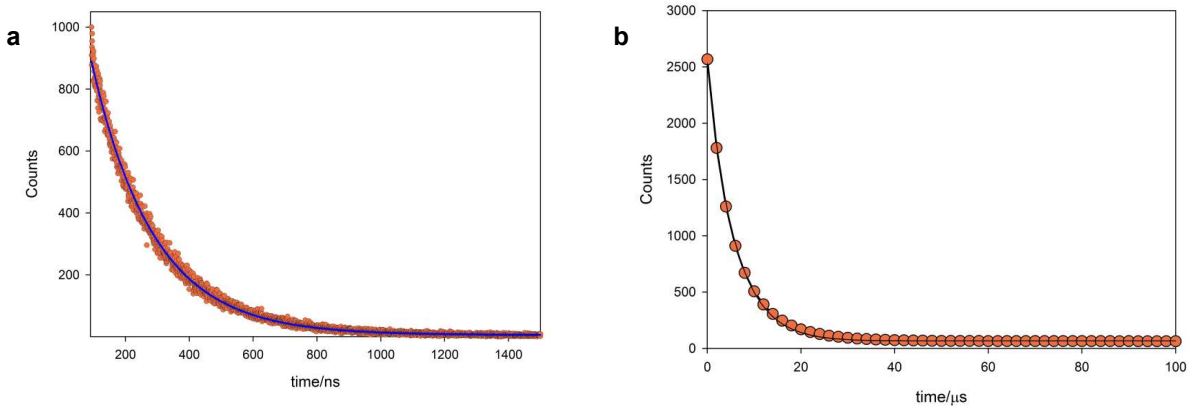


Figure S5. (a) Emission intensity decay of **IrS** at room temperature in CH_2Cl_2 (orange dots) and (b) at 77 K in CH_2Cl_2:CH_3Cl 1:1 (v/v) (orange dots) upon excitation at 400 nm. The blue and black curves represent the mathematical fit of the experimental data.

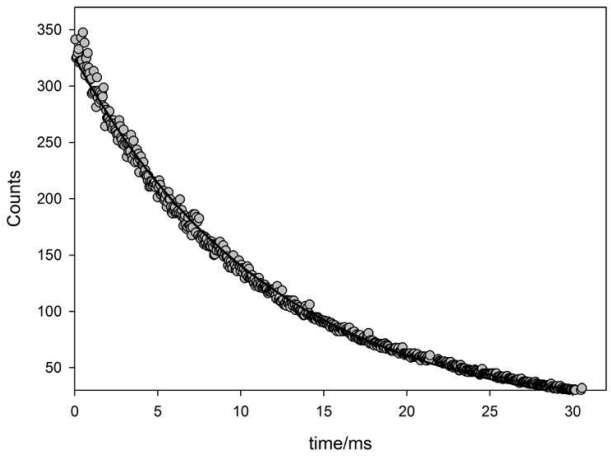


Figure S6. Emission intensity decay at 77K of **1** (grey dots) CH_2Cl_2:CH_3Cl 1:1 (v/v) (setup parameters: λ_{exc} 350 nm, λ_{em} 550 nm, integration time 0.1 s, cycle time 60 ms, first delay time 0.05 ms, gate time 20.00 ms, delay time interval 0.05 ms). The black curve represents the mathematical fit of the experimental data.

IV. Procedures for the Electrochemical Measurements

The electrochemical experiments were carried out in argon-purged dichloromethane (Hi-Dry anhydrous solvent) solution at 298 K. In the cyclic voltammetry (CV) the working electrode was a glassy carbon electrode (0.08 cm^2), the counter electrode was a Pt spiral. The potentials reported are referred to SCE; Ferrocene and decamethylferrocene were used as standards. The concentration of the compounds examined was of the order of 1 mM; tetrabutylammonium hexafluorophosphate ($TBAPF_6^-$) 0.1M was added as supporting electrolyte. Cyclic voltammograms were obtained with scan rates in the range 0.01–1 V s^{-1}. The estimated experimental error on the $E_{1/2}$ value is ± 10 mV.

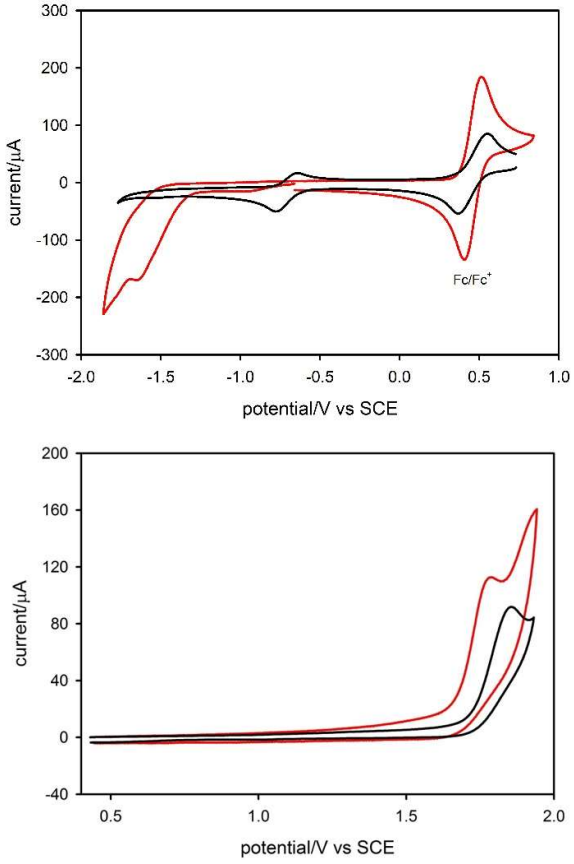


Figure S7. Cyclic voltammetry of argon-purged CH_2Cl_2 solutions of **RhS** (1mM,) (red line) and **Rh-1** (1mM) (black line) in the presence of 0.1M $TBAPF_6$. Scan rate=0.5Vs^{-1}; scan rate for **RhS** reduction (left red line) 2.0Vs^{-1}; working electrode: glassy carbon.

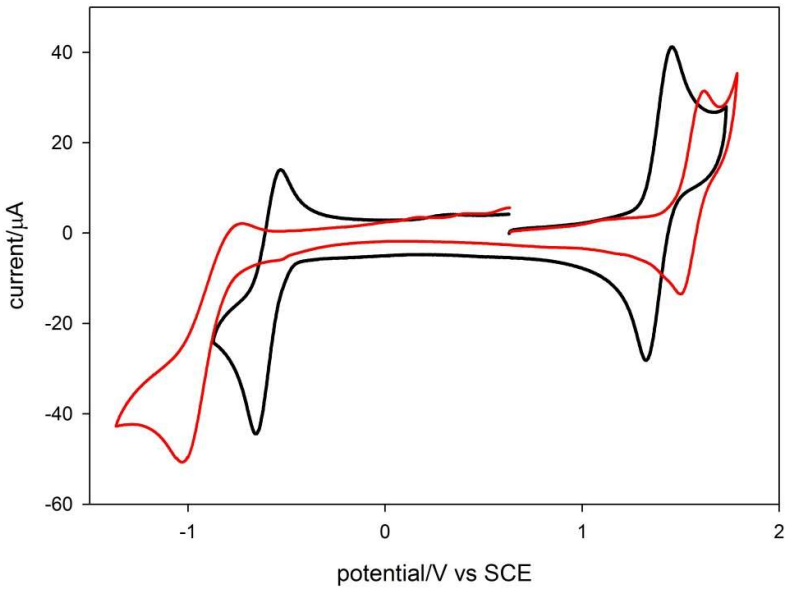


Figure S8. Cyclic voltammetry of an argon-purged solution of **IrS** (1mM) (red line) and a solution of **Ir-1** (1mM) (black line) in CH_2Cl_2 in the presence 0.1M $TBAPF_6$. Scan rate=0.5Vs^{-1}; working electrode: glassy carbon.

Table S7. Reduction and oxidation potentials estimated from cyclic voltammetry of an argon-purged solution of the metal complexes **RhS, Rh-1, IrS** and **Ir-1** in CH_2Cl_2 and 0.1 M tetraethylammonium hexafluorophosphate ($TEAPF_6$).

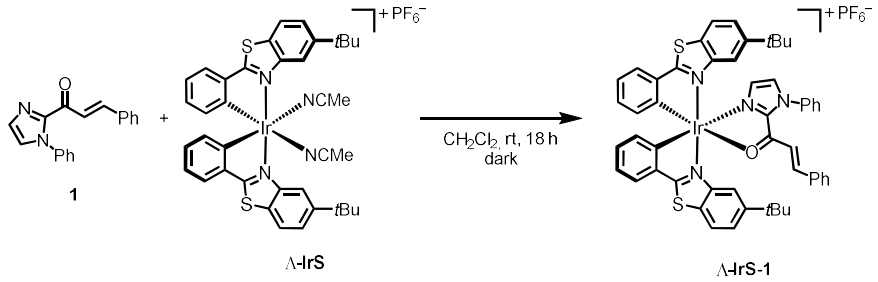
	E_{pa}^{ox} (V vs SCE)		$E_{1/2}^{red}$ (V vs SCE)
RhS	+1.76		-1.55
Rh-1	+1.41		-0.71
	$E_{1/2}^{ox}$ (V vs SCE)	$E_{1/2}^{red}$ (V vs SCE)	$\Delta E_{1/2}$ (V)
IrS	+1.56	-0.88	2.44
Ir-1	+1.39	-0.59	1.98

V. Procedures for the Synthesis of Substrates and Metal Complexes

1. Synthesis of Substrates and Complexes

Chiral Lewis acid catalysts Λ-**IrS**[S28] and Λ-**RhS**[S29], 2-acyl imidazole substrate **1**[S30] and Rh-substrate complex **Rh-1**[S30] were prepared according to previously reported procedures. (*E*)-Methyl cinnamate (**4**) was purchased commercially and used without further purification.

Synthesis of Iridium Substrate Complex Ir-1

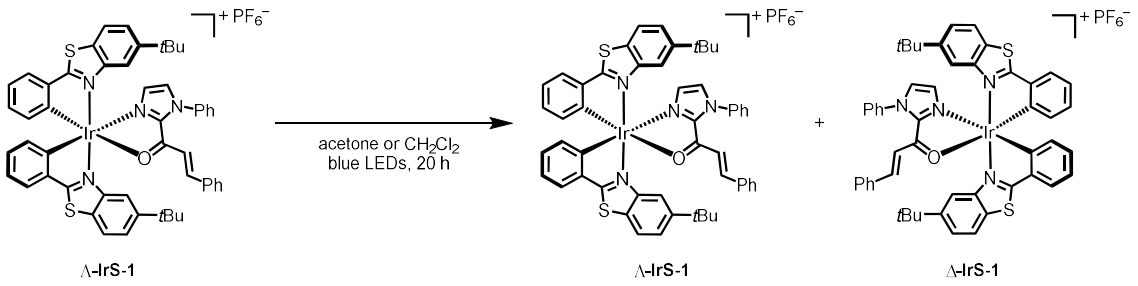


Enantiopure Λ-**Ir-1** was prepared according to a slightly modified reported procedure. A flame dried Schlenk tube was charged with Λ-**IrS** (30.0 mg, 31.5 µmol, 1.00 eq.) and 2-acyl imidazole **1** (8.6 mg, 31.5 µmol, 1.00 eq.). Afterwards, CH_2Cl_2 (1.0 mL) was added and the resulting mixture was stirred in the dark for 18 h at rt under inert gas atmosphere. The solvent was evaporated under vacuum and the precipitate was redissolved in CH_2Cl_2 (0.1 mL). *n*-Hexane was added dropwise until precipitation was complete. The clear solution was carefully decantated and the precipitate was again dissolved in CH_2Cl_2 (0.1 mL). The precipitation was repeated one time. Afterwards, the precipitate was dried under vacuum to afford Λ-**Ir-1** as an orange solid (31.9 mg, 27.9 µmol, 88%).

^{1}H NMR (300 MHz, CD_2Cl_2): δ = 7.93 (d, J = 8.6 Hz, 2H), 7.83 (s, 2H), 7.67 (dd, J = 7.6, 1.3 Hz, 4H), 7.59 (dd, J = 8.6, 1.8 Hz, 2H), 7.47–7.35 (m, 9H), 7.09–7.03 (m, 4H), 7.00 (dd, J = 7.5, 1.1 Hz, 1H), 6.91 (dt, J = 7.5, 1.4 Hz, 2H), 6.57 (d, J = 7.2 Hz, 2H), 1.14 (s, 18H) ppm. **^{13}C NMR** (75 MHz, CD_2Cl_2): δ = 181.9, 152.3, 150.4, 149.1, 141.5, 138.8, 136.0, 133.3, 132.3, 131.9, 130.7, 129.5, 129.3, 126.6, 124.7, 123.5, 123.2, 121.7, 121.2, 116.2, 35.2, 31.3 ppm. **^{19}F NMR** (282 MHz, CD_2Cl_2): -73.4 (d, J = 710.3 Hz, 6F) ppm. **IR** (neat): $\tilde{\nu}$ = 3135, 3051, 2959, 1586, 1512, 1442, 1408, 1362, 1292, 1248, 1160, 1109, 1065, 1025, 997, 933, 834, 755, 687, 554, 522, 461 cm^{-1}.

2. Stability of Λ-Ir-Complexes under Irradiation

Procedure for Photoracemization Experiments



A flame dried Schlenk tube was charged with Λ-**Ir-1** (2.0 mg, 1.74 µmol) under inert gas atmosphere and acetone or CH_2Cl_2 (8.8 mL, 0.2 mM) was added. The resulting mixture was degassed via freeze-pump-thaw thoroughly for three cycles. CD spectra were measured before and after stirring at rt for 20 h under inert gas atmosphere in front of blue LEDs (10 cm distance). The CD spectra are shown in

.

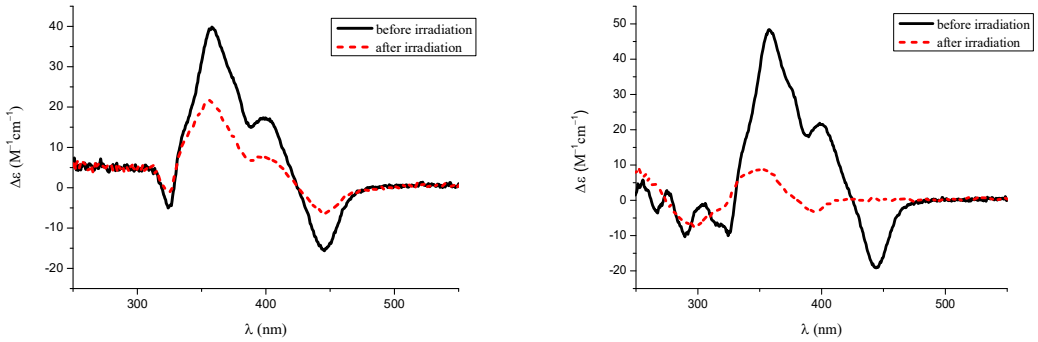


Figure S9. Left) CD spectra of Λ-**Ir-1** in acetone (0.2 mM) before and after irradiation for 20 h at rt. Right) CD spectra of Λ-**Ir-1** in CH_2Cl_2 (0.2 mM) before and after irradiation for 20 h at rt.

As can be seen by the CD spectra in Figure S9, a racemization upon irradiation of Λ-**Ir-1** for 20 h with acetone as solvent can be observed. When the same experiment is performed in CH_2Cl_2, a major change of the CD spectrum is noticed indicating major decomposition of iridium-substrate complex Λ-**Ir-1**. ^{1}H-NMR spectra of the complex after irradiation seem to support that acetone as solvent results in racemization, whereas CH_2Cl_2 leads to major decomposition. The ^{1}H-NMR spectra are shown in Figure S10.

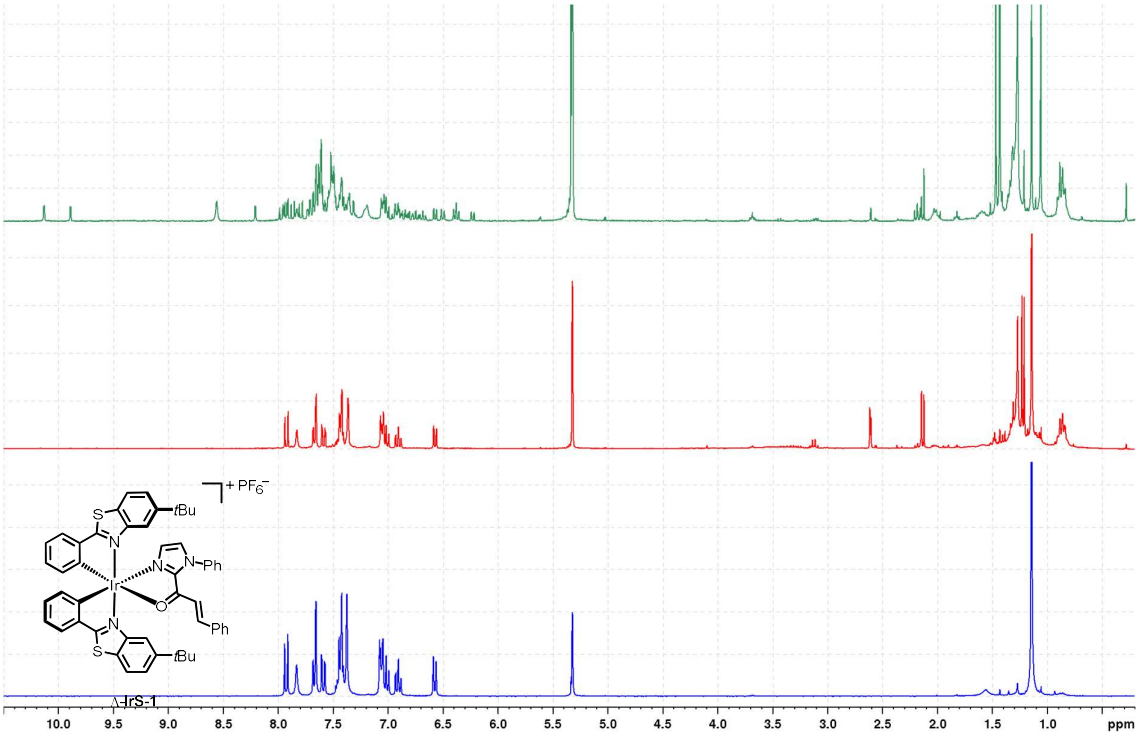
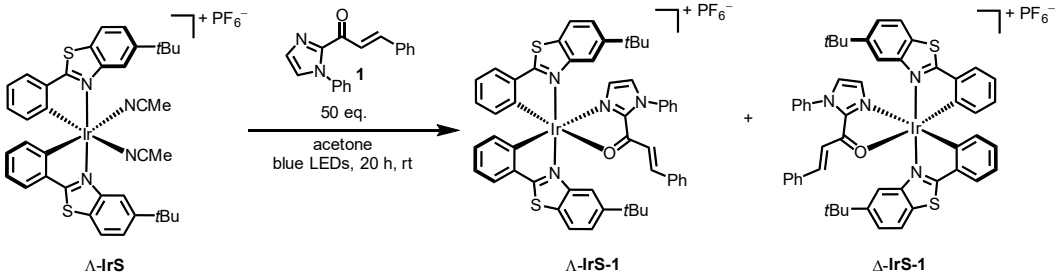


Figure S10. ^{1}H-NMR spectra (300 MHz, rt, CD_2Cl_2) of Λ-**Ir-1** (blue) and Λ-**Ir-1** after irradiation with blue LEDs for 20 h in acetone (red) and in CH_2Cl_2 (green).

Stability of IrS in Presence of Substrate



According to the above described procedure for photoracemization experiments, Λ-**IrS** (2.0 mg, 2.10 µmol, 1.00 eq.) was irradiated in presence of 2-acyl imidazole **1** (28.8 mg, 0.11 mmol, 50.0 eq.) with blue LEDs for 20 h at rt in acetone (10.5 mL). CD spectra before and after irradiation were measured and are shown in Figure S10.

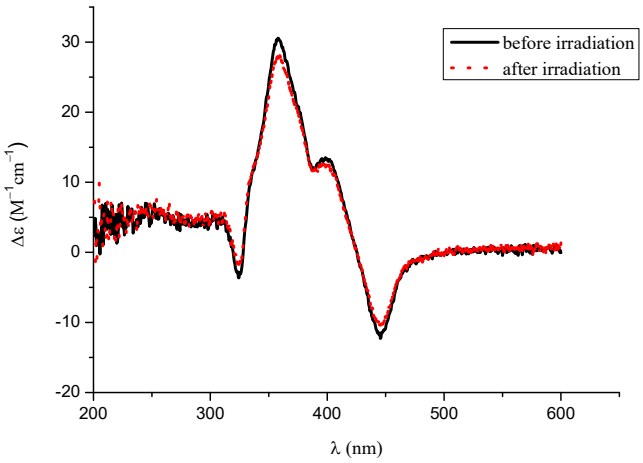
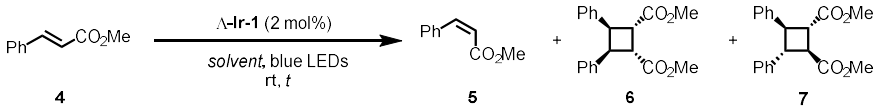


Figure S11. CD spectra of a mixture of Λ-**IrS** with 50 eq. of 2-acyl imidazole **1** in acetone (0.2 mM) before and after irradiation.

The CD spectrum before irradiation in Figure S11 strongly resembles the CD spectrum of Λ-**Ir-1** (Figure S9) indicating that the Ir-substrate complex is formed rather quickly. Comparison of the spectra before and after illumination imply that there is almost no racemization occurring when the catalyst is irradiated in presence of a large excess of substrate showing that the stereogenic center of the complex is stabilized under these conditions.

3. Evaluating Photosensitization with Ir-1 in a [2+2] Photocycloaddition

Procedure for the Λ-Ir-1 catalyzed [2+2] photocycloaddition of methyl cinnamate (4)



4 5 6 7

Reaction conditions were chosen analogous to the rhodium catalyzed [2+2] photocycloaddition.[S1] A flame dried Schlenk flask was charged with (*E*)-methyl cinnamate (**4**, 16.2 mg, 0.10 mmol, 1.00 eq.) and Λ-**Ir-1** (2 mol%) under inert gas atmosphere. The indicated solvent (0.5 mL) was added and the resulting mixture was degassed thoroughly via freeze-pump-thaw for three cycles. Afterwards, the mixture was stirred at rt under inert gas atmosphere for the indicated time. Subsequently, the solvent was evaporated under vacuum (DMF was coevaporated with toluene) and the precipitate was submitted to ^{1}H-NMR measurement. Signal assignment of the [2+2] photocycloadducts was done by comparison with the literature.[S31] The results are summarized in Table S8.

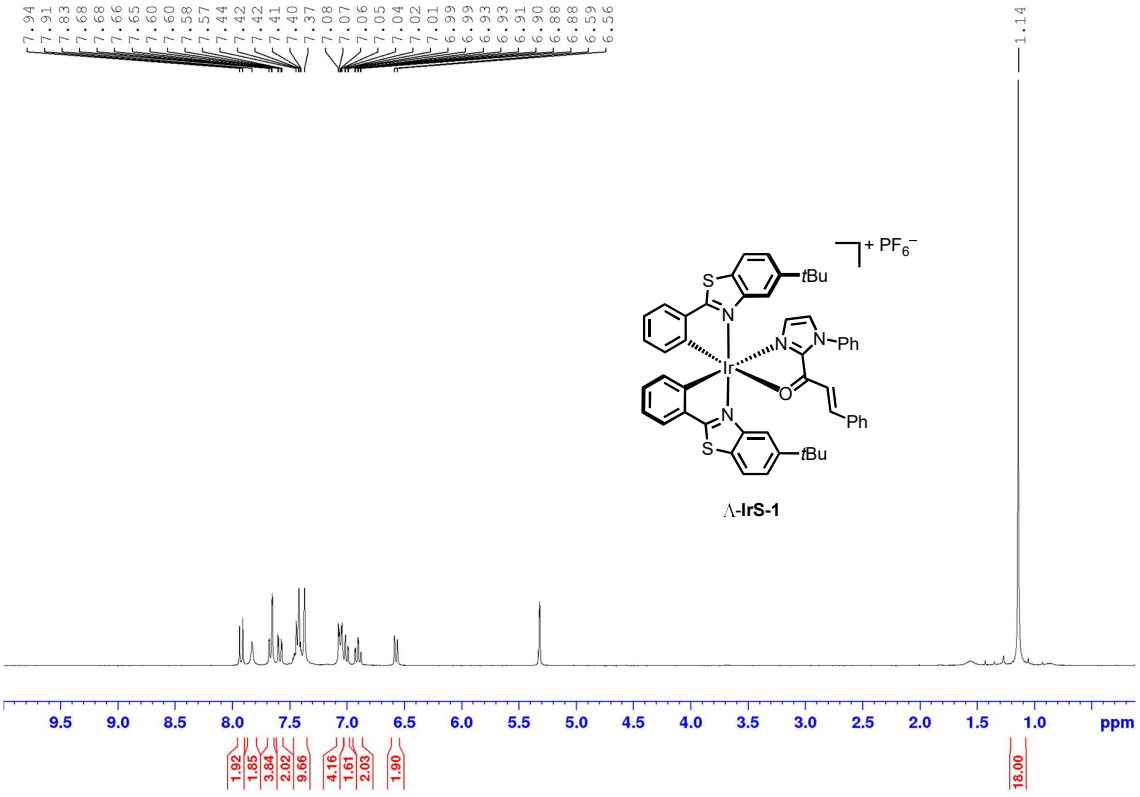
Table S8. Results of the [2+2] photocycloaddition of methyl cinnamate (**4**).

Entry	Solvent	*t* (h)	Conversion (%)[a]	Yield of 5 (%)[a]	Yield of 6 + 7 (%)[a,b]
1	Acetone	20	70.4	60.1	10.3
2[c]	Acetone	20	0	–	–
3	DMF	44	50.4	16.4	34.0
4[c]	DMF	44	0	–	–

[a] Yield determined by ^{1}H-NMR of the crude mixture after solvent evaporation. [b] Combined ^{1}H-NMR yields of the two diastereomers δ- and β-truxinate. [c] Reaction was performed without catalyst.

The results show that Λ-**Ir-1** is capable of acting as a photosensitizer to promote the [2+2] photocycloaddition of (*E*)-methyl cinnamate (**4**) as well as its photoisomerization to the (*Z*)-isomer **5**. Control reactions under the same conditions without catalyst showed no conversion of the starting material.

4. NMR Spectra



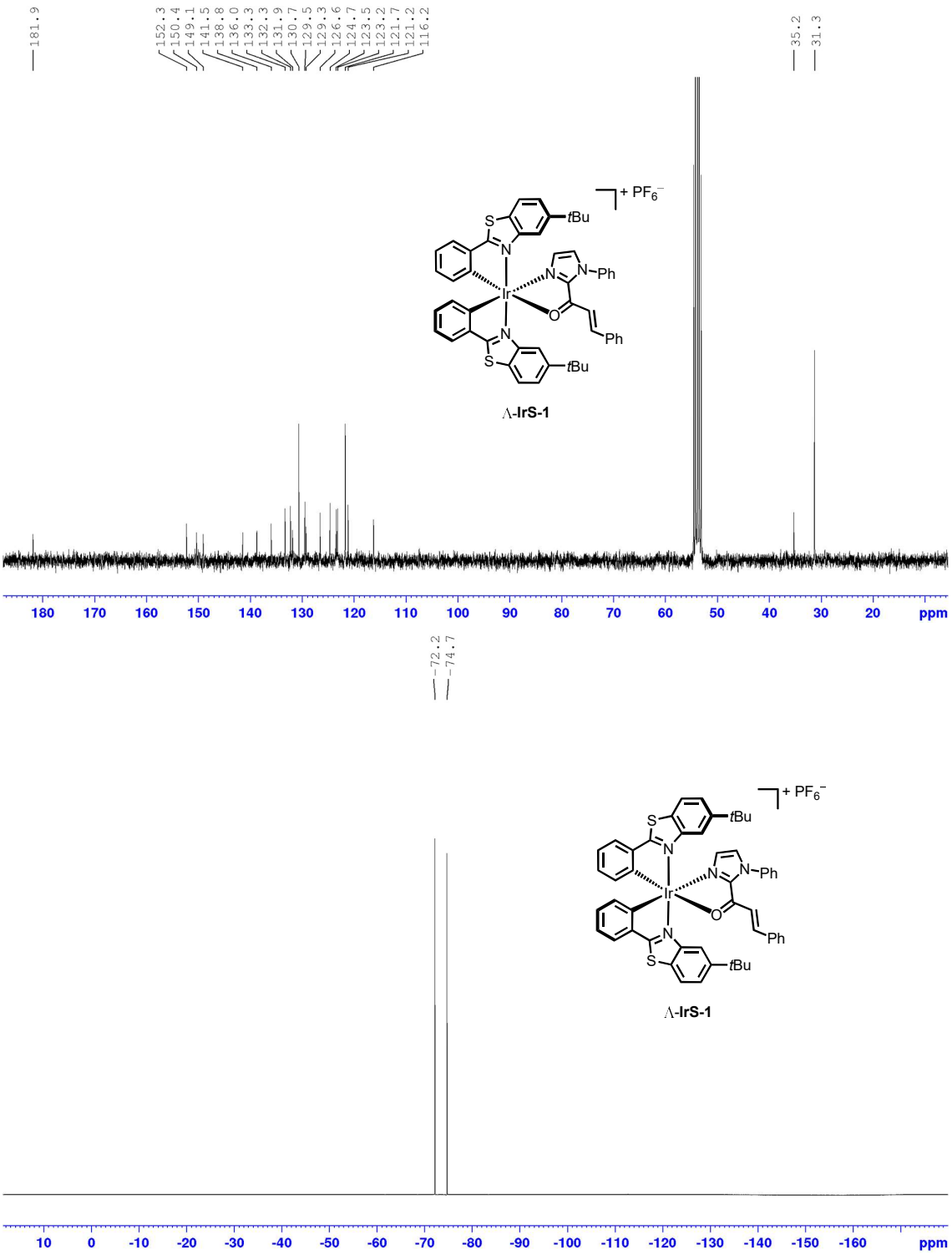


Figure S12. ^{1}H-(300 MHz, rt) and ^{13}C-(75 MHz, rt) and ^{19}F-(282 MHz, rt) NMR spectra of Λ-**Ir-1** in CD_2Cl_2.

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