

Supporting Information

**The Crystalline Sponge Method: Quantum Chemical *In Silico*
Derivation and Analysis of Guest Binding Energies**

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Computational Details

Crystal structure data were downloaded free of charge as a CIF from The Cambridge Crystallographic Data Centre (CCDC) website (<https://www.ccdc.cam.ac.uk/>). Structures were simplified for calculations by deleting the lowest-occupancy atom(s) in each disordered pair/triplet in Olex2 to eliminate positional disorder.¹ The resulting structures were subsequently written as a CIF with Olex2 for use as input.

Gas-phase geometry-optimisation and single-point energy (SPE) calculations were performed using the Cambridge Serial Total Energy Package (CASTEP) in the BIOVIA Materials Studio 2019 suite.² For calculations, all target and solvent molecules were included and assumed to be at full occupancy. Calculations were performed using DFT-D2 as implemented by Grimme³ with a PBE GGA functional.⁴ A plane-wave basis set with tabulated ultrasoft pseudopotentials,^{5,6} and a Pulay density-mixing scheme were employed for all calculations.⁷ Geometry optimisations utilized a variant of the BFGS quasi-Newton minimiser.⁸ Prior to execution of geometry optimisation calculations, unit cells were reduced to primitive unit cells where symmetry was reduced to triclinic *P*1. Geometry optimisations were performed in two rounds, with the first using CASTEP “express” settings followed by a round using tighter convergence criteria. Unit cell parameters were not optimized, and no other geometric constraints were applied for any geometry optimization calculations. Round one of the geometry optimisation was performed with a plane-wave basis set energy cut-off of 300 eV using a standard FFT grid (grid size: 1.5, maximum g-vector size: 13.3104 1/Å) and utilising the following convergence tolerances: energy of 0.001 eV/cell, maximum force of 100.0 eV/Å, maximum stress of 100.0 GPa, and maximum displacement of 100.0 Å for a maximum of 200 iterations. Electronically, the first round of calculations were run with a medium energy cutoff, an SCF tolerance of 1.0×10^{-4} eV/cell over a maximum of 100 SCF cycles with a convergence window of 2 and a coarse k-point set (1 x 1 x 1). Typically, first round jobs could be completed via running parallel on 40 cores. Round two of the geometry optimisation was performed with a plane-wave basis set energy cut-off of 340 eV using a standard FFT grid (grid size: 1.5, maximum g-vector size: 14.1700 1/Å) and utilising the following convergence tolerances: energy of 1.0×10^{-5} eV/atom, maximum force of 0.05 eV/Å, maximum stress of 0.1 GPa, and maximum displacement of 0.002 Å for a maximum of 200 iterations. Electronically, the second round of calculations was run with a fine energy cutoff, an SCF tolerance of 1.0×10^{-6} eV/atom over a maximum of 100 SCF cycles with a convergence window of 3 and a medium k-point set (1 x 1 x 1). Typically, second round jobs could be completed via running parallel on 55–100 cores. The final geometry optimised structure was utilized for SPE calculations, which were performed using the same criteria as in the second round of geometry optimisations. In order to obtain the SPE for the guest alone, the framework and all ancillary guests were deleted, leaving only the guest of interest. The SPE calculation was then performed on this new structure file containing only the guest of interest. The inverse was then completed to obtain the SPE for the host and ancillary guests (i.e., the guest of interest was deleted) and the SPE calculation was performed on the new structure file without the guest.

For asymmetric unit comparison (computed versus experiment), the geometry optimised structure file (.xsd) was exported as a CIF through Materials Studio. The geometry optimised structure was then compared to the experimental structure (without hydrogens and disordered atoms) and RMSD values were generated via a Structure Overlay calculation performed in Mercury.⁹

Averaged non-H *B*-factors for each guest were calculated by averaging the U_{eq} values obtained from the respective CIFs. All standard uncertainties were also appropriately averaged by summing the squares of all individual standard uncertainties followed by taking the square root of the resulting value and subsequently dividing by the quantity of values averaged. The averaged U_{eq} values with standard uncertainties were then scaled to averaged *B*-factor values by multiplying by $8\pi^2$.

Hirshfeld surfaces for Figures 2 and 3 were constructed using *CrystalExplorer 17.5* (revision: f4e298a, build: 2017-05-01 03:35).^{10,11} Default settings within the program were used to generate and visualize the Hirshfeld surfaces in high resolution.

All calculations were performed using computing resources maintained by Pfizer's High Performance Computing facility. CASTEP jobs were specifically executed on the Delta cluster. Delta's computational resources are scheduled and managed with Slurm. Application environments are accessed with Lmod. Remote access is provided with SSH and NICE when GPU accelerated graphical environments are required. All nodes run Red Hat Enterprise Linux 7. CPU nodes feature 2 x Intel® Xeon® Gold 6148 CPUs @ 2.40GHz and 192 GB of memory. GPU nodes feature 2 x Intel® Xeon® Gold 6140 CPUs @ 2.30GHz, 4 x Nvidia V100, and 384 GB memory. All nodes are connected by non-blocking EDR Infiniband.

Computational Data

Table S1. Primitive unit cell parameters of geometry-optimised structures

Target@host	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>a</i> (°)	<i>β</i> (°)	<i>γ</i> (°)	Volume (Å ³)
<i>trans</i> -anethole@1a	18.762201	18.762201	32.550200	102.260188	102.260188	47.503908	8217.977160
(+)-artemisinin@1a	19.128243	19.128243	35.233000	106.650483	106.650483	45.717697	8771.526472
4-(trifluoromethyl)phenyl azide@1a	19.150577	19.150577	30.941500	100.885704	100.885704	45.732789	7953.442709
vanillin@1a	14.922300	18.907800	32.591000	102.728100	91.7744000	110.79630	8324.809739
(1 <i>R</i>)-(-)-menthyl acetate@1b	18.482509	18.482509	33.787000	103.698739	103.698739	46.493204	8088.315649
(1 <i>R</i>)-(-)-menthyl acetate@1c	18.181356	18.181356	33.897000	103.997709	103.997709	46.649388	7860.186160
chloroform@1a	18.827922	18.827922	31.081000	100.142208	100.142208	46.057496	7786.729747

Table S2. Real and reciprocal lattice matrices of geometry-optimised structures

Target@host	Real Lattice (Å)			Reciprocal Lattice (1/Å)		
<i>trans</i> -anethole@1a	16.7044375	-7.5569999	-3.9841801	0.188069347	-0.415719555	0.000000000
	16.7044375	7.5569999	-3.9841801	0.188069347	0.415719555	0.000000000
	0.0000000	0.0000000	32.5501998	0.046039788	-0.000000000	0.193030622
(+)artemisinin@1a	16.7521934	-7.4306000	-5.4808657	0.187533213	-0.422791250	0.000000000
	16.7521934	7.4306000	-5.4808657	0.187533213	0.422791250	0.000000000
	0.0000000	0.0000000	35.2329999	0.058345549	-0.000000000	0.178332397
4-(trifluoromethyl)phenyl azide@1a	17.2709999	-7.4415999	-3.6165947	0.181899871	-0.422166292	0.000000000
	17.2709999	7.4415999	-3.6165947	0.181899871	0.422166292	0.000000000
	0.0000000	0.0000000	30.9414998	0.042522703	0.000000000	0.203066605
vanillin@1a	13.8497214	-5.5359513	-0.4620567	0.453668716	0.000000000	0.000000000
	0.0000000	18.4431711	-4.1658538	0.136174409	0.340678144	0.000000000
	0.0000000	0.0000000	32.5909999	0.023837972	0.043546235	0.192788970
(1 <i>R</i>)-(-)-menthyl acetate@1b	16.4082439	-7.2948499	-4.3769682	0.191464282	-0.430658982	0.000000000
	16.4082439	7.2948499	-4.3769682	0.191464282	0.430658982	0.000000000
	0.0000000	0.0000000	33.7869998	0.049606836	0.000000000	0.185964583
(1 <i>R</i>)-(-)-menthyl acetate@1c	16.1058809	-7.1987500	-4.3977627	0.195058728	-0.436408080	0.000000000
	16.1058809	7.1987500	-4.3977627	0.195058728	0.436408080	0.000000000
	0.0000000	0.0000000	33.8969999	0.050613447	0.000000000	0.185361104
chloroform@1a	17.0073536	-7.3653499	-3.3154452	0.184719665	-0.426536781	0.000000000
	17.0073536	7.3653499	-3.3154452	0.184719665	0.426536781	0.000000000
	0.0000000	0.0000000	31.0809998	0.039408509	0.000000000	0.202155187

Table S3. Dispersion-corrected SPE values

Target@host	E_{system} (eV)	Specific Molecule + Identifying Atom ^a	E_{guest} (eV)	$E_{\text{framework + ancillary guests}}$ (eV)
<i>trans</i> -anethole@1a	-91096.06450515	oxygen O1 (A)	-8716.202254073	-82374.15873094
		oxygen O2 (B)	-8716.002781276	-82374.72804829
		oxygen O3 (C)	-8715.860473120	-82375.98385724
(+) -artemisinin@1a	-77473.07655431	artemisinin (D)	-9721.315513490	-67749.49205686
		methyl <i>tert</i> -butyl ether (E)	-2810.908247633	-74660.84723345
4-(trifluoromethyl)phenyl azide@1a	-86349.34822945	4-(trifluoromethyl)phenyl azide (F)	-15784.58242957	-70560.81645002
		methyl <i>tert</i> -butyl ether (G)	-5621.632844729	-80724.60418295
vanillin@1a	-86361.82127863	vanillin C73 (H)	-5354.133358011	-81004.32635454
		vanillin C81 (I)	-5354.478877421	-81005.21417489
		vanillin C89 (J)	-5354.480315080	-81005.89707043
		vanillin C97 (K)	-5354.421015291	-81004.54463821
(1R)-(-)-menthyl acetate@1b	-84148.39120818	menthyl acetate O1 (L)	-6179.023415139	-77966.34283358
		menthyl acetate O3 (M)	-6178.978349088	-77966.35628883
		chloroform C97 (N)	-2791.612621387	-81355.59556125
		chloroform C98 (O)	-2791.597330020	-81356.11769262
(1R)-(-)-menthyl acetate@1c	-82378.89997767	menthyl acetate O1 (P)	-6178.840997281	-76197.16148950
		menthyl acetate O3 (Q)	-6178.871931031	-76197.15129303
		chloroform C109 (R)	-2791.595050487	-79586.07000691
chloroform@1a	-81691.98068097	chloroform C37 (S)	-5583.400829553	-76106.50148923
		chloroform C38 (T)	-5583.279469098	-76106.94577670
		chloroform C39 (U)	-5583.285362603	-76106.46338912

^a Based on atom labels in the CIF

Table S4. Fractional atomic coordinates of the optimised structure of *trans*-anethole@**1a**

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----x					
x	H	1	-0.020399	1.035709	0.562237	x
x	H	2	-0.154464	1.159725	0.512755	x
x	H	3	0.040956	1.188376	0.486545	x
x	H	4	0.168128	1.060813	0.535783	x
x	H	5	-0.078949	1.483107	0.385877	x
x	H	6	-0.088038	1.401174	0.433832	x
x	H	7	-0.288406	1.405327	0.338337	x
x	H	8	-0.264458	1.478363	0.292127	x
x	H	9	-0.620707	1.494919	0.384636	x
x	H	10	-0.459568	1.448605	0.383406	x
x	H	11	-0.370340	1.334073	0.503092	x
x	H	12	-0.535801	1.389496	0.501041	x
x	H	13	-0.555722	1.268198	0.418356	x
x	H	14	-0.520518	1.130494	0.366800	x
x	H	15	-0.808336	1.336812	0.305211	x
x	H	16	-0.827157	1.467637	0.355482	x
x	H	17	-0.991712	1.296547	0.160386	x
x	H	18	-0.870472	1.269162	0.221153	x
x	H	19	-0.715180	0.962633	0.196313	x
x	H	20	-0.844843	1.002295	0.138307	x
x	H	21	-0.340497	0.654335	0.233793	x
x	H	22	-0.500607	0.825544	0.227915	x
x	H	23	-0.417574	0.905344	0.350360	x
x	H	24	-0.261925	0.732856	0.351974	x
x	H	25	0.620974	0.867626	0.519940	x
x	H	26	0.582236	0.841263	0.555270	x
x	H	27	0.652659	0.875721	0.574348	x
x	H	28	0.509289	1.044109	0.547612	x
x	H	29	0.412237	0.976254	0.568607	x
x	H	30	0.247032	1.094695	0.578773	x
x	H	31	0.085765	1.260905	0.573955	x
x	H	32	0.222590	1.357956	0.548006	x
x	H	33	0.382254	1.192963	0.552415	x
x	H	34	-0.027963	1.380594	0.525824	x
x	H	35	-0.086454	1.505956	0.540241	x
x	H	36	-0.043027	1.428216	0.580247	x
x	H	37	-0.081807	0.629304	0.525344	x
x	H	38	-0.183114	0.683990	0.551822	x
x	H	39	-0.079257	0.662142	0.581093	x
x	H	40	-0.217051	0.811612	0.514523	x
x	H	41	-0.098945	0.806271	0.597126	x

x H	42	-0.305620	0.964148	0.513370	x
x H	43	-0.376673	1.130550	0.507271	x
x H	44	-0.170718	1.101393	0.608502	x
x H	45	-0.098044	0.934893	0.613427	x
x H	46	-0.305740	1.266231	0.615320	x
x H	47	-0.349448	1.344685	0.575601	x
x H	48	-0.224743	1.235946	0.580309	x
x H	49	0.007979	1.261928	0.320537	x
x H	50	-0.023714	1.239826	0.266869	x
x H	51	0.055325	1.263173	0.279556	x
x H	52	0.122688	1.069882	0.266156	x
x H	53	0.191736	1.134600	0.347102	x
x H	54	0.256142	0.918020	0.268224	x
x H	55	0.402191	0.748096	0.281861	x
x H	56	0.476511	0.850360	0.399693	x
x H	57	0.331394	1.018327	0.386236	x
x H	58	0.620916	0.694772	0.392288	x
x H	59	0.631797	0.590852	0.387294	x
x H	60	0.533415	0.703908	0.412993	x
x H	61	-1.035709	0.020399	-0.062237	x
x H	62	-1.159725	0.154464	-0.012755	x
x H	63	-1.188376	-0.040956	0.013455	x
x H	64	-1.060813	-0.168128	-0.035783	x
x H	65	-1.483107	0.078949	0.114123	x
x H	66	-1.401174	0.088038	0.066168	x
x H	67	-1.405327	0.288406	0.161663	x
x H	68	-1.478363	0.264458	0.207873	x
x H	69	-1.494919	0.620707	0.115364	x
x H	70	-1.448605	0.459568	0.116594	x
x H	71	-1.334073	0.370340	-0.003092	x
x H	72	-1.389496	0.535801	-0.001041	x
x H	73	-1.268198	0.555722	0.081644	x
x H	74	-1.130494	0.520518	0.133200	x
x H	75	-1.336812	0.808336	0.194789	x
x H	76	-1.467637	0.827157	0.144518	x
x H	77	-1.296547	0.991712	0.339614	x
x H	78	-1.269162	0.870472	0.278847	x
x H	79	-0.962633	0.715180	0.303687	x
x H	80	-1.002295	0.844843	0.361693	x
x H	81	-0.654335	0.340497	0.266207	x
x H	82	-0.825544	0.500607	0.272085	x
x H	83	-0.905344	0.417574	0.149640	x
x H	84	-0.732856	0.261925	0.148026	x
x H	85	-0.867626	-0.620974	-0.019940	x
x H	86	-0.841263	-0.582236	-0.055270	x
x H	87	-0.875721	-0.652659	-0.074348	x

x H	88	-1.044109	-0.509289	-0.047612	x
x H	89	-0.976254	-0.412237	-0.068607	x
x H	90	-1.094695	-0.247032	-0.078773	x
x H	91	-1.260905	-0.085765	-0.073955	x
x H	92	-1.357956	-0.222590	-0.048006	x
x H	93	-1.192963	-0.382254	-0.052415	x
x H	94	-1.380594	0.027963	-0.025824	x
x H	95	-1.505956	0.086454	-0.040241	x
x H	96	-1.428216	0.043027	-0.080247	x
x H	97	-0.629304	0.081807	-0.025344	x
x H	98	-0.683990	0.183114	-0.051822	x
x H	99	-0.662142	0.079257	-0.081093	x
x H	100	-0.811612	0.217051	-0.014523	x
x H	101	-0.806271	0.098945	-0.097126	x
x H	102	-0.964148	0.305620	-0.013370	x
x H	103	-1.130550	0.376673	-0.007271	x
x H	104	-1.101393	0.170718	-0.108502	x
x H	105	-0.934893	0.098044	-0.113427	x
x H	106	-1.266231	0.305740	-0.115320	x
x H	107	-1.344685	0.349448	-0.075601	x
x H	108	-1.235946	0.224743	-0.080309	x
x H	109	-1.261928	-0.007979	0.179463	x
x H	110	-1.239826	0.023714	0.233131	x
x H	111	-1.263173	-0.055325	0.220444	x
x H	112	-1.069882	-0.122688	0.233844	x
x H	113	-1.134600	-0.191736	0.152898	x
x H	114	-0.918020	-0.256142	0.231776	x
x H	115	-0.748096	-0.402191	0.218139	x
x H	116	-0.850360	-0.476511	0.100307	x
x H	117	-1.018327	-0.331394	0.113764	x
x H	118	-0.694772	-0.620916	0.107712	x
x H	119	-0.590852	-0.631797	0.112706	x
x H	120	-0.703908	-0.533415	0.087007	x
x H	121	0.020399	-1.035709	-0.562237	x
x H	122	0.154464	-1.159725	-0.512755	x
x H	123	-0.040956	-1.188376	-0.486545	x
x H	124	-0.168128	-1.060813	-0.535783	x
x H	125	0.078949	-1.483107	-0.385877	x
x H	126	0.088038	-1.401174	-0.433832	x
x H	127	0.288406	-1.405327	-0.338337	x
x H	128	0.264458	-1.478363	-0.292127	x
x H	129	0.620707	-1.494919	-0.384636	x
x H	130	0.459568	-1.448605	-0.383406	x
x H	131	0.370340	-1.334073	-0.503092	x
x H	132	0.535801	-1.389496	-0.501041	x
x H	133	0.555722	-1.268198	-0.418356	x

x H	134	0.520518	-1.130494	-0.366800	x
x H	135	0.808336	-1.336812	-0.305211	x
x H	136	0.827157	-1.467637	-0.355482	x
x H	137	0.991712	-1.296547	-0.160386	x
x H	138	0.870472	-1.269162	-0.221153	x
x H	139	0.715180	-0.962633	-0.196313	x
x H	140	0.844843	-1.002295	-0.138307	x
x H	141	0.340497	-0.654335	-0.233793	x
x H	142	0.500607	-0.825544	-0.227915	x
x H	143	0.417574	-0.905344	-0.350360	x
x H	144	0.261925	-0.732856	-0.351974	x
x H	145	-0.620974	-0.867626	-0.519940	x
x H	146	-0.582236	-0.841263	-0.555270	x
x H	147	-0.652659	-0.875721	-0.574348	x
x H	148	-0.509289	-1.044109	-0.547612	x
x H	149	-0.412237	-0.976254	-0.568607	x
x H	150	-0.247032	-1.094695	-0.578773	x
x H	151	-0.085765	-1.260905	-0.573955	x
x H	152	-0.222590	-1.357956	-0.548006	x
x H	153	-0.382254	-1.192963	-0.552415	x
x H	154	0.027963	-1.380594	-0.525824	x
x H	155	0.086454	-1.505956	-0.540241	x
x H	156	0.043027	-1.428216	-0.580247	x
x H	157	0.081807	-0.629304	-0.525344	x
x H	158	0.183114	-0.683990	-0.551822	x
x H	159	0.079257	-0.662142	-0.581093	x
x H	160	0.217051	-0.811612	-0.514523	x
x H	161	0.098945	-0.806271	-0.597126	x
x H	162	0.305620	-0.964148	-0.513370	x
x H	163	0.376673	-1.130550	-0.507271	x
x H	164	0.170718	-1.101393	-0.608502	x
x H	165	0.098044	-0.934893	-0.613427	x
x H	166	0.305740	-1.266231	-0.615320	x
x H	167	0.349448	-1.344685	-0.575601	x
x H	168	0.224743	-1.235946	-0.580309	x
x H	169	-0.007979	-1.261928	-0.320537	x
x H	170	0.023714	-1.239826	-0.266869	x
x H	171	-0.055325	-1.263173	-0.279556	x
x H	172	-0.122688	-1.069882	-0.266156	x
x H	173	-0.191736	-1.134600	-0.347102	x
x H	174	-0.256142	-0.918020	-0.268224	x
x H	175	-0.402191	-0.748096	-0.281861	x
x H	176	-0.476511	-0.850360	-0.399693	x
x H	177	-0.331394	-1.018327	-0.386236	x
x H	178	-0.620916	-0.694772	-0.392288	x
x H	179	-0.631797	-0.590852	-0.387294	x

x H	180	-0.533415	-0.703908	-0.412993	x
x H	181	1.035709	-0.020399	1.062237	x
x H	182	1.159725	-0.154464	1.012755	x
x H	183	1.188376	0.040956	0.986545	x
x H	184	1.060813	0.168128	1.035783	x
x H	185	1.483107	-0.078949	0.885877	x
x H	186	1.401174	-0.088038	0.933832	x
x H	187	1.405327	-0.288406	0.838337	x
x H	188	1.478363	-0.264458	0.792127	x
x H	189	1.494919	-0.620707	0.884636	x
x H	190	1.448605	-0.459568	0.883406	x
x H	191	1.334073	-0.370340	1.003092	x
x H	192	1.389496	-0.535801	1.001041	x
x H	193	1.268198	-0.555722	0.918356	x
x H	194	1.130494	-0.520518	0.866800	x
x H	195	1.336812	-0.808336	0.805211	x
x H	196	1.467637	-0.827157	0.855482	x
x H	197	1.296547	-0.991712	0.660386	x
x H	198	1.269162	-0.870472	0.721153	x
x H	199	0.962633	-0.715180	0.696313	x
x H	200	1.002295	-0.844843	0.638307	x
x H	201	0.654335	-0.340497	0.733793	x
x H	202	0.825544	-0.500607	0.727915	x
x H	203	0.905344	-0.417574	0.850360	x
x H	204	0.732856	-0.261925	0.851974	x
x H	205	0.867626	0.620974	1.019940	x
x H	206	0.841263	0.582236	1.055270	x
x H	207	0.875721	0.652659	1.074348	x
x H	208	1.044109	0.509289	1.047612	x
x H	209	0.976254	0.412237	1.068607	x
x H	210	1.094695	0.247032	1.078773	x
x H	211	1.260905	0.085765	1.073955	x
x H	212	1.357956	0.222590	1.048006	x
x H	213	1.192963	0.382254	1.052415	x
x H	214	1.380594	-0.027963	1.025824	x
x H	215	1.505956	-0.086454	1.040241	x
x H	216	1.428216	-0.043027	1.080247	x
x H	217	0.629304	-0.081807	1.025344	x
x H	218	0.683990	-0.183114	1.051822	x
x H	219	0.662142	-0.079257	1.081093	x
x H	220	0.811612	-0.217051	1.014523	x
x H	221	0.806271	-0.098945	1.097126	x
x H	222	0.964148	-0.305620	1.013370	x
x H	223	1.130550	-0.376673	1.007271	x
x H	224	1.101393	-0.170718	1.108502	x
x H	225	0.934893	-0.098044	1.113427	x

x H	226	1.266231	-0.305740	1.115320	x
x H	227	1.344685	-0.349448	1.075601	x
x H	228	1.235946	-0.224743	1.080309	x
x H	229	1.261928	0.007979	0.820537	x
x H	230	1.239826	-0.023714	0.766869	x
x H	231	1.263173	0.055325	0.779556	x
x H	232	1.069882	0.122688	0.766156	x
x H	233	1.134600	0.191736	0.847102	x
x H	234	0.918020	0.256142	0.768224	x
x H	235	0.748096	0.402191	0.781861	x
x H	236	0.850360	0.476511	0.899693	x
x H	237	1.018327	0.331394	0.886236	x
x H	238	0.694772	0.620916	0.892288	x
x H	239	0.590852	0.631797	0.887294	x
x H	240	0.703908	0.533415	0.912993	x
x C	1	-0.010714	1.071822	0.544729	x
x C	2	-0.084145	1.140203	0.517428	x
x C	3	-0.067708	1.185696	0.496955	x
x C	4	0.024460	1.156694	0.502889	x
x C	5	0.094898	1.086765	0.530422	x
x C	6	-0.147822	1.262731	0.469870	x
x C	7	-0.306029	1.354660	0.442938	x
x C	8	-0.204190	1.356822	0.417501	x
x C	9	-0.123264	1.463034	0.376337	x
x C	10	-0.128894	1.418217	0.402876	x
x C	11	-0.189758	1.397690	0.389486	x
x C	12	-0.240291	1.420257	0.349382	x
x C	13	-0.228601	1.461890	0.324056	x
x C	14	-0.562746	1.459860	0.410208	x
x C	15	-0.474493	1.434640	0.409807	x
x C	16	-0.403383	1.388523	0.443441	x
x C	17	-0.424926	1.372130	0.477002	x
x C	18	-0.515628	1.401318	0.475810	x
x C	19	-0.608483	1.280261	0.392018	x
x C	20	-0.589879	1.203979	0.363811	x
x C	21	-0.662373	1.222600	0.332044	x
x C	22	-0.749308	1.318767	0.329046	x
x C	23	-0.761104	1.391787	0.357359	x
x C	24	-0.649125	1.142564	0.303349	x
x C	25	-0.561631	0.980969	0.284250	x
x C	26	-0.708334	1.091767	0.248701	x
x C	27	-0.929430	1.223955	0.169790	x
x C	28	-0.861787	1.208065	0.203329	x
x C	29	-0.783584	1.113155	0.213882	x
x C	30	-0.776240	1.037522	0.189752	x
x C	31	-0.847188	1.059097	0.157222	x

x C	32	-0.361630	0.712452	0.258946	x
x C	33	-0.449496	0.806736	0.255944	x
x C	34	-0.471025	0.878766	0.288545	x
x C	35	-0.403091	0.851985	0.323869	x
x C	36	-0.316802	0.756041	0.325003	x
x C	37	0.593521	0.889352	0.550951	x
x C	38	0.503310	0.993575	0.554207	x
x C	39	0.417536	1.028223	0.563279	x
x C	40	0.326560	1.129325	0.564273	x
x C	41	0.241278	1.152561	0.571296	x
x C	42	0.150466	1.246052	0.568946	x
x C	43	0.144049	1.319610	0.559470	x
x C	44	0.228949	1.299581	0.555101	x
x C	45	0.318163	1.206324	0.557162	x
x C	46	-0.029405	1.432440	0.549980	x
x C	47	-0.125186	0.684734	0.550937	x
x C	48	-0.167738	0.782952	0.543294	x
x C	49	-0.150826	0.837226	0.569129	x
x C	50	-0.195007	0.935590	0.563771	x
x C	51	-0.274691	0.993079	0.534051	x
x C	52	-0.315598	1.086793	0.530547	x
x C	53	-0.279538	1.127475	0.557427	x
x C	54	-0.200568	1.072086	0.587271	x
x C	55	-0.159520	0.977358	0.589968	x
x C	56	-0.299526	1.269006	0.582910	x
x C	57	0.036101	1.225717	0.289501	x
x C	58	0.121509	1.119358	0.291407	x
x C	59	0.195486	1.083020	0.322111	x
x C	60	0.281617	0.981634	0.326864	x
x C	61	0.303766	0.903672	0.297282	x
x C	62	0.385337	0.808485	0.304510	x
x C	63	0.447745	0.787742	0.341795	x
x C	64	0.429087	0.864031	0.370745	x
x C	65	0.346939	0.959182	0.363010	x
x C	66	0.580578	0.669792	0.387328	x
x C	67	-1.071822	0.010714	-0.044729	x
x C	68	-1.140203	0.084145	-0.017428	x
x C	69	-1.185696	0.067708	0.003045	x
x C	70	-1.156694	-0.024460	-0.002889	x
x C	71	-1.086765	-0.094898	-0.030422	x
x C	72	-1.262731	0.147822	0.030130	x
x C	73	-1.354660	0.306029	0.057062	x
x C	74	-1.356822	0.204190	0.082499	x
x C	75	-1.463034	0.123264	0.123663	x
x C	76	-1.418217	0.128894	0.097124	x
x C	77	-1.397690	0.189758	0.110514	x

x C	78	-1.420257	0.240291	0.150618	x
x C	79	-1.461890	0.228601	0.175944	x
x C	80	-1.459860	0.562746	0.089792	x
x C	81	-1.434640	0.474493	0.090193	x
x C	82	-1.388523	0.403383	0.056559	x
x C	83	-1.372130	0.424926	0.022998	x
x C	84	-1.401318	0.515628	0.024190	x
x C	85	-1.280261	0.608483	0.107982	x
x C	86	-1.203979	0.589879	0.136189	x
x C	87	-1.222600	0.662373	0.167956	x
x C	88	-1.318767	0.749308	0.170954	x
x C	89	-1.391787	0.761104	0.142641	x
x C	90	-1.142564	0.649125	0.196651	x
x C	91	-0.980969	0.561631	0.215750	x
x C	92	-1.091767	0.708334	0.251299	x
x C	93	-1.223955	0.929430	0.330210	x
x C	94	-1.208065	0.861787	0.296671	x
x C	95	-1.113155	0.783584	0.286118	x
x C	96	-1.037522	0.776240	0.310248	x
x C	97	-1.059097	0.847188	0.342778	x
x C	98	-0.712452	0.361630	0.241054	x
x C	99	-0.806736	0.449496	0.244056	x
x C	100	-0.878766	0.471025	0.211455	x
x C	101	-0.851985	0.403091	0.176131	x
x C	102	-0.756041	0.316802	0.174997	x
x C	103	-0.889352	-0.593521	-0.050951	x
x C	104	-0.993575	-0.503310	-0.054207	x
x C	105	-1.028223	-0.417536	-0.063279	x
x C	106	-1.129325	-0.326560	-0.064273	x
x C	107	-1.152561	-0.241278	-0.071296	x
x C	108	-1.246052	-0.150466	-0.068946	x
x C	109	-1.319610	-0.144049	-0.059470	x
x C	110	-1.299581	-0.228949	-0.055101	x
x C	111	-1.206324	-0.318163	-0.057162	x
x C	112	-1.432440	0.029405	-0.049980	x
x C	113	-0.684734	0.125186	-0.050937	x
x C	114	-0.782952	0.167738	-0.043294	x
x C	115	-0.837226	0.150826	-0.069129	x
x C	116	-0.935590	0.195007	-0.063771	x
x C	117	-0.993079	0.274691	-0.034051	x
x C	118	-1.086793	0.315598	-0.030547	x
x C	119	-1.127475	0.279538	-0.057427	x
x C	120	-1.072086	0.200568	-0.087271	x
x C	121	-0.977358	0.159520	-0.089968	x
x C	122	-1.269006	0.299526	-0.082910	x
x C	123	-1.225717	-0.036101	0.210499	x

x C	124	-1.119358	-0.121509	0.208593	x
x C	125	-1.083020	-0.195486	0.177889	x
x C	126	-0.981634	-0.281617	0.173136	x
x C	127	-0.903672	-0.303766	0.202718	x
x C	128	-0.808485	-0.385337	0.195490	x
x C	129	-0.787742	-0.447745	0.158205	x
x C	130	-0.864031	-0.429087	0.129255	x
x C	131	-0.959182	-0.346939	0.136990	x
x C	132	-0.669792	-0.580578	0.112672	x
x C	133	0.010714	-1.071822	-0.544729	x
x C	134	0.084145	-1.140203	-0.517428	x
x C	135	0.067708	-1.185696	-0.496955	x
x C	136	-0.024460	-1.156694	-0.502889	x
x C	137	-0.094898	-1.086765	-0.530422	x
x C	138	0.147822	-1.262731	-0.469870	x
x C	139	0.306029	-1.354660	-0.442938	x
x C	140	0.204190	-1.356822	-0.417501	x
x C	141	0.123264	-1.463034	-0.376337	x
x C	142	0.128894	-1.418217	-0.402876	x
x C	143	0.189758	-1.397690	-0.389486	x
x C	144	0.240291	-1.420257	-0.349382	x
x C	145	0.228601	-1.461890	-0.324056	x
x C	146	0.562746	-1.459860	-0.410208	x
x C	147	0.474493	-1.434640	-0.409807	x
x C	148	0.403383	-1.388523	-0.443441	x
x C	149	0.424926	-1.372130	-0.477002	x
x C	150	0.515628	-1.401318	-0.475810	x
x C	151	0.608483	-1.280261	-0.392018	x
x C	152	0.589879	-1.203979	-0.363811	x
x C	153	0.662373	-1.222600	-0.332044	x
x C	154	0.749308	-1.318767	-0.329046	x
x C	155	0.761104	-1.391787	-0.357359	x
x C	156	0.649125	-1.142564	-0.303349	x
x C	157	0.561631	-0.980969	-0.284250	x
x C	158	0.708334	-1.091767	-0.248701	x
x C	159	0.929430	-1.223955	-0.169790	x
x C	160	0.861787	-1.208065	-0.203329	x
x C	161	0.783584	-1.113155	-0.213882	x
x C	162	0.776240	-1.037522	-0.189752	x
x C	163	0.847188	-1.059097	-0.157222	x
x C	164	0.361630	-0.712452	-0.258946	x
x C	165	0.449496	-0.806736	-0.255944	x
x C	166	0.471025	-0.878766	-0.288545	x
x C	167	0.403091	-0.851985	-0.323869	x
x C	168	0.316802	-0.756041	-0.325003	x
x C	169	-0.593521	-0.889352	-0.550951	x

x C	170	-0.503310	-0.993575	-0.554207	x
x C	171	-0.417536	-1.028223	-0.563279	x
x C	172	-0.326560	-1.129325	-0.564273	x
x C	173	-0.241278	-1.152561	-0.571296	x
x C	174	-0.150466	-1.246052	-0.568946	x
x C	175	-0.144049	-1.319610	-0.559470	x
x C	176	-0.228949	-1.299581	-0.555101	x
x C	177	-0.318163	-1.206324	-0.557162	x
x C	178	0.029405	-1.432440	-0.549980	x
x C	179	0.125186	-0.684734	-0.550937	x
x C	180	0.167738	-0.782952	-0.543294	x
x C	181	0.150826	-0.837226	-0.569129	x
x C	182	0.195007	-0.935590	-0.563771	x
x C	183	0.274691	-0.993079	-0.534051	x
x C	184	0.315598	-1.086793	-0.530547	x
x C	185	0.279538	-1.127475	-0.557427	x
x C	186	0.200568	-1.072086	-0.587271	x
x C	187	0.159520	-0.977358	-0.589968	x
x C	188	0.299526	-1.269006	-0.582910	x
x C	189	-0.036101	-1.225717	-0.289501	x
x C	190	-0.121509	-1.119358	-0.291407	x
x C	191	-0.195486	-1.083020	-0.322111	x
x C	192	-0.281617	-0.981634	-0.326864	x
x C	193	-0.303766	-0.903672	-0.297282	x
x C	194	-0.385337	-0.808485	-0.304510	x
x C	195	-0.447745	-0.787742	-0.341795	x
x C	196	-0.429087	-0.864031	-0.370745	x
x C	197	-0.346939	-0.959182	-0.363010	x
x C	198	-0.580578	-0.669792	-0.387328	x
x C	199	1.071822	-0.010714	1.044729	x
x C	200	1.140203	-0.084145	1.017428	x
x C	201	1.185696	-0.067708	0.996955	x
x C	202	1.156694	0.024460	1.002889	x
x C	203	1.086765	0.094898	1.030422	x
x C	204	1.262731	-0.147822	0.969870	x
x C	205	1.354660	-0.306029	0.942938	x
x C	206	1.356822	-0.204190	0.917501	x
x C	207	1.463034	-0.123264	0.876337	x
x C	208	1.418217	-0.128894	0.902876	x
x C	209	1.397690	-0.189758	0.889486	x
x C	210	1.420257	-0.240291	0.849382	x
x C	211	1.461890	-0.228601	0.824056	x
x C	212	1.459860	-0.562746	0.910208	x
x C	213	1.434640	-0.474493	0.909807	x
x C	214	1.388523	-0.403383	0.943441	x
x C	215	1.372130	-0.424926	0.977002	x

x C	216	1.401318	-0.515628	0.975810	x
x C	217	1.280261	-0.608483	0.892018	x
x C	218	1.203979	-0.589879	0.863811	x
x C	219	1.222600	-0.662373	0.832044	x
x C	220	1.318767	-0.749308	0.829046	x
x C	221	1.391787	-0.761104	0.857359	x
x C	222	1.142564	-0.649125	0.803349	x
x C	223	0.980969	-0.561631	0.784250	x
x C	224	1.091767	-0.708334	0.748701	x
x C	225	1.223955	-0.929430	0.669790	x
x C	226	1.208065	-0.861787	0.703329	x
x C	227	1.113155	-0.783584	0.713882	x
x C	228	1.037522	-0.776240	0.689752	x
x C	229	1.059097	-0.847188	0.657222	x
x C	230	0.712452	-0.361630	0.758946	x
x C	231	0.806736	-0.449496	0.755944	x
x C	232	0.878766	-0.471025	0.788545	x
x C	233	0.851985	-0.403091	0.823869	x
x C	234	0.756041	-0.316802	0.825003	x
x C	235	0.889352	0.593521	1.050951	x
x C	236	0.993575	0.503310	1.054207	x
x C	237	1.028223	0.417536	1.063279	x
x C	238	1.129325	0.326560	1.064273	x
x C	239	1.152561	0.241278	1.071296	x
x C	240	1.246052	0.150466	1.068946	x
x C	241	1.319610	0.144049	1.059470	x
x C	242	1.299581	0.228949	1.055101	x
x C	243	1.206324	0.318163	1.057162	x
x C	244	1.432440	-0.029405	1.049980	x
x C	245	0.684734	-0.125186	1.050937	x
x C	246	0.782952	-0.167738	1.043294	x
x C	247	0.837226	-0.150826	1.069129	x
x C	248	0.935590	-0.195007	1.063771	x
x C	249	0.993079	-0.274691	1.034051	x
x C	250	1.086793	-0.315598	1.030547	x
x C	251	1.127475	-0.279538	1.057427	x
x C	252	1.072086	-0.200568	1.087271	x
x C	253	0.977358	-0.159520	1.089968	x
x C	254	1.269006	-0.299526	1.082910	x
x C	255	1.225717	0.036101	0.789501	x
x C	256	1.119358	0.121509	0.791407	x
x C	257	1.083020	0.195486	0.822111	x
x C	258	0.981634	0.281617	0.826864	x
x C	259	0.903672	0.303766	0.797282	x
x C	260	0.808485	0.385337	0.804510	x
x C	261	0.787742	0.447745	0.841795	x

x C	262	0.864031	0.429087	0.870745	x
x C	263	0.959182	0.346939	0.863010	x
x C	264	0.669792	0.580578	0.887328	x
x N	1	-0.172093	1.484417	0.337398	x
x N	2	0.077039	1.046894	0.552062	x
x N	3	-0.583397	1.443782	0.442732	x
x N	4	-0.129190	1.296595	0.445137	x
x N	5	-0.236327	1.294379	0.471687	x
x N	6	-0.292561	1.384257	0.413445	x
x N	7	-0.692426	1.373116	0.389050	x
x N	8	-0.720650	1.166959	0.272424	x
x N	9	-0.567557	1.050712	0.310323	x
x N	10	-0.630697	0.997629	0.253703	x
x N	11	-0.295499	0.686860	0.292919	x
x N	12	-0.923166	1.150854	0.147180	x
x N	13	-1.484417	0.172093	0.162602	x
x N	14	-1.046894	-0.077039	-0.052062	x
x N	15	-1.443782	0.583397	0.057268	x
x N	16	-1.296595	0.129190	0.054863	x
x N	17	-1.294379	0.236327	0.028313	x
x N	18	-1.384257	0.292561	0.086555	x
x N	19	-1.373116	0.692426	0.110950	x
x N	20	-1.166959	0.720650	0.227576	x
x N	21	-1.050712	0.567557	0.189677	x
x N	22	-0.997629	0.630697	0.246297	x
x N	23	-0.686860	0.295499	0.207081	x
x N	24	-1.150854	0.923166	0.352820	x
x N	25	0.172093	-1.484417	-0.337398	x
x N	26	-0.077039	-1.046894	-0.552062	x
x N	27	0.583397	-1.443782	-0.442732	x
x N	28	0.129190	-1.296595	-0.445137	x
x N	29	0.236327	-1.294379	-0.471687	x
x N	30	0.292561	-1.384257	-0.413445	x
x N	31	0.692426	-1.373116	-0.389050	x
x N	32	0.720650	-1.166959	-0.272424	x
x N	33	0.567557	-1.050712	-0.310323	x
x N	34	0.630697	-0.997629	-0.253703	x
x N	35	0.295499	-0.686860	-0.292919	x
x N	36	0.923166	-1.150854	-0.147180	x
x N	37	1.484417	-0.172093	0.837398	x
x N	38	1.046894	0.077039	1.052062	x
x N	39	1.443782	-0.583397	0.942732	x
x N	40	1.296595	-0.129190	0.945137	x
x N	41	1.294379	-0.236327	0.971687	x
x N	42	1.384257	-0.292561	0.913445	x
x N	43	1.373116	-0.692426	0.889050	x

x N	44	1.166959	-0.720650	0.772424	x
x N	45	1.050712	-0.567557	0.810323	x
x N	46	0.997629	-0.630697	0.753703	x
x N	47	0.686860	-0.295499	0.792919	x
x N	48	1.150854	-0.923166	0.647180	x
x O	1	0.059847	1.412602	0.553754	x
x O	2	-0.328077	1.222589	0.552767	x
x O	3	0.524690	0.691215	0.346904	x
x O	4	-1.412602	-0.059847	-0.053754	x
x O	5	-1.222589	0.328077	-0.052767	x
x O	6	-0.691215	-0.524690	0.153096	x
x O	7	-0.059847	-1.412602	-0.553754	x
x O	8	0.328077	-1.222589	-0.552767	x
x O	9	-0.524690	-0.691215	-0.346904	x
x O	10	1.412602	0.059847	1.053754	x
x O	11	1.222589	-0.328077	1.052767	x
x O	12	0.691215	0.524690	0.846904	x
x Zn	1	-0.161537	1.545919	0.293639	x
x Zn	2	0.174166	0.966458	0.602152	x
x Zn	3	-0.715839	1.480023	0.437086	x
x Zn	4	-1.545919	0.161537	0.206361	x
x Zn	5	-0.966458	-0.174166	-0.102152	x
x Zn	6	-1.480023	0.715839	0.062914	x
x Zn	7	0.161537	-1.545919	-0.293639	x
x Zn	8	-0.174166	-0.966458	-0.602152	x
x Zn	9	0.715839	-1.480023	-0.437086	x
x Zn	10	1.545919	-0.161537	0.793639	x
x Zn	11	0.966458	0.174166	1.102152	x
x Zn	12	1.480023	-0.715839	0.937086	x
x I	1	-0.150634	1.449980	0.222754	x
x I	2	-0.028704	1.550176	0.329277	x
x I	3	0.347891	0.859692	0.582767	x
x I	4	0.105906	0.905324	0.629971	x
x I	5	-0.842286	1.635828	0.398762	x
x I	6	-0.716259	1.428209	0.503843	x
x I	7	-1.449980	0.150634	0.277246	x
x I	8	-1.550176	0.028704	0.170723	x
x I	9	-0.859692	-0.347891	-0.082767	x
x I	10	-0.905324	-0.105906	-0.129971	x
x I	11	-1.635828	0.842286	0.101238	x
x I	12	-1.428209	0.716259	-0.003843	x
x I	13	0.150634	-1.449980	-0.222754	x
x I	14	0.028704	-1.550176	-0.329277	x
x I	15	-0.347891	-0.859692	-0.582767	x
x I	16	-0.105906	-0.905324	-0.629971	x
x I	17	0.842286	-1.635828	-0.398762	x

x I	18	0.716259	-1.428209	-0.503843	x
x I	19	1.449980	-0.150634	0.722754	x
x I	20	1.550176	-0.028704	0.829277	x
x I	21	0.859692	0.347891	1.082767	x
x I	22	0.905324	0.105906	1.129971	x
x I	23	1.635828	-0.842286	0.898762	x
x I	24	1.428209	-0.716259	1.003843	x

Table S5. Fractional atomic coordinates of the optimised structure of (+)-artemisinin@**1a**

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----					x
x	H	1	-1.213154	1.491774	-0.145004	x
x	H	2	-1.095408	1.431368	-0.083182	x
x	H	3	-1.315235	1.713389	-0.018840	x
x	H	4	-1.426504	1.762557	-0.083075	x
x	H	5	-0.677082	1.132623	0.077052	x
x	H	6	-0.820837	1.314887	0.080412	x
x	H	7	-0.940665	1.262121	-0.036130	x
x	H	8	-0.792256	1.081424	-0.034719	x
x	H	9	-1.237838	1.886938	0.117158	x
x	H	10	-1.221753	1.763521	0.060587	x
x	H	11	-0.930523	1.539573	0.117733	x
x	H	12	-0.958234	1.669937	0.172170	x
x	H	13	-0.777965	0.987036	0.043768	x
x	H	14	-0.800742	0.939351	0.095707	x
x	H	15	-0.494031	0.771955	0.139806	x
x	H	16	-0.482992	0.827645	0.087075	x
x	H	17	-0.936391	0.837914	0.247319	x
x	H	18	-0.784564	0.802009	0.242691	x
x	H	19	-0.891395	0.848381	0.118851	x
x	H	20	-1.038401	0.882623	0.128298	x
x	H	21	-0.293508	0.638532	0.286347	x
x	H	22	-0.438343	0.742711	0.236678	x
x	H	23	-0.531345	0.596198	0.243138	x
x	H	24	-0.376472	0.490424	0.290348	x
x	H	25	-0.395571	0.663692	0.356136	x
x	H	26	-0.455693	0.780895	0.418795	x
x	H	27	-0.166098	0.568840	0.480554	x
x	H	28	-0.117950	0.457395	0.416248	x
x	H	29	-0.742960	1.195853	0.582731	x
x	H	30	-0.561443	1.052913	0.585550	x
x	H	31	-0.615155	0.946220	0.465248	x
x	H	32	-0.796012	1.092117	0.468141	x
x	H	33	0.011087	0.631785	0.617427	x
x	H	34	-0.114375	0.650219	0.561214	x
x	H	35	-0.334264	0.943753	0.618005	x
x	H	36	-0.201724	0.916064	0.670851	x
x	H	37	-0.037109	0.934878	0.749489	x
x	H	38	-0.073576	1.089118	0.748219	x
x	H	39	-0.036887	0.996476	0.623283	x
x	H	40	-0.003328	0.847434	0.629115	x
x	H	41	-0.287004	1.615946	0.770471	x

x H	42	-0.183044	1.467213	0.720632	x
x H	43	-0.264642	1.337661	0.756619	x
x H	44	-0.370397	1.493954	0.803342	x
x H	45	0.128441	1.092832	0.555833	x
x H	46	0.068216	1.077355	0.604668	x
x H	47	-0.136563	1.392200	0.631908	x
x H	48	-0.072012	1.397751	0.581056	x
x H	49	0.228888	0.284371	0.248990	x
x H	50	0.126175	0.304138	0.254138	x
x H	51	0.241873	0.217828	0.281140	x
x H	52	0.129494	0.374738	0.324405	x
x H	53	0.294413	0.349109	0.307322	x
x H	54	0.186436	0.536421	0.319774	x
x H	55	0.009797	0.626404	0.305870	x
x H	56	0.020574	0.567825	0.340787	x
x H	57	0.024606	0.482711	0.272423	x
x H	58	0.120883	0.469289	0.264430	x
x H	59	0.364882	0.196041	0.323503	x
x H	60	0.282631	0.253555	0.358056	x
x H	61	0.445980	0.176819	0.392644	x
x H	62	0.456741	0.240481	0.369948	x
x H	63	0.393533	0.355701	0.480184	x
x H	64	0.500558	0.253097	0.455855	x
x H	65	0.418641	0.243243	0.462269	x
x H	66	0.137227	0.439757	0.381559	x
x H	67	0.198972	0.606735	0.387021	x
x H	68	-0.019475	0.755096	0.353816	x
x H	69	0.075665	0.720057	0.331986	x
x H	70	0.056459	0.778790	0.382174	x
x H	71	-0.327514	0.881659	0.373788	x
x H	72	-0.213177	0.822547	0.359581	x
x H	73	-0.246165	0.753144	0.355479	x
x H	74	-0.536246	0.909786	0.308043	x
x H	75	-0.517986	0.993994	0.320069	x
x H	76	-0.461110	0.905792	0.353198	x
x H	77	-0.221001	0.694480	0.283059	x
x H	78	-0.187160	0.761790	0.284926	x
x H	79	-0.285009	0.782156	0.248903	x
x H	80	-0.401440	0.963313	0.272988	x
x H	81	-0.301214	0.943352	0.306538	x
x H	82	-0.412555	1.006755	0.324936	x
x H	83	-1.491774	1.213154	0.145004	x
x H	84	-1.431368	1.095408	0.083182	x
x H	85	-1.713389	1.315235	0.018840	x
x H	86	-1.762557	1.426504	0.083075	x
x H	87	-1.132623	0.677082	-0.077052	x

x H	88	-1.314887	0.820837	-0.080412	x
x H	89	-1.262121	0.940665	0.036130	x
x H	90	-1.081424	0.792256	0.034719	x
x H	91	-1.886938	1.237838	-0.117158	x
x H	92	-1.763521	1.221753	-0.060587	x
x H	93	-1.539573	0.930523	-0.117733	x
x H	94	-1.669937	0.958234	-0.172170	x
x H	95	-0.987036	0.777965	-0.043768	x
x H	96	-0.939351	0.800742	-0.095707	x
x H	97	-0.771955	0.494031	-0.139806	x
x H	98	-0.827645	0.482992	-0.087075	x
x H	99	-0.837914	0.936391	-0.247319	x
x H	100	-0.802009	0.784564	-0.242691	x
x H	101	-0.848381	0.891395	-0.118851	x
x H	102	-0.882623	1.038401	-0.128298	x
x H	103	-0.638532	0.293508	-0.286347	x
x H	104	-0.742711	0.438343	-0.236678	x
x H	105	-0.596198	0.531345	-0.243138	x
x H	106	-0.490424	0.376472	-0.290348	x
x H	107	-0.663692	0.395571	-0.356136	x
x H	108	-0.780895	0.455693	-0.418795	x
x H	109	-0.568840	0.166098	-0.480554	x
x H	110	-0.457395	0.117950	-0.416248	x
x H	111	-1.195853	0.742960	-0.582731	x
x H	112	-1.052913	0.561443	-0.585550	x
x H	113	-0.946220	0.615155	-0.465248	x
x H	114	-1.092117	0.796012	-0.468141	x
x H	115	-0.631785	-0.011087	-0.617427	x
x H	116	-0.650219	0.114375	-0.561214	x
x H	117	-0.943753	0.334264	-0.618005	x
x H	118	-0.916064	0.201724	-0.670851	x
x H	119	-0.934878	0.037109	-0.749489	x
x H	120	-1.089118	0.073576	-0.748219	x
x H	121	-0.996476	0.036887	-0.623283	x
x H	122	-0.847434	0.003328	-0.629115	x
x H	123	-1.615946	0.287004	-0.770471	x
x H	124	-1.467213	0.183044	-0.720632	x
x H	125	-1.337661	0.264642	-0.756619	x
x H	126	-1.493954	0.370397	-0.803342	x
x H	127	-1.092832	-0.128441	-0.555833	x
x H	128	-1.077355	-0.068216	-0.604668	x
x H	129	-1.392200	0.136563	-0.631908	x
x H	130	-1.397751	0.072012	-0.581056	x
x H	131	-0.284371	-0.228888	-0.248990	x
x H	132	-0.304138	-0.126175	-0.254138	x
x H	133	-0.217828	-0.241873	-0.281140	x

x H	134	-0.374738	-0.129494	-0.324405	x
x H	135	-0.349109	-0.294413	-0.307322	x
x H	136	-0.536421	-0.186436	-0.319774	x
x H	137	-0.626404	-0.009797	-0.305870	x
x H	138	-0.567825	-0.020574	-0.340787	x
x H	139	-0.482711	-0.024606	-0.272423	x
x H	140	-0.469289	-0.120883	-0.264430	x
x H	141	-0.196041	-0.364882	-0.323503	x
x H	142	-0.253555	-0.282631	-0.358056	x
x H	143	-0.176819	-0.445980	-0.392644	x
x H	144	-0.240481	-0.456741	-0.369948	x
x H	145	-0.355701	-0.393533	-0.480184	x
x H	146	-0.253097	-0.500558	-0.455855	x
x H	147	-0.243243	-0.418641	-0.462269	x
x H	148	-0.439757	-0.137227	-0.381559	x
x H	149	-0.606735	-0.198972	-0.387021	x
x H	150	-0.755096	0.019475	-0.353816	x
x H	151	-0.720057	-0.075665	-0.331986	x
x H	152	-0.778790	-0.056459	-0.382174	x
x H	153	-0.881659	0.327514	-0.373788	x
x H	154	-0.822547	0.213177	-0.359581	x
x H	155	-0.753144	0.246165	-0.355479	x
x H	156	-0.909786	0.536246	-0.308043	x
x H	157	-0.993994	0.517986	-0.320069	x
x H	158	-0.905792	0.461110	-0.353198	x
x H	159	-0.694480	0.221001	-0.283059	x
x H	160	-0.761790	0.187160	-0.284926	x
x H	161	-0.782156	0.285009	-0.248903	x
x H	162	-0.963313	0.401440	-0.272988	x
x H	163	-0.943352	0.301214	-0.306538	x
x H	164	-1.006755	0.412555	-0.324936	x
x C	1	-1.233388	1.538874	-0.116553	x
x C	2	-1.167810	1.505204	-0.082075	x
x C	3	-1.196015	1.568023	-0.046168	x
x C	4	-1.290113	1.662232	-0.046261	x
x C	5	-1.352144	1.690297	-0.081999	x
x C	6	-0.737851	1.164611	0.052891	x
x C	7	-0.817233	1.265530	0.054341	x
x C	8	-0.892991	1.302561	0.022338	x
x C	9	-0.884253	1.235840	-0.010353	x
x C	10	-0.802848	1.136223	-0.009755	x
x C	11	-1.171130	1.809081	0.115776	x
x C	12	-1.161368	1.740702	0.084454	x
x C	13	-1.073683	1.641842	0.084224	x
x C	14	-0.999316	1.615634	0.116099	x
x C	15	-1.014647	1.688112	0.146739	x

x C	16	-1.124583	1.534556	-0.009607	x
x C	17	-0.980017	1.409455	0.022391	x
x C	18	-1.062485	1.568258	0.050851	x
x C	19	-0.717170	0.939972	0.065826	x
x C	20	-0.729500	0.913510	0.094508	x
x C	21	-0.648430	0.851830	0.121728	x
x C	22	-0.558301	0.820219	0.119134	x
x C	23	-0.551730	0.849962	0.089875	x
x C	24	-0.923073	0.839894	0.219691	x
x C	25	-0.839914	0.820206	0.216866	x
x C	26	-0.826921	0.822828	0.180465	x
x C	27	-0.899181	0.846348	0.147816	x
x C	28	-0.980153	0.864477	0.152796	x
x C	29	-0.346685	0.629861	0.275159	x
x C	30	-0.427123	0.687057	0.247308	x
x C	31	-0.494009	0.674140	0.234928	x
x C	32	-0.478416	0.605223	0.251454	x
x C	33	-0.394568	0.548234	0.277935	x
x C	34	-0.654865	0.817199	0.152014	x
x C	35	-0.736891	0.800083	0.178085	x
x C	36	-0.580724	0.732303	0.205192	x
x C	37	-0.347499	0.644901	0.384383	x
x C	38	-0.380545	0.709957	0.419114	x
x C	39	-0.314856	0.684160	0.454299	x
x C	40	-0.219011	0.591966	0.453568	x
x C	41	-0.191720	0.530057	0.417794	x
x C	42	-0.711290	1.138357	0.557559	x
x C	43	-0.610535	1.059402	0.558650	x
x C	44	-0.574381	0.987861	0.525235	x
x C	45	-0.641158	1.000158	0.491766	x
x C	46	-0.740726	1.079999	0.493135	x
x C	47	-0.066275	0.699717	0.615969	x
x C	48	-0.135837	0.710367	0.584994	x
x C	49	-0.233996	0.799243	0.584795	x
x C	50	-0.258634	0.874033	0.616346	x
x C	51	-0.184942	0.858453	0.646222	x
x C	52	-0.346504	0.755193	0.491035	x
x C	53	-0.468577	0.899715	0.524358	x
x C	54	-0.308844	0.812718	0.551701	x
x C	55	-0.036887	0.951619	0.722390	x
x C	56	-0.056708	1.036102	0.721564	x
x C	57	-0.056186	1.052981	0.685640	x
x C	58	-0.035785	0.984240	0.651860	x
x C	59	-0.018066	0.902251	0.654787	x
x C	60	-0.280083	1.552611	0.766072	x
x C	61	-0.223011	1.470733	0.738860	x

x C	62	-0.216749	1.391889	0.735093	x
x C	63	-0.269288	1.398599	0.758688	x
x C	64	-0.326400	1.483744	0.784733	x
x C	65	0.067871	1.157932	0.572265	x
x C	66	0.035021	1.149192	0.599567	x
x C	67	-0.039025	1.233836	0.621803	x
x C	68	-0.078879	1.325032	0.615086	x
x C	69	-0.044120	1.328433	0.586853	x
x C	70	-0.080157	1.143701	0.683155	x
x C	71	-0.154794	1.302802	0.707032	x
x C	72	-0.073012	1.228352	0.652762	x
x C	73	0.192815	0.289524	0.270323	x
x C	74	0.165049	0.372829	0.303840	x
x C	75	0.256232	0.354906	0.327973	x
x C	76	0.228005	0.443909	0.359281	x
x C	77	0.151357	0.541814	0.341782	x
x C	78	0.060484	0.557934	0.319608	x
x C	79	0.090033	0.471704	0.287398	x
x C	80	0.326833	0.258838	0.346872	x
x C	81	0.404587	0.245914	0.380847	x
x C	82	0.363776	0.328809	0.416291	x
x C	83	0.423106	0.293276	0.456367	x
x C	84	0.190962	0.448292	0.393888	x
x C	85	0.095845	0.628860	0.410133	x
x C	86	0.128220	0.625583	0.374826	x
x C	87	0.055978	0.725796	0.359795	x
x C	88	-0.322721	0.847571	0.309259	x
x C	89	-0.274828	0.825197	0.352216	x
x C	90	-0.482536	0.917994	0.321521	x
x C	91	-0.249579	0.766300	0.279671	x
x C	92	-0.362187	0.946521	0.303281	x
x C	93	-1.538874	1.233388	0.116553	x
x C	94	-1.505204	1.167810	0.082075	x
x C	95	-1.568023	1.196015	0.046168	x
x C	96	-1.662232	1.290113	0.046261	x
x C	97	-1.690297	1.352144	0.081999	x
x C	98	-1.164611	0.737851	-0.052891	x
x C	99	-1.265530	0.817233	-0.054341	x
x C	100	-1.302561	0.892991	-0.022338	x
x C	101	-1.235840	0.884253	0.010353	x
x C	102	-1.136223	0.802848	0.009755	x
x C	103	-1.809081	1.171130	-0.115776	x
x C	104	-1.740702	1.161368	-0.084454	x
x C	105	-1.641842	1.073683	-0.084224	x
x C	106	-1.615634	0.999316	-0.116099	x
x C	107	-1.688112	1.014647	-0.146739	x

x C	108	-1.534556	1.124583	0.009607	x
x C	109	-1.409455	0.980017	-0.022391	x
x C	110	-1.568258	1.062485	-0.050851	x
x C	111	-0.939972	0.717170	-0.065826	x
x C	112	-0.913510	0.729500	-0.094508	x
x C	113	-0.851830	0.648430	-0.121728	x
x C	114	-0.820219	0.558301	-0.119134	x
x C	115	-0.849962	0.551730	-0.089875	x
x C	116	-0.839894	0.923073	-0.219691	x
x C	117	-0.820206	0.839914	-0.216866	x
x C	118	-0.822828	0.826921	-0.180465	x
x C	119	-0.846348	0.899181	-0.147816	x
x C	120	-0.864477	0.980153	-0.152796	x
x C	121	-0.629861	0.346685	-0.275159	x
x C	122	-0.687057	0.427123	-0.247308	x
x C	123	-0.674140	0.494009	-0.234928	x
x C	124	-0.605223	0.478416	-0.251454	x
x C	125	-0.548234	0.394568	-0.277935	x
x C	126	-0.817199	0.654865	-0.152014	x
x C	127	-0.800083	0.736891	-0.178085	x
x C	128	-0.732303	0.580724	-0.205192	x
x C	129	-0.644901	0.347499	-0.384383	x
x C	130	-0.709957	0.380545	-0.419114	x
x C	131	-0.684160	0.314856	-0.454299	x
x C	132	-0.591966	0.219011	-0.453568	x
x C	133	-0.530057	0.191720	-0.417794	x
x C	134	-1.138357	0.711290	-0.557559	x
x C	135	-1.059402	0.610535	-0.558650	x
x C	136	-0.987861	0.574381	-0.525235	x
x C	137	-1.000158	0.641158	-0.491766	x
x C	138	-1.079999	0.740726	-0.493135	x
x C	139	-0.699717	0.066275	-0.615969	x
x C	140	-0.710367	0.135837	-0.584994	x
x C	141	-0.799243	0.233996	-0.584795	x
x C	142	-0.874033	0.258634	-0.616346	x
x C	143	-0.858453	0.184942	-0.646222	x
x C	144	-0.755193	0.346504	-0.491035	x
x C	145	-0.899715	0.468577	-0.524358	x
x C	146	-0.812718	0.308844	-0.551701	x
x C	147	-0.951619	0.036887	-0.722390	x
x C	148	-1.036102	0.056708	-0.721564	x
x C	149	-1.052981	0.056186	-0.685640	x
x C	150	-0.984240	0.035785	-0.651860	x
x C	151	-0.902251	0.018066	-0.654787	x
x C	152	-1.552611	0.280083	-0.766072	x
x C	153	-1.470733	0.223011	-0.738860	x

x C	154	-1.391889	0.216749	-0.735093	x
x C	155	-1.398599	0.269288	-0.758688	x
x C	156	-1.483744	0.326400	-0.784733	x
x C	157	-1.157932	-0.067871	-0.572265	x
x C	158	-1.149192	-0.035021	-0.599567	x
x C	159	-1.233836	0.039025	-0.621803	x
x C	160	-1.325032	0.078879	-0.615086	x
x C	161	-1.328433	0.044120	-0.586853	x
x C	162	-1.143701	0.080157	-0.683155	x
x C	163	-1.302802	0.154794	-0.707032	x
x C	164	-1.228352	0.073012	-0.652762	x
x C	165	-0.289524	-0.192815	-0.270323	x
x C	166	-0.372829	-0.165049	-0.303840	x
x C	167	-0.354906	-0.256232	-0.327973	x
x C	168	-0.443909	-0.228005	-0.359281	x
x C	169	-0.541814	-0.151357	-0.341782	x
x C	170	-0.557934	-0.060484	-0.319608	x
x C	171	-0.471704	-0.090033	-0.287398	x
x C	172	-0.258838	-0.326833	-0.346872	x
x C	173	-0.245914	-0.404587	-0.380847	x
x C	174	-0.328809	-0.363776	-0.416291	x
x C	175	-0.293276	-0.423106	-0.456367	x
x C	176	-0.448292	-0.190962	-0.393888	x
x C	177	-0.628860	-0.095845	-0.410133	x
x C	178	-0.625583	-0.128220	-0.374826	x
x C	179	-0.725796	-0.055978	-0.359795	x
x C	180	-0.847571	0.322721	-0.309259	x
x C	181	-0.825197	0.274828	-0.352216	x
x C	182	-0.917994	0.482536	-0.321521	x
x C	183	-0.766300	0.249579	-0.279671	x
x C	184	-0.946521	0.362187	-0.303281	x
x N	1	-1.324024	1.630005	-0.116861	x
x N	2	-0.730650	1.100100	0.021497	x
x N	3	-1.098791	1.783853	0.146522	x
x N	4	-1.051058	1.436714	-0.008801	x
x N	5	-0.981873	1.472010	0.052977	x
x N	6	-1.134653	1.603210	0.019615	x
x N	7	-0.629792	0.909196	0.063403	x
x N	8	-0.992329	0.861370	0.188051	x
x N	9	-0.329239	0.560094	0.289713	x
x N	10	-0.737574	0.835026	0.149654	x
x N	11	-0.659430	0.745774	0.205501	x
x N	12	-0.575533	0.768264	0.179488	x
x N	13	-0.254493	0.556519	0.383486	x
x N	14	-0.776102	1.148347	0.525596	x
x N	15	-0.089719	0.772985	0.646053	x

x N	16	-0.443561	0.830631	0.492514	x
x N	17	-0.404067	0.894694	0.554723	x
x N	18	-0.276025	0.741819	0.520123	x
x N	19	-0.017694	0.885438	0.689641	x
x N	20	-0.331062	1.559236	0.788827	x
x N	21	0.028981	1.246348	0.565882	x
x N	22	-0.132670	1.221092	0.710891	x
x N	23	-0.125707	1.309855	0.678908	x
x N	24	-0.049957	1.143963	0.652984	x
x N	25	-1.630005	1.324024	0.116861	x
x N	26	-1.100100	0.730650	-0.021497	x
x N	27	-1.783853	1.098791	-0.146522	x
x N	28	-1.436714	1.051058	0.008801	x
x N	29	-1.472010	0.981873	-0.052977	x
x N	30	-1.603210	1.134653	-0.019615	x
x N	31	-0.909196	0.629792	-0.063403	x
x N	32	-0.861370	0.992329	-0.188051	x
x N	33	-0.560094	0.329239	-0.289713	x
x N	34	-0.835026	0.737574	-0.149654	x
x N	35	-0.745774	0.659430	-0.205501	x
x N	36	-0.768264	0.575533	-0.179488	x
x N	37	-0.556519	0.254493	-0.383486	x
x N	38	-1.148347	0.776102	-0.525596	x
x N	39	-0.772985	0.089719	-0.646053	x
x N	40	-0.830631	0.443561	-0.492514	x
x N	41	-0.894694	0.404067	-0.554723	x
x N	42	-0.741819	0.276025	-0.520123	x
x N	43	-0.885438	0.017694	-0.689641	x
x N	44	-1.559236	0.331062	-0.788827	x
x N	45	-1.246348	-0.028981	-0.565882	x
x N	46	-1.221092	0.132670	-0.710891	x
x N	47	-1.309855	0.125707	-0.678908	x
x N	48	-1.143963	0.049957	-0.652984	x
x O	1	0.316317	0.430117	0.371918	x
x O	2	0.359914	0.403404	0.413223	x
x O	3	0.264463	0.374577	0.418778	x
x O	4	0.136527	0.542024	0.419846	x
x O	5	0.038259	0.704326	0.431798	x
x O	6	-0.401369	0.846294	0.298775	x
x O	7	-0.430117	-0.316317	-0.371918	x
x O	8	-0.403404	-0.359914	-0.413223	x
x O	9	-0.374577	-0.264463	-0.418778	x
x O	10	-0.542024	-0.136527	-0.419846	x
x O	11	-0.704326	-0.038259	-0.431798	x
x O	12	-0.846294	0.401369	-0.298775	x
x Zn	1	-1.414409	1.682609	-0.170171	x

x Zn	2	-0.611559	0.948358	0.018711	x
x Zn	3	-1.117849	0.892718	0.191888	x
x Zn	4	-0.203769	0.470807	0.329665	x
x Zn	5	-0.926341	1.262934	0.523326	x
x Zn	6	0.018153	0.755956	0.691468	x
x Zn	7	-1.682609	1.414409	0.170171	x
x Zn	8	-0.948358	0.611559	-0.018711	x
x Zn	9	-0.892718	1.117849	-0.191888	x
x Zn	10	-0.470807	0.203769	-0.329665	x
x Zn	11	-1.262934	0.926341	-0.523326	x
x Zn	12	-0.755956	-0.018153	-0.691468	x
x I	1	-1.405650	1.806028	-0.178533	x
x I	2	-1.574289	1.725821	-0.172462	x
x I	3	-0.627978	0.872061	-0.052355	x
x I	4	-0.447716	0.907708	0.047410	x
x I	5	-1.263106	1.059224	0.164932	x
x I	6	-1.107356	0.858735	0.258917	x
x I	7	-0.152071	0.304002	0.321205	x
x I	8	-0.085832	0.491165	0.324457	x
x I	9	-1.007503	1.248172	0.452529	x
x I	10	-0.970541	1.429820	0.547783	x
x I	11	-0.018904	0.770077	0.758830	x
x I	12	0.185772	0.608596	0.666113	x
x I	13	-1.806028	1.405650	0.178533	x
x I	14	-1.725821	1.574289	0.172462	x
x I	15	-0.872061	0.627978	0.052355	x
x I	16	-0.907708	0.447716	-0.047410	x
x I	17	-1.059224	1.263106	-0.164932	x
x I	18	-0.858735	1.107356	-0.258917	x
x I	19	-0.304002	0.152071	-0.321205	x
x I	20	-0.491165	0.085832	-0.324457	x
x I	21	-1.248172	1.007503	-0.452529	x
x I	22	-1.429820	0.970541	-0.547783	x
x I	23	-0.770077	0.018904	-0.758830	x
x I	24	-0.608596	-0.185772	-0.666113	x

Table S6. Fractional atomic coordinates of the optimised structure of 4-(trifluoromethyl)phenyl azide@**1a**

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	H	1	0.168324	1.519516	0.834785	x
x	H	2	0.207308	1.398528	0.770671	x
x	H	3	0.512098	1.215168	0.818142	x
x	H	4	0.462365	1.344127	0.878669	x
x	H	5	0.239637	1.087861	0.562492	x
x	H	6	0.374698	1.059498	0.613217	x
x	H	7	0.157121	1.297290	0.700784	x
x	H	8	0.030375	1.313541	0.647591	x
x	H	9	0.840363	0.893650	0.762023	x
x	H	10	0.664266	1.052662	0.757274	x
x	H	11	0.597095	0.897051	0.672814	x
x	H	12	0.775850	0.743765	0.680583	x
x	H	13	0.046266	1.111360	0.621334	x
x	H	14	0.090968	0.953802	0.625142	x
x	H	15	0.148370	0.883463	0.488343	x
x	H	16	0.097440	1.046207	0.489153	x
x	H	17	0.096644	0.555260	0.653237	x
x	H	18	0.171158	0.563481	0.598168	x
x	H	19	0.025962	0.856047	0.654392	x
x	H	20	-0.039043	0.834947	0.708931	x
x	H	21	0.481123	0.485415	0.435895	x
x	H	22	0.354806	0.636502	0.484365	x
x	H	23	0.292554	0.479085	0.520746	x
x	H	24	0.421562	0.335060	0.471981	x
x	H	25	0.194702	0.381154	0.618378	x
x	H	26	0.283046	0.390930	0.632922	x
x	H	27	0.320513	0.274374	0.626792	x
x	H	28	0.198753	0.294591	0.542167	x
x	H	29	0.327680	0.194440	0.548921	x
x	H	30	0.274688	0.265077	0.502865	x
x	H	31	0.395961	0.282439	0.525049	x
x	H	32	0.441074	0.223168	0.574566	x
x	H	33	0.391056	0.344715	0.577137	x
x	H	34	0.106327	0.441545	0.509301	x
x	H	35	0.073759	0.553131	0.533070	x
x	H	36	0.088465	0.476415	0.566918	x
x	H	37	0.102497	1.347319	0.414846	x
x	H	38	0.185281	1.177120	0.421467	x
x	H	39	0.465726	1.083699	0.422844	x

x H	40	0.384081	1.253131	0.416777	x
x H	41	-1.519516	-0.168324	-0.334785	x
x H	42	-1.398528	-0.207308	-0.270671	x
x H	43	-1.215168	-0.512098	-0.318142	x
x H	44	-1.344127	-0.462365	-0.378669	x
x H	45	-1.087861	-0.239637	-0.062492	x
x H	46	-1.059498	-0.374698	-0.113217	x
x H	47	-1.297290	-0.157121	-0.200784	x
x H	48	-1.313541	-0.030375	-0.147591	x
x H	49	-0.893650	-0.840363	-0.262023	x
x H	50	-1.052662	-0.664266	-0.257274	x
x H	51	-0.897051	-0.597095	-0.172814	x
x H	52	-0.743765	-0.775850	-0.180583	x
x H	53	-1.111360	-0.046266	-0.121334	x
x H	54	-0.953802	-0.090968	-0.125142	x
x H	55	-0.883463	-0.148370	0.011657	x
x H	56	-1.046207	-0.097440	0.010847	x
x H	57	-0.555260	-0.096644	-0.153237	x
x H	58	-0.563481	-0.171158	-0.098168	x
x H	59	-0.856047	-0.025962	-0.154392	x
x H	60	-0.834947	0.039043	-0.208931	x
x H	61	-0.485415	-0.481123	0.064105	x
x H	62	-0.636502	-0.354806	0.015635	x
x H	63	-0.479085	-0.292554	-0.020746	x
x H	64	-0.335060	-0.421562	0.028019	x
x H	65	-0.381154	-0.194702	-0.118378	x
x H	66	-0.390930	-0.283046	-0.132922	x
x H	67	-0.274374	-0.320513	-0.126792	x
x H	68	-0.294591	-0.198753	-0.042167	x
x H	69	-0.194440	-0.327680	-0.048921	x
x H	70	-0.265077	-0.274688	-0.002865	x
x H	71	-0.282439	-0.395961	-0.025049	x
x H	72	-0.223168	-0.441074	-0.074566	x
x H	73	-0.344715	-0.391056	-0.077137	x
x H	74	-0.441545	-0.106327	-0.009301	x
x H	75	-0.553131	-0.073759	-0.033070	x
x H	76	-0.476415	-0.088465	-0.066918	x
x H	77	-1.347319	-0.102497	0.085154	x
x H	78	-1.177120	-0.185281	0.078533	x
x H	79	-1.083699	-0.465726	0.077156	x
x H	80	-1.253131	-0.384081	0.083223	x
x H	81	-0.168324	-1.519516	-0.834785	x
x H	82	-0.207308	-1.398528	-0.770671	x
x H	83	-0.512098	-1.215168	-0.818142	x
x H	84	-0.462365	-1.344127	-0.878669	x
x H	85	-0.239637	-1.087861	-0.562492	x

x H	86	-0.374698	-1.059498	-0.613217	x
x H	87	-0.157121	-1.297290	-0.700784	x
x H	88	-0.030375	-1.313541	-0.647591	x
x H	89	-0.840363	-0.893650	-0.762023	x
x H	90	-0.664266	-1.052662	-0.757274	x
x H	91	-0.597095	-0.897051	-0.672814	x
x H	92	-0.775850	-0.743765	-0.680583	x
x H	93	-0.046266	-1.111360	-0.621334	x
x H	94	-0.090968	-0.953802	-0.625142	x
x H	95	-0.148370	-0.883463	-0.488343	x
x H	96	-0.097440	-1.046207	-0.489153	x
x H	97	-0.096644	-0.555260	-0.653237	x
x H	98	-0.171158	-0.563481	-0.598168	x
x H	99	-0.025962	-0.856047	-0.654392	x
x H	100	0.039043	-0.834947	-0.708931	x
x H	101	-0.481123	-0.485415	-0.435895	x
x H	102	-0.354806	-0.636502	-0.484365	x
x H	103	-0.292554	-0.479085	-0.520746	x
x H	104	-0.421562	-0.335060	-0.471981	x
x H	105	-0.194702	-0.381154	-0.618378	x
x H	106	-0.283046	-0.390930	-0.632922	x
x H	107	-0.320513	-0.274374	-0.626792	x
x H	108	-0.198753	-0.294591	-0.542167	x
x H	109	-0.327680	-0.194440	-0.548921	x
x H	110	-0.274688	-0.265077	-0.502865	x
x H	111	-0.395961	-0.282439	-0.525049	x
x H	112	-0.441074	-0.223168	-0.574566	x
x H	113	-0.391056	-0.344715	-0.577137	x
x H	114	-0.106327	-0.441545	-0.509301	x
x H	115	-0.073759	-0.553131	-0.533070	x
x H	116	-0.088465	-0.476415	-0.566918	x
x H	117	-0.102497	-1.347319	-0.414846	x
x H	118	-0.185281	-1.177120	-0.421467	x
x H	119	-0.465726	-1.083699	-0.422844	x
x H	120	-0.384081	-1.253131	-0.416777	x
x H	121	1.519516	0.168324	1.334785	x
x H	122	1.398528	0.207308	1.270671	x
x H	123	1.215168	0.512098	1.318142	x
x H	124	1.344127	0.462365	1.378669	x
x H	125	1.087861	0.239637	1.062492	x
x H	126	1.059498	0.374698	1.113217	x
x H	127	1.297290	0.157121	1.200784	x
x H	128	1.313541	0.030375	1.147591	x
x H	129	0.893650	0.840363	1.262023	x
x H	130	1.052662	0.664266	1.257274	x
x H	131	0.897051	0.597095	1.172814	x

x H	132	0.743765	0.775850	1.180583	x
x H	133	1.111360	0.046266	1.121334	x
x H	134	0.953802	0.090968	1.125142	x
x H	135	0.883463	0.148370	0.988343	x
x H	136	1.046207	0.097440	0.989153	x
x H	137	0.555260	0.096644	1.153237	x
x H	138	0.563481	0.171158	1.098168	x
x H	139	0.856047	0.025962	1.154392	x
x H	140	0.834947	-0.039043	1.208931	x
x H	141	0.485415	0.481123	0.935895	x
x H	142	0.636502	0.354806	0.984365	x
x H	143	0.479085	0.292554	1.020746	x
x H	144	0.335060	0.421562	0.971981	x
x H	145	0.381154	0.194702	1.118378	x
x H	146	0.390930	0.283046	1.132922	x
x H	147	0.274374	0.320513	1.126792	x
x H	148	0.294591	0.198753	1.042167	x
x H	149	0.194440	0.327680	1.048921	x
x H	150	0.265077	0.274688	1.002865	x
x H	151	0.282439	0.395961	1.025049	x
x H	152	0.223168	0.441074	1.074566	x
x H	153	0.344715	0.391056	1.077137	x
x H	154	0.441545	0.106327	1.009301	x
x H	155	0.553131	0.073759	1.033070	x
x H	156	0.476415	0.088465	1.066918	x
x H	157	1.347319	0.102497	0.914846	x
x H	158	1.177120	0.185281	0.921467	x
x H	159	1.083699	0.465726	0.922844	x
x H	160	1.253131	0.384081	0.916777	x
x C	1	0.243502	1.451060	0.829828	x
x C	2	0.265526	1.383547	0.794403	x
x C	3	0.363543	1.297528	0.788958	x
x C	4	0.435428	1.282126	0.820160	x
x C	5	0.407953	1.353499	0.854147	x
x C	6	0.224905	1.131979	0.593671	x
x C	7	0.299268	1.116888	0.621749	x
x C	8	0.275888	1.176186	0.661129	x
x C	9	0.177924	1.248847	0.670735	x
x C	10	0.107698	1.258440	0.641591	x
x C	11	0.784105	0.898814	0.741481	x
x C	12	0.686904	0.985931	0.739200	x
x C	13	0.617316	0.987078	0.714117	x
x C	14	0.649281	0.899317	0.692067	x
x C	15	0.747958	0.814281	0.696355	x
x C	16	0.392373	1.223324	0.751637	x
x C	17	0.352309	1.163706	0.691942	x

x C	18	0.512156	1.078261	0.714470	x
x C	19	0.068178	1.059069	0.592658	x
x C	20	0.091948	0.972766	0.594407	x
x C	21	0.120278	0.908457	0.556496	x
x C	22	0.124356	0.933384	0.518018	x
x C	23	0.096985	1.022242	0.518306	x
x C	24	0.084105	0.620050	0.652658	x
x C	25	0.124785	0.625174	0.622199	x
x C	26	0.103719	0.711327	0.622473	x
x C	27	0.043557	0.788294	0.653883	x
x C	28	0.006889	0.777124	0.683623	x
x C	29	0.436872	0.488549	0.455287	x
x C	30	0.367698	0.570905	0.481846	x
x C	31	0.313521	0.568992	0.505223	x
x C	32	0.332918	0.483240	0.502525	x
x C	33	0.403096	0.403951	0.475291	x
x C	34	0.147985	0.815007	0.557888	x
x C	35	0.143275	0.721290	0.589985	x
x C	36	0.238428	0.655519	0.533303	x
x C	37	0.269012	0.346724	0.613789	x
x C	38	0.269639	0.268866	0.538143	x
x C	39	0.384155	0.293746	0.560036	x
x C	40	0.283345	0.334677	0.564950	x
x C	41	0.116334	0.477067	0.538917	x
x C	42	0.237792	1.311388	0.414443	x
x C	43	0.182070	1.289282	0.415674	x
x C	44	0.228673	1.193384	0.419165	x
x C	45	0.330650	1.118583	0.420679	x
x C	46	0.386082	1.140834	0.420081	x
x C	47	0.340178	1.236451	0.416869	x
x C	48	0.379361	1.014712	0.421120	x
x C	49	-1.451060	-0.243502	-0.329828	x
x C	50	-1.383547	-0.265526	-0.294403	x
x C	51	-1.297528	-0.363543	-0.288958	x
x C	52	-1.282126	-0.435428	-0.320160	x
x C	53	-1.353499	-0.407953	-0.354147	x
x C	54	-1.131979	-0.224905	-0.093671	x
x C	55	-1.116888	-0.299268	-0.121749	x
x C	56	-1.176186	-0.275888	-0.161129	x
x C	57	-1.248847	-0.177924	-0.170735	x
x C	58	-1.258440	-0.107698	-0.141591	x
x C	59	-0.898814	-0.784105	-0.241481	x
x C	60	-0.985931	-0.686904	-0.239200	x
x C	61	-0.987078	-0.617316	-0.214117	x
x C	62	-0.899317	-0.649281	-0.192067	x
x C	63	-0.814281	-0.747958	-0.196355	x

x C	64	-1.223324	-0.392373	-0.251637	x
x C	65	-1.163706	-0.352309	-0.191942	x
x C	66	-1.078261	-0.512156	-0.214470	x
x C	67	-1.059069	-0.068178	-0.092658	x
x C	68	-0.972766	-0.091948	-0.094407	x
x C	69	-0.908457	-0.120278	-0.056496	x
x C	70	-0.933384	-0.124356	-0.018018	x
x C	71	-1.022242	-0.096985	-0.018306	x
x C	72	-0.620050	-0.084105	-0.152658	x
x C	73	-0.625174	-0.124785	-0.122199	x
x C	74	-0.711327	-0.103719	-0.122473	x
x C	75	-0.788294	-0.043557	-0.153883	x
x C	76	-0.777124	-0.006889	-0.183623	x
x C	77	-0.488549	-0.436872	0.044713	x
x C	78	-0.570905	-0.367698	0.018154	x
x C	79	-0.568992	-0.313521	-0.005223	x
x C	80	-0.483240	-0.332918	-0.002525	x
x C	81	-0.403951	-0.403096	0.024709	x
x C	82	-0.815007	-0.147985	-0.057888	x
x C	83	-0.721290	-0.143275	-0.089985	x
x C	84	-0.655519	-0.238428	-0.033303	x
x C	85	-0.346724	-0.269012	-0.113789	x
x C	86	-0.268866	-0.269639	-0.038143	x
x C	87	-0.293746	-0.384155	-0.060036	x
x C	88	-0.334677	-0.283345	-0.064950	x
x C	89	-0.477067	-0.116334	-0.038917	x
x C	90	-1.311388	-0.237792	0.085557	x
x C	91	-1.289282	-0.182070	0.084326	x
x C	92	-1.193384	-0.228673	0.080835	x
x C	93	-1.118583	-0.330650	0.079321	x
x C	94	-1.140834	-0.386082	0.079919	x
x C	95	-1.236451	-0.340178	0.083131	x
x C	96	-1.014712	-0.379361	0.078880	x
x C	97	-0.243502	-1.451060	-0.829828	x
x C	98	-0.265526	-1.383547	-0.794403	x
x C	99	-0.363543	-1.297528	-0.788958	x
x C	100	-0.435428	-1.282126	-0.820160	x
x C	101	-0.407953	-1.353499	-0.854147	x
x C	102	-0.224905	-1.131979	-0.593671	x
x C	103	-0.299268	-1.116888	-0.621749	x
x C	104	-0.275888	-1.176186	-0.661129	x
x C	105	-0.177924	-1.248847	-0.670735	x
x C	106	-0.107698	-1.258440	-0.641591	x
x C	107	-0.784105	-0.898814	-0.741481	x
x C	108	-0.686904	-0.985931	-0.739200	x
x C	109	-0.617316	-0.987078	-0.714117	x

x C	110	-0.649281	-0.899317	-0.692067	x
x C	111	-0.747958	-0.814281	-0.696355	x
x C	112	-0.392373	-1.223324	-0.751637	x
x C	113	-0.352309	-1.163706	-0.691942	x
x C	114	-0.512156	-1.078261	-0.714470	x
x C	115	-0.068178	-1.059069	-0.592658	x
x C	116	-0.091948	-0.972766	-0.594407	x
x C	117	-0.120278	-0.908457	-0.556496	x
x C	118	-0.124356	-0.933384	-0.518018	x
x C	119	-0.096985	-1.022242	-0.518306	x
x C	120	-0.084105	-0.620050	-0.652658	x
x C	121	-0.124785	-0.625174	-0.622199	x
x C	122	-0.103719	-0.711327	-0.622473	x
x C	123	-0.043557	-0.788294	-0.653883	x
x C	124	-0.006889	-0.777124	-0.683623	x
x C	125	-0.436872	-0.488549	-0.455287	x
x C	126	-0.367698	-0.570905	-0.481846	x
x C	127	-0.313521	-0.568992	-0.505223	x
x C	128	-0.332918	-0.483240	-0.502525	x
x C	129	-0.403096	-0.403951	-0.475291	x
x C	130	-0.147985	-0.815007	-0.557888	x
x C	131	-0.143275	-0.721290	-0.589985	x
x C	132	-0.238428	-0.655519	-0.533303	x
x C	133	-0.269012	-0.346724	-0.613789	x
x C	134	-0.269639	-0.268866	-0.538143	x
x C	135	-0.384155	-0.293746	-0.560036	x
x C	136	-0.283345	-0.334677	-0.564950	x
x C	137	-0.116334	-0.477067	-0.538917	x
x C	138	-0.237792	-1.311388	-0.414443	x
x C	139	-0.182070	-1.289282	-0.415674	x
x C	140	-0.228673	-1.193384	-0.419165	x
x C	141	-0.330650	-1.118583	-0.420679	x
x C	142	-0.386082	-1.140834	-0.420081	x
x C	143	-0.340178	-1.236451	-0.416869	x
x C	144	-0.379361	-1.014712	-0.421120	x
x C	145	1.451060	0.243502	1.329828	x
x C	146	1.383547	0.265526	1.294403	x
x C	147	1.297528	0.363543	1.288958	x
x C	148	1.282126	0.435428	1.320160	x
x C	149	1.353499	0.407953	1.354147	x
x C	150	1.131979	0.224905	1.093671	x
x C	151	1.116888	0.299268	1.121749	x
x C	152	1.176186	0.275888	1.161129	x
x C	153	1.248847	0.177924	1.170735	x
x C	154	1.258440	0.107698	1.141591	x
x C	155	0.898814	0.784105	1.241481	x

x C	156	0.985931	0.686904	1.239200	x
x C	157	0.987078	0.617316	1.214117	x
x C	158	0.899317	0.649281	1.192067	x
x C	159	0.814281	0.747958	1.196355	x
x C	160	1.223324	0.392373	1.251637	x
x C	161	1.163706	0.352309	1.191942	x
x C	162	1.078261	0.512156	1.214470	x
x C	163	1.059069	0.068178	1.092658	x
x C	164	0.972766	0.091948	1.094407	x
x C	165	0.908457	0.120278	1.056496	x
x C	166	0.933384	0.124356	1.018018	x
x C	167	1.022242	0.096985	1.018306	x
x C	168	0.620050	0.084105	1.152658	x
x C	169	0.625174	0.124785	1.122199	x
x C	170	0.711327	0.103719	1.122473	x
x C	171	0.788294	0.043557	1.153883	x
x C	172	0.777124	0.006889	1.183623	x
x C	173	0.488549	0.436872	0.955287	x
x C	174	0.570905	0.367698	0.981846	x
x C	175	0.568992	0.313521	1.005223	x
x C	176	0.483240	0.332918	1.002525	x
x C	177	0.403951	0.403096	0.975291	x
x C	178	0.815007	0.147985	1.057888	x
x C	179	0.721290	0.143275	1.089985	x
x C	180	0.655519	0.238428	1.033303	x
x C	181	0.346724	0.269012	1.113789	x
x C	182	0.268866	0.269639	1.038143	x
x C	183	0.293746	0.384155	1.060036	x
x C	184	0.334677	0.283345	1.064950	x
x C	185	0.477067	0.116334	1.038917	x
x C	186	1.311388	0.237792	0.914443	x
x C	187	1.289282	0.182070	0.915674	x
x C	188	1.193384	0.228673	0.919165	x
x C	189	1.118583	0.330650	0.920679	x
x C	190	1.140834	0.386082	0.920081	x
x C	191	1.236451	0.340178	0.916869	x
x C	192	1.014712	0.379361	0.921120	x
x N	1	0.313694	1.437292	0.859054	x
x N	2	0.130523	1.201086	0.603452	x
x N	3	0.815021	0.813637	0.720566	x
x N	4	0.321583	1.233120	0.725671	x
x N	5	0.447048	1.083594	0.685254	x
x N	6	0.488585	1.148622	0.746392	x
x N	7	0.069116	1.084551	0.555035	x
x N	8	0.025663	0.694658	0.682955	x
x N	9	0.453671	0.406494	0.451530	x

x N	10	0.113743	0.808844	0.589700	x
x N	11	0.207838	0.641681	0.563541	x
x N	12	0.207025	0.741930	0.527602	x
x N	13	0.025972	1.555706	0.416925	x
x N	14	0.107807	1.479110	0.414646	x
x N	15	0.198083	1.406168	0.411962	x
x N	16	-1.437292	-0.313694	-0.359054	x
x N	17	-1.201086	-0.130523	-0.103452	x
x N	18	-0.813637	-0.815021	-0.220566	x
x N	19	-1.233120	-0.321583	-0.225671	x
x N	20	-1.083594	-0.447048	-0.185254	x
x N	21	-1.148622	-0.488585	-0.246392	x
x N	22	-1.084551	-0.069116	-0.055035	x
x N	23	-0.694658	-0.025663	-0.182955	x
x N	24	-0.406494	-0.453671	0.048470	x
x N	25	-0.808844	-0.113743	-0.089700	x
x N	26	-0.641681	-0.207838	-0.063541	x
x N	27	-0.741930	-0.207025	-0.027602	x
x N	28	-1.555706	-0.025972	0.083075	x
x N	29	-1.479110	-0.107807	0.085354	x
x N	30	-1.406168	-0.198083	0.088038	x
x N	31	-0.313694	-1.437292	-0.859054	x
x N	32	-0.130523	-1.201086	-0.603452	x
x N	33	-0.815021	-0.813637	-0.720566	x
x N	34	-0.321583	-1.233120	-0.725671	x
x N	35	-0.447048	-1.083594	-0.685254	x
x N	36	-0.488585	-1.148622	-0.746392	x
x N	37	-0.069116	-1.084551	-0.555035	x
x N	38	-0.025663	-0.694658	-0.682955	x
x N	39	-0.453671	-0.406494	-0.451530	x
x N	40	-0.113743	-0.808844	-0.589700	x
x N	41	-0.207838	-0.641681	-0.563541	x
x N	42	-0.207025	-0.741930	-0.527602	x
x N	43	-0.025972	-1.555706	-0.416925	x
x N	44	-0.107807	-1.479110	-0.414646	x
x N	45	-0.198083	-1.406168	-0.411962	x
x N	46	1.437292	0.313694	1.359054	x
x N	47	1.201086	0.130523	1.103452	x
x N	48	0.813637	0.815021	1.220566	x
x N	49	1.233120	0.321583	1.225671	x
x N	50	1.083594	0.447048	1.185254	x
x N	51	1.148622	0.488585	1.246392	x
x N	52	1.084551	0.069116	1.055035	x
x N	53	0.694658	0.025663	1.182955	x
x N	54	0.406494	0.453671	0.951530	x
x N	55	0.808844	0.113743	1.089700	x

x N	56	0.641681	0.207838	1.063541	x
x N	57	0.741930	0.207025	1.027602	x
x N	58	1.555706	0.025972	0.916925	x
x N	59	1.479110	0.107807	0.914646	x
x N	60	1.406168	0.198083	0.911962	x
x O	1	0.215761	0.431108	0.547868	x
x O	2	-0.431108	-0.215761	-0.047868	x
x O	3	-0.215761	-0.431108	-0.547868	x
x O	4	0.431108	0.215761	1.047868	x
x F	1	0.330276	1.005975	0.442804	x
x F	2	0.385753	0.971976	0.378685	x
x F	3	0.473744	0.956417	0.440087	x
x F	4	-1.005975	-0.330276	0.057196	x
x F	5	-0.971976	-0.385753	0.121315	x
x F	6	-0.956417	-0.473744	0.059913	x
x F	7	-0.330276	-1.005975	-0.442804	x
x F	8	-0.385753	-0.971976	-0.378685	x
x F	9	-0.473744	-0.956417	-0.440087	x
x F	10	1.005975	0.330276	0.942804	x
x F	11	0.971976	0.385753	0.878685	x
x F	12	0.956417	0.473744	0.940087	x
x Zn	1	0.286866	1.547159	0.906110	x
x Zn	2	0.023848	1.220703	0.557787	x
x Zn	3	-0.036204	0.688397	0.729552	x
x Zn	4	-1.547159	-0.286866	-0.406110	x
x Zn	5	-1.220703	-0.023848	-0.057787	x
x Zn	6	-0.688397	0.036204	-0.229552	x
x Zn	7	-0.286866	-1.547159	-0.906110	x
x Zn	8	-0.023848	-1.220703	-0.557787	x
x Zn	9	0.036204	-0.688397	-0.729552	x
x Zn	10	1.547159	0.286866	1.406110	x
x Zn	11	1.220703	0.023848	1.057787	x
x Zn	12	0.688397	-0.036204	1.229552	x
x I	1	0.325507	1.625665	0.870470	x
x I	2	0.137953	1.626974	0.946954	x
x I	3	-0.135342	1.341455	0.598533	x
x I	4	0.048536	1.237250	0.482855	x
x I	5	0.019627	0.719875	0.807025	x
x I	6	-0.007684	0.536054	0.703822	x
x I	7	-1.625665	-0.325507	-0.370470	x
x I	8	-1.626974	-0.137953	-0.446954	x
x I	9	-1.341455	0.135342	-0.098533	x
x I	10	-1.237250	-0.048536	0.017145	x
x I	11	-0.719875	-0.019627	-0.307025	x
x I	12	-0.536054	0.007684	-0.203822	x
x I	13	-0.325507	-1.625665	-0.870470	x

x I	14	-0.137953	-1.626974	-0.946954	x
x I	15	0.135342	-1.341455	-0.598533	x
x I	16	-0.048536	-1.237250	-0.482855	x
x I	17	-0.019627	-0.719875	-0.807025	x
x I	18	0.007684	-0.536054	-0.703822	x
x I	19	1.625665	0.325507	1.370470	x
x I	20	1.626974	0.137953	1.446954	x
x I	21	1.341455	-0.135342	1.098533	x
x I	22	1.237250	0.048536	0.982855	x
x I	23	0.719875	0.019627	1.307025	x
x I	24	0.536054	-0.007684	1.203822	x

Table S7. Fractional atomic coordinates of the optimised structure of vanillin@1a

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----					x
x	H	1	1.031368	0.179077	0.132639	x
x	H	2	0.986899	0.268294	0.188782	x
x	H	3	1.287810	0.420110	0.215083	x
x	H	4	1.319425	0.326303	0.154238	x
x	H	5	0.724835	0.482590	0.327502	x
x	H	6	0.902398	0.508518	0.333579	x
x	H	7	0.847011	0.325353	0.219336	x
x	H	8	0.671842	0.306606	0.217866	x
x	H	9	1.470461	0.667655	0.353539	x
x	H	10	1.348702	0.560045	0.297744	x
x	H	11	1.125748	0.603239	0.368041	x
x	H	12	1.254582	0.705812	0.422105	x
x	H	13	0.427431	0.378580	0.340872	x
x	H	14	0.353302	0.299212	0.391972	x
x	H	15	0.495290	0.142365	0.340688	x
x	H	16	0.556622	0.223630	0.288684	x
x	H	17	0.034072	0.090853	0.538042	x
x	H	18	0.145712	0.048667	0.490232	x
x	H	19	0.264886	0.284218	0.475495	x
x	H	20	0.154125	0.318575	0.526195	x
x	H	21	0.496611	-0.120921	0.379914	x
x	H	22	0.459071	-0.003221	0.375242	x
x	H	23	0.346107	-0.005736	0.495122	x
x	H	24	0.390367	-0.122183	0.495952	x
x	H	25	-0.012208	0.311060	0.667739	x
x	H	26	0.094485	0.365593	0.737204	x
x	H	27	0.315188	0.304833	0.672558	x
x	H	28	0.203417	0.258071	0.605499	x
x	H	29	0.438994	0.690276	0.923627	x
x	H	30	0.470030	0.582596	0.874490	x
x	H	31	0.182969	0.510474	0.810960	x
x	H	32	0.163929	0.623721	0.861286	x
x	H	33	0.613186	0.251732	0.734519	x
x	H	34	0.458542	0.276935	0.734430	x
x	H	35	0.604050	0.486527	0.832597	x
x	H	36	0.754204	0.454081	0.828305	x
x	H	37	0.391591	0.826756	0.875603	x
x	H	38	0.545762	0.939276	0.874683	x
x	H	39	0.610393	0.964184	1.007876	x
x	H	40	0.450921	0.852824	1.003897	x
x	H	41	0.921571	1.340073	0.860532	x

x H	42	0.910516	1.265644	0.916862	x
x H	43	0.655817	1.086015	0.841276	x
x H	44	0.680775	1.163017	0.786892	x
x H	45	1.000360	1.032818	1.072864	x
x H	46	0.854103	1.004026	1.021582	x
x H	47	1.011420	1.214147	0.984144	x
x H	48	1.154196	1.231784	1.034095	x
x H	49	0.403701	0.087373	0.205607	x
x H	50	0.307485	0.147661	0.234618	x
x H	51	0.219448	-0.014956	0.339092	x
x H	52	0.328234	-0.038993	0.285438	x
x H	53	0.191496	0.195378	0.230351	x
x H	54	0.292499	0.265918	0.266394	x
x H	55	0.175238	0.271389	0.269955	x
x H	56	0.139180	0.143143	0.353067	x
x H	57	0.423388	0.423938	0.600383	x
x H	58	0.256801	0.493523	0.545311	x
x H	59	0.461145	0.381991	0.454254	x
x H	60	0.470351	0.388250	0.531907	x
x H	61	0.138572	0.541716	0.460211	x
x H	62	0.126254	0.483099	0.498262	x
x H	63	0.222278	0.577767	0.507575	x
x H	64	0.303647	0.456251	0.408360	x
x H	65	1.013272	0.093483	0.208769	x
x H	66	0.768140	0.101199	0.186068	x
x H	67	0.928688	0.221638	0.334625	x
x H	68	1.010349	0.160561	0.279336	x
x H	69	0.559225	0.156486	0.200428	x
x H	70	0.671087	0.161661	0.179728	x
x H	71	0.593403	0.072613	0.191750	x
x H	72	0.694917	0.220477	0.308301	x
x H	73	0.067304	0.287252	0.426821	x
x H	74	0.007654	0.070111	0.375803	x
x H	75	-0.202854	0.142406	0.479873	x
x H	76	-0.059349	0.246193	0.464099	x
x H	77	-0.128151	-0.136259	0.345639	x
x H	78	-0.015910	-0.060473	0.371246	x
x H	79	-0.089334	-0.043046	0.332703	x
x H	80	-0.267827	-0.058225	0.429431	x
x H	81	-1.031368	-0.179077	-0.132639	x
x H	82	-0.986899	-0.268294	-0.188782	x
x H	83	-1.287810	-0.420110	-0.215083	x
x H	84	-1.319425	-0.326303	-0.154238	x
x H	85	-0.724835	-0.482590	-0.327502	x
x H	86	-0.902398	-0.508518	-0.333579	x
x H	87	-0.847011	-0.325353	-0.219336	x

x H	88	-0.671842	-0.306606	-0.217866	x
x H	89	-1.470461	-0.667655	-0.353539	x
x H	90	-1.348702	-0.560045	-0.297744	x
x H	91	-1.125748	-0.603239	-0.368041	x
x H	92	-1.254582	-0.705812	-0.422105	x
x H	93	-0.427431	-0.378580	-0.340872	x
x H	94	-0.353302	-0.299212	-0.391972	x
x H	95	-0.495290	-0.142365	-0.340688	x
x H	96	-0.556622	-0.223630	-0.288684	x
x H	97	-0.034072	-0.090853	-0.538042	x
x H	98	-0.145712	-0.048667	-0.490232	x
x H	99	-0.264886	-0.284218	-0.475495	x
x H	100	-0.154125	-0.318575	-0.526195	x
x H	101	-0.496611	0.120921	-0.379914	x
x H	102	-0.459071	0.003221	-0.375242	x
x H	103	-0.346107	0.005736	-0.495122	x
x H	104	-0.390367	0.122183	-0.495952	x
x H	105	0.012208	-0.311060	-0.667739	x
x H	106	-0.094485	-0.365593	-0.737204	x
x H	107	-0.315188	-0.304833	-0.672558	x
x H	108	-0.203417	-0.258071	-0.605499	x
x H	109	-0.438994	-0.690276	-0.923627	x
x H	110	-0.470030	-0.582596	-0.874490	x
x H	111	-0.182969	-0.510474	-0.810960	x
x H	112	-0.163929	-0.623721	-0.861286	x
x H	113	-0.613186	-0.251732	-0.734519	x
x H	114	-0.458542	-0.276935	-0.734430	x
x H	115	-0.604050	-0.486527	-0.832597	x
x H	116	-0.754204	-0.454081	-0.828305	x
x H	117	-0.391591	-0.826756	-0.875603	x
x H	118	-0.545762	-0.939276	-0.874683	x
x H	119	-0.610393	-0.964184	-1.007876	x
x H	120	-0.450921	-0.852824	-1.003897	x
x H	121	-0.921571	-1.340073	-0.860532	x
x H	122	-0.910516	-1.265644	-0.916862	x
x H	123	-0.655817	-1.086015	-0.841276	x
x H	124	-0.680775	-1.163017	-0.786892	x
x H	125	-1.000360	-1.032818	-1.072864	x
x H	126	-0.854103	-1.004026	-1.021582	x
x H	127	-1.011420	-1.214147	-0.984144	x
x H	128	-1.154196	-1.231784	-1.034095	x
x H	129	-0.403701	-0.087373	-0.205607	x
x H	130	-0.307485	-0.147661	-0.234618	x
x H	131	-0.219448	0.014956	-0.339092	x
x H	132	-0.328234	0.038993	-0.285438	x
x H	133	-0.191496	-0.195378	-0.230351	x

x H	134	-0.292499	-0.265918	-0.266394	x
x H	135	-0.175238	-0.271389	-0.269955	x
x H	136	-0.139180	-0.143143	-0.353067	x
x H	137	-0.423388	-0.423938	-0.600383	x
x H	138	-0.256801	-0.493523	-0.545311	x
x H	139	-0.461145	-0.381991	-0.454254	x
x H	140	-0.470351	-0.388250	-0.531907	x
x H	141	-0.138572	-0.541716	-0.460211	x
x H	142	-0.126254	-0.483099	-0.498262	x
x H	143	-0.222278	-0.577767	-0.507575	x
x H	144	-0.303647	-0.456251	-0.408360	x
x H	145	-1.013272	-0.093483	-0.208769	x
x H	146	-0.768140	-0.101199	-0.186068	x
x H	147	-0.928688	-0.221638	-0.334625	x
x H	148	-1.010349	-0.160561	-0.279336	x
x H	149	-0.559225	-0.156486	-0.200428	x
x H	150	-0.671087	-0.161661	-0.179728	x
x H	151	-0.593403	-0.072613	-0.191750	x
x H	152	-0.694917	-0.220477	-0.308301	x
x H	153	-0.067304	-0.287252	-0.426821	x
x H	154	-0.007654	-0.070111	-0.375803	x
x H	155	0.202854	-0.142406	-0.479873	x
x H	156	0.059349	-0.246193	-0.464099	x
x H	157	0.128151	0.136259	-0.345639	x
x H	158	0.015910	0.060473	-0.371246	x
x H	159	0.089334	0.043046	-0.332703	x
x H	160	0.267827	0.058225	-0.429431	x
x C	1	1.085948	0.233756	0.150837	x
x C	2	1.061666	0.283047	0.182688	x
x C	3	1.134228	0.351224	0.206460	x
x C	4	1.229205	0.368163	0.196739	x
x C	5	1.247413	0.316636	0.163632	x
x C	6	0.755337	0.449291	0.304302	x
x C	7	0.853559	0.463096	0.307503	x
x C	8	0.888687	0.418888	0.276617	x
x C	9	0.822735	0.361201	0.243853	x
x C	10	0.726030	0.350404	0.242843	x
x C	11	1.393184	0.651244	0.355395	x
x C	12	1.325455	0.592238	0.324418	x
x C	13	1.227319	0.573072	0.328808	x
x C	14	1.201307	0.615563	0.363930	x
x C	15	1.272756	0.673020	0.393897	x
x C	16	1.109367	0.403464	0.241145	x
x C	17	0.992951	0.433697	0.276067	x
x C	18	1.151490	0.508153	0.297793	x
x C	19	0.440236	0.325850	0.342045	x

x C	20	0.400359	0.282205	0.370440	x
x C	21	0.421556	0.216142	0.370827	x
x C	22	0.480041	0.194784	0.341763	x
x C	23	0.515025	0.240098	0.313529	x
x C	24	0.087039	0.131311	0.523392	x
x C	25	0.147467	0.108247	0.496649	x
x C	26	0.213231	0.163981	0.479230	x
x C	27	0.214821	0.240171	0.488968	x
x C	28	0.153989	0.259476	0.516738	x
x C	29	0.463613	-0.093292	0.404712	x
x C	30	0.443282	-0.028244	0.402440	x
x C	31	0.399858	0.004234	0.434914	x
x C	32	0.381051	-0.028783	0.469562	x
x C	33	0.404401	-0.093397	0.469970	x
x C	34	0.381513	0.169449	0.401266	x
x C	35	0.283532	0.145097	0.452451	x
x C	36	0.370640	0.069639	0.431256	x
x C	37	0.061309	0.312024	0.670195	x
x C	38	0.120063	0.340801	0.708691	x
x C	39	0.213057	0.338925	0.709847	x
x C	40	0.243246	0.306842	0.672572	x
x C	41	0.181369	0.281293	0.635397	x
x C	42	0.383855	0.649075	0.898286	x
x C	43	0.400747	0.588850	0.871055	x
x C	44	0.327740	0.537295	0.839298	x
x C	45	0.241142	0.549543	0.835562	x
x C	46	0.229829	0.611575	0.863414	x
x C	47	0.606847	0.302316	0.756150	x
x C	48	0.522134	0.316554	0.756117	x
x C	49	0.519377	0.383393	0.783877	x
x C	50	0.603625	0.433918	0.810546	x
x C	51	0.686327	0.416065	0.808758	x
x C	52	0.283210	0.375662	0.748360	x
x C	53	0.341071	0.472406	0.809014	x
x C	54	0.428990	0.399519	0.783299	x
x C	55	0.441553	0.860299	0.904157	x
x C	56	0.526162	0.922248	0.903926	x
x C	57	0.588008	0.961412	0.941855	x
x C	58	0.562505	0.935984	0.978280	x
x C	59	0.475754	0.874555	0.976313	x
x C	60	0.864874	1.283087	0.857718	x
x C	61	0.858003	1.242153	0.888693	x
x C	62	0.781919	1.170562	0.883472	x
x C	63	0.715871	1.141648	0.846757	x
x C	64	0.728579	1.184806	0.816607	x
x C	65	1.000080	1.070144	1.051691	x

x C	66	0.919652	1.054906	1.023762	x
x C	67	0.922462	1.107083	0.999016	x
x C	68	1.007399	1.172323	1.002844	x
x C	69	1.085693	1.182896	1.030621	x
x C	70	0.680226	1.026314	0.943006	x
x C	71	0.771819	1.124588	0.915453	x
x C	72	0.837413	1.094923	0.970016	x
x C	73	0.392783	0.046673	0.226727	x
x C	74	0.325600	0.054145	0.257250	x
x C	75	0.288276	0.113212	0.258047	x
x C	76	0.229500	0.127348	0.288380	x
x C	77	0.205009	0.080600	0.317873	x
x C	78	0.240251	0.020437	0.316131	x
x C	79	0.300038	0.007109	0.286211	x
x C	80	0.214531	0.231916	0.262958	x
x C	81	0.371603	0.447499	0.588577	x
x C	82	0.365536	0.442915	0.543104	x
x C	83	0.301418	0.470397	0.524754	x
x C	84	0.296804	0.467068	0.481976	x
x C	85	0.355746	0.435528	0.456540	x
x C	86	0.417372	0.406732	0.474470	x
x C	87	0.422428	0.410757	0.517607	x
x C	88	0.177265	0.525252	0.483278	x
x C	89	0.942487	0.094183	0.197163	x
x C	90	0.893625	0.128038	0.229572	x
x C	91	0.801334	0.127677	0.218697	x
x C	92	0.756459	0.160975	0.249472	x
x C	93	0.803063	0.194895	0.291444	x
x C	94	0.894274	0.195098	0.302128	x
x C	95	0.939063	0.161044	0.271187	x
x C	96	0.619891	0.136797	0.200998	x
x C	97	0.059863	0.228183	0.408037	x
x C	98	-0.018800	0.164877	0.417844	x
x C	99	-0.038915	0.085652	0.398147	x
x C	100	-0.117252	0.028446	0.407936	x
x C	101	-0.178084	0.049635	0.436939	x
x C	102	-0.156380	0.127828	0.457094	x
x C	103	-0.076836	0.185012	0.447931	x
x C	104	-0.090443	-0.073229	0.358096	x
x C	105	-1.085948	-0.233756	-0.150837	x
x C	106	-1.061666	-0.283047	-0.182688	x
x C	107	-1.134228	-0.351224	-0.206460	x
x C	108	-1.229205	-0.368163	-0.196739	x
x C	109	-1.247413	-0.316636	-0.163632	x
x C	110	-0.755337	-0.449291	-0.304302	x
x C	111	-0.853559	-0.463096	-0.307503	x

x C	112	-0.888687	-0.418888	-0.276617	x
x C	113	-0.822735	-0.361201	-0.243853	x
x C	114	-0.726030	-0.350404	-0.242843	x
x C	115	-1.393184	-0.651244	-0.355395	x
x C	116	-1.325455	-0.592238	-0.324418	x
x C	117	-1.227319	-0.573072	-0.328808	x
x C	118	-1.201307	-0.615563	-0.363930	x
x C	119	-1.272756	-0.673020	-0.393897	x
x C	120	-1.109367	-0.403464	-0.241145	x
x C	121	-0.992951	-0.433697	-0.276067	x
x C	122	-1.151490	-0.508153	-0.297793	x
x C	123	-0.440236	-0.325850	-0.342045	x
x C	124	-0.400359	-0.282205	-0.370440	x
x C	125	-0.421556	-0.216142	-0.370827	x
x C	126	-0.480041	-0.194784	-0.341763	x
x C	127	-0.515025	-0.240098	-0.313529	x
x C	128	-0.087039	-0.131311	-0.523392	x
x C	129	-0.147467	-0.108247	-0.496649	x
x C	130	-0.213231	-0.163981	-0.479230	x
x C	131	-0.214821	-0.240171	-0.488968	x
x C	132	-0.153989	-0.259476	-0.516738	x
x C	133	-0.463613	0.093292	-0.404712	x
x C	134	-0.443282	0.028244	-0.402440	x
x C	135	-0.399858	-0.004234	-0.434914	x
x C	136	-0.381051	0.028783	-0.469562	x
x C	137	-0.404401	0.093397	-0.469970	x
x C	138	-0.381513	-0.169449	-0.401266	x
x C	139	-0.283532	-0.145097	-0.452451	x
x C	140	-0.370640	-0.069639	-0.431256	x
x C	141	-0.061309	-0.312024	-0.670195	x
x C	142	-0.120063	-0.340801	-0.708691	x
x C	143	-0.213057	-0.338925	-0.709847	x
x C	144	-0.243246	-0.306842	-0.672572	x
x C	145	-0.181369	-0.281293	-0.635397	x
x C	146	-0.383855	-0.649075	-0.898286	x
x C	147	-0.400747	-0.588850	-0.871055	x
x C	148	-0.327740	-0.537295	-0.839298	x
x C	149	-0.241142	-0.549543	-0.835562	x
x C	150	-0.229829	-0.611575	-0.863414	x
x C	151	-0.606847	-0.302316	-0.756150	x
x C	152	-0.522134	-0.316554	-0.756117	x
x C	153	-0.519377	-0.383393	-0.783877	x
x C	154	-0.603625	-0.433918	-0.810546	x
x C	155	-0.686327	-0.416065	-0.808758	x
x C	156	-0.283210	-0.375662	-0.748360	x
x C	157	-0.341071	-0.472406	-0.809014	x

x C	158	-0.428990	-0.399519	-0.783299	x
x C	159	-0.441553	-0.860299	-0.904157	x
x C	160	-0.526162	-0.922248	-0.903926	x
x C	161	-0.588008	-0.961412	-0.941855	x
x C	162	-0.562505	-0.935984	-0.978280	x
x C	163	-0.475754	-0.874555	-0.976313	x
x C	164	-0.864874	-1.283087	-0.857718	x
x C	165	-0.858003	-1.242153	-0.888693	x
x C	166	-0.781919	-1.170562	-0.883472	x
x C	167	-0.715871	-1.141648	-0.846757	x
x C	168	-0.728579	-1.184806	-0.816607	x
x C	169	-1.000080	-1.070144	-1.051691	x
x C	170	-0.919652	-1.054906	-1.023762	x
x C	171	-0.922462	-1.107083	-0.999016	x
x C	172	-1.007399	-1.172323	-1.002844	x
x C	173	-1.085693	-1.182896	-1.030621	x
x C	174	-0.680226	-1.026314	-0.943006	x
x C	175	-0.771819	-1.124588	-0.915453	x
x C	176	-0.837413	-1.094923	-0.970016	x
x C	177	-0.392783	-0.046673	-0.226727	x
x C	178	-0.325600	-0.054145	-0.257250	x
x C	179	-0.288276	-0.113212	-0.258047	x
x C	180	-0.229500	-0.127348	-0.288380	x
x C	181	-0.205009	-0.080600	-0.317873	x
x C	182	-0.240251	-0.020437	-0.316131	x
x C	183	-0.300038	-0.007109	-0.286211	x
x C	184	-0.214531	-0.231916	-0.262958	x
x C	185	-0.371603	-0.447499	-0.588577	x
x C	186	-0.365536	-0.442915	-0.543104	x
x C	187	-0.301418	-0.470397	-0.524754	x
x C	188	-0.296804	-0.467068	-0.481976	x
x C	189	-0.355746	-0.435528	-0.456540	x
x C	190	-0.417372	-0.406732	-0.474470	x
x C	191	-0.422428	-0.410757	-0.517607	x
x C	192	-0.177265	-0.525252	-0.483278	x
x C	193	-0.942487	-0.094183	-0.197163	x
x C	194	-0.893625	-0.128038	-0.229572	x
x C	195	-0.801334	-0.127677	-0.218697	x
x C	196	-0.756459	-0.160975	-0.249472	x
x C	197	-0.803063	-0.194895	-0.291444	x
x C	198	-0.894274	-0.195098	-0.302128	x
x C	199	-0.939063	-0.161044	-0.271187	x
x C	200	-0.619891	-0.136797	-0.200998	x
x C	201	-0.059863	-0.228183	-0.408037	x
x C	202	0.018800	-0.164877	-0.417844	x
x C	203	0.038915	-0.085652	-0.398147	x

x C	204	0.117252	-0.028446	-0.407936	x
x C	205	0.178084	-0.049635	-0.436939	x
x C	206	0.156380	-0.127828	-0.457094	x
x C	207	0.076836	-0.185012	-0.447931	x
x C	208	0.090443	0.073229	-0.358096	x
x N	1	1.177166	0.250160	0.141293	x
x N	2	0.691725	0.393356	0.272441	x
x N	3	1.367749	0.691002	0.389868	x
x N	4	1.015251	0.384188	0.245631	x
x N	5	1.058519	0.495076	0.304107	x
x N	6	1.180727	0.466164	0.265818	x
x N	7	0.496521	0.305180	0.313774	x
x N	8	0.090699	0.205805	0.533791	x
x N	9	0.444048	-0.125986	0.438050	x
x N	10	0.320073	0.190429	0.425932	x
x N	11	0.307380	0.084865	0.457005	x
x N	12	0.407816	0.108653	0.402117	x
x N	13	0.091926	0.283274	0.633900	x
x N	14	0.300267	0.660709	0.894589	x
x N	15	0.688051	0.350803	0.782043	x
x N	16	0.269825	0.433024	0.776738	x
x N	17	0.422914	0.458367	0.813699	x
x N	18	0.360028	0.354740	0.750828	x
x N	19	0.415643	0.837557	0.939969	x
x N	20	0.801012	1.255188	0.822194	x
x N	21	1.082223	1.132897	1.055029	x
x N	22	0.685747	1.067144	0.913679	x
x N	23	0.850112	1.140324	0.942529	x
x N	24	0.753000	1.038662	0.972491	x
x N	25	-1.177166	-0.250160	-0.141293	x
x N	26	-0.691725	-0.393356	-0.272441	x
x N	27	-1.367749	-0.691002	-0.389868	x
x N	28	-1.015251	-0.384188	-0.245631	x
x N	29	-1.058519	-0.495076	-0.304107	x
x N	30	-1.180727	-0.466164	-0.265818	x
x N	31	-0.496521	-0.305180	-0.313774	x
x N	32	-0.090699	-0.205805	-0.533791	x
x N	33	-0.444048	0.125986	-0.438050	x
x N	34	-0.320073	-0.190429	-0.425932	x
x N	35	-0.307380	-0.084865	-0.457005	x
x N	36	-0.407816	-0.108653	-0.402117	x
x N	37	-0.091926	-0.283274	-0.633900	x
x N	38	-0.300267	-0.660709	-0.894589	x
x N	39	-0.688051	-0.350803	-0.782043	x
x N	40	-0.269825	-0.433024	-0.776738	x
x N	41	-0.422914	-0.458367	-0.813699	x

x N	42	-0.360028	-0.354740	-0.750828	x
x N	43	-0.415643	-0.837557	-0.939969	x
x N	44	-0.801012	-1.255188	-0.822194	x
x N	45	-1.082223	-1.132897	-1.055029	x
x N	46	-0.685747	-1.067144	-0.913679	x
x N	47	-0.850112	-1.140324	-0.942529	x
x N	48	-0.753000	-1.038662	-0.972491	x
x O	1	0.436078	0.000739	0.222872	x
x O	2	0.191165	0.184080	0.292562	x
x O	3	0.147770	0.091491	0.347912	x
x O	4	0.324350	0.474677	0.613591	x
x O	5	0.237722	0.490356	0.459649	x
x O	6	0.350783	0.433295	0.414464	x
x O	7	0.911595	0.068634	0.159082	x
x O	8	0.667387	0.165621	0.243556	x
x O	9	0.759020	0.228412	0.321497	x
x O	10	0.116224	0.223416	0.381013	x
x O	11	-0.144521	-0.049951	0.390749	x
x O	12	-0.258459	-0.004404	0.445338	x
x O	13	-0.436078	-0.000739	-0.222872	x
x O	14	-0.191165	-0.184080	-0.292562	x
x O	15	-0.147770	-0.091491	-0.347912	x
x O	16	-0.324350	-0.474677	-0.613591	x
x O	17	-0.237722	-0.490356	-0.459649	x
x O	18	-0.350783	-0.433295	-0.414464	x
x O	19	-0.911595	-0.068634	-0.159082	x
x O	20	-0.667387	-0.165621	-0.243556	x
x O	21	-0.759020	-0.228412	-0.321497	x
x O	22	-0.116224	-0.223416	-0.381013	x
x O	23	0.144521	0.049951	-0.390749	x
x O	24	0.258459	0.004404	-0.445338	x
x Zn	1	1.203333	0.162752	0.098279	x
x Zn	2	1.470923	0.774725	0.437849	x
x Zn	3	0.543345	0.367514	0.267916	x
x Zn	4	0.003631	0.240733	0.575664	x
x Zn	5	0.810923	0.320973	0.778156	x
x Zn	6	0.281215	0.750912	0.938118	x
x Zn	7	-1.203333	-0.162752	-0.098279	x
x Zn	8	-1.470923	-0.774725	-0.437849	x
x Zn	9	-0.543345	-0.367514	-0.267916	x
x Zn	10	-0.003631	-0.240733	-0.575664	x
x Zn	11	-0.810923	-0.320973	-0.778156	x
x Zn	12	-0.281215	-0.750912	-0.938118	x
x I	1	1.181625	0.057093	0.137671	x
x I	2	1.350981	0.229209	0.063901	x
x I	3	1.427425	0.732125	0.506563	x

x I	4	1.635306	0.793176	0.409401	x
x I	5	0.459716	0.268758	0.197344	x
x I	6	0.494305	0.485936	0.289472	x
x I	7	-0.139513	0.120288	0.582371	x
x I	8	-0.005542	0.369813	0.562291	x
x I	9	0.790469	0.231432	0.702713	x
x I	10	0.959903	0.447145	0.804181	x
x I	11	0.267455	0.718198	1.010466	x
x I	12	0.158233	0.785433	0.897353	x
x I	13	-1.181625	-0.057093	-0.137671	x
x I	14	-1.350981	-0.229209	-0.063901	x
x I	15	-1.427425	-0.732125	-0.506563	x
x I	16	-1.635306	-0.793176	-0.409401	x
x I	17	-0.459716	-0.268758	-0.197344	x
x I	18	-0.494305	-0.485936	-0.289472	x
x I	19	0.139513	-0.120288	-0.582371	x
x I	20	0.005542	-0.369813	-0.562291	x
x I	21	-0.790469	-0.231432	-0.702713	x
x I	22	-0.959903	-0.447145	-0.804181	x
x I	23	-0.267455	-0.718198	-1.010466	x
x I	24	-0.158233	-0.785433	-0.897353	x

Table S8. Fractional atomic coordinates of the optimised structure of (1*R*)-(-)-menthyl acetate@**1b**

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----x					
x	H	1	-0.214128	1.130578	0.653845	x
x	H	2	-0.050082	1.083930	0.651748	x
x	H	3	0.083279	0.882573	0.742368	x
x	H	4	-0.085877	0.937887	0.741405	x
x	H	5	0.397984	1.000761	0.618949	x
x	H	6	0.382862	0.928940	0.667546	x
x	H	7	0.102565	1.036288	0.598506	x
x	H	8	0.132618	1.097060	0.550244	x
x	H	9	0.478644	0.596256	0.806198	x
x	H	10	0.320511	0.718938	0.760472	x
x	H	11	0.460972	0.816256	0.738114	x
x	H	12	0.610169	0.694612	0.785414	x
x	H	13	0.188016	1.296641	0.597547	x
x	H	14	0.028444	1.477307	0.597336	x
x	H	15	-0.071275	1.395852	0.481493	x
x	H	16	0.094545	1.217432	0.485909	x
x	H	17	-0.398258	2.052302	0.615289	x
x	H	18	0.923423	0.734936	0.108525	x
x	H	19	-0.378966	1.921868	0.561737	x
x	H	20	-0.084840	1.699736	0.623461	x
x	H	21	-0.115553	1.838258	0.674206	x
x	H	22	-0.366606	1.614935	0.363272	x
x	H	23	-0.246989	1.558521	0.426462	x
x	H	24	-0.459583	1.859094	0.485310	x
x	H	25	-0.571390	1.904615	0.419562	x
x	H	26	-0.547228	1.631811	0.297267	x
x	H	27	-0.429756	1.472380	0.251288	x
x	H	28	-0.294935	1.583765	0.239456	x
x	H	29	-0.410445	1.733051	0.287624	x
x	H	30	-0.007231	0.922829	0.147798	x
x	H	31	-0.055003	1.087893	0.146906	x
x	H	32	-0.259412	1.218549	0.235844	x
x	H	33	-0.200643	1.047973	0.234874	x
x	H	34	-0.094753	1.506556	0.120460	x
x	H	35	-0.162321	1.493059	0.171655	x
x	H	36	-0.114899	1.247087	0.091819	x
x	H	37	-0.053646	1.273308	0.042270	x
x	H	38	0.089489	1.219811	-0.019809	x
x	H	39	0.268480	1.053868	-0.023300	x
x	H	40	0.347609	1.158881	0.091086	x

x H	41	0.166942	1.320314	0.089848	x
x H	42	0.777358	0.551062	-0.080811	x
x H	43	0.730115	0.664786	-0.015201	x
x H	44	0.427994	0.871005	-0.073844	x
x H	45	0.485904	0.750186	-0.136579	x
x H	46	0.708067	1.014942	0.169124	x
x H	47	0.570096	1.045067	0.118440	x
x H	48	0.792230	0.752035	0.056304	x
x H	49	0.631892	0.907255	0.761487	x
x H	50	0.751359	0.686692	0.768132	x
x H	51	0.891951	0.660093	0.749032	x
x H	52	0.808051	0.789110	0.742559	x
x H	53	0.828944	0.685727	0.675667	x
x H	54	0.789897	0.637396	0.694906	x
x H	55	0.663735	0.856463	0.682829	x
x H	56	0.605365	0.762299	0.714163	x
x H	57	0.525579	0.891649	0.707267	x
x H	58	0.371377	0.983824	0.799148	x
x H	59	0.395844	1.037739	0.845116	x
x H	60	0.468210	0.904905	0.836724	x
x H	61	0.910111	0.674395	0.861673	x
x H	62	0.943502	0.658902	0.813295	x
x H	63	0.899837	0.601704	0.819634	x
x H	64	0.733631	0.771710	0.834809	x
x H	65	0.817311	0.852684	0.812592	x
x H	66	0.792401	0.861512	0.861945	x
x H	67	0.691858	0.925983	0.822729	x
x H	68	0.687249	0.741783	0.618829	x
x H	69	0.560091	0.832236	0.630211	x
x H	70	0.639481	0.706436	0.641650	x
x H	71	-0.208410	0.764428	0.256423	x
x H	72	-0.412722	0.824730	0.243941	x
x H	73	-0.462182	0.951909	0.202295	x
x H	74	-0.342523	0.913609	0.217818	x
x H	75	-0.497642	1.001168	0.275482	x
x H	76	-0.467819	1.064763	0.262167	x
x H	77	-0.294394	0.943703	0.293691	x
x H	78	-0.357219	0.843724	0.315761	x
x H	79	-0.237611	0.808175	0.329783	x
x H	80	-0.155650	0.531624	0.312118	x
x H	81	-0.026447	0.472239	0.315863	x
x H	82	-0.091501	0.472194	0.267629	x
x H	83	-0.473264	0.850946	0.156197	x
x H	84	-0.468174	0.775483	0.183255	x
x H	85	-0.406246	0.722536	0.138096	x
x H	86	-0.283639	0.669597	0.199807	x

x H	87	-0.311747	0.815948	0.155884	x
x H	88	-0.246054	0.687087	0.139489	x
x H	89	-0.198819	0.721502	0.184658	x
x H	90	-0.422650	1.091211	0.338743	x
x H	91	-0.328785	0.985376	0.367095	x
x H	92	-0.447818	1.021466	0.350234	x
x H	93	-0.443420	1.253643	0.257235	x
x H	94	-0.486671	0.705752	0.049876	x
x H	95	-1.130578	0.214128	-0.653845	x
x H	96	-1.083930	0.050082	-0.651748	x
x H	97	-0.882573	-0.083279	-0.742368	x
x H	98	-0.937887	0.085877	-0.741405	x
x H	99	-1.000761	-0.397984	-0.618949	x
x H	100	-0.928940	-0.382862	-0.667546	x
x H	101	-1.036288	-0.102565	-0.598506	x
x H	102	-1.097060	-0.132618	-0.550244	x
x H	103	-0.596256	-0.478644	-0.806198	x
x H	104	-0.718938	-0.320511	-0.760472	x
x H	105	-0.816256	-0.460972	-0.738114	x
x H	106	-0.694612	-0.610169	-0.785414	x
x H	107	-1.296641	-0.188016	-0.597547	x
x H	108	-1.477307	-0.028444	-0.597336	x
x H	109	-1.395852	0.071275	-0.481493	x
x H	110	-1.217432	-0.094545	-0.485909	x
x H	111	-2.052302	0.398258	-0.615289	x
x H	112	-0.734936	-0.923423	-0.108525	x
x H	113	-1.921868	0.378966	-0.561737	x
x H	114	-1.699736	0.084840	-0.623461	x
x H	115	-1.838258	0.115553	-0.674206	x
x H	116	-1.614935	0.366606	-0.363272	x
x H	117	-1.558521	0.246989	-0.426462	x
x H	118	-1.859094	0.459583	-0.485310	x
x H	119	-1.904615	0.571390	-0.419562	x
x H	120	-1.631811	0.547228	-0.297267	x
x H	121	-1.472380	0.429756	-0.251288	x
x H	122	-1.583765	0.294935	-0.239456	x
x H	123	-1.733051	0.410445	-0.287624	x
x H	124	-0.922829	0.007231	-0.147798	x
x H	125	-1.087893	0.055003	-0.146906	x
x H	126	-1.218549	0.259412	-0.235844	x
x H	127	-1.047973	0.200643	-0.234874	x
x H	128	-1.506556	0.094753	-0.120460	x
x H	129	-1.493059	0.162321	-0.171655	x
x H	130	-1.247087	0.114899	-0.091819	x
x H	131	-1.273308	0.053646	-0.042270	x
x H	132	-1.219811	-0.089489	0.019809	x

x H	133	-1.053868	-0.268480	0.023300	x
x H	134	-1.158881	-0.347609	-0.091086	x
x H	135	-1.320314	-0.166942	-0.089848	x
x H	136	-0.551062	-0.777358	0.080811	x
x H	137	-0.664786	-0.730115	0.015201	x
x H	138	-0.871005	-0.427994	0.073844	x
x H	139	-0.750186	-0.485904	0.136579	x
x H	140	-1.014942	-0.708067	-0.169124	x
x H	141	-1.045067	-0.570096	-0.118440	x
x H	142	-0.752035	-0.792230	-0.056304	x
x H	143	-0.907255	-0.631892	-0.761487	x
x H	144	-0.686692	-0.751359	-0.768132	x
x H	145	-0.660093	-0.891951	-0.749032	x
x H	146	-0.789110	-0.808051	-0.742559	x
x H	147	-0.685727	-0.828944	-0.675667	x
x H	148	-0.637396	-0.789897	-0.694906	x
x H	149	-0.856463	-0.663735	-0.682829	x
x H	150	-0.762299	-0.605365	-0.714163	x
x H	151	-0.891649	-0.525579	-0.707267	x
x H	152	-0.983824	-0.371377	-0.799148	x
x H	153	-1.037739	-0.395844	-0.845116	x
x H	154	-0.904905	-0.468210	-0.836724	x
x H	155	-0.674395	-0.910111	-0.861673	x
x H	156	-0.658902	-0.943502	-0.813295	x
x H	157	-0.601704	-0.899837	-0.819634	x
x H	158	-0.771710	-0.733631	-0.834809	x
x H	159	-0.852684	-0.817311	-0.812592	x
x H	160	-0.861512	-0.792401	-0.861945	x
x H	161	-0.925983	-0.691858	-0.822729	x
x H	162	-0.741783	-0.687249	-0.618829	x
x H	163	-0.832236	-0.560091	-0.630211	x
x H	164	-0.706436	-0.639481	-0.641650	x
x H	165	-0.764428	0.208410	-0.256423	x
x H	166	-0.824730	0.412722	-0.243941	x
x H	167	-0.951909	0.462182	-0.202295	x
x H	168	-0.913609	0.342523	-0.217818	x
x H	169	-1.001168	0.497642	-0.275482	x
x H	170	-1.064763	0.467819	-0.262167	x
x H	171	-0.943703	0.294394	-0.293691	x
x H	172	-0.843724	0.357219	-0.315761	x
x H	173	-0.808175	0.237611	-0.329783	x
x H	174	-0.531624	0.155650	-0.312118	x
x H	175	-0.472239	0.026447	-0.315863	x
x H	176	-0.472194	0.091501	-0.267629	x
x H	177	-0.850946	0.473264	-0.156197	x
x H	178	-0.775483	0.468174	-0.183255	x

x H	179	-0.722536	0.406246	-0.138096	x
x H	180	-0.669597	0.283639	-0.199807	x
x H	181	-0.815948	0.311747	-0.155884	x
x H	182	-0.687087	0.246054	-0.139489	x
x H	183	-0.721502	0.198819	-0.184658	x
x H	184	-1.091211	0.422650	-0.338743	x
x H	185	-0.985376	0.328785	-0.367095	x
x H	186	-1.021466	0.447818	-0.350234	x
x H	187	-1.253643	0.443420	-0.257235	x
x H	188	-0.705752	0.486671	-0.049876	x
x C	1	-0.145584	1.075566	0.672532	x
x C	2	-0.055717	1.050142	0.671804	x
x C	3	0.028686	0.978689	0.696752	x
x C	4	0.018664	0.938209	0.722756	x
x C	5	-0.073434	0.967456	0.722103	x
x C	6	0.335717	1.003876	0.614949	x
x C	7	0.326737	0.964549	0.641617	x
x C	8	0.242076	0.976199	0.635962	x
x C	9	0.169408	1.025806	0.603124	x
x C	10	0.184990	1.060517	0.577051	x
x C	11	0.469945	0.647304	0.790379	x
x C	12	0.384069	0.713979	0.765248	x
x C	13	0.380864	0.774972	0.745712	x
x C	14	0.462437	0.768655	0.752686	x
x C	15	0.544949	0.701751	0.778693	x
x C	16	0.128019	0.942822	0.694840	x
x C	17	0.228585	0.939902	0.665484	x
x C	18	0.293379	0.845933	0.717688	x
x C	19	0.128099	1.322222	0.572518	x
x C	20	0.039566	1.422084	0.572200	x
x C	21	-0.033652	1.450043	0.538902	x
x C	22	-0.015367	1.375744	0.507697	x
x C	23	0.074960	1.277768	0.509937	x
x C	24	-0.330029	1.973292	0.615445	x
x C	25	0.844039	0.802013	0.109327	x
x C	26	-0.318491	1.900778	0.585787	x
x C	27	-0.229652	1.800647	0.588328	x
x C	28	-0.154928	1.776842	0.620385	x
x C	29	-0.171560	1.853618	0.648593	x
x C	30	-0.384963	1.666484	0.391039	x
x C	31	-0.318779	1.635166	0.426425	x
x C	32	-0.343945	1.704641	0.460956	x
x C	33	-0.436684	1.802925	0.458989	x
x C	34	-0.499166	1.828647	0.422534	x
x C	35	-0.126052	1.556359	0.534871	x
x C	36	-0.215941	1.721429	0.557640	x

x C	37	-0.270929	1.675899	0.497905	x
x C	38	-0.488639	1.616260	0.284116	x
x C	39	-0.425000	1.529688	0.258527	x
x C	40	-0.354224	1.516998	0.241852	x
x C	41	-0.349260	1.591246	0.251810	x
x C	42	-0.413021	1.674154	0.278408	x
x C	43	-0.062729	0.990829	0.166610	x
x C	44	-0.089189	1.081365	0.166306	x
x C	45	-0.161470	1.165341	0.191139	x
x C	46	-0.203079	1.154385	0.216221	x
x C	47	-0.171566	1.061067	0.215600	x
x C	48	-0.101518	1.450962	0.115226	x
x C	49	-0.139098	1.443241	0.143332	x
x C	50	-0.144547	1.369459	0.134871	x
x C	51	-0.111958	1.305564	0.098463	x
x C	52	-0.077366	1.319159	0.071501	x
x C	53	-0.282909	1.427270	0.214787	x
x C	54	-0.193791	1.263674	0.190285	x
x C	55	-0.184815	1.358863	0.163720	x
x C	56	0.149716	1.201708	0.003966	x
x C	57	0.247796	1.111093	0.002387	x
x C	58	0.321034	1.094246	0.033774	x
x C	59	0.292376	1.169593	0.066163	x
x C	60	0.192831	1.258479	0.065726	x
x C	61	0.701185	0.623016	-0.077939	x
x C	62	0.674594	0.686246	-0.041652	x
x C	63	0.575418	0.777512	-0.039762	x
x C	64	0.505601	0.800561	-0.073945	x
x C	65	0.537805	0.733733	-0.109090	x
x C	66	0.724044	0.959033	0.143381	x
x C	67	0.647267	0.975334	0.115309	x
x C	68	0.671074	0.900667	0.083303	x
x C	69	0.771235	0.812426	0.080348	x
x C	70	0.427146	1.000708	0.031264	x
x C	71	0.546428	0.851527	-0.003376	x
x C	72	0.591996	0.913373	0.053136	x
x C	73	0.639451	0.841932	0.758645	x
x C	74	0.747448	0.750237	0.771509	x
x C	75	0.813055	0.725504	0.740780	x
x C	76	0.780360	0.704057	0.697012	x
x C	77	0.670604	0.792552	0.683714	x
x C	78	0.603673	0.823550	0.715177	x
x C	79	0.501574	0.961171	0.801546	x
x C	80	0.430949	0.972047	0.822325	x
x C	81	0.890129	0.668976	0.828411	x
x C	82	0.782187	0.763243	0.816760	x

x C	83	0.769799	0.856308	0.828865	x
x C	84	0.637097	0.767367	0.641122	x
x C	85	-0.267735	0.773684	0.265749	x
x C	86	-0.355294	0.815301	0.232276	x
x C	87	-0.400358	0.920267	0.227106	x
x C	88	-0.436793	0.990391	0.266661	x
x C	89	-0.351785	0.947911	0.301782	x
x C	90	-0.302248	0.841035	0.306091	x
x C	91	-0.129605	0.611737	0.290016	x
x C	92	-0.099049	0.516486	0.297175	x
x C	93	-0.424749	0.775357	0.165829	x
x C	94	-0.329299	0.745895	0.191553	x
x C	95	-0.267709	0.742368	0.166562	x
x C	96	-0.389693	1.015388	0.341785	x
x C	97	-0.422755	1.257617	0.290410	x
x C	98	-0.412988	0.630293	0.046584	x
x C	99	-1.075566	0.145584	-0.672532	x
x C	100	-1.050142	0.055717	-0.671804	x
x C	101	-0.978689	-0.028686	-0.696752	x
x C	102	-0.938209	-0.018664	-0.722756	x
x C	103	-0.967456	0.073434	-0.722103	x
x C	104	-1.003876	-0.335717	-0.614949	x
x C	105	-0.964549	-0.326737	-0.641617	x
x C	106	-0.976199	-0.242076	-0.635962	x
x C	107	-1.025806	-0.169408	-0.603124	x
x C	108	-1.060517	-0.184990	-0.577051	x
x C	109	-0.647304	-0.469945	-0.790379	x
x C	110	-0.713979	-0.384069	-0.765248	x
x C	111	-0.774972	-0.380864	-0.745712	x
x C	112	-0.768655	-0.462437	-0.752686	x
x C	113	-0.701751	-0.544949	-0.778693	x
x C	114	-0.942822	-0.128019	-0.694840	x
x C	115	-0.939902	-0.228585	-0.665484	x
x C	116	-0.845933	-0.293379	-0.717688	x
x C	117	-1.322222	-0.128099	-0.572518	x
x C	118	-1.422084	-0.039566	-0.572200	x
x C	119	-1.450043	0.033652	-0.538902	x
x C	120	-1.375744	0.015367	-0.507697	x
x C	121	-1.277768	-0.074960	-0.509937	x
x C	122	-1.973292	0.330029	-0.615445	x
x C	123	-0.802013	-0.844039	-0.109327	x
x C	124	-1.900778	0.318491	-0.585787	x
x C	125	-1.800647	0.229652	-0.588328	x
x C	126	-1.776842	0.154928	-0.620385	x
x C	127	-1.853618	0.171560	-0.648593	x
x C	128	-1.666484	0.384963	-0.391039	x

x C	129	-1.635166	0.318779	-0.426425	x
x C	130	-1.704641	0.343945	-0.460956	x
x C	131	-1.802925	0.436684	-0.458989	x
x C	132	-1.828647	0.499166	-0.422534	x
x C	133	-1.556359	0.126052	-0.534871	x
x C	134	-1.721429	0.215941	-0.557640	x
x C	135	-1.675899	0.270929	-0.497905	x
x C	136	-1.616260	0.488639	-0.284116	x
x C	137	-1.529688	0.425000	-0.258527	x
x C	138	-1.516998	0.354224	-0.241852	x
x C	139	-1.591246	0.349260	-0.251810	x
x C	140	-1.674154	0.413021	-0.278408	x
x C	141	-0.990829	0.062729	-0.166610	x
x C	142	-1.081365	0.089189	-0.166306	x
x C	143	-1.165341	0.161470	-0.191139	x
x C	144	-1.154385	0.203079	-0.216221	x
x C	145	-1.061067	0.171566	-0.215600	x
x C	146	-1.450962	0.101518	-0.115226	x
x C	147	-1.443241	0.139098	-0.143332	x
x C	148	-1.369459	0.144547	-0.134871	x
x C	149	-1.305564	0.111958	-0.098463	x
x C	150	-1.319159	0.077366	-0.071501	x
x C	151	-1.427270	0.282909	-0.214787	x
x C	152	-1.263674	0.193791	-0.190285	x
x C	153	-1.358863	0.184815	-0.163720	x
x C	154	-1.201708	-0.149716	-0.003966	x
x C	155	-1.111093	-0.247796	-0.002387	x
x C	156	-1.094246	-0.321034	-0.033774	x
x C	157	-1.169593	-0.292376	-0.066163	x
x C	158	-1.258479	-0.192831	-0.065726	x
x C	159	-0.623016	-0.701185	0.077939	x
x C	160	-0.686246	-0.674594	0.041652	x
x C	161	-0.777512	-0.575418	0.039762	x
x C	162	-0.800561	-0.505601	0.073945	x
x C	163	-0.733733	-0.537805	0.109090	x
x C	164	-0.959033	-0.724044	-0.143381	x
x C	165	-0.975334	-0.647267	-0.115309	x
x C	166	-0.900667	-0.671074	-0.083303	x
x C	167	-0.812426	-0.771235	-0.080348	x
x C	168	-1.000708	-0.427146	-0.031264	x
x C	169	-0.851527	-0.546428	0.003376	x
x C	170	-0.913373	-0.591996	-0.053136	x
x C	171	-0.841932	-0.639451	-0.758645	x
x C	172	-0.750237	-0.747448	-0.771509	x
x C	173	-0.725504	-0.813055	-0.740780	x
x C	174	-0.704057	-0.780360	-0.697012	x

x C	175	-0.792552	-0.670604	-0.683714	x
x C	176	-0.823550	-0.603673	-0.715177	x
x C	177	-0.961171	-0.501574	-0.801546	x
x C	178	-0.972047	-0.430949	-0.822325	x
x C	179	-0.668976	-0.890129	-0.828411	x
x C	180	-0.763243	-0.782187	-0.816760	x
x C	181	-0.856308	-0.769799	-0.828865	x
x C	182	-0.767367	-0.637097	-0.641122	x
x C	183	-0.773684	0.267735	-0.265749	x
x C	184	-0.815301	0.355294	-0.232276	x
x C	185	-0.920267	0.400358	-0.227106	x
x C	186	-0.990391	0.436793	-0.266661	x
x C	187	-0.947911	0.351785	-0.301782	x
x C	188	-0.841035	0.302248	-0.306091	x
x C	189	-0.611737	0.129605	-0.290016	x
x C	190	-0.516486	0.099049	-0.297175	x
x C	191	-0.775357	0.424749	-0.165829	x
x C	192	-0.745895	0.329299	-0.191553	x
x C	193	-0.742368	0.267709	-0.166562	x
x C	194	-1.015388	0.389693	-0.341785	x
x C	195	-1.257617	0.422755	-0.290410	x
x C	196	-0.630293	0.412988	-0.046584	x
x N	1	-0.153968	1.033837	0.696967	x
x N	2	0.266468	1.050192	0.582869	x
x N	3	0.548991	0.641259	0.796964	x
x N	4	0.136329	0.975189	0.665936	x
x N	5	0.309791	0.874181	0.690233	x
x N	6	0.204147	0.878257	0.721563	x
x N	7	0.146369	1.251074	0.541866	x
x N	8	-0.257733	1.950458	0.646336	x
x N	9	-0.473661	1.761888	0.388935	x
x N	10	-0.134712	1.625241	0.563921	x
x N	11	-0.285602	1.750509	0.524953	x
x N	12	-0.192839	1.577434	0.501795	x
x N	13	-0.482116	1.687035	0.294342	x
x N	14	-0.103180	0.980566	0.190906	x
x N	15	-0.071937	1.390605	0.079671	x
x N	16	-0.257245	1.340408	0.217190	x
x N	17	-0.158129	1.269789	0.162038	x
x N	18	-0.247007	1.439857	0.189289	x
x N	19	0.122416	1.274808	0.035122	x
x N	20	0.634206	0.646633	-0.111382	x
x N	21	0.820990	0.873856	0.140410	x
x N	22	0.448103	0.927859	0.001208	x
x N	23	0.620952	0.840665	0.021877	x
x N	24	0.495813	0.996818	0.058274	x

x N	25	-1.033837	0.153968	-0.696967	x
x N	26	-1.050192	-0.266468	-0.582869	x
x N	27	-0.641259	-0.548991	-0.796964	x
x N	28	-0.975189	-0.136329	-0.665936	x
x N	29	-0.874181	-0.309791	-0.690233	x
x N	30	-0.878257	-0.204147	-0.721563	x
x N	31	-1.251074	-0.146369	-0.541866	x
x N	32	-1.950458	0.257733	-0.646336	x
x N	33	-1.761888	0.473661	-0.388935	x
x N	34	-1.625241	0.134712	-0.563921	x
x N	35	-1.750509	0.285602	-0.524953	x
x N	36	-1.577434	0.192839	-0.501795	x
x N	37	-1.687035	0.482116	-0.294342	x
x N	38	-0.980566	0.103180	-0.190906	x
x N	39	-1.390605	0.071937	-0.079671	x
x N	40	-1.340408	0.257245	-0.217190	x
x N	41	-1.269789	0.158129	-0.162038	x
x N	42	-1.439857	0.247007	-0.189289	x
x N	43	-1.274808	-0.122416	-0.035122	x
x N	44	-0.646633	-0.634206	0.111382	x
x N	45	-0.873856	-0.820990	-0.140410	x
x N	46	-0.927859	-0.448103	-0.001208	x
x N	47	-0.840665	-0.620952	-0.021877	x
x N	48	-0.996818	-0.495813	-0.058274	x
x O	1	0.573066	0.864752	0.785800	x
x O	2	0.494295	1.031012	0.798416	x
x O	3	-0.225212	0.674478	0.272097	x
x O	4	-0.075559	0.631107	0.298627	x
x O	5	-0.864752	-0.573066	-0.785800	x
x O	6	-1.031012	-0.494295	-0.798416	x
x O	7	-0.674478	0.225212	-0.272097	x
x O	8	-0.631107	0.075559	-0.298627	x
x Cl	1	-0.390848	1.332196	0.302797	x
x Cl	2	-0.527889	1.311547	0.314736	x
x Cl	3	-0.318521	1.133053	0.302394	x
x Cl	4	-0.322449	0.642253	0.060126	x
x Cl	5	-0.409917	0.579330	-0.004893	x
x Cl	6	-0.397468	0.559434	0.080362	x
x Cl	7	-1.332196	0.390848	-0.302797	x
x Cl	8	-1.311547	0.527889	-0.314736	x
x Cl	9	-1.133053	0.318521	-0.302394	x
x Cl	10	-0.642253	0.322449	-0.060126	x
x Cl	11	-0.579330	0.409917	0.004893	x
x Cl	12	-0.559434	0.397468	-0.080362	x
x Zn	1	-0.283081	1.060435	0.692222	x
x Zn	2	0.283369	1.104137	0.542112	x

x Zn	3	0.931941	0.846244	0.185958	x
x Zn	4	-0.569789	1.812710	0.335332	x
x Zn	5	-0.025492	1.409268	0.035794	x
x Zn	6	0.674106	0.545989	-0.163862	x
x Zn	7	-1.060435	0.283081	-0.692222	x
x Zn	8	-1.104137	-0.283369	-0.542112	x
x Zn	9	-0.846244	-0.931941	-0.185958	x
x Zn	10	-1.812710	0.569789	-0.335332	x
x Zn	11	-1.409268	0.025492	-0.035794	x
x Zn	12	-0.545989	-0.674106	0.163862	x
x Br	1	-0.269750	1.004141	0.752178	x
x Br	2	-0.415395	1.214663	0.664673	x
x Br	3	0.410437	1.104420	0.577000	x
x Br	4	0.283393	1.027769	0.475544	x
x Br	5	1.082303	0.720441	0.153977	x
x Br	6	0.889085	0.839848	0.244819	x
x Br	7	-0.568863	1.933777	0.322064	x
x Br	8	-0.713435	1.838820	0.334825	x
x Br	9	-0.032903	1.543604	0.064533	x
x Br	10	-0.105510	1.400258	-0.028180	x
x Br	11	0.810040	0.502989	-0.189727	x
x Br	12	0.668989	0.428683	-0.152554	x
x Br	13	-1.004141	0.269750	-0.752178	x
x Br	14	-1.214663	0.415395	-0.664673	x
x Br	15	-1.104420	-0.410437	-0.577000	x
x Br	16	-1.027769	-0.283393	-0.475544	x
x Br	17	-0.720441	-1.082303	-0.153977	x
x Br	18	-0.839848	-0.889085	-0.244819	x
x Br	19	-1.933777	0.568863	-0.322064	x
x Br	20	-1.838820	0.713435	-0.334825	x
x Br	21	-1.543604	0.032903	-0.064533	x
x Br	22	-1.400258	0.105510	0.028180	x
x Br	23	-0.502989	-0.810040	0.189727	x
x Br	24	-0.428683	-0.668989	0.152554	x

Table S9. Fractional atomic coordinates of the optimised structure of (1*R*)-(-)-menthyl acetate@**1c**

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----x					
x	H	1	0.817519	0.955211	1.136341	x
x	H	2	0.692872	1.003998	1.074383	x
x	H	3	0.915498	0.699563	1.016754	x
x	H	4	1.031433	0.661152	1.081190	x
x	H	5	0.240675	1.261927	0.910851	x
x	H	6	0.405544	1.078105	0.910716	x
x	H	7	0.513037	1.165278	1.022768	x
x	H	8	0.342746	1.345799	1.019058	x
x	H	9	0.846154	0.502673	0.883785	x
x	H	10	0.826985	0.631929	0.939237	x
x	H	11	0.521971	0.857552	0.882601	x
x	H	12	0.553681	0.721253	0.829006	x
x	H	13	0.041416	1.557084	0.887333	x
x	H	14	0.055740	1.628041	0.837600	x
x	H	15	0.337600	1.527289	0.907079	x
x	H	16	0.308815	1.465819	0.955843	x
x	H	17	-0.060738	1.977741	0.701322	x
x	H	18	0.098220	1.859369	0.748570	x
x	H	19	-0.027727	1.736468	0.762774	x
x	H	20	-0.177208	1.854235	0.713875	x
x	H	21	0.654366	1.429426	0.845137	x
x	H	22	0.486514	1.481285	0.849647	x
x	H	23	0.347675	1.688992	0.760744	x
x	H	24	0.520721	1.627647	0.758587	x
x	H	25	-0.334498	2.014806	0.579481	x
x	H	26	-0.292170	1.899483	0.514510	x
x	H	27	0.008695	1.675836	0.574196	x
x	H	28	-0.044128	1.798490	0.637028	x
x	H	29	-0.279954	1.555211	0.323891	x
x	H	30	-0.139126	1.522772	0.375173	x
x	H	31	-0.363524	1.819143	0.438313	x
x	H	32	-0.496754	1.838559	0.384680	x
x	H	33	0.348604	1.317296	0.515541	x
x	H	34	0.170473	1.490225	0.520802	x
x	H	35	0.082191	1.403651	0.401815	x
x	H	36	0.263056	1.238419	0.400325	x
x	H	37	-0.576679	1.657991	0.345466	x
x	H	38	-0.524983	1.490243	0.349601	x
x	H	39	-0.320273	1.353199	0.259491	x
x	H	40	-0.380507	1.526766	0.258538	x

x H	41	-0.550024	1.302992	0.447610	x
x H	42	-0.489708	1.338363	0.401361	x
x H	43	-0.360605	1.046498	0.334119	x
x H	44	-0.431308	1.025098	0.380972	x
x H	45	-0.022974	0.963584	0.201401	x
x H	46	-0.149173	1.118127	0.248561	x
x H	47	-0.245054	0.965804	0.261828	x
x H	48	-0.120402	0.820904	0.213262	x
x H	49	0.199656	1.341125	0.756780	x
x H	50	0.324495	1.118211	0.766589	x
x H	51	0.469626	1.095520	0.753287	x
x H	52	0.382269	1.224466	0.743436	x
x H	53	0.419050	1.107242	0.678467	x
x H	54	0.377822	1.059674	0.697664	x
x H	55	0.247599	1.277977	0.679264	x
x H	56	0.184965	1.184483	0.709874	x
x H	57	0.103981	1.313896	0.700161	x
x H	58	-0.063162	1.423122	0.798417	x
x H	59	-0.023301	1.461478	0.845776	x
x H	60	0.039629	1.329754	0.830829	x
x H	61	0.460061	1.117250	0.866185	x
x H	62	0.450512	1.041106	0.824838	x
x H	63	0.509949	1.085106	0.819834	x
x H	64	0.285656	1.219659	0.831703	x
x H	65	0.393985	1.281282	0.813828	x
x H	66	0.353359	1.303807	0.861591	x
x H	67	0.262113	1.364056	0.818755	x
x H	68	0.286580	1.144956	0.618403	x
x H	69	0.154574	1.239194	0.625211	x
x H	70	0.232177	1.116740	0.641804	x
x H	71	-0.777168	1.274677	0.318234	x
x H	72	-0.655550	1.238825	0.329452	x
x H	73	-0.720936	1.381988	0.295000	x
x H	74	-0.925614	1.437087	0.280100	x
x H	75	-0.899834	1.506228	0.267577	x
x H	76	-0.777717	1.359026	0.219645	x
x H	77	-0.899048	1.396484	0.206118	x
x H	78	-0.842561	1.261374	0.244749	x
x H	79	-0.633343	1.196964	0.256306	x
x H	80	-0.593425	0.962062	0.304862	x
x H	81	-0.460555	0.896819	0.310923	x
x H	82	-0.523918	0.899601	0.261653	x
x H	83	-0.901501	1.216071	0.182038	x
x H	84	-0.905120	1.293823	0.156702	x
x H	85	-0.838108	1.164247	0.137446	x
x H	86	-0.714811	1.108033	0.199887	x

x H	87	-0.739854	1.255494	0.157210	x
x H	88	-0.671531	1.124358	0.141487	x
x H	89	-0.626889	1.162045	0.187170	x
x H	90	-0.842995	1.525081	0.344495	x
x H	91	-0.865243	1.450851	0.355171	x
x H	92	-0.743218	1.412972	0.369453	x
x H	93	0.315591	0.886304	0.743503	x
x H	94	-0.955211	-0.817519	-1.136341	x
x H	95	-1.003998	-0.692872	-1.074383	x
x H	96	-0.699563	-0.915498	-1.016754	x
x H	97	-0.661152	-1.031433	-1.081190	x
x H	98	-1.261927	-0.240675	-0.910851	x
x H	99	-1.078105	-0.405544	-0.910716	x
x H	100	-1.165278	-0.513037	-1.022768	x
x H	101	-1.345799	-0.342746	-1.019058	x
x H	102	-0.502673	-0.846154	-0.883785	x
x H	103	-0.631929	-0.826985	-0.939237	x
x H	104	-0.857552	-0.521971	-0.882601	x
x H	105	-0.721253	-0.553681	-0.829006	x
x H	106	-1.557084	-0.041416	-0.887333	x
x H	107	-1.628041	-0.055740	-0.837600	x
x H	108	-1.527289	-0.337600	-0.907079	x
x H	109	-1.465819	-0.308815	-0.955843	x
x H	110	-1.977741	0.060738	-0.701322	x
x H	111	-1.859369	-0.098220	-0.748570	x
x H	112	-1.736468	0.027727	-0.762774	x
x H	113	-1.854235	0.177208	-0.713875	x
x H	114	-1.429426	-0.654366	-0.845137	x
x H	115	-1.481285	-0.486514	-0.849647	x
x H	116	-1.688992	-0.347675	-0.760744	x
x H	117	-1.627647	-0.520721	-0.758587	x
x H	118	-2.014806	0.334498	-0.579481	x
x H	119	-1.899483	0.292170	-0.514510	x
x H	120	-1.675836	-0.008695	-0.574196	x
x H	121	-1.798490	0.044128	-0.637028	x
x H	122	-1.555211	0.279954	-0.323891	x
x H	123	-1.522772	0.139126	-0.375173	x
x H	124	-1.819143	0.363524	-0.438313	x
x H	125	-1.838559	0.496754	-0.384680	x
x H	126	-1.317296	-0.348604	-0.515541	x
x H	127	-1.490225	-0.170473	-0.520802	x
x H	128	-1.403651	-0.082191	-0.401815	x
x H	129	-1.238419	-0.263056	-0.400325	x
x H	130	-1.657991	0.576679	-0.345466	x
x H	131	-1.490243	0.524983	-0.349601	x
x H	132	-1.353199	0.320273	-0.259491	x

x H	133	-1.526766	0.380507	-0.258538	x
x H	134	-1.302992	0.550024	-0.447610	x
x H	135	-1.338363	0.489708	-0.401361	x
x H	136	-1.046498	0.360605	-0.334119	x
x H	137	-1.025098	0.431308	-0.380972	x
x H	138	-0.963584	0.022974	-0.201401	x
x H	139	-1.118127	0.149173	-0.248561	x
x H	140	-0.965804	0.245054	-0.261828	x
x H	141	-0.820904	0.120402	-0.213262	x
x H	142	-1.341125	-0.199656	-0.756780	x
x H	143	-1.118211	-0.324495	-0.766589	x
x H	144	-1.095520	-0.469626	-0.753287	x
x H	145	-1.224466	-0.382269	-0.743436	x
x H	146	-1.107242	-0.419050	-0.678467	x
x H	147	-1.059674	-0.377822	-0.697664	x
x H	148	-1.277977	-0.247599	-0.679264	x
x H	149	-1.184483	-0.184965	-0.709874	x
x H	150	-1.313896	-0.103981	-0.700161	x
x H	151	-1.423122	0.063162	-0.798417	x
x H	152	-1.461478	0.023301	-0.845776	x
x H	153	-1.329754	-0.039629	-0.830829	x
x H	154	-1.117250	-0.460061	-0.866185	x
x H	155	-1.041106	-0.450512	-0.824838	x
x H	156	-1.085106	-0.509949	-0.819834	x
x H	157	-1.219659	-0.285656	-0.831703	x
x H	158	-1.281282	-0.393985	-0.813828	x
x H	159	-1.303807	-0.353359	-0.861591	x
x H	160	-1.364056	-0.262113	-0.818755	x
x H	161	-1.144956	-0.286580	-0.618403	x
x H	162	-1.239194	-0.154574	-0.625211	x
x H	163	-1.116740	-0.232177	-0.641804	x
x H	164	-1.274677	0.777168	-0.318234	x
x H	165	-1.238825	0.655550	-0.329452	x
x H	166	-1.381988	0.720936	-0.295000	x
x H	167	-1.437087	0.925614	-0.280100	x
x H	168	-1.506228	0.899834	-0.267577	x
x H	169	-1.359026	0.777717	-0.219645	x
x H	170	-1.396484	0.899048	-0.206118	x
x H	171	-1.261374	0.842561	-0.244749	x
x H	172	-1.196964	0.633343	-0.256306	x
x H	173	-0.962062	0.593425	-0.304862	x
x H	174	-0.896819	0.460555	-0.310923	x
x H	175	-0.899601	0.523918	-0.261653	x
x H	176	-1.216071	0.901501	-0.182038	x
x H	177	-1.293823	0.905120	-0.156702	x
x H	178	-1.164247	0.838108	-0.137446	x

x H	179	-1.108033	0.714811	-0.199887	x
x H	180	-1.255494	0.739854	-0.157210	x
x H	181	-1.124358	0.671531	-0.141487	x
x H	182	-1.162045	0.626889	-0.187170	x
x H	183	-1.525081	0.842995	-0.344495	x
x H	184	-1.450851	0.865243	-0.355171	x
x H	185	-1.412972	0.743218	-0.369453	x
x H	186	-0.886304	-0.315591	-0.743503	x
x C	1	0.836792	0.900579	1.109294	x
x C	2	0.767588	0.927822	1.074584	x
x C	3	0.794169	0.855700	1.040478	x
x C	4	0.890816	0.758257	1.042495	x
x C	5	0.955858	0.736345	1.078448	x
x C	6	0.303964	1.236666	0.934601	x
x C	7	0.394429	1.135990	0.934673	x
x C	8	0.471558	1.109366	0.966598	x
x C	9	0.454604	1.184941	0.997349	x
x C	10	0.362115	1.283727	0.995502	x
x C	11	0.775659	0.582227	0.885048	x
x C	12	0.764059	0.654239	0.915866	x
x C	13	0.672243	0.755188	0.915523	x
x C	14	0.594635	0.779985	0.884167	x
x C	15	0.612042	0.703955	0.854181	x
x C	16	0.719014	0.882453	1.004100	x
x C	17	0.566927	1.002262	0.969564	x
x C	18	0.659100	0.834714	0.946660	x
x C	19	0.104152	1.554642	0.890957	x
x C	20	0.112701	1.593413	0.863668	x
x C	21	0.197278	1.584165	0.869110	x
x C	22	0.270448	1.536496	0.902397	x
x C	23	0.255473	1.501622	0.928961	x
x C	24	-0.048572	1.921870	0.715582	x
x C	25	0.038022	1.857269	0.741522	x
x C	26	0.046838	1.789240	0.759120	x
x C	27	-0.031908	1.788813	0.750025	x
x C	28	-0.114863	1.853367	0.722905	x
x C	29	0.584086	1.486310	0.827081	x
x C	30	0.492325	1.514327	0.829071	x
x C	31	0.405338	1.588716	0.805282	x
x C	32	0.414638	1.630154	0.779099	x
x C	33	0.509133	1.597604	0.778265	x
x C	34	0.208350	1.622299	0.839138	x
x C	35	0.137927	1.716727	0.786130	x
x C	36	0.305464	1.623848	0.808563	x
x C	37	-0.259170	1.939171	0.577087	x
x C	38	-0.235320	1.874588	0.540994	x

x C	39	-0.138083	1.777609	0.539562	x
x C	40	-0.067371	1.750529	0.574184	x
x C	41	-0.096835	1.818892	0.609249	x
x C	42	-0.295245	1.611314	0.349848	x
x C	43	-0.217264	1.593679	0.378380	x
x C	44	-0.241187	1.668834	0.410864	x
x C	45	-0.342516	1.758462	0.413904	x
x C	46	-0.416503	1.770081	0.384298	x
x C	47	0.286818	1.341906	0.491033	x
x C	48	0.189499	1.436000	0.493738	x
x C	49	0.113606	1.459548	0.461660	x
x C	50	0.139329	1.388470	0.427293	x
x C	51	0.239071	1.296658	0.426387	x
x C	52	-0.111120	1.704177	0.502520	x
x C	53	-0.160249	1.653188	0.441856	x
x C	54	0.007149	1.555469	0.465545	x
x C	55	-0.520045	1.587964	0.327260	x
x C	56	-0.491757	1.496065	0.329126	x
x C	57	-0.417930	1.409830	0.304945	x
x C	58	-0.377820	1.419689	0.278385	x
x C	59	-0.409683	1.513938	0.278085	x
x C	60	-0.508323	1.248803	0.421829	x
x C	61	-0.473999	1.267580	0.396729	x
x C	62	-0.418726	1.193437	0.364775	x
x C	63	-0.401229	1.104191	0.359214	x
x C	64	-0.440180	1.091964	0.384902	x
x C	65	-0.074492	0.968778	0.215589	x
x C	66	-0.142942	1.052485	0.241469	x
x C	67	-0.204943	1.052015	0.258800	x
x C	68	-0.196870	0.967785	0.249217	x
x C	69	-0.128440	0.887724	0.222328	x
x C	70	-0.380651	1.309091	0.307958	x
x C	71	-0.380397	1.207730	0.336178	x
x C	72	-0.280712	1.140651	0.285655	x
x C	73	0.209777	1.273306	0.754173	x
x C	74	0.318404	1.184357	0.770533	x
x C	75	0.390171	1.158284	0.742336	x
x C	76	0.366087	1.128066	0.698294	x
x C	77	0.256299	1.212594	0.681389	x
x C	78	0.182295	1.247184	0.710310	x
x C	79	0.072997	1.391966	0.798693	x
x C	80	0.003203	1.401610	0.820164	x
x C	81	0.446978	1.105807	0.832699	x
x C	82	0.344078	1.202475	0.816547	x
x C	83	0.337781	1.293173	0.828138	x
x C	84	0.230643	1.176983	0.639219	x

x C	85	-0.724127	1.273866	0.307257	x
x C	86	-0.776320	1.383582	0.304185	x
x C	87	-0.866211	1.429098	0.270746	x
x C	88	-0.833486	1.362500	0.229711	x
x C	89	-0.785594	1.254349	0.233363	x
x C	90	-0.694589	1.208819	0.266072	x
x C	91	-0.556927	1.037871	0.285507	x
x C	92	-0.532630	0.943998	0.291493	x
x C	93	-0.856616	1.216740	0.165647	x
x C	94	-0.759860	1.185550	0.192130	x
x C	95	-0.695591	1.181564	0.168347	x
x C	96	-0.808738	1.446962	0.345728	x
x C	97	0.306113	0.865214	0.710648	x
x C	98	-0.900579	-0.836792	-1.109294	x
x C	99	-0.927822	-0.767588	-1.074584	x
x C	100	-0.855700	-0.794169	-1.040478	x
x C	101	-0.758257	-0.890816	-1.042495	x
x C	102	-0.736345	-0.955858	-1.078448	x
x C	103	-1.236666	-0.303964	-0.934601	x
x C	104	-1.135990	-0.394429	-0.934673	x
x C	105	-1.109366	-0.471558	-0.966598	x
x C	106	-1.184941	-0.454604	-0.997349	x
x C	107	-1.283727	-0.362115	-0.995502	x
x C	108	-0.582227	-0.775659	-0.885048	x
x C	109	-0.654239	-0.764059	-0.915866	x
x C	110	-0.755188	-0.672243	-0.915523	x
x C	111	-0.779985	-0.594635	-0.884167	x
x C	112	-0.703955	-0.612042	-0.854181	x
x C	113	-0.882453	-0.719014	-1.004100	x
x C	114	-1.002262	-0.566927	-0.969564	x
x C	115	-0.834714	-0.659100	-0.946660	x
x C	116	-1.554642	-0.104152	-0.890957	x
x C	117	-1.593413	-0.112701	-0.863668	x
x C	118	-1.584165	-0.197278	-0.869110	x
x C	119	-1.536496	-0.270448	-0.902397	x
x C	120	-1.501622	-0.255473	-0.928961	x
x C	121	-1.921870	0.048572	-0.715582	x
x C	122	-1.857269	-0.038022	-0.741522	x
x C	123	-1.789240	-0.046838	-0.759120	x
x C	124	-1.788813	0.031908	-0.750025	x
x C	125	-1.853367	0.114863	-0.722905	x
x C	126	-1.486310	-0.584086	-0.827081	x
x C	127	-1.514327	-0.492325	-0.829071	x
x C	128	-1.588716	-0.405338	-0.805282	x
x C	129	-1.630154	-0.414638	-0.779099	x
x C	130	-1.597604	-0.509133	-0.778265	x

x C	131	-1.622299	-0.208350	-0.839138	x
x C	132	-1.716727	-0.137927	-0.786130	x
x C	133	-1.623848	-0.305464	-0.808563	x
x C	134	-1.939171	0.259170	-0.577087	x
x C	135	-1.874588	0.235320	-0.540994	x
x C	136	-1.777609	0.138083	-0.539562	x
x C	137	-1.750529	0.067371	-0.574184	x
x C	138	-1.818892	0.096835	-0.609249	x
x C	139	-1.611314	0.295245	-0.349848	x
x C	140	-1.593679	0.217264	-0.378380	x
x C	141	-1.668834	0.241187	-0.410864	x
x C	142	-1.758462	0.342516	-0.413904	x
x C	143	-1.770081	0.416503	-0.384298	x
x C	144	-1.341906	-0.286818	-0.491033	x
x C	145	-1.436000	-0.189499	-0.493738	x
x C	146	-1.459548	-0.113606	-0.461660	x
x C	147	-1.388470	-0.139329	-0.427293	x
x C	148	-1.296658	-0.239071	-0.426387	x
x C	149	-1.704177	0.111120	-0.502520	x
x C	150	-1.653188	0.160249	-0.441856	x
x C	151	-1.555469	-0.007149	-0.465545	x
x C	152	-1.587964	0.520045	-0.327260	x
x C	153	-1.496065	0.491757	-0.329126	x
x C	154	-1.409830	0.417930	-0.304945	x
x C	155	-1.419689	0.377820	-0.278385	x
x C	156	-1.513938	0.409683	-0.278085	x
x C	157	-1.248803	0.508323	-0.421829	x
x C	158	-1.267580	0.473999	-0.396729	x
x C	159	-1.193437	0.418726	-0.364775	x
x C	160	-1.104191	0.401229	-0.359214	x
x C	161	-1.091964	0.440180	-0.384902	x
x C	162	-0.968778	0.074492	-0.215589	x
x C	163	-1.052485	0.142942	-0.241469	x
x C	164	-1.052015	0.204943	-0.258800	x
x C	165	-0.967785	0.196870	-0.249217	x
x C	166	-0.887724	0.128440	-0.222328	x
x C	167	-1.309091	0.380651	-0.307958	x
x C	168	-1.207730	0.380397	-0.336178	x
x C	169	-1.140651	0.280712	-0.285655	x
x C	170	-1.273306	-0.209777	-0.754173	x
x C	171	-1.184357	-0.318404	-0.770533	x
x C	172	-1.158284	-0.390171	-0.742336	x
x C	173	-1.128066	-0.366087	-0.698294	x
x C	174	-1.212594	-0.256299	-0.681389	x
x C	175	-1.247184	-0.182295	-0.710310	x
x C	176	-1.391966	-0.072997	-0.798693	x

x C	177	-1.401610	-0.003203	-0.820164	x
x C	178	-1.105807	-0.446978	-0.832699	x
x C	179	-1.202475	-0.344078	-0.816547	x
x C	180	-1.293173	-0.337781	-0.828138	x
x C	181	-1.176983	-0.230643	-0.639219	x
x C	182	-1.273866	0.724127	-0.307257	x
x C	183	-1.383582	0.776320	-0.304185	x
x C	184	-1.429098	0.866211	-0.270746	x
x C	185	-1.362500	0.833486	-0.229711	x
x C	186	-1.254349	0.785594	-0.233363	x
x C	187	-1.208819	0.694589	-0.266072	x
x C	188	-1.037871	0.556927	-0.285507	x
x C	189	-0.943998	0.532630	-0.291493	x
x C	190	-1.216740	0.856616	-0.165647	x
x C	191	-1.185550	0.759860	-0.192130	x
x C	192	-1.181564	0.695591	-0.168347	x
x C	193	-1.446962	0.808738	-0.345728	x
x C	194	-0.865214	-0.306113	-0.710648	x
x N	1	0.929342	0.805702	1.111615	x
x N	2	0.287968	1.309444	0.964469	x
x N	3	0.700962	0.606347	0.854664	x
x N	4	0.638926	0.982031	1.000459	x
x N	5	0.573538	0.931810	0.941718	x
x N	6	0.733174	0.805844	0.977922	x
x N	7	0.173944	1.509984	0.923385	x
x N	8	-0.123465	1.919335	0.706027	x
x N	9	0.592474	1.527742	0.802237	x
x N	10	0.125032	1.685388	0.813841	x
x N	11	0.227021	1.686213	0.781459	x
x N	12	0.299773	1.591500	0.838580	x
x N	13	-0.191696	1.911556	0.610907	x
x N	14	-0.393357	1.698052	0.352751	x
x N	15	0.311561	1.273125	0.457794	x
x N	16	-0.187966	1.723199	0.474686	x
x N	17	-0.063628	1.568426	0.435761	x
x N	18	-0.012050	1.621456	0.499166	x
x N	19	-0.478676	1.596425	0.302463	x
x N	20	-0.492026	1.162595	0.416144	x
x N	21	-0.067929	0.887886	0.205848	x
x N	22	-0.415011	1.301148	0.336275	x
x N	23	-0.312459	1.124876	0.311876	x
x N	24	-0.313714	1.231350	0.281951	x
x N	25	-0.805702	-0.929342	-1.111615	x
x N	26	-1.309444	-0.287968	-0.964469	x
x N	27	-0.606347	-0.700962	-0.854664	x
x N	28	-0.982031	-0.638926	-1.000459	x

x N	29	-0.931810	-0.573538	-0.941718	x
x N	30	-0.805844	-0.733174	-0.977922	x
x N	31	-1.509984	-0.173944	-0.923385	x
x N	32	-1.919335	0.123465	-0.706027	x
x N	33	-1.527742	-0.592474	-0.802237	x
x N	34	-1.685388	-0.125032	-0.813841	x
x N	35	-1.686213	-0.227021	-0.781459	x
x N	36	-1.591500	-0.299773	-0.838580	x
x N	37	-1.911556	0.191696	-0.610907	x
x N	38	-1.698052	0.393357	-0.352751	x
x N	39	-1.273125	-0.311561	-0.457794	x
x N	40	-1.723199	0.187966	-0.474686	x
x N	41	-1.568426	0.063628	-0.435761	x
x N	42	-1.621456	0.012050	-0.499166	x
x N	43	-1.596425	0.478676	-0.302463	x
x N	44	-1.162595	0.492026	-0.416144	x
x N	45	-0.887886	0.067929	-0.205848	x
x N	46	-1.301148	0.415011	-0.336275	x
x N	47	-1.124876	0.312459	-0.311876	x
x N	48	-1.231350	0.313714	-0.281951	x
x O	1	0.137690	1.297495	0.778718	x
x O	2	0.071348	1.461000	0.799345	x
x O	3	-0.656109	1.109230	0.271269	x
x O	4	-0.495343	1.049012	0.292104	x
x O	5	-1.297495	-0.137690	-0.778718	x
x O	6	-1.461000	-0.071348	-0.799345	x
x O	7	-1.109230	0.656109	-0.271269	x
x O	8	-1.049012	0.495343	-0.292104	x
x Cl	1	1.140633	0.776825	1.158674	x
x Cl	2	1.073410	0.630958	1.184745	x
x Cl	3	0.161845	1.530751	1.026258	x
x Cl	4	0.026766	1.464601	0.934651	x
x Cl	5	0.851814	0.349196	0.834382	x
x Cl	6	0.724540	0.544256	0.752738	x
x Cl	7	-0.277571	2.149368	0.666573	x
x Cl	8	-0.362910	2.001859	0.671706	x
x Cl	9	-0.448269	1.707980	0.250903	x
x Cl	10	-0.652022	1.856624	0.333491	x
x Cl	11	-0.537579	1.014624	0.420155	x
x Cl	12	-0.465385	1.130884	0.518561	x
x Cl	13	0.223732	0.841099	0.702845	x
x Cl	14	0.428528	0.754396	0.696564	x
x Cl	15	0.253320	0.968149	0.684594	x
x Cl	16	-0.776825	-1.140633	-1.158674	x
x Cl	17	-0.630958	-1.073410	-1.184745	x
x Cl	18	-1.530751	-0.161845	-1.026258	x

x Cl	19	-1.464601	-0.026766	-0.934651	x
x Cl	20	-0.349196	-0.851814	-0.834382	x
x Cl	21	-0.544256	-0.724540	-0.752738	x
x Cl	22	-2.149368	0.277571	-0.666573	x
x Cl	23	-2.001859	0.362910	-0.671706	x
x Cl	24	-1.707980	0.448269	-0.250903	x
x Cl	25	-1.856624	0.652022	-0.333491	x
x Cl	26	-1.014624	0.537579	-0.420155	x
x Cl	27	-1.130884	0.465385	-0.518561	x
x Cl	28	-0.841099	-0.223732	-0.702845	x
x Cl	29	-0.754396	-0.428528	-0.696564	x
x Cl	30	-0.968149	-0.253320	-0.684594	x
x Zn	1	1.030157	0.767052	1.165520	x
x Zn	2	0.152953	1.459055	0.964586	x
x Zn	3	0.727702	0.495694	0.807623	x
x Zn	4	-0.247908	2.009261	0.664415	x
x Zn	5	-0.506796	1.728633	0.307315	x
x Zn	6	-0.541802	1.135845	0.456421	x
x Zn	7	-0.767052	-1.030157	-1.165520	x
x Zn	8	-1.459055	-0.152953	-0.964586	x
x Zn	9	-0.495694	-0.727702	-0.807623	x
x Zn	10	-2.009261	0.247908	-0.664415	x
x Zn	11	-1.728633	0.506796	-0.307315	x
x Zn	12	-1.135845	0.541802	-0.456421	x

Table S10. Fractional atomic coordinates of the optimised structure of chloroform@1a

x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	x
x	-----					x
x	H	1	0.864956	0.969811	0.863412	x
x	H	2	0.734988	1.021034	0.802854	x
x	H	3	0.884925	0.713593	0.774956	x
x	H	4	1.004124	0.675543	0.840192	x
x	H	5	0.235798	1.286025	0.681620	x
x	H	6	0.389650	1.106240	0.671161	x
x	H	7	0.549119	1.168787	0.757279	x
x	H	8	0.388311	1.346498	0.764951	x
x	H	9	0.807840	0.529922	0.656982	x
x	H	10	0.785780	0.663505	0.707347	x
x	H	11	0.561392	0.870948	0.612172	x
x	H	12	0.595737	0.729217	0.564824	x
x	H	13	0.561955	0.589928	0.490652	x
x	H	14	0.392888	0.649044	0.487826	x
x	H	15	0.450463	0.597453	0.624518	x
x	H	16	0.616097	0.541311	0.622260	x
x	H	17	-0.162436	0.916330	0.464783	x
x	H	18	-0.019167	0.789219	0.515140	x
x	H	19	0.141643	0.852178	0.478550	x
x	H	20	-0.008019	0.976983	0.429323	x
x	H	21	0.327099	0.481509	0.713502	x
x	H	22	0.351340	0.542444	0.657115	x
x	H	23	0.067561	0.663884	0.594752	x
x	H	24	0.056459	0.593340	0.651660	x
x	H	25	0.144457	1.386453	0.471925	x
x	H	26	0.111820	1.358026	0.637796	x
x	H	27	0.612131	0.639191	0.430152	x
x	H	28	-0.969811	-0.864956	-0.363412	x
x	H	29	-1.021034	-0.734988	-0.302854	x
x	H	30	-0.713593	-0.884925	-0.274956	x
x	H	31	-0.675543	-1.004124	-0.340192	x
x	H	32	-1.286025	-0.235798	-0.181620	x
x	H	33	-1.106240	-0.389650	-0.171161	x
x	H	34	-1.168787	-0.549119	-0.257279	x
x	H	35	-1.346498	-0.388311	-0.264951	x
x	H	36	-0.529922	-0.807840	-0.156982	x
x	H	37	-0.663505	-0.785780	-0.207347	x
x	H	38	-0.870948	-0.561392	-0.112172	x
x	H	39	-0.729217	-0.595737	-0.064824	x
x	H	40	-0.589928	-0.561955	0.009348	x
x	H	41	-0.649044	-0.392888	0.012174	x

x H	42	-0.597453	-0.450463	-0.124518	x
x H	43	-0.541311	-0.616097	-0.122260	x
x H	44	-0.916330	0.162436	0.035217	x
x H	45	-0.789219	0.019167	-0.015140	x
x H	46	-0.852178	-0.141643	0.021450	x
x H	47	-0.976983	0.008019	0.070677	x
x H	48	-0.481509	-0.327099	-0.213502	x
x H	49	-0.542444	-0.351340	-0.157115	x
x H	50	-0.663884	-0.067561	-0.094752	x
x H	51	-0.593340	-0.056459	-0.151660	x
x H	52	-1.386453	-0.144457	0.028075	x
x H	53	-1.358026	-0.111820	-0.137796	x
x H	54	-0.639191	-0.612131	0.069848	x
x H	55	-0.864956	-0.969811	-0.863412	x
x H	56	-0.734988	-1.021034	-0.802854	x
x H	57	-0.884925	-0.713593	-0.774956	x
x H	58	-1.004124	-0.675543	-0.840192	x
x H	59	-0.235798	-1.286025	-0.681620	x
x H	60	-0.389650	-1.106240	-0.671161	x
x H	61	-0.549119	-1.168787	-0.757279	x
x H	62	-0.388311	-1.346498	-0.764951	x
x H	63	-0.807840	-0.529922	-0.656982	x
x H	64	-0.785780	-0.663505	-0.707347	x
x H	65	-0.561392	-0.870948	-0.612172	x
x H	66	-0.595737	-0.729217	-0.564824	x
x H	67	-0.561955	-0.589928	-0.490652	x
x H	68	-0.392888	-0.649044	-0.487826	x
x H	69	-0.450463	-0.597453	-0.624518	x
x H	70	-0.616097	-0.541311	-0.622260	x
x H	71	0.162436	-0.916330	-0.464783	x
x H	72	0.019167	-0.789219	-0.515140	x
x H	73	-0.141643	-0.852178	-0.478550	x
x H	74	0.008019	-0.976983	-0.429323	x
x H	75	-0.327099	-0.481509	-0.713502	x
x H	76	-0.351340	-0.542444	-0.657115	x
x H	77	-0.067561	-0.663884	-0.594752	x
x H	78	-0.056459	-0.593340	-0.651660	x
x H	79	-0.144457	-1.386453	-0.471925	x
x H	80	-0.111820	-1.358026	-0.637796	x
x H	81	-0.612131	-0.639191	-0.430152	x
x H	82	0.969811	0.864956	1.363412	x
x H	83	1.021034	0.734988	1.302854	x
x H	84	0.713593	0.884925	1.274956	x
x H	85	0.675543	1.004124	1.340192	x
x H	86	1.286025	0.235798	1.181620	x
x H	87	1.106240	0.389650	1.171161	x

x H	88	1.168787	0.549119	1.257279	x
x H	89	1.346498	0.388311	1.264951	x
x H	90	0.529922	0.807840	1.156982	x
x H	91	0.663505	0.785780	1.207347	x
x H	92	0.870948	0.561392	1.112172	x
x H	93	0.729217	0.595737	1.064824	x
x H	94	0.589928	0.561955	0.990652	x
x H	95	0.649044	0.392888	0.987826	x
x H	96	0.597453	0.450463	1.124518	x
x H	97	0.541311	0.616097	1.122260	x
x H	98	0.916330	-0.162436	0.964783	x
x H	99	0.789219	-0.019167	1.015140	x
x H	100	0.852178	0.141643	0.978550	x
x H	101	0.976983	-0.008019	0.929323	x
x H	102	0.481509	0.327099	1.213502	x
x H	103	0.542444	0.351340	1.157115	x
x H	104	0.663884	0.067561	1.094752	x
x H	105	0.593340	0.056459	1.151660	x
x H	106	1.386453	0.144457	0.971925	x
x H	107	1.358026	0.111820	1.137796	x
x H	108	0.639191	0.612131	0.930152	x
x C	1	0.865895	0.915598	0.843367	x
x C	2	0.794986	0.943425	0.809099	x
x C	3	0.800942	0.870586	0.783459	x
x C	4	0.877421	0.772311	0.794354	x
x C	5	0.943972	0.750556	0.830025	x
x C	6	0.724654	0.898227	0.747462	x
x C	7	0.660378	0.856111	0.691711	x
x C	8	0.574776	1.017941	0.712404	x
x C	9	0.307086	1.256956	0.697361	x
x C	10	0.392590	1.157435	0.691612	x
x C	11	0.481794	1.123948	0.713319	x
x C	12	0.481024	1.192826	0.739663	x
x C	13	0.393098	1.290741	0.743774	x
x C	14	0.754182	0.606784	0.648838	x
x C	15	0.741339	0.680707	0.676370	x
x C	16	0.672224	0.777354	0.663314	x
x C	17	0.617207	0.796403	0.623054	x
x C	18	0.635028	0.718374	0.596904	x
x C	19	0.533941	0.592421	0.519267	x
x C	20	0.441409	0.624342	0.517837	x
x C	21	0.411654	0.624329	0.555922	x
x C	22	0.473817	0.595386	0.594357	x
x C	23	0.564325	0.565231	0.593358	x
x C	24	0.316335	0.653525	0.556720	x
x C	25	0.156888	0.740078	0.530643	x

x C	26	0.221684	0.645640	0.587885	x
x C	27	-0.093309	0.899175	0.468859	x
x C	28	-0.014604	0.830116	0.496912	x
x C	29	0.071381	0.812592	0.501024	x
x C	30	0.075288	0.864964	0.476328	x
x C	31	-0.006323	0.933209	0.449044	x
x C	32	0.272664	0.520236	0.685961	x
x C	33	0.285199	0.555090	0.655235	x
x C	34	0.211194	0.607219	0.621427	x
x C	35	0.126778	0.623060	0.620330	x
x C	36	0.120227	0.584281	0.651714	x
x C	37	0.133542	1.337831	0.455272	x
x C	38	0.120523	1.338309	0.602496	x
x C	39	0.541324	0.698002	0.412822	x
x C	40	-0.915598	-0.865895	-0.343367	x
x C	41	-0.943425	-0.794986	-0.309099	x
x C	42	-0.870586	-0.800942	-0.283459	x
x C	43	-0.772311	-0.877421	-0.294354	x
x C	44	-0.750556	-0.943972	-0.330025	x
x C	45	-0.898227	-0.724654	-0.247462	x
x C	46	-0.856111	-0.660378	-0.191711	x
x C	47	-1.017941	-0.574776	-0.212404	x
x C	48	-1.256956	-0.307086	-0.197361	x
x C	49	-1.157435	-0.392590	-0.191612	x
x C	50	-1.123948	-0.481794	-0.213319	x
x C	51	-1.192826	-0.481024	-0.239663	x
x C	52	-1.290741	-0.393098	-0.243774	x
x C	53	-0.606784	-0.754182	-0.148838	x
x C	54	-0.680707	-0.741339	-0.176370	x
x C	55	-0.777354	-0.672224	-0.163314	x
x C	56	-0.796403	-0.617207	-0.123054	x
x C	57	-0.718374	-0.635028	-0.096904	x
x C	58	-0.592421	-0.533941	-0.019267	x
x C	59	-0.624342	-0.441409	-0.017837	x
x C	60	-0.624329	-0.411654	-0.055922	x
x C	61	-0.595386	-0.473817	-0.094357	x
x C	62	-0.565231	-0.564325	-0.093358	x
x C	63	-0.653525	-0.316335	-0.056720	x
x C	64	-0.740078	-0.156888	-0.030643	x
x C	65	-0.645640	-0.221684	-0.087885	x
x C	66	-0.899175	0.093309	0.031141	x
x C	67	-0.830116	0.014604	0.003088	x
x C	68	-0.812592	-0.071381	-0.001024	x
x C	69	-0.864964	-0.075288	0.023672	x
x C	70	-0.933209	0.006323	0.050956	x
x C	71	-0.520236	-0.272664	-0.185961	x

x C	72	-0.555090	-0.285199	-0.155235	x
x C	73	-0.607219	-0.211194	-0.121427	x
x C	74	-0.623060	-0.126778	-0.120330	x
x C	75	-0.584281	-0.120227	-0.151714	x
x C	76	-1.337831	-0.133542	0.044728	x
x C	77	-1.338309	-0.120523	-0.102496	x
x C	78	-0.698002	-0.541324	0.087178	x
x C	79	-0.865895	-0.915598	-0.843367	x
x C	80	-0.794986	-0.943425	-0.809099	x
x C	81	-0.800942	-0.870586	-0.783459	x
x C	82	-0.877421	-0.772311	-0.794354	x
x C	83	-0.943972	-0.750556	-0.830025	x
x C	84	-0.724654	-0.898227	-0.747462	x
x C	85	-0.660378	-0.856111	-0.691711	x
x C	86	-0.574776	-1.017941	-0.712404	x
x C	87	-0.307086	-1.256956	-0.697361	x
x C	88	-0.392590	-1.157435	-0.691612	x
x C	89	-0.481794	-1.123948	-0.713319	x
x C	90	-0.481024	-1.192826	-0.739663	x
x C	91	-0.393098	-1.290741	-0.743774	x
x C	92	-0.754182	-0.606784	-0.648838	x
x C	93	-0.741339	-0.680707	-0.676370	x
x C	94	-0.672224	-0.777354	-0.663314	x
x C	95	-0.617207	-0.796403	-0.623054	x
x C	96	-0.635028	-0.718374	-0.596904	x
x C	97	-0.533941	-0.592421	-0.519267	x
x C	98	-0.441409	-0.624342	-0.517837	x
x C	99	-0.411654	-0.624329	-0.555922	x
x C	100	-0.473817	-0.595386	-0.594357	x
x C	101	-0.564325	-0.565231	-0.593358	x
x C	102	-0.316335	-0.653525	-0.556720	x
x C	103	-0.156888	-0.740078	-0.530643	x
x C	104	-0.221684	-0.645640	-0.587885	x
x C	105	0.093309	-0.899175	-0.468859	x
x C	106	0.014604	-0.830116	-0.496912	x
x C	107	-0.071381	-0.812592	-0.501024	x
x C	108	-0.075288	-0.864964	-0.476328	x
x C	109	0.006323	-0.933209	-0.449044	x
x C	110	-0.272664	-0.520236	-0.685961	x
x C	111	-0.285199	-0.555090	-0.655235	x
x C	112	-0.211194	-0.607219	-0.621427	x
x C	113	-0.126778	-0.623060	-0.620330	x
x C	114	-0.120227	-0.584281	-0.651714	x
x C	115	-0.133542	-1.337831	-0.455272	x
x C	116	-0.120523	-1.338309	-0.602496	x
x C	117	-0.541324	-0.698002	-0.412822	x

x C	118	0.915598	0.865895	1.343367	x
x C	119	0.943425	0.794986	1.309099	x
x C	120	0.870586	0.800942	1.283459	x
x C	121	0.772311	0.877421	1.294354	x
x C	122	0.750556	0.943972	1.330025	x
x C	123	0.898227	0.724654	1.247462	x
x C	124	0.856111	0.660378	1.191711	x
x C	125	1.017941	0.574776	1.212404	x
x C	126	1.256956	0.307086	1.197361	x
x C	127	1.157435	0.392590	1.191612	x
x C	128	1.123948	0.481794	1.213319	x
x C	129	1.192826	0.481024	1.239663	x
x C	130	1.290741	0.393098	1.243774	x
x C	131	0.606784	0.754182	1.148838	x
x C	132	0.680707	0.741339	1.176370	x
x C	133	0.777354	0.672224	1.163314	x
x C	134	0.796403	0.617207	1.123054	x
x C	135	0.718374	0.635028	1.096904	x
x C	136	0.592421	0.533941	1.019267	x
x C	137	0.624342	0.441409	1.017837	x
x C	138	0.624329	0.411654	1.055922	x
x C	139	0.595386	0.473817	1.094357	x
x C	140	0.565231	0.564325	1.093358	x
x C	141	0.653525	0.316335	1.056720	x
x C	142	0.740078	0.156888	1.030643	x
x C	143	0.645640	0.221684	1.087885	x
x C	144	0.899175	-0.093309	0.968859	x
x C	145	0.830116	-0.014604	0.996912	x
x C	146	0.812592	0.071381	1.001024	x
x C	147	0.864964	0.075288	0.976328	x
x C	148	0.933209	-0.006323	0.949044	x
x C	149	0.520236	0.272664	1.185961	x
x C	150	0.555090	0.285199	1.155235	x
x C	151	0.607219	0.211194	1.121427	x
x C	152	0.623060	0.126778	1.120330	x
x C	153	0.584281	0.120227	1.151714	x
x C	154	1.337831	0.133542	0.955272	x
x C	155	1.338309	0.120523	1.102496	x
x C	156	0.698002	0.541324	0.912822	x
x N	1	0.938894	0.820941	0.853920	x
x N	2	0.648409	0.995127	0.741828	x
x N	3	0.578579	0.951629	0.684956	x
x N	4	0.732499	0.826094	0.723945	x
x N	5	0.306724	1.323219	0.722899	x
x N	6	0.702847	0.624941	0.609430	x
x N	7	0.594639	0.562630	0.556350	x

x N	8	0.243132	0.713182	0.526636	x
x N	9	0.142694	0.707210	0.560085	x
x N	10	0.309637	0.617492	0.587922	x
x N	11	-0.089569	0.950351	0.445415	x
x N	12	0.192034	0.533271	0.684160	x
x N	13	-0.820941	-0.938894	-0.353920	x
x N	14	-0.995127	-0.648409	-0.241828	x
x N	15	-0.951629	-0.578579	-0.184956	x
x N	16	-0.826094	-0.732499	-0.223945	x
x N	17	-1.323219	-0.306724	-0.222899	x
x N	18	-0.624941	-0.702847	-0.109430	x
x N	19	-0.562630	-0.594639	-0.056350	x
x N	20	-0.713182	-0.243132	-0.026636	x
x N	21	-0.707210	-0.142694	-0.060085	x
x N	22	-0.617492	-0.309637	-0.087922	x
x N	23	-0.950351	0.089569	0.054585	x
x N	24	-0.533271	-0.192034	-0.184160	x
x N	25	-0.938894	-0.820941	-0.853920	x
x N	26	-0.648409	-0.995127	-0.741828	x
x N	27	-0.578579	-0.951629	-0.684956	x
x N	28	-0.732499	-0.826094	-0.723945	x
x N	29	-0.306724	-1.323219	-0.722899	x
x N	30	-0.702847	-0.624941	-0.609430	x
x N	31	-0.594639	-0.562630	-0.556350	x
x N	32	-0.243132	-0.713182	-0.526636	x
x N	33	-0.142694	-0.707210	-0.560085	x
x N	34	-0.309637	-0.617492	-0.587922	x
x N	35	0.089569	-0.950351	-0.445415	x
x N	36	-0.192034	-0.533271	-0.684160	x
x N	37	0.820941	0.938894	1.353920	x
x N	38	0.995127	0.648409	1.241828	x
x N	39	0.951629	0.578579	1.184956	x
x N	40	0.826094	0.732499	1.223945	x
x N	41	1.323219	0.306724	1.222899	x
x N	42	0.624941	0.702847	1.109430	x
x N	43	0.562630	0.594639	1.056350	x
x N	44	0.713182	0.243132	1.026636	x
x N	45	0.707210	0.142694	1.060085	x
x N	46	0.617492	0.309637	1.087922	x
x N	47	0.950351	-0.089569	0.945415	x
x N	48	0.533271	0.192034	1.184160	x
x Cl	1	0.016893	1.388507	0.466935	x
x Cl	2	0.136746	1.334139	0.398040	x
x Cl	3	0.230843	1.219348	0.475359	x
x Cl	4	0.178739	1.372823	0.587173	x
x Cl	5	0.196145	1.207745	0.593629	x

x Cl	6	0.001236	1.403613	0.576830	x
x Cl	7	0.468949	0.801549	0.450385	x
x Cl	8	0.567456	0.724680	0.369251	x
x Cl	9	0.483662	0.652577	0.392843	x
x Cl	10	-1.388507	-0.016893	0.033065	x
x Cl	11	-1.334139	-0.136746	0.101960	x
x Cl	12	-1.219348	-0.230843	0.024641	x
x Cl	13	-1.372823	-0.178739	-0.087173	x
x Cl	14	-1.207745	-0.196145	-0.093629	x
x Cl	15	-1.403613	-0.001236	-0.076830	x
x Cl	16	-0.801549	-0.468949	0.049615	x
x Cl	17	-0.724680	-0.567456	0.130749	x
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x Cl	19	-0.016893	-1.388507	-0.466935	x
x Cl	20	-0.136746	-1.334139	-0.398040	x
x Cl	21	-0.230843	-1.219348	-0.475359	x
x Cl	22	-0.178739	-1.372823	-0.587173	x
x Cl	23	-0.196145	-1.207745	-0.593629	x
x Cl	24	-0.001236	-1.403613	-0.576830	x
x Cl	25	-0.468949	-0.801549	-0.450385	x
x Cl	26	-0.567456	-0.724680	-0.369251	x
x Cl	27	-0.483662	-0.652577	-0.392843	x
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x Cl	29	1.334139	0.136746	0.898040	x
x Cl	30	1.219348	0.230843	0.975359	x
x Cl	31	1.372823	0.178739	1.087173	x
x Cl	32	1.207745	0.196145	1.093629	x
x Cl	33	1.403613	0.001236	1.076830	x
x Cl	34	0.801549	0.468949	0.950385	x
x Cl	35	0.724680	0.567456	0.869251	x
x Cl	36	0.652577	0.483662	0.892843	x
x Zn	1	1.046912	0.790183	0.902438	x
x Zn	2	0.733338	0.512637	0.564874	x
x Zn	3	0.181248	0.474438	0.731352	x
x Zn	4	-0.790183	-1.046912	-0.402438	x
x Zn	5	-0.512637	-0.733338	-0.064874	x
x Zn	6	-0.474438	-0.181248	-0.231352	x
x Zn	7	-1.046912	-0.790183	-0.902438	x
x Zn	8	-0.733338	-0.512637	-0.564874	x
x Zn	9	-0.181248	-0.474438	-0.731352	x
x Zn	10	0.790183	1.046912	1.402438	x
x Zn	11	0.512637	0.733338	1.064874	x
x Zn	12	0.474438	0.181248	1.231352	x
x I	1	1.127108	0.637378	0.940136	x
x I	2	1.127096	0.826794	0.863766	x
x I	3	0.850389	0.351116	0.601725	x

x I	4	0.764657	0.541246	0.494904	x
x I	5	0.213839	0.531862	0.807123	x
x I	6	0.024691	0.505250	0.707889	x
x I	7	-0.637378	-1.127108	-0.440136	x
x I	8	-0.826794	-1.127096	-0.363766	x
x I	9	-0.351116	-0.850389	-0.101725	x
x I	10	-0.541246	-0.764657	0.005096	x
x I	11	-0.531862	-0.213839	-0.307123	x
x I	12	-0.505250	-0.024691	-0.207889	x
x I	13	-1.127108	-0.637378	-0.940136	x
x I	14	-1.127096	-0.826794	-0.863766	x
x I	15	-0.850389	-0.351116	-0.601725	x
x I	16	-0.764657	-0.541246	-0.494904	x
x I	17	-0.213839	-0.531862	-0.807123	x
x I	18	-0.024691	-0.505250	-0.707889	x
x I	19	0.637378	1.127108	1.440136	x
x I	20	0.826794	1.127096	1.363766	x
x I	21	0.351116	0.850389	1.101725	x
x I	22	0.541246	0.764657	0.994904	x
x I	23	0.531862	0.213839	1.307123	x
x I	24	0.505250	0.024691	1.207889	x

Additional Figures

Figure S1. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of (+)-artemisinin@**1a**. Hydrogen atoms have been omitted.

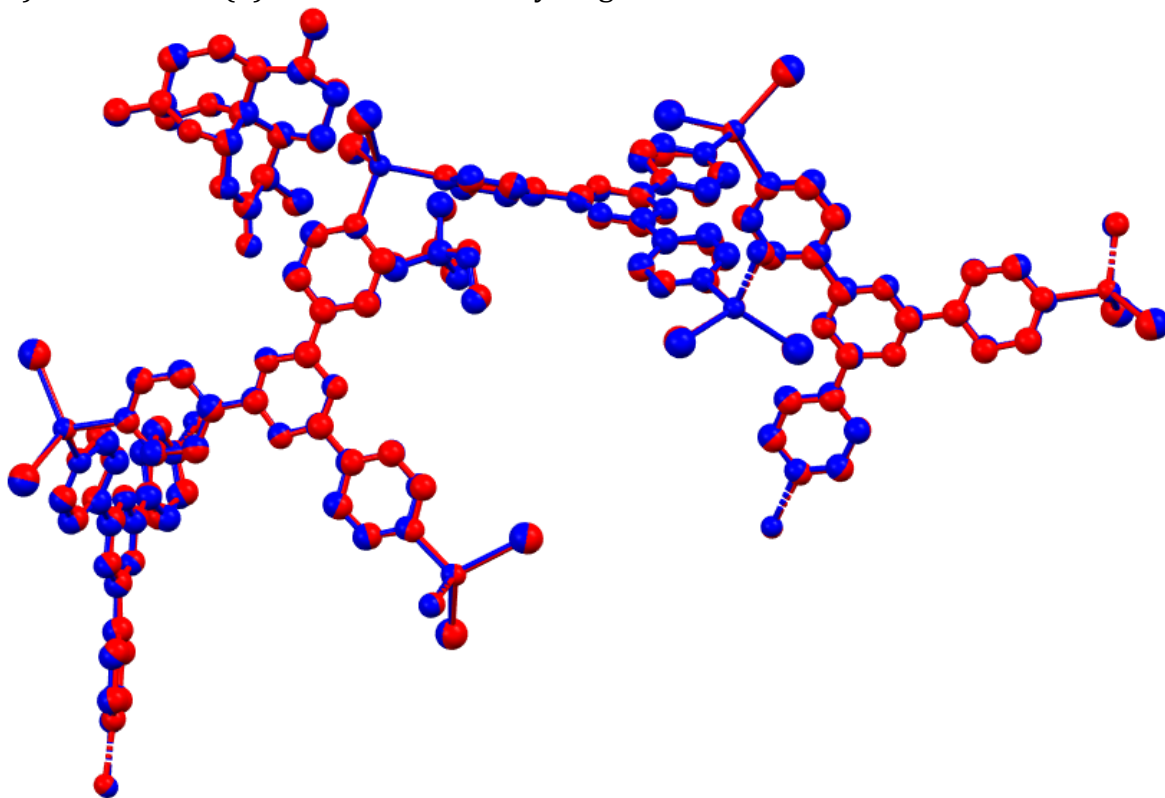


Figure S2. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of 4-(trifluoromethyl)phenyl azide@**1a**. Hydrogen atoms have been omitted.

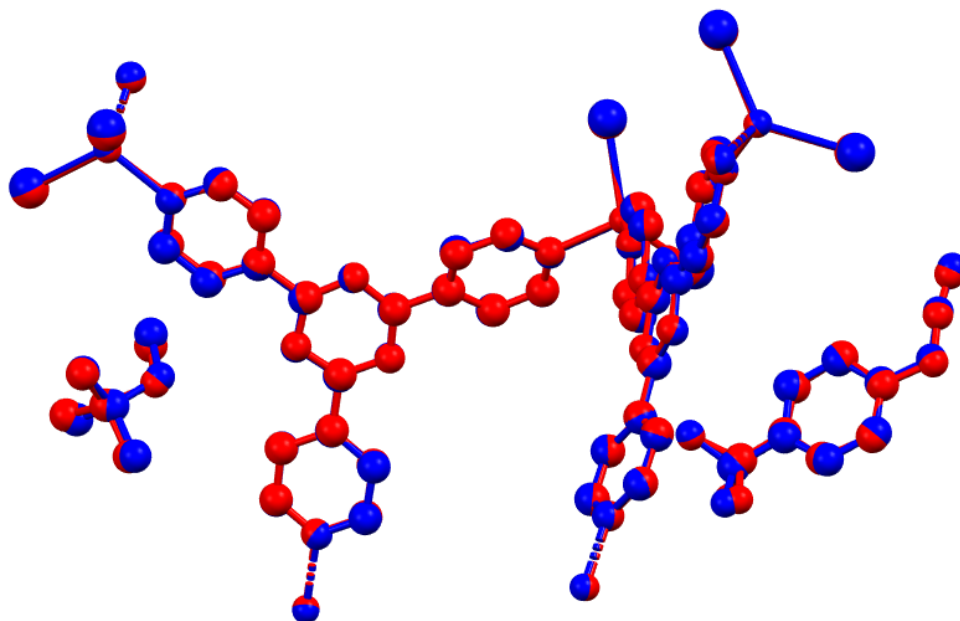


Figure S3. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of vanillin@1a. Hydrogen atoms have been omitted.

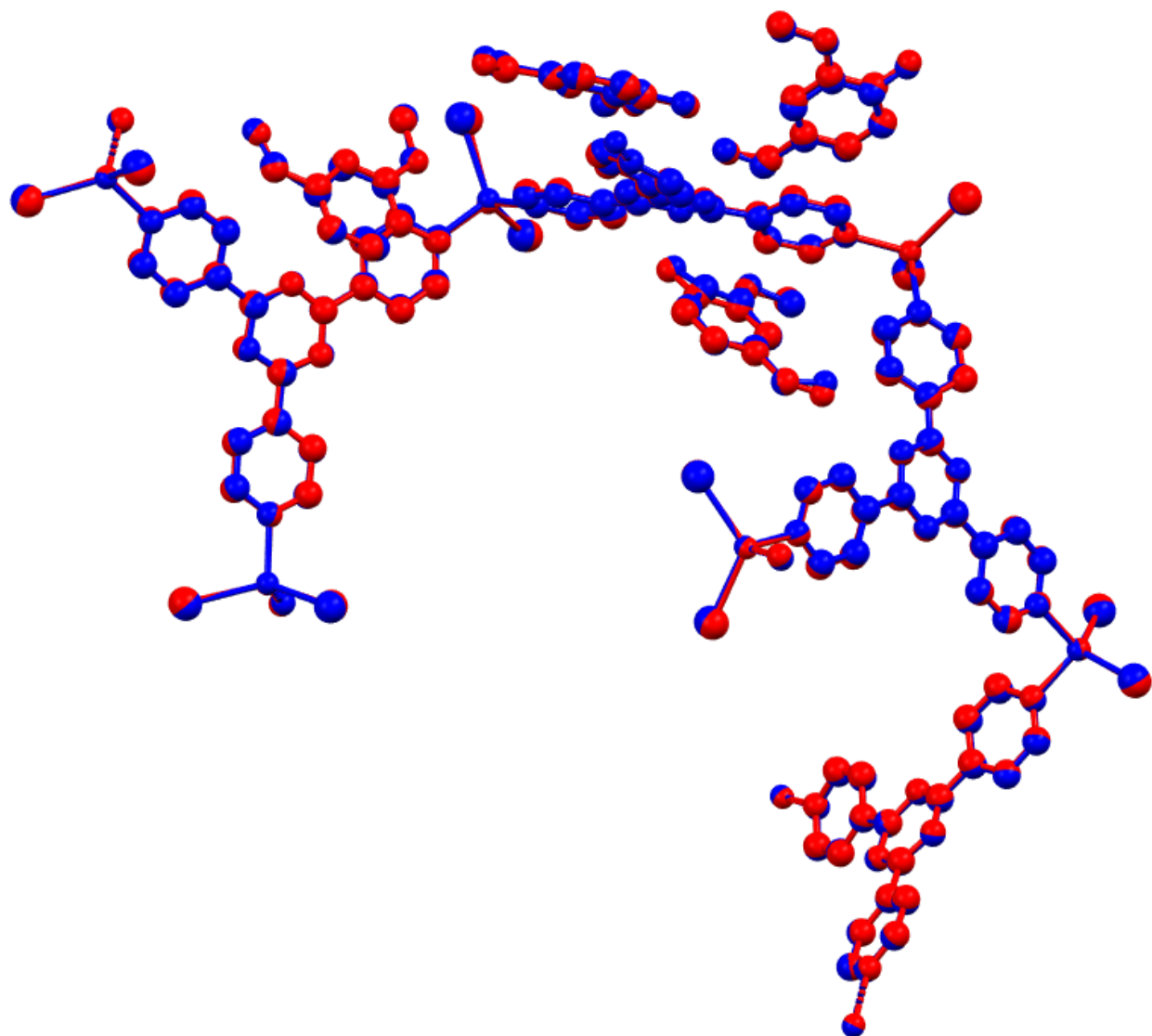


Figure S4. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of (1*R*)-(-)-menthyl acetate@**1b**. Hydrogen atoms have been omitted.

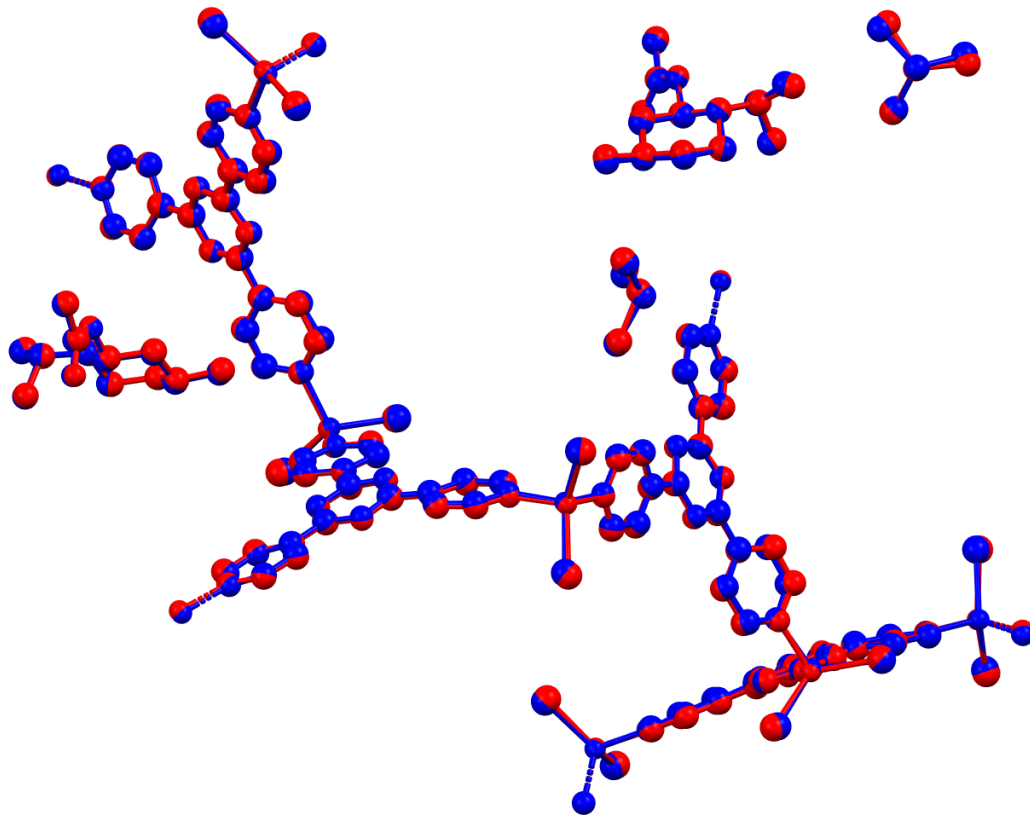


Figure S5. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of (1*R*)-(-)-menthyl acetate@**1c**. Hydrogen atoms have been omitted.

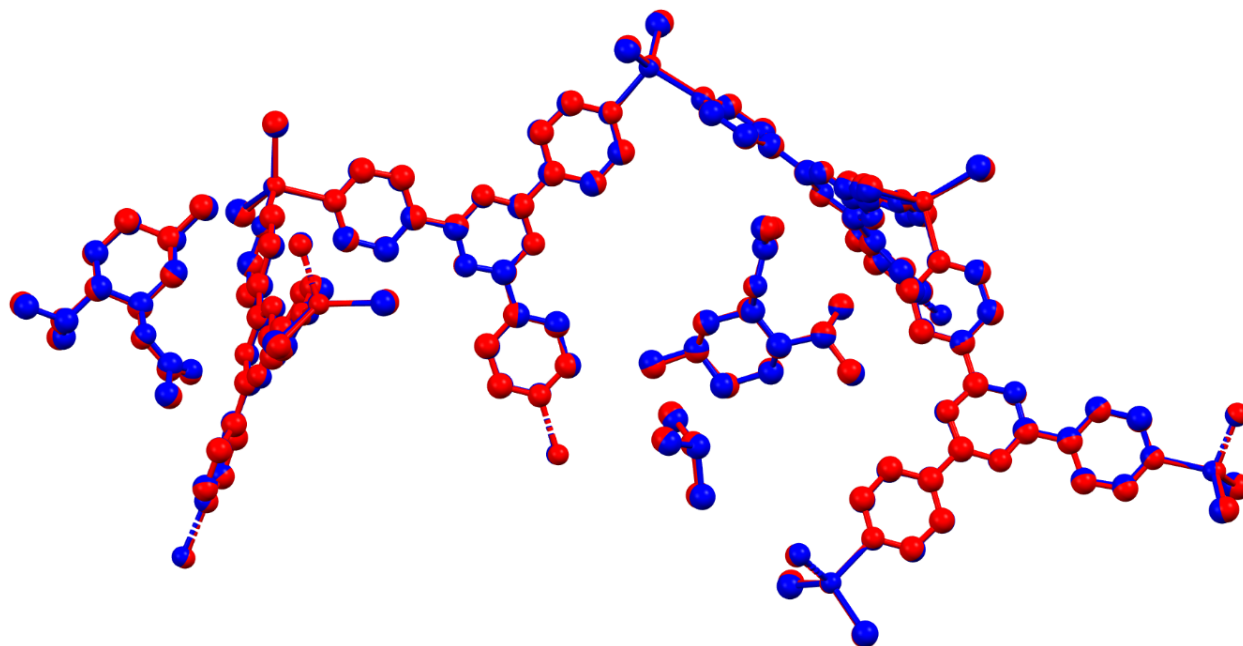


Figure S6. Overlay of the experimental (blue) and computationally geometry optimised (red) structures of chloroform@**1a**. Hydrogen atoms have been omitted.

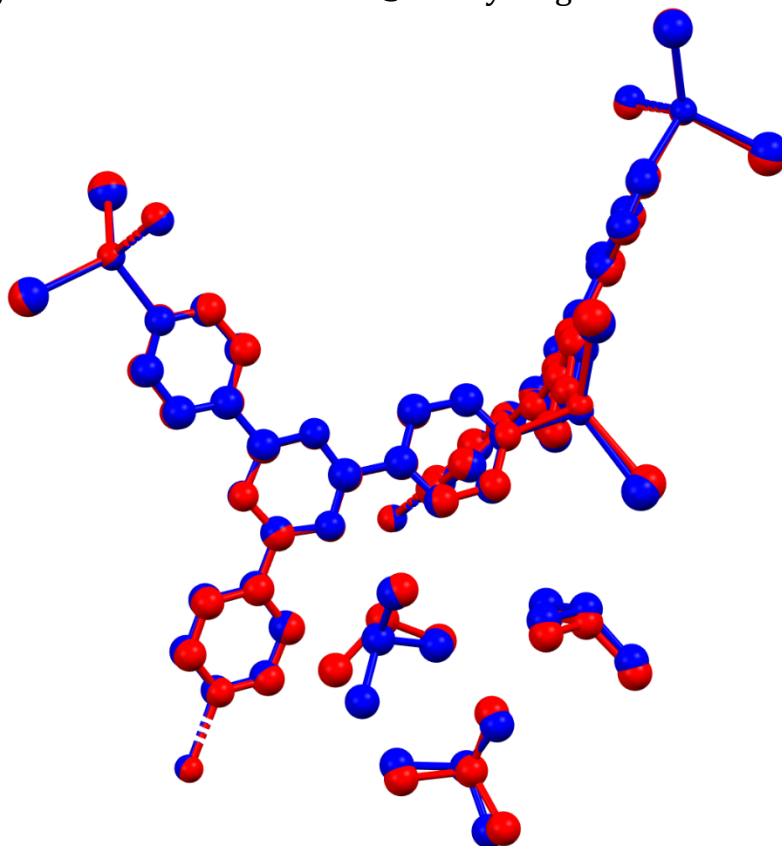


Figure S8. Experimental crystallographic packing models illustrating possible contacts (in Å) forged by (a) **E** in (+)-artemisinin@**1a** and (b) **G** in 4-(trifluoromethyl)phenyl azide@**1a**. Extraneous atoms are hidden for clarity. Guest ellipsoids are shown at 50% probability.

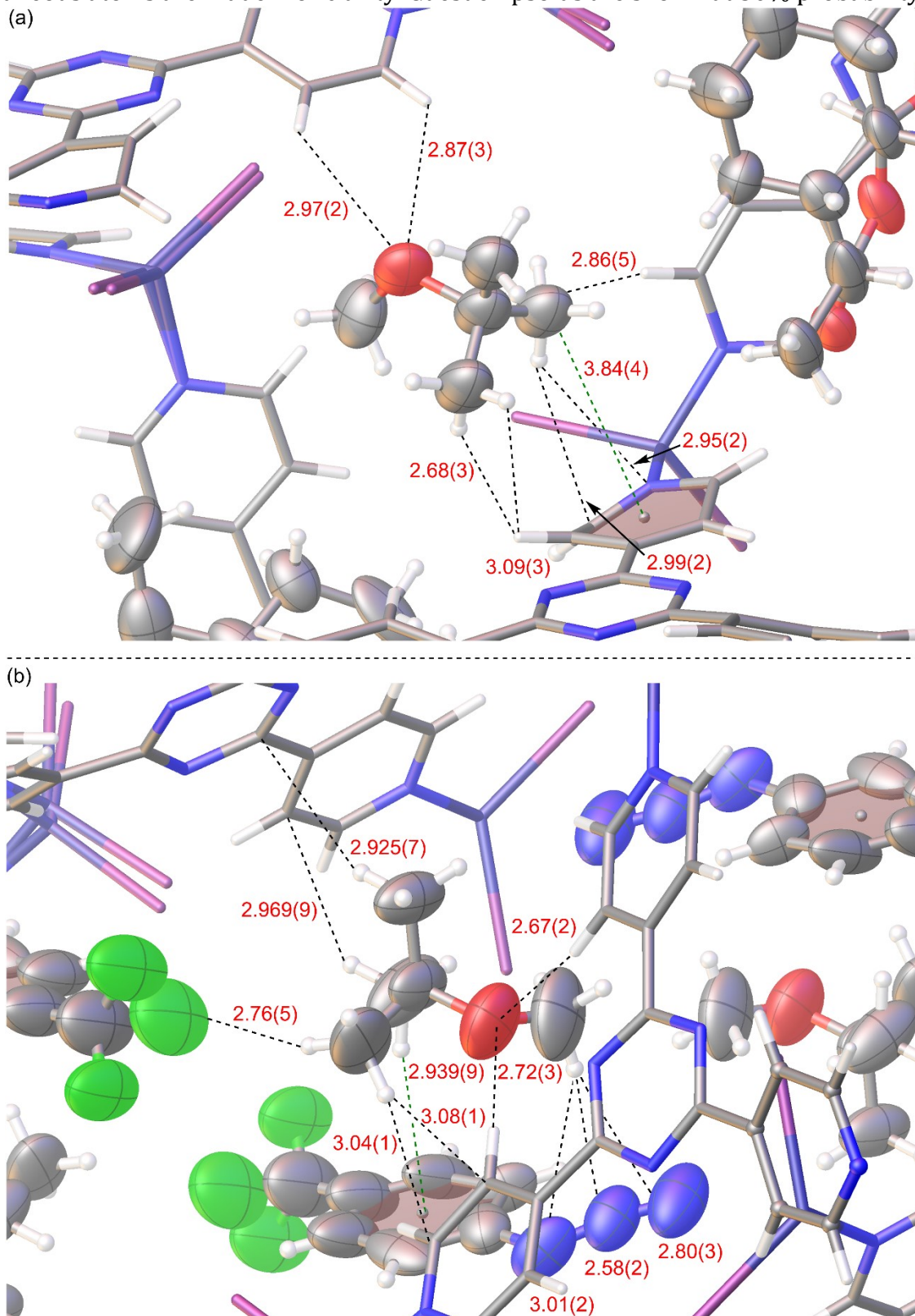


Figure S9. Experimental crystallographic packing model illustrating possible contacts (in Å) forged by **H** in vanillin@**1a**. Extraneous atoms are hidden for clarity. Guest ellipsoids are shown at 50% probability.

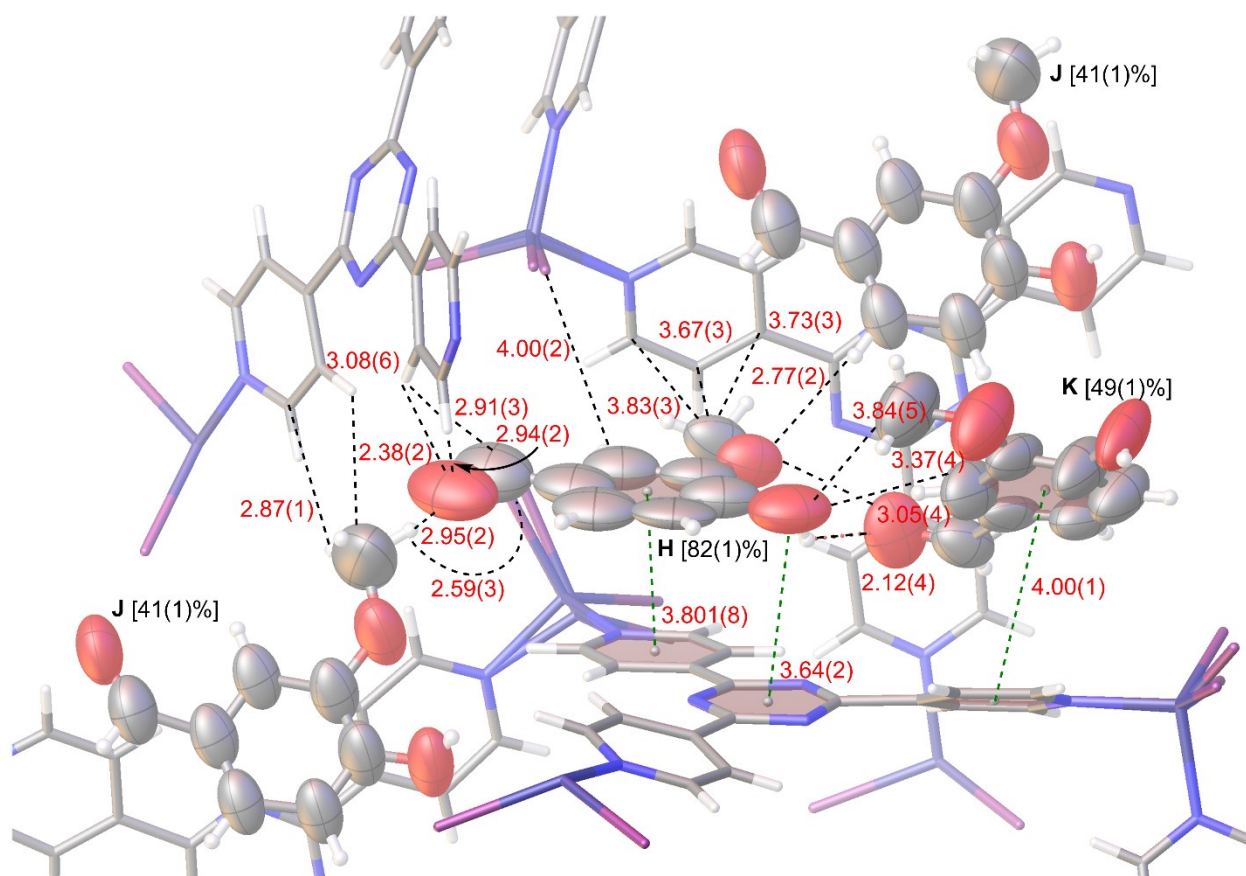


Figure S10. Experimental crystallographic packing model illustrating possible contacts (in Å) forged by **K** (centre) in vanillin@**1a**. Extraneous atoms are hidden for clarity. Guest ellipsoids are shown at 50% probability.

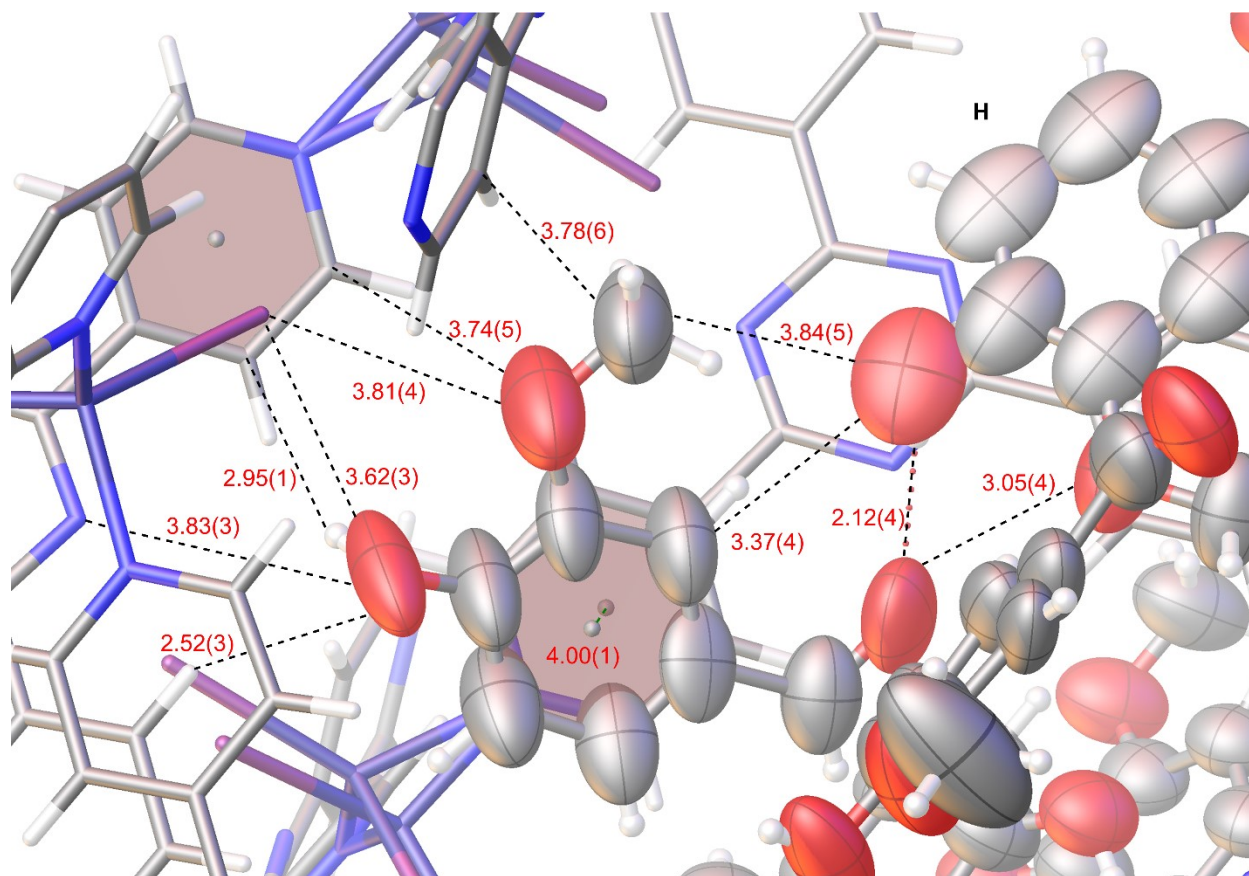


Figure S11. Experimental crystallographic packing models illustrating possible contacts (in Å) in (1*R*)-(-)-menthyl acetate@**1b** forged by (a) **N** and (b) **O**. Extraneous atoms are hidden for clarity. Guest ellipsoids are shown at 50% probability.

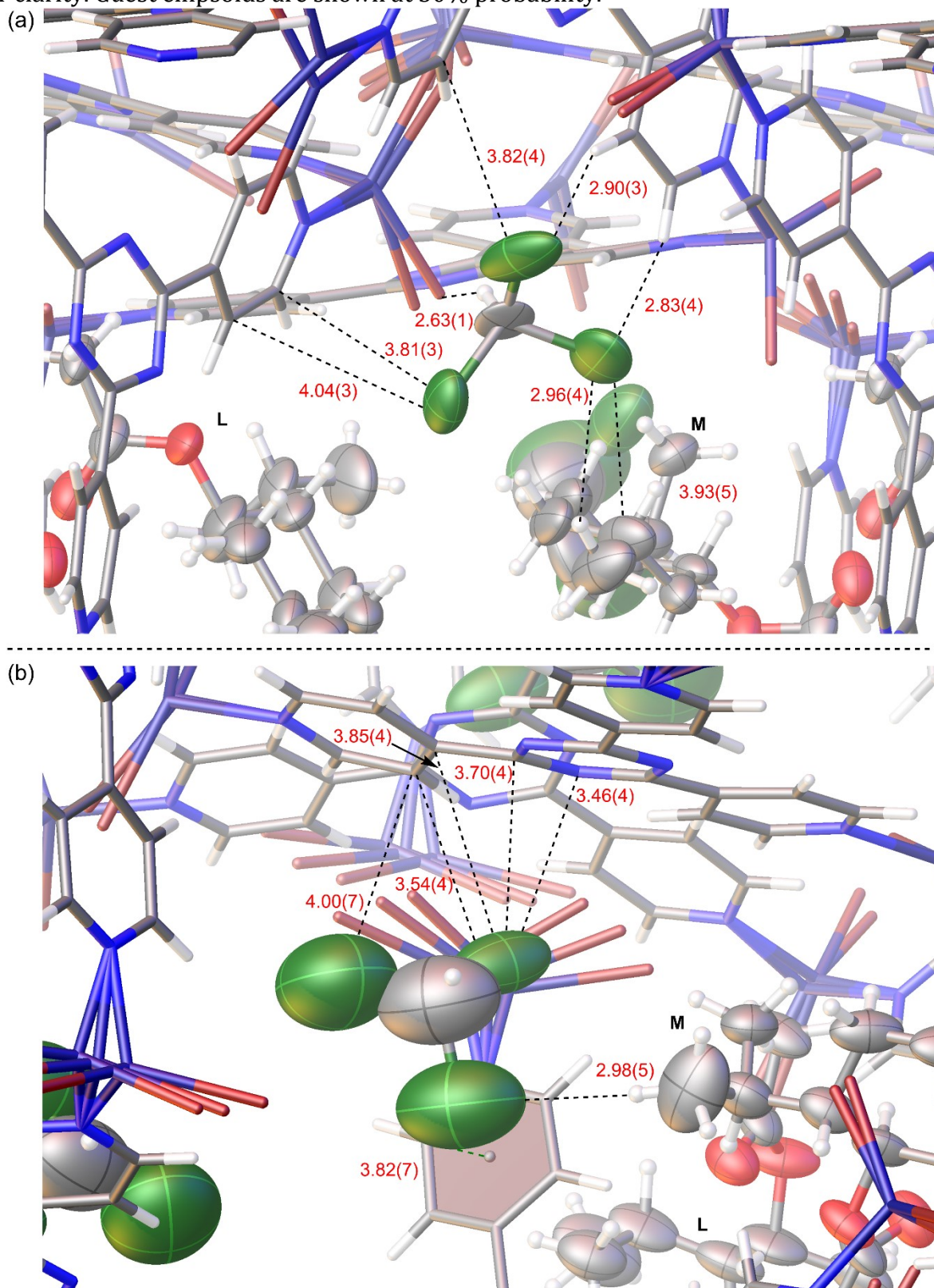
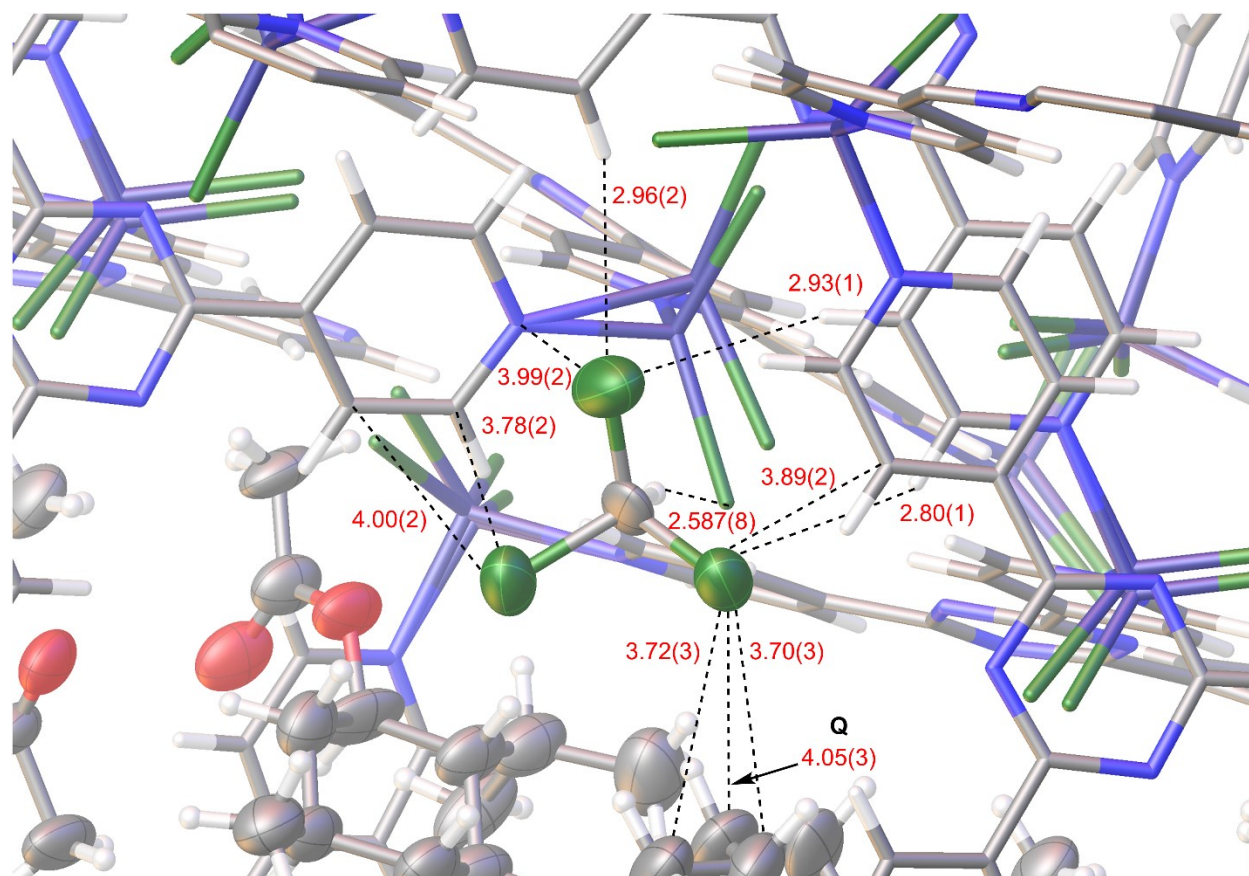


Figure S12. Experimental crystallographic packing model illustrating possible contacts (in Å) forged by **R** in (1*R*)-(-)-menthyl acetate@**1c**. Extraneous atoms are hidden for clarity. Guest ellipsoids are shown at 50% probability.



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