

Supporting Information

Lacking of ESIPT Band of Aromatic ortho-Aminoaldehyde Derivatives

Triggered by the N-H Vibration

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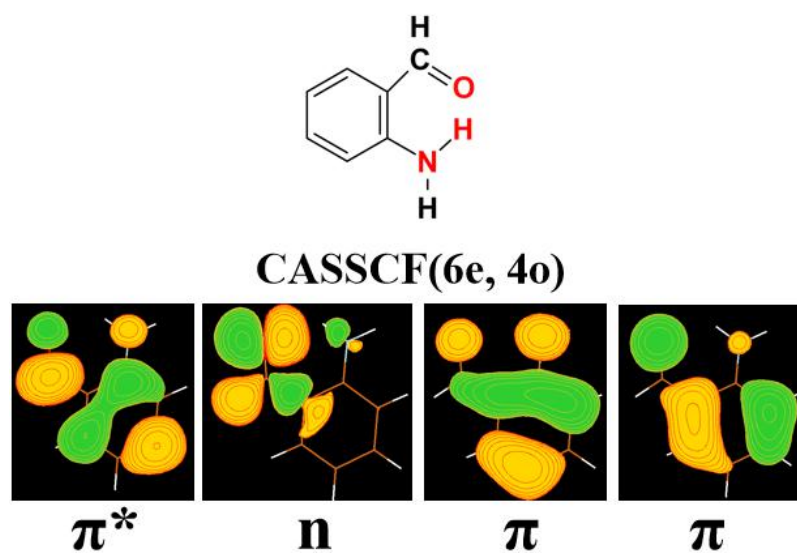


Figure S1: Active spaces used in the CASSCF and NEVPT2 calculations of 2-aminobenzaldehyde (a simplified model of A₁).

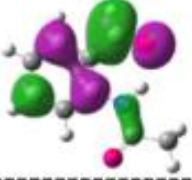
		Hole	Electron	Weight
A₁	T₃(³$\pi\pi^*$)			0.987
	T₂(³$n\pi^*$)			0.998
	T₁(³$\pi\pi^*$)			0.915
K₁	T₃(³$n\pi^*$)			0.972
	T₂(³$\pi\pi^*$)			0.982
	T₁(³$\pi\pi^*$)			0.872

Figure S2: Leading NTOs involved in three low-lying triplet excited states for A₁ and K₁ molecules with isovalue=0.02.

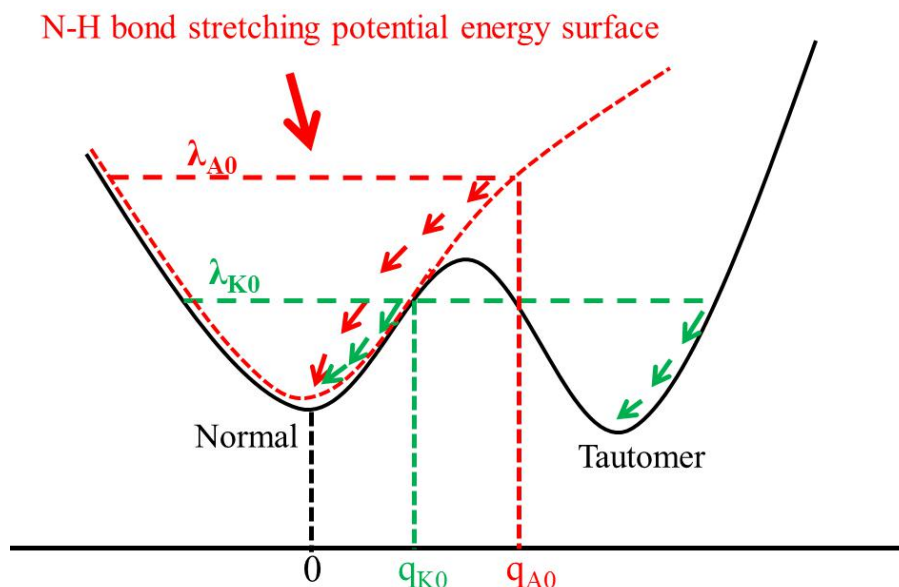


Figure S3: Schematic diagram for helping to understand only one normal emission band of aromatic ortho-aminoaldehyde derivatives triggered by the N-H vibration. And the linear couplings (g_T) for the high frequency modes are obtained from the anharmonic displacement of the N-H vibration.

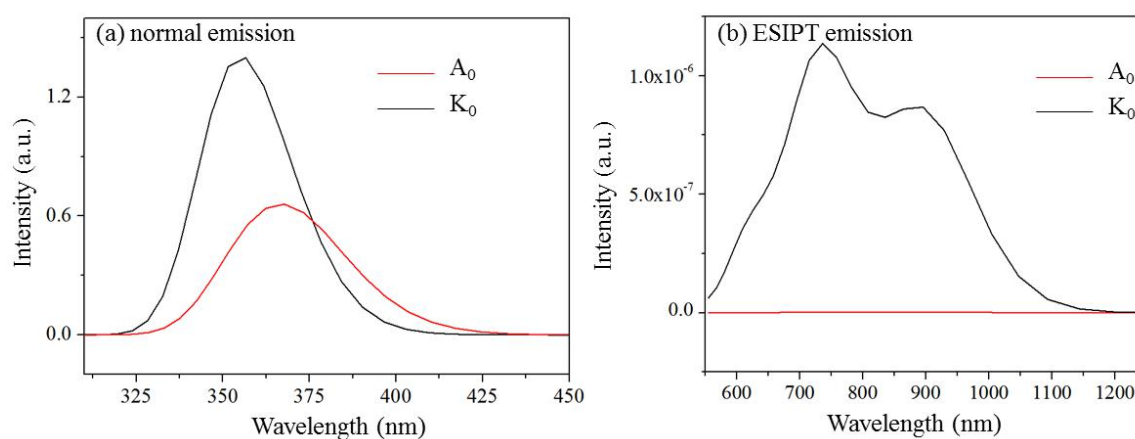


Figure S4: The gaussian expansion spectra of A_0 and K_0 molecules with the ezFCF software for (a) normal emission and (b) ESIPT emission. The width for the gaussian kernel is 0.1 eV.

Table S1: The reorganization energies of $\lambda_{\text{NH}}^{\text{D}}$, $\lambda_{\text{tot}}^{\text{D}}$, and $\lambda_{\text{other}}^{\text{D}}$ (in kcal/mol) for the *o*-aminoaldehydes (A₀-A₅) and *o*-aminoketones derivatives (K₀-K₁₀) computed at the CAM-B3LYP/6-31+G* level of theory using the Dushin (D) program. By means of electronic structure calculations, the total reorganization energy of $\lambda_{\text{tot}}^{\text{ele}}$ (in kcal/mol) can be calculated as $\lambda_{\text{tot}}^{\text{ele}} = (E_{\text{GS}})_{\text{T}} - (E_{\text{GS}})_{\text{G}}$. $(E_{\text{GS}})_{\text{T}}$ and $(E_{\text{GS}})_{\text{G}}$ (in a.u.) represent the absolute energies the optimized ground state geometry (G) and the excited state tautomer structure (T), respectively.

Molecules	$\lambda_{\text{NH}}^{\text{D}}$	$\lambda_{\text{tot}}^{\text{D}}$	$\lambda_{\text{other}}^{\text{D}}$	$(E_{\text{GS}})_{\text{G}}$	$(E_{\text{GS}})_{\text{T}}$	$\lambda_{\text{tot}}^{\text{ele}}$
A ₀	173.4	194.8	21.4	-514.0554636	-514.0100247	28.5
A ₁	155.9	176.2	20.3	-553.3551037	-553.3092337	28.8
A ₂	138.4	158.6	20.2	-3124.581381	-3124.535951	28.5
A ₃	156.6	178.0	21.3	-747.3717048	-747.325411	29.0
A ₄	153.2	173.6	20.3	-785.4419646	-785.3958636	28.9
A ₅	158.4	179.0	20.6	-821.3751933	-821.3292059	28.9
K ₀	153.0	174.9	21.9	-630.7421802	-630.700972	25.9
K ₁	142.3	163.7	21.4	-670.041692	-669.9996444	26.4
K ₂	115.2	135.3	20.1	-3241.268319	-3241.227848	25.4
K ₃	148.3	170.8	22.5	-938.0615473	-938.0189016	26.8
K ₄	122.6	143.7	21.1	-3509.288396	-3509.247551	25.6
K ₅	139.6	160.9	21.4	-902.1282463	-902.0862292	26.4
K ₆	139.7	160.4	20.7	-864.0580404	-864.0163803	26.1
K ₇	131.0	152.3	21.3	-592.6527171	-592.6102271	26.7
K ₈	118.6	139.0	20.4	-3163.879369	-3163.837274	26.4
K ₉	135.3	156.6	21.3	-860.6725152	-860.6296663	26.9
K ₁₀	121.5	142.4	20.9	-3431.899451	-3431.857184	26.5

Table S2: The minimum energy paths (MEP) for A₀ and K₀ molecules.

A ₀		K ₀	
Distance of N-H (Å)	Relative Energy (kcal/mol)	Distance of N-H (Å)	Relative Energy (kcal/mol)
0.9	15.7	1.052	0.0
1.0	1.0	1.152	3.8
1.0	0.0	1.252	4.6
1.1	1.0	1.352	4.3
1.2	5.1	1.452	1.9
1.3	6.1	1.552	1.2
1.4	6.0	1.620	0.9
1.5	3.7	1.752	1.0
1.6	2.6	1.952	2.7
1.8	3.3	2.252	7.0
1.9	3.9		
2.0	4.7		
2.1	5.8		
2.3	8.6		

Table S3: The electronic structure energies ($(E_{GS})_T$ and $(E_{GS})_G$) for the *o*-aminoaldehydes (A₁-A₅) and *o*-aminoketones derivatives (K₁-K₁₀) computed using 10 kinds of functionals (CAM-B3LYP, B3LYP, B3PW91, BHandHYP, HSE06, LC-BLYP, M06-2x, PBE0, wB97XD, and X3LYP, respectively) with the 6-31+G* basis set. $(E_{GS})_G$ and $(E_{GS})_T$ represent the ground state energies of optimized ground state geometry (G) and the excited state tautomer structure (T), respectively, and λ_{tot}^{ele} can be calculated by the formula of $\lambda_{tot}^{ele} = (E_{GS})_T - (E_{GS})_G$.

Molecules		CAM-B3LYP	B3LYP	B3PW91	BHandHYP	HSE06	LC-BLYP	M06-2x	PBE0	wB97XD	X3LYP
A ₁	$(E_{GS})_G$	-553.3551037	-553.6302436	-553.4124099	-553.3026532	-553.0434053	-552.1358909	-553.3886716	-552.9956765	-553.442423	-553.3872745
	$(E_{GS})_T$	-553.3092337	-553.5885693	-553.3710417	-553.2530778	-553.0011015	-552.0849339	-553.3437322	-552.9531736	-553.3959655	-553.3452352
A ₂	$(E_{GS})_G$	-3124.581381	-3124.756929	-3124.524274	-3124.375584	-3123.820647	-3122.867101	-3124.593138	-3123.797795	-3124.594798	-3124.408781
	$(E_{GS})_T$	-3124.535951	-3124.715441	-3124.483511	-3124.326279	-3123.779007	-3122.817079	-3124.548791	-3123.756018	-3124.548818	-3124.36695
A ₃	$(E_{GS})_G$	-747.3717048	-747.7608022	-747.4733534	-747.3120024	-746.9601851	-745.6636826	-747.4338077	-746.897402	-747.5178029	-747.41917
	$(E_{GS})_T$	-747.325411	-747.7183977	-747.4314542	-747.2620102	-746.9174767	-745.6126968	-747.3887802	-746.8545099	-747.4706696	-747.3764407
A ₄	$(E_{GS})_G$	-785.4419646	-785.8475978	-785.5511464	-785.3795222	-785.0150792	-783.6453624	-785.5155096	-784.9501252	-785.5984164	-785.4897126
	$(E_{GS})_T$	-785.3958636	-785.8056069	-785.5096195	-785.3295792	-784.9726919	-783.5943281	-785.4707035	-784.9075443	-785.5521285	-785.4473742
A ₅	$(E_{GS})_G$	-821.3751933	-821.7808488	-821.4613644	-821.2974728	-820.9152361	-819.5608092	-821.4354059	-820.8455755	-821.5095862	-821.4202799
	$(E_{GS})_T$	-821.3292059	-821.7390715	-821.4199252	-821.2478116	-820.8728958	-819.5097122	-821.390489	-820.8030291	-821.4631503	-821.3781437
K ₁	$(E_{GS})_G$	-670.041692	-670.3829335	-670.1270625	-669.9839971	-669.6718967	-668.5333248	-670.0916468	-669.6153808	-670.166721	-670.0803234
	$(E_{GS})_T$	-669.9996444	-670.3448612	-670.0893905	-669.9386498	-669.6332865	-668.4866529	-670.0508676	-669.5766212	-670.1242801	-670.0418816
K ₂	$(E_{GS})_G$	-3241.268319	-3241.509672	-3241.239408	-3241.056992	-3240.450022	-3239.265244	-3241.297676	-3240.418323	-3241.320033	-3241.101999
	$(E_{GS})_T$	-3241.227848	-3241.472925	-3241.203432	-3241.013093	-3240.41316	-3239.22062	-3241.258431	-3240.381396	-3241.279122	-3241.064913
K ₃	$(E_{GS})_G$	-938.0615473	-938.5332604	-938.1758167	-937.9786102	-937.5435031	-935.9580634	-938.1383171	-937.4650707	-938.2339492	-938.113041

K ₄	(E _{GS}) _T	-938.0189016	-938.4946589	-938.1375553	-937.9325883	-937.504378	-935.9107537	-938.0970694	-937.4257715	-938.1910697	-938.0740839
	(E _{GS}) _G	-3509.288396	-3509.660199	-3509.288358	-3509.051852	-3508.32185	-3506.690272	-3509.344616	-3508.268235	-3509.387539	-3509.134928
K ₅	(E _{GS}) _T	-3509.247551	-3509.623079	-3509.25189	-3509.007482	-3508.284668	-3506.645271	-3509.305422	-3508.230952	-3509.346737	-3509.097515
	(E _{GS}) _G	-902.1282463	-902.5999148	-902.265492	-902.0605692	-901.643242	-900.042553	-902.2183155	-901.5695136	-902.3226454	-902.1823807
K ₆	(E _{GS}) _T	-902.0862292	-902.5618674	-902.2279224	-902.0150824	-901.6048424	-899.9959953	-902.1778239	-901.5309514	-902.2804727	-902.1439899
	(E _{GS}) _G	-864.0580404	-864.51318	-864.187773	-863.9931253	-863.5884185	-862.0609475	-864.1366808	-863.5168624	-864.242075	-864.1118974
K ₇	(E _{GS}) _T	-864.0163803	-864.4755866	-864.1504979	-863.9481414	-863.5502665	-862.0145201	-864.0962647	-863.4785348	-864.2000588	-864.0739515
	(E _{GS}) _G	-592.6527171	-592.9519652	-592.72055	-592.5979095	-592.3201261	-591.3339855	-592.6903025	-592.2692853	-592.7538819	-592.6873874
K ₈	(E _{GS}) _T	-592.6102271	-592.9136908	-592.6827312	-592.5517789	-592.2813039	-591.2865774	-592.6488977	-592.2303276	-592.7109514	-592.6487225
	(E _{GS}) _G	-3163.879369	-3164.079269	-3163.833035	-3163.671436	-3163.097984	-3162.065773	-3163.895356	-3163.072016	-3163.906926	-3163.709511
K ₉	(E _{GS}) _T	-3163.837274	-3164.040893	-3163.795512	-3163.625393	-3163.05953	-3162.019033	-3163.854281	-3163.033483	-3163.864238	-3163.67077
	(E _{GS}) _G	-860.6725152	-861.1022443	-860.7692535	-860.5924781	-860.1916779	-858.7586485	-860.7368972	-860.1189205	-860.821021	-860.7200559
K ₁₀	(E _{GS}) _T	-860.6296663	-861.0637001	-860.7311523	-860.5459752	-860.1525999	-858.7107967	-860.6951247	-860.0796817	-860.7776098	-860.6811185
	(E _{GS}) _G	-3431.899451	-3432.22959	-3431.881775	-3431.666073	-3430.969593	-3429.490519	-3431.942058	-3430.921707	-3431.974225	-3431.742231
	(E _{GS}) _T	-3431.857184	-3432.191285	-3431.84429	-3431.620036	-3430.93126	-3429.44383	-3431.90111	-3430.88327	-3431.931469	-3431.703581

Table S4: The corrected reorganization energies (kcal/mol) of the N-H vibration ($\lambda_{\text{NH}}^{\text{ele}} = \lambda_{\text{tot}}^{\text{ele}} - \lambda_{\text{other}}^{\text{D}}$) for the *o*-aminoaldehydes (A₁-A₅) and *o*-aminoketones derivatives (K₁-K₁₀) computed with 10 kinds of functionals (CAM-B3LYP, B3LYP, B3PW91, BHandHYP, HSE06, LC-BLYP, M06-2x, PBE0, wB97XD, and X3LYP, respectively) with the 6-31+G* basis set.

Molecules	CAM-B3LYP	B3LYP	B3PW91	BHandHYP	HSE06	LC-BLYP	M06-2x	PBE0	PBE0	wB97XD	X3LYP
A ₁	8.4838837	5.851019913	5.658978635	10.80906427	6.246076363	11.67604652	7.899894029	8.039450998	6.370956501	8.852580966	6.080052905
A ₂	8.307591047	5.834354508	5.379139929	10.73924877	5.929930556	11.18984488	7.628248721	7.697425423	6.015397419	8.653047852	6.049439836
A ₃	7.749822438	5.309233362	4.992214055	10.07062613	5.499960634	10.69413073	6.955216565	7.471897631	5.615256812	8.27659261	5.51306367
A ₄	8.62883851	6.049729112	5.758540626	11.03974636	6.298453996	11.72457815	7.816270791	7.874578393	6.419958757	8.746133307	6.267767501
A ₅	8.257553374	5.61567164	5.40353561	10.56292722	5.968950358	11.46388851	7.585792624	7.711080643	6.098292091	8.538990354	5.840890627
K ₁	4.985289476	2.490802311	2.239564878	7.055916854	2.82831233	7.887122875	4.189332574	5.035014623	2.922032831	5.232113004	2.722644666
K ₂	5.2962	2.958953093	2.475243284	7.446942263	3.031430498	7.901924663	4.52660485	5.174897981	3.072093146	5.571911008	3.171666433
K ₃	4.260603207	1.722864288	1.509395426	6.379201842	2.051383343	7.187331182	3.383341717	4.385832868	2.160623422	4.407335753	1.945982371
K ₄	4.530771452	2.193026873	1.78400958	6.742675176	2.232158396	7.138677912	3.494112382	4.234542806	2.2951604	4.503788522	2.376774351
K ₅	4.966150421	2.475102011	2.175289656	7.143439438	2.696129858	7.815393461	4.008861326	4.853167873	2.798168632	5.063782192	2.690638518
K ₆	5.442129351	2.890213726	2.690457213	7.527819479	3.2407565	8.433669697	4.661503146	5.435630857	3.350964826	5.665609507	3.111447397
K ₇	5.3628999	2.717618317	2.431729781	7.64736888	3.061301152	8.449061851	4.681956169	5.418607728	3.146352602	5.639282287	2.962601359
K ₈	6.01503345	3.680871953	3.145787901	8.491865621	3.729798908	8.929735824	5.375406232	6.072996549	3.779811454	6.386908426	3.910145281
K ₉	5.588113239	2.886858392	2.608879619	7.881054859	3.221839545	8.727457918	4.912707911	5.879222658	3.322689187	5.9410029	3.133589676
K ₁₀	5.622463162	3.136845851	2.622174699	7.989054376	3.15435338	8.398034018	4.795367331	5.579309299	3.219846599	5.929792459	3.352809693

Table S5: The absolute energies of $(E_{ES})_N$ and $(E_{ES})_b$ (in a.u.) for the *o*-aminoaldehydes (A_1 - A_5) and *o*-aminoketones derivatives (K_1 - K_{10}) computed using 10 kinds of functionals (CAM-B3LYP, B3LYP, B3PW91, BHandHYP, HSE06, LC-BLYP, M06-2x, PBE0, wB97XD, and X3LYP) with the 6-31+G* basis set. $(E_{ES})_N$ and $(E_{ES})_b$ represent the excited state (ES) energies of normal structure (N) and the highest point (b) along MEP, respectively.

Molecules		CAM-B3LYP	B3LYP	B3PW91	BHandHYP	HSE06	LC-BLYP	M06-2x	PBE0	wB97XD	X3LYP
A_1	$(E_{ES})_N$	-553.2159471	-553.5014013	-553.2826742	-553.1531197	-552.9111587	-551.9817255	-553.2449341	-552.8623345	-553.3003317	-553.2572067
	$(E_{ES})_b$	-553.2077711	-553.4925855	-553.2751857	-553.1430157	-552.9035284	-551.9734619	-553.2391254	-552.8550382	-553.2909814	-553.2484733
A_2	$(E_{ES})_N$	-3124.447142	-3124.634885	-3124.40167	-3124.231281	-3123.695835	-3122.717221	-3124.455257	-3123.671499	-3124.457539	-3124.285453
	$(E_{ES})_b$	-3124.437451	-3124.623756	-3124.391855	-3124.219371	-3123.685827	-3122.707792	-3124.447664	-3123.661946	-3124.44663	-3124.274434
A_3	$(E_{ES})_N$	-747.2325161	-747.6318179	-747.3436061	-747.1626027	-746.8280055	-745.5098879	-747.2903858	-746.7641219	-747.3754744	-747.2889801
	$(E_{ES})_b$	-747.2241256	-747.6227218	-747.335877	-747.1522424	-746.8201774	-745.5014871	-747.2843728	-746.7566341	-747.3659436	-747.2799813
A_4	$(E_{ES})_N$	-785.3033925	-785.7196435	-785.4223233	-785.2307215	-784.8837693	-783.4918194	-785.3727219	-784.8176368	-785.457216	-785.360509
	$(E_{ES})_b$	-785.2948079	-785.7103489	-785.4144561	-785.2201534	-784.8758022	-783.483359	-785.3666448	-784.8100087	-785.4476988	-785.3513118
A_5	$(E_{ES})_N$	-821.2357187	-821.6557091	-821.335893	-821.1477916	-820.7882324	-819.4064883	-821.2915942	-820.7128312	-821.3673663	-821.2922117
	$(E_{ES})_b$	-821.2274814	-821.644762	-821.3262249	-821.1375472	-820.7780818	-819.3980465	-821.2857239	-820.7051627	-821.3580694	-821.2821062
K_1	$(E_{ES})_N$	-669.9022395	-670.2547249	-669.9982843	-669.8346846	-669.5406263	-668.3790779	-669.9495546	-669.4829755	-670.0248716	-669.9508469
	$(E_{ES})_b$	-669.8968786	-670.2489802	-669.9937371	-669.8272771	-669.535802	-668.3733847	-669.9455395	-669.4784836	-670.0183905	-669.9451274
K_2	$(E_{ES})_N$	-3241.13248	-3241.386025	-3241.115481	-3240.911483	-3240.323882	-3239.114387	-3241.159645	-3240.290793	-3241.181672	-3240.977066
	$(E_{ES})_b$	-3241.126415	-3241.378968	-3241.109546	-3240.903596	-3240.3177	-3239.108069	-3241.15518	-3240.285014	-3241.174403	-3240.970078
K_3	$(E_{ES})_N$	-937.9219912	-938.4055056	-938.0474527	-937.8293204	-937.4129214	-935.8038523	-937.9962883	-937.3328243	-938.0921315	-937.9839095
	$(E_{ES})_b$	-937.916743	-938.3999072	-938.0430173	-937.8218248	-937.4080139	-935.7982671	-937.992116	-937.3285236	-938.0858186	-937.9783747

K ₄	(E _{ES}) _N	-3509.152589	-3509.536955	-3509.164777	-3508.906442	-3508.196343	-3506.539651	-3509.207006	-3508.140922	-3509.249613	-3509.01035
	(E _{ES}) _b	-3509.146503	-3509.529887	-3509.158854	-3508.898469	-3508.190033	-3506.533172	-3509.202436	-3508.135242	-3509.242344	-3509.003383
K ₅	(E _{ES}) _N	-901.9894522	-902.4726204	-902.1375348	-901.9120459	-901.5128359	-899.8889225	-902.07672	-901.437922	-902.1815471	-902.0538224
	(E _{ES}) _b	-901.9840894	-902.4669461	-902.1330569	-901.9044274	-901.5081044	-899.8834786	-902.0729022	-901.4335184	-902.1753523	-902.0481714
K ₆	(E _{ES}) _N	-863.9185899	-864.3848498	-864.0589002	-863.8439345	-863.4571518	-861.9069634	-863.9943849	-863.3844567	-864.099765	-863.9823356
	(E _{ES}) _b	-863.9133526	-864.3793443	-864.0545783	-863.8364667	-863.4525495	-861.9015756	-863.9906337	-863.3801717	-864.0935986	-863.9768407
K ₇	(E _{ES}) _N	-592.51129	-592.8210514	-592.5888433	-592.4461295	-592.1858745	-591.1775387	-592.5445776	-592.1339517	-592.6095366	-592.5552183
	(E _{ES}) _b	-592.5056595	-592.8152546	-592.58433	-592.4383604	-592.1810915	-591.1715578	-592.5410156	-592.1294883	-592.6029646	-592.549433
K ₈	(E _{ES}) _N	-3163.74274	-3163.954701	-3163.707991	-3163.524574	-3162.970716	-3161.913341	-3163.755197	-3162.943309	-3163.767132	-3163.58365
	(E _{ES}) _b	-3163.735883	-3163.947805	-3163.702298	-3163.515753	-3162.964676	-3161.906925	-3163.75047	-3162.937651	-3163.759923	-3163.576763
K ₉	(E _{ES}) _N	-860.5313383	-860.9731425	-860.6396916	-860.4410854	-860.0603595	-858.6026673	-860.5917732	-859.9843129	-860.677183	-860.5890003
	(E _{ES}) _b	-860.525683	-860.9668928	-860.6344886	-860.4333983	-860.0544305	-858.5969497	-860.5881023	-859.9799872	-860.6708275	-860.5831953
K ₁₀	(E _{ES}) _N	-3431.762852	-3432.106408	-3431.758491	-3431.519607	-3430.844712	-3429.338534	-3431.802431	-3430.793654	-3431.834885	-3431.617278
	(E _{ES}) _b	-3431.756279	-3432.098169	-3431.751298	-3431.510986	-3430.836945	-3429.331763	-3431.797857	-3430.787311	-3431.827205	-3431.6094

Table S6: The energy difference of zero-point vibrational energy (Δ ZPVE) between the excited state normal structure (N) and the structure with the highest point (b) along MEP for the *o*-aminoaldehydes (A₁-A₅) and *o*-aminoketones derivatives (K₁-K₁₀) computed at the CAM-B3LYP/6-31+G* level of theory.

Molecules	(ZPVE) _N (a.u)	(ZPVE) _b (a.u)	Δ ZPVE
A ₁	0.156521108	0.1590914	1.6
A ₂	0.147321957	0.1497975	1.4
A ₃	0.256412406	0.2588003	1.5
A ₄	0.264311504	0.266732	1.5
A ₅	0.238033924	0.2404578	1.5
K ₁	0.222342958	0.2246257	1.4
K ₂	0.212719629	0.2153457	1.6
K ₃	0.303678594	0.3060217	1.5
K ₄	0.294247864	0.2966987	1.5
K ₅	0.329938256	0.3323098	1.5
K ₆	0.321960758	0.3243133	1.5
K ₇	0.184864036	0.1869787	1.3
K ₈	0.175582438	0.1777665	1.4
K ₉	0.266202795	0.2683068	1.3
K ₁₀	0.256749958	0.2591088	1.5

Table S7: The proton transfer barrier (E_b) (in kcal/mol) with zero-point vibrational energy (ZPVE) correction computed using $E_b = (E_{ES})_b - (E_{ES})_N + \Delta ZPVE$. Ten kinds of functionals (CAM-B3LYP, B3LYP, B3PW91, BHandHYP, HSE06, LC-BLYP, M06-2x, PBE0, wB97XD, and X3LYP, respectively) were used to calculate the E_b value of each system (A_1 - A_5 and K_1 - K_{10}). The basis set of 6-31+G* was used for all the calculations.

Molecules		CAM-B3LYP	B3LYP	B3PW91	BHandHYP	HSE06	LC-BLYP	M06-2x	PBE0	wB97XD	X3LYP
A_1	E_b	6.7	7.1	6.3	8.0	6.4	6.8	5.3	6.2	7.5	7.1
A_2	E_b	7.6	8.5	7.7	9.0	7.8	7.5	6.3	7.5	8.4	8.5
A_3	E_b	6.8	7.2	6.4	8.0	6.4	6.8	5.3	6.2	7.5	7.1
A_4	E_b	6.9	7.4	6.5	8.2	6.5	6.8	5.3	6.3	7.5	7.3
A_5	E_b	6.7	8.4	7.6	7.9	7.9	6.8	5.2	6.3	7.4	7.9
K_1	E_b	4.8	5.0	4.3	6.1	4.5	5.0	3.9	4.2	5.5	5.0
K_2	E_b	5.5	6.1	5.4	6.6	5.5	5.6	4.5	5.3	6.2	6.1
K_3	E_b	4.8	5.0	4.3	6.2	4.5	5.0	4.1	4.2	5.4	4.9
K_4	E_b	5.4	6.0	5.3	6.5	5.5	5.6	4.4	5.1	6.1	5.9
K_5	E_b	4.9	5.1	4.3	6.3	4.5	4.9	3.9	4.3	5.4	5.0
K_6	E_b	4.8	4.9	4.2	6.2	4.4	4.9	3.8	4.2	5.3	4.9
K_7	E_b	4.9	5.0	4.2	6.2	4.3	5.1	3.6	4.1	5.5	5.0
K_8	E_b	5.7	5.7	4.9	6.9	5.2	5.4	4.3	4.9	5.9	5.7
K_9	E_b	4.9	5.3	4.6	6.2	5.1	4.9	3.6	4.0	5.3	5.0
K_{10}	E_b	5.6	6.7	6.0	6.9	6.4	5.7	4.4	5.5	6.3	6.4

Table S8: The average values ($\lambda_{\text{NH}}^{\text{avg}}$) of reorganization energy of the N-H vibration and the average values ($E_{\text{b}}^{\text{avg}}$) of the proton transfer barrier for *o*-aminoaldehyde derivatives (A₁-A₅) and *o*-aminoketone derivatives (K₁-K₁₀). The average values are calculated by the formula of $X^{\text{avg}} = \sum_i^M X_i / M$ ($X = \lambda_{\text{NH}}$ or E_{b} ; i = functional (X3LYP, PBE0, B3LYP, B3PW91, BHandHYP, LC-BLYP, CAM-B3LYP, wB97XD, M06-2x, and HSE06). The SD^{λ} and SD^{b} are calculated by the formula of standard deviation (SD) $\text{SD}^X = \{ (\sum_i^M [(X_i - \bar{X})^2] / (M-1))^{1/2} / M$ ($X = \lambda_{\text{NH}}$ or E_{b} ; i = functional. The unit of energy is kcal/mol.

Molecules	$\lambda_{\text{NH}}^{\text{avg}}$	SD^{λ}	$E_{\text{b}}^{\text{avg}}$	SD^{b}
A ₁	7.79	3.37	6.73	2.36
A ₂	8.34	2.27	7.69	2.67
A ₃	7.07	2.97	6.76	2.26
A ₄	7.88	3.39	6.86	2.42
A ₅	7.53	3.13	7.21	2.59
K ₁	4.26	2.45	4.84	1.74
K ₂	4.55	2.47	5.68	1.99
K ₃	3.5	2.33	4.5	2.33
K ₄	3.73	2.31	5.58	1.95
K ₅	4.18	2.46	4.84	1.75
K ₆	4.7	2.57	4.76	1.72
K ₇	4.61	2.63	4.77	1.76
K ₈	4.82	2.65	5.99	2.13
K ₉	5.34	2.27	5.46	1.95
K ₁₀	4.82	2.65	5.99	2.13

Table S9: $(E_{ES})_G$ and $(E_{ES})_T$ represent the excited state energies of the optimized ground state geometry (G) and the optimized excited state tautomer structure (T), respectively, and $\lambda_{tot}^{ele}(ES)$ can be calculated by the formula of $\lambda_{tot}^{ele}(ES) = (E_{ES})_G - (E_{ES})_T$.

	$(E_{ES})_G$ (a.u.)	$(E_{ES})_T$ (a.u.)	$\lambda_{tot}^{ele}(ES)$ (kcal/mol)	$^a\lambda_{tot}^{ele}(GS)$ (kcal/mol)
A ₀	-513.868841	-513.9095592	25.6	28.5
A ₁	-553.1681923	-553.2091391	25.7	28.8
A ₂	-3124.395466	-3124.438103	26.8	28.5
A ₃	-747.1850833	-747.2254829	25.4	29.0
A ₄	-785.25542	-785.2960813	25.5	28.9
A ₅	-821.1885222	-821.2289784	25.4	28.9
K ₀	-630.5597252	-630.5996058	25.0	25.9
K ₁	-669.8593289	-669.8990396	24.9	26.4
K ₂	-3241.0852	-3241.12722	26.4	25.4
K ₃	-937.8793003	-937.9190484	24.9	26.8
K ₄	-3509.105507	-3509.147639	26.4	25.6
K ₅	-901.9460397	-901.9859736	25.1	26.4
K ₆	-863.8757658	-863.9149303	24.6	26.1
K ₇	-592.4646907	-592.507627	26.9	26.7
K ₈	-3163.69272	-3163.73719	27.9	26.4
K ₉	-860.4847791	-860.5273773	26.7	26.9
K ₁₀	-3431.712909	-3431.757203	27.8	26.5

^asee Table S1

Table S10: The total reorganization energies (in kcal/mol) from GS and ES surface computed with electronic structure methods (ADC2 and TDDFT) and Dushin for A₀ and K₀ molecules, respectively.

Method	A ₀		K ₀	
	GS	ES	GS	ES
ADC2 ^a /6-31+G*	31.7	34.6	28.8	37.2
CAM-B3LYP/6-31+G*	28.5	25.6	25.9	25.0
Dushin	194.8	219.2	174.9	175.1

^aThe absolute energies computed with ADC2 of ground and excited states for normal structure of A₀ are -512.7257698 a.u. and -512.5400360 a.u., respectively, for tautomer structure of A₀ are -512.6752668 a.u. and -512.5951521 a.u., respectively, for normal structure of K₀ are -629.0704771 a.u. and -628.8852579 a.u., respectively, for tautomer structure of K₀ are -629.0246474 a.u. and -628.9445327 a.u., respectively. The ADC2 calculations were performed with Molpro2012 Package.

Cartesian Coordinates of All Optimized Structures

In xyz format (unit: Ångstrom)

(A₀)_G

C	2.40608500	0.44298800	0.00000000
C	1.14636500	1.03222900	0.00000000
C	0.00000000	0.23143700	0.00000000
C	0.14701900	-1.17825500	0.00000000
C	1.43051200	-1.73884800	0.00000000
C	2.56297800	-0.94198700	0.00000000
H	3.28175600	1.08506500	0.00000000
H	1.04274100	2.10736700	0.00000000
H	1.52431900	-2.82150800	0.00000000
H	3.55187200	-1.38739000	0.00000000
C	-0.97877200	-2.11343700	0.00000000
H	-0.69362500	-3.17972600	0.00000000
O	-2.16744500	-1.81163600	0.00000000
C	-1.68582200	2.06371300	0.00000000
N	-1.29418200	0.76078500	0.00000000
O	-0.95764300	3.04523300	0.00000000
H	-2.03494300	0.05970400	0.00000000
H	-2.78232900	2.15517700	0.00000000

(A₀)_N

C	2.38358500	0.74319800	0.00000000
C	1.06053600	1.17134800	0.00000000
C	0.00000000	0.23247500	0.00000000
C	0.26241300	-1.21323700	0.00000000
C	1.60682700	-1.58708800	0.00000000
C	2.64645300	-0.63953600	0.00000000
H	3.19321800	1.46239200	0.00000000
H	0.81589600	2.22425800	0.00000000
H	1.85740100	-2.64401300	0.00000000
H	3.67312600	-0.99151700	0.00000000
C	-0.77605300	-2.19734400	0.00000000
H	-0.44044400	-3.24365800	0.00000000
O	-2.02415700	-1.94910700	0.00000000
C	-1.90551300	1.83434300	0.00000000
N	-1.31503400	0.58090400	0.00000000
O	-1.30303900	2.89260100	0.00000000
H	-1.94490700	-0.25587500	0.00000000
H	-3.00097900	1.76918100	0.00000000

(A₀)_T

C	2.44867400	0.47828900	0.00000000
C	1.16538600	1.05283700	0.00000000
C	0.00000000	0.25499700	0.00000000
C	0.14263600	-1.19665300	0.00000000
C	1.42951100	-1.72996800	0.00000000
C	2.57636800	-0.90307400	0.00000000
H	3.32497400	1.11611600	0.00000000
H	1.04774100	2.12720700	0.00000000
H	1.55799400	-2.80873000	0.00000000
H	3.55761600	-1.36594700	0.00000000
C	-0.96540700	-2.07818500	0.00000000
H	-0.81430200	-3.15339700	0.00000000
O	-2.22703900	-1.69669100	0.00000000
C	-1.67234700	2.00601800	0.00000000
N	-1.28797600	0.69423600	0.00000000
O	-0.95344500	3.00641700	0.00000000
H	-2.19600200	-0.67128200	0.00000000
H	-2.76725000	2.11300800	0.00000000

(A₀)_b

C	2.39118400	0.74330400	0.00000000
C	1.05918600	1.17358500	0.00000000
C	0.00000000	0.23845200	0.00000000
C	0.28719100	-1.19455900	0.00000000
C	1.62352700	-1.58003600	0.00000000
C	2.66477900	-0.62501100	0.00000000
H	3.19627500	1.46838900	0.00000000
H	0.81648100	2.22708900	0.00000000
H	1.87482600	-2.63693400	0.00000000
H	3.69253500	-0.97332600	0.00000000
C	-0.76572000	-2.15193100	0.00000000
H	-0.52860400	-3.21548700	0.00000000
O	-2.02335600	-1.81697100	0.00000000
C	-1.91403100	1.76251700	0.00000000
N	-1.32955200	0.52076300	0.00000000
O	-1.33379500	2.84252900	0.00000000
H	-1.95293100	-0.62002600	0.00000000
H	-3.01120800	1.70256300	0.00000000

(A₁)_G

C	1.94146700	-1.91984200	-0.00013500
C	0.59636200	-1.56918100	0.00005200

C	0.22211500	-0.22023500	0.00004500
C	1.23982400	0.76886200	-0.00014900
C	2.58616000	0.37974400	-0.00033200
C	2.94897200	-0.95573600	-0.00032800
H	2.20406300	-2.97361900	-0.00012800
H	-0.16969600	-2.32988200	0.00019800
H	3.34942900	1.15349300	-0.00047800
H	3.99413700	-1.24555300	-0.00047200
C	0.97674900	2.20702600	-0.00016800
H	1.88010200	2.84115600	-0.00033900
O	-0.12791000	2.74156000	0.00000300
C	-2.25662600	-0.54204700	0.00041500
N	-1.10631200	0.20578700	0.00022000
O	-2.27381500	-1.76759000	0.00014900
H	-1.21204900	1.21948200	0.00017100
C	-3.51937300	0.28773800	0.00021400
H	-3.56041800	0.93086300	0.88498800
H	-3.55956300	0.93199800	-0.88377000
H	-4.38191600	-0.37818000	-0.00061000

(A₁)_N

C	2.02837700	-1.90373400	-0.00009100
C	0.67188200	-1.58605700	0.00004100
C	0.24846500	-0.23622500	0.00006200
C	1.22228500	0.86497900	-0.00003000
C	2.56629500	0.49084000	-0.00019600
C	2.96732400	-0.85832900	-0.00021400
H	2.34867800	-2.93831000	-0.00010500
H	-0.08139000	-2.36071600	0.00011900
H	3.32651400	1.26665000	-0.00030700
H	4.02827900	-1.08737600	-0.00032500
C	0.84538900	2.24648900	-0.00000500
H	1.67702800	2.96486500	-0.00038700
O	-0.34933600	2.68683000	-0.00021900
C	-2.22540200	-0.61035000	0.00018000
N	-1.05417500	0.15384300	0.00013700
O	-2.20905100	-1.83101500	0.00000500
H	-1.14676300	1.19613700	0.00027300
C	-3.47963300	0.21769900	0.00031400
H	-3.51575400	0.86363100	0.88409100
H	-3.51542900	0.86455500	-0.88279600
H	-4.34472400	-0.44473800	-0.00017400

(A₁)_T

C	2.04626200	-1.87801300	-0.00011700
C	0.67280600	-1.56853900	-0.00004700
C	0.21803100	-0.23249400	-0.00004700
C	1.20606800	0.84281900	-0.00011000
C	2.55509700	0.49871100	-0.00019000
C	2.97746200	-0.85143400	-0.00019400
H	2.36359400	-2.91451000	-0.00011700
H	-0.06503400	-2.35768200	0.00000700
H	3.30473600	1.28513400	-0.00025300
H	4.04029800	-1.06957200	-0.00025500
C	0.84485700	2.21315900	-0.00008500
H	1.60942700	2.98468600	-0.00010500
O	-0.39495700	2.65715400	-0.00001400
C	-2.18403000	-0.61595500	0.00006700
N	-1.07155400	0.19663300	-0.00000800
O	-2.16699000	-1.85056500	0.00028700
H	-0.97587200	1.80107700	-0.00002800
C	-3.48216900	0.15415900	0.00030200
H	-3.54031800	0.80145600	0.88186700
H	-3.54030200	0.80211500	-0.88077100
H	-4.32637000	-0.53633100	0.00006200

(A₁)_b

C	2.10225200	-1.83140500	-0.00011100
C	0.72482000	-1.56253400	-0.00006700
C	0.24661900	-0.23448300	-0.00003100
C	1.19748100	0.87578200	0.00001000
C	2.55331500	0.56834900	-0.00003500
C	3.00460900	-0.77188500	-0.00011000
H	2.45299800	-2.85676000	-0.00012800
H	0.00427100	-2.36784400	-0.00011300
H	3.28328800	1.37315200	0.00000700
H	4.07255000	-0.96445600	-0.00016900
C	0.74949900	2.22613200	0.00009100
H	1.47303300	3.03972900	-0.00003300
O	-0.51370100	2.55362500	0.00026500
C	-2.17133100	-0.63921800	0.00003100
N	-1.05027000	0.17011300	-0.00009600
O	-2.13764600	-1.86899400	0.00059200
H	-1.02483300	1.51627100	0.00011900
C	-3.46479100	0.13377700	-0.00048200
H	-3.52286800	0.78087600	0.88131300
H	-3.52223900	0.78100200	-0.88219700
H	-4.30836600	-0.55688800	-0.00075800

(A₂)_G

C	0.91431900	-1.33181100	0.00007200
C	-0.47228000	-1.29183200	0.00024100
C	-1.14861100	-0.06519400	0.00019300
C	-0.38294100	1.12757500	-0.00003700
C	1.01538100	1.06498200	-0.00019700
C	1.65797600	-0.15586000	-0.00014200
H	1.41634800	-2.29325300	0.00011100
H	-1.03946400	-2.21041900	0.00041000
H	1.58544200	1.98869500	-0.00036500
C	-0.96790700	2.47104700	-0.00009400
H	-0.23482300	3.29577300	-0.00033200
O	-2.16508900	2.73192900	0.00000500
C	-3.47973600	-0.95779800	0.00065900
N	-2.53632500	0.04118600	0.00036500
O	-3.20493500	-2.15132300	0.00030300
H	-2.87658000	1.00166600	0.00027000
C	-4.90121600	-0.44873400	0.00041800
H	-5.09182100	0.16636900	0.88548100
H	-5.09094700	0.16866500	-0.88322500
H	-5.58281800	-1.29888200	-0.00098400
Br	3.54912100	-0.23502900	-0.00037300

(A₂)_N

C	0.96039700	-1.38680700	0.00006200
C	-0.43059400	-1.33590900	0.00027400
C	-1.11359500	-0.10284000	0.00030600
C	-0.37723900	1.16879200	0.00012400
C	1.01458200	1.07926200	-0.00008800
C	1.66032100	-0.16767600	-0.00011100
H	1.48470100	-2.33309500	0.00003300
H	-1.00979300	-2.24803200	0.00041700
H	1.60861700	1.98713800	-0.00024900
C	-1.01601900	2.45038000	0.00010900
H	-0.33954600	3.31667700	-0.00054000
O	-2.27004300	2.64909800	-0.00031500
C	-3.45881300	-0.96447800	0.00068700
N	-2.46866500	0.02016800	0.00048300
O	-3.19613500	-2.15647900	0.00015300
H	-2.77074800	1.01878100	0.00055600
C	-4.85481800	-0.40775400	0.00043300
H	-5.02029700	0.21683400	0.88456800
H	-5.01931600	0.21904500	-0.88230700

H	-5.56835400	-1.23114800	-0.00095200
Br	3.52398500	-0.20074700	-0.00041100

(A₂)_T

C	0.96149000	-1.37553600	-0.00013900
C	-0.44119400	-1.33157200	0.00013700
C	-1.14711400	-0.11212400	0.00018900
C	-0.38512400	1.13523300	0.00005700
C	1.00382200	1.06913700	-0.00023200
C	1.66333800	-0.17937200	-0.00042900
H	1.47940500	-2.32642100	-0.00008100
H	-1.00731700	-2.25168000	0.00028500
H	1.59172300	1.98110100	-0.00025000
C	-1.00972900	2.40864700	-0.00006800
H	-0.41262000	3.31647200	-0.00024400
O	-2.30889800	2.59070400	-0.00009100
C	-3.42721900	-0.94868700	0.00021900
N	-2.49268100	0.06363600	0.00027700
O	-3.16770700	-2.15498800	0.00020200
H	-2.70472900	1.62339400	0.00003400
C	-4.85005100	-0.44652100	0.00036700
H	-5.03324700	0.17693500	0.88195500
H	-5.03321200	0.17748200	-0.88083800
H	-5.54291900	-1.28867100	0.00011300
Br	3.53472000	-0.19014300	-0.00012600

(A₂)_b

C	0.97437000	-1.37646800	0.00034300
C	-0.42505000	-1.34162700	0.00055600
C	-1.12584400	-0.11991300	0.00057200
C	-0.37952000	1.13838300	0.00040700
C	1.00851100	1.07829500	0.00019300
C	1.66800300	-0.16914100	0.00020000
H	1.50177900	-2.32167200	0.00029600
H	-0.99125200	-2.26194700	0.00067800
H	1.59393600	1.99162400	-0.00018500
C	-1.05152600	2.39315100	0.00029800
H	-0.47661700	3.31827400	0.00054200
O	-2.34806300	2.49964500	-0.00013600
C	-3.43362000	-0.93501200	0.00004500
N	-2.47119200	0.05656900	0.00064300
O	-3.18421300	-2.13930700	0.00020500
H	-2.67936700	1.38364300	0.00018100
C	-4.84223400	-0.40064400	-0.00114600

H	-5.01229700	0.22800000	0.87937000
H	-5.01200000	0.22427900	-0.88442900
H	-5.55154500	-1.22854300	0.00032900
Br	3.53786800	-0.17755700	-0.00030400

(A₃)_G

C	3.71253900	-1.60345200	0.50090900
C	2.37339600	-1.48272900	0.14714100
C	1.82972800	-0.22200000	-0.12374600
C	2.67009000	0.91745700	-0.03000000
C	4.01488400	0.75967600	0.32987800
C	4.54630700	-0.49021200	0.59694400
H	4.10933600	-2.59331600	0.70592100
H	1.74207600	-2.35573400	0.07813700
H	4.64114800	1.64540700	0.39642000
H	5.58890000	-0.60028200	0.87488500
C	2.22087900	2.28471800	-0.29083400
H	3.00108800	3.05658900	-0.17320000
O	1.08843200	2.62507100	-0.61795800
C	-0.50173600	-0.94897800	-0.64554400
C	-4.35192700	-0.22687100	-0.56365700
C	-2.81387200	-0.25055300	1.26394500
C	-4.61916700	0.97652000	0.36884000
H	-4.37326500	0.04598100	-1.62328200
C	-3.68860000	0.71967100	1.52816700
H	-4.38092500	1.93594000	-0.11040400
H	-3.72448600	1.29207500	2.45097600
N	0.49531100	-0.02374800	-0.48411900
O	-0.34956600	-2.15409700	-0.47044100
C	-1.83870500	-0.37474800	-1.06983300
H	-1.80029100	0.71775300	-1.13116900
C	-2.98224300	-0.80928000	-0.13280100
H	-5.12662900	-0.98456500	-0.40888400
H	-3.00025500	-1.90400700	-0.12771900
H	-5.66917400	1.03720800	0.67569100
H	-2.03226600	-0.58846200	1.93933600
H	-2.03923600	-0.75386200	-2.07881800
H	0.25642800	0.95241000	-0.64833400

(A₃)_N

C	3.70724000	-1.86760600	0.11554300
C	2.36953200	-1.54746400	-0.10539600
C	1.94029400	-0.19968500	-0.09166800
C	2.89277700	0.89768000	0.12997900

C	4.21488300	0.52005000	0.36682600
C	4.62091000	-0.82721500	0.35533900
H	4.03184600	-2.90082900	0.10610200
H	1.63371800	-2.31938100	-0.27928500
H	4.95547600	1.29248300	0.55355700
H	5.66660000	-1.05875200	0.53153800
C	2.51596600	2.27914300	0.11540700
H	3.32513700	2.99361500	0.32150900
O	1.34467900	2.72356500	-0.11195700
C	-0.50355900	-0.57159900	-0.47790600
C	-4.29066700	0.36800400	-0.86014900
C	-3.28398000	-0.95541200	0.85685600
C	-4.86563200	0.76364200	0.51920500
H	-4.05216400	1.23581100	-1.48278500
C	-4.25461800	-0.25752400	1.44596600
H	-4.57216100	1.77950900	0.81718500
H	-4.56429200	-0.37353900	2.48097400
N	0.64883700	0.19097600	-0.26083900
O	-0.48491900	-1.79200200	-0.48810700
C	-1.73619000	0.26455300	-0.72617800
H	-1.72636200	1.13777800	-0.06231200
C	-3.04871100	-0.51430800	-0.57247600
H	-5.03114000	-0.22633400	-1.40440700
H	-3.00852800	-1.37128500	-1.25270700
H	-5.96096700	0.74282900	0.53158600
H	-2.68581000	-1.72596200	1.33366100
H	-1.65447800	0.65881700	-1.74944400
H	0.55372100	1.23234800	-0.24687200

(A₃)_T

C	3.67556700	-1.90327600	0.07790400
C	2.32603200	-1.54290400	-0.09864000
C	1.91399000	-0.19344900	-0.07278400
C	2.92312700	0.84159100	0.13458600
C	4.24698600	0.44752800	0.30878400
C	4.62588900	-0.91498800	0.28111000
H	3.95991400	-2.94907100	0.05420000
H	1.57380600	-2.30205200	-0.25646600
H	5.01008300	1.20427900	0.46812800
H	5.67046400	-1.17341100	0.41998100
C	2.60715200	2.22279100	0.16170900
H	3.38600300	2.96295800	0.32136400
O	1.39607700	2.71320800	-0.00158400
C	-0.47449600	-0.48667700	-0.42848700

C	-4.27549300	0.44454400	-0.87134200
C	-3.33578800	-1.03049700	0.75499400
C	-4.91748500	0.70393700	0.51089500
H	-4.01894800	1.36960600	-1.39731300
C	-4.34101000	-0.40006100	1.36254900
H	-4.64473900	1.68756500	0.91764100
H	-4.69739700	-0.61731400	2.36595300
N	0.64984800	0.28310200	-0.22128600
O	-0.49505100	-1.71940500	-0.47929500
C	-1.72646900	0.34577300	-0.62634700
H	-1.74717700	1.13602700	0.13442400
C	-3.03561900	-0.45025400	-0.61088400
H	-4.98488600	-0.10007100	-1.50279500
H	-2.95465400	-1.23922000	-1.36625300
H	-6.01229000	0.67971000	0.47041900
H	-2.75004100	-1.83800300	1.18304600
H	-1.61753700	0.86274200	-1.59062000
H	0.79596300	1.87976100	-0.12995500

(A₃)_b

C	3.72002200	-1.86304400	0.08740500
C	2.36713500	-1.53876900	-0.09867300
C	1.93510000	-0.19544400	-0.07392800
C	2.90986400	0.87290600	0.13872600
C	4.23914600	0.51075500	0.32439300
C	4.64379700	-0.84392300	0.29869000
H	4.03510000	-2.89973800	0.06689600
H	1.63024100	-2.31253200	-0.25975300
H	4.98453800	1.28355100	0.49019900
H	5.69281500	-1.07969400	0.44555400
C	2.51082900	2.23855400	0.15431600
H	3.25064600	3.01979900	0.32208000
O	1.27591100	2.61808300	-0.02871500
C	-0.46979200	-0.50158300	-0.44150600
C	-4.26408500	0.44368100	-0.86106800
C	-3.31720500	-1.03787800	0.75634400
C	-4.89740600	0.69998200	0.52570100
H	-4.00759100	1.36966000	-1.38523700
C	-4.31689900	-0.40616700	1.37144100
H	-4.62242900	1.68249000	0.93347100
H	-4.66720100	-0.62490700	2.37659700
N	0.66429700	0.26026600	-0.22517400
O	-0.47700900	-1.72981100	-0.49766600
C	-1.71491400	0.33739500	-0.63460600

H	-1.72952700	1.12929500	0.12484900
C	-3.02581600	-0.45605800	-0.61090700
H	-4.97817400	-0.09668800	-1.49066100
H	-2.95230000	-1.24329300	-1.36874700
H	-5.99236900	0.67578500	0.49156100
H	-2.73094000	-1.84795300	1.17889200
H	-1.60787400	0.85133600	-1.60080900
H	0.73511700	1.60239900	-0.15559500

(A₄)_G

C	-3.72113300	-1.83805400	0.22558400
C	-2.37374000	-1.54691400	0.04646800
C	-1.95201600	-0.21749300	-0.07495800
C	-2.92534400	0.81385500	-0.01095600
C	-4.27517300	0.48428500	0.17044600
C	-4.68478000	-0.83227600	0.28960500
H	-4.02077700	-2.87794400	0.31653700
H	-1.64208200	-2.33914200	-0.00206300
H	-5.00385300	1.28938700	0.21603900
H	-5.73245800	-1.07557100	0.42938400
C	-2.61154800	2.23737000	-0.12369700
H	-3.48418900	2.90909700	-0.04715600
O	-1.49700700	2.72319400	-0.29020400
C	0.49753600	-0.64331200	-0.33694400
N	-0.61944700	0.15105000	-0.25921700
O	0.46166900	-1.86732900	-0.26916800
H	-0.48084600	1.15748000	-0.33265700
C	1.78917400	0.14496600	-0.46653700
C	2.89884600	-0.59910200	-1.25643000
C	2.46739400	0.35566400	0.94565900
C	4.08149500	-0.65998500	-0.24146500
H	2.57006600	-1.60909000	-1.51327300
C	3.56348500	1.37805200	0.70380300
H	1.76414900	0.57984600	1.75006600
C	4.52413700	0.77269800	-0.00273100
H	4.86473600	-1.36912700	-0.51525800
H	3.49553600	2.42897900	0.96544500
H	5.40942200	1.22984600	-0.43307400
C	3.30491900	-0.93142000	1.06034400
H	2.70668000	-1.84610800	1.02592900
H	3.94395500	-0.93329900	1.94784500
H	3.16570500	-0.07703500	-2.17849400
H	1.56327700	1.11840200	-0.90890600

(A₄)_N

C	-3.77365900	-1.81496900	0.27542500
C	-2.41605900	-1.55931800	0.09707600
C	-1.94791100	-0.23387100	-0.06271900
C	-2.87426100	0.90699800	-0.02515500
C	-4.22434900	0.59278100	0.13421000
C	-4.67017600	-0.73286400	0.28715000
H	-4.12810200	-2.83125200	0.39621500
H	-1.69694700	-2.36510400	0.06579500
H	-4.95216400	1.39911000	0.15127000
H	-5.73195300	-0.91462900	0.42008100
C	-2.44839300	2.26883400	-0.14640900
H	-3.24986600	3.02034200	-0.12070200
O	-1.24338000	2.65799400	-0.27813800
C	0.48689300	-0.71952600	-0.38478700
N	-0.64600200	0.09541800	-0.27410100
O	0.41464300	-1.93768000	-0.32288200
H	-0.51526100	1.13030400	-0.34227000
C	1.76557700	0.06877000	-0.53317300
C	2.91803900	-0.72779500	-1.19880500
C	2.37579200	0.41984400	0.88888300
C	4.04770800	-0.68817900	-0.12472500
H	2.60936400	-1.75896200	-1.38698400
C	3.47686100	1.42397300	0.60384100
H	1.63515700	0.71210800	1.63539100
C	4.47280000	0.76382700	0.00356500
H	4.84562200	-1.41306800	-0.29431200
H	3.39080300	2.49337200	0.76496300
H	5.37679800	1.18645600	-0.42281000
C	3.20834600	-0.84680900	1.15677300
H	2.61683100	-1.76713000	1.17739600
H	3.80187300	-0.76565700	2.07145100
H	3.22618500	-0.28133300	-2.14697200
H	1.54032400	0.99482000	-1.06854900

(A₄)_T

C	-3.79753300	-1.78730700	0.21140300
C	-2.42438100	-1.54640100	0.01594700
C	-1.91453300	-0.23516200	-0.09347300
C	-2.84632600	0.88636900	-0.01065900
C	-4.19677000	0.60980900	0.18577600
C	-4.67425800	-0.71681200	0.29513900
H	-4.15812300	-2.80636500	0.29263600
H	-1.72968000	-2.37066100	-0.05518700

H	-4.90343000	1.43219000	0.25640600
H	-5.73607400	-0.88307500	0.44377700
C	-2.42864900	2.23613200	-0.11911100
H	-3.15147700	3.04427500	-0.05282200
O	-1.18153600	2.61677400	-0.30177900
C	0.45386400	-0.73225600	-0.35346000
N	-0.61926300	0.13076900	-0.28285000
O	0.38643400	-1.95738400	-0.21378000
H	-0.64631600	1.73062500	-0.34255900
C	1.76702400	-0.00356300	-0.57369000
C	2.92135000	-0.89098300	-1.10323900
C	2.35101700	0.52106200	0.80090500
C	4.02713900	-0.73459200	-0.01399100
H	2.59719700	-1.93249900	-1.16701400
C	3.48022300	1.46202300	0.42362800
H	1.59656800	0.91789300	1.48250000
C	4.47866100	0.71463900	-0.05942100
H	4.81511600	-1.48826200	-0.06662300
H	3.41320100	2.54504700	0.44287800
H	5.40081600	1.06468600	-0.51247800
C	3.15308200	-0.71291300	1.25421200
H	2.54205200	-1.61278200	1.37402800
H	3.72563900	-0.52638200	2.16738400
H	3.26473100	-0.57464500	-2.09157400
H	1.56597400	0.84916900	-1.22673200

(A₄)_b

C	-3.81870200	-1.75726700	0.24784300
C	-2.44727000	-1.54159100	0.04264600
C	-1.93185900	-0.23421800	-0.08888900
C	-2.83908200	0.90999300	-0.01633500
C	-4.19045400	0.65475300	0.18864400
C	-4.67884800	-0.66546700	0.31915200
H	-4.19812300	-2.76753700	0.34701700
H	-1.76036200	-2.37325000	-0.02075900
H	-4.88737600	1.48593000	0.25085000
H	-5.74181000	-0.81726800	0.47614500
C	-2.35434300	2.24118100	-0.14769400
H	-3.04612800	3.08061300	-0.09553100
O	-1.09331300	2.52098300	-0.33175900
C	0.45247100	-0.72942200	-0.38447600
N	-0.63590300	0.12054700	-0.28978300
O	0.37617200	-1.95394200	-0.28940900
H	-0.62030200	1.46433200	-0.35246100

C	1.75785500	0.01646000	-0.57006300
C	2.91779500	-0.84719600	-1.12670500
C	2.33212700	0.49006000	0.82820300
C	4.01568800	-0.72986900	-0.02494700
H	2.59751800	-1.88629900	-1.23425000
C	3.46047100	1.44738800	0.49245500
H	1.57361500	0.85946300	1.52069700
C	4.46338300	0.72117100	-0.01265200
H	4.80573800	-1.47906900	-0.10199200
H	3.38981800	2.52849600	0.55324200
H	5.38748000	1.09021400	-0.44603900
C	3.13420400	-0.75891900	1.23795600
H	2.52517600	-1.66442400	1.32061200
H	3.70070900	-0.60572800	2.16085200
H	3.26530500	-0.49049400	-2.09949300
H	1.55657000	0.89251100	-1.19189500

(A₅)_G

O	-0.27990400	-2.29537100	-0.33137300
O	-2.40213300	-0.05990900	1.08561400
O	1.30813700	2.26356400	-1.60242400
H	0.44310200	0.63943300	-1.28884300
N	0.61255600	-0.23570100	-0.79638800
C	-0.35552300	-1.19966200	-0.87609000
C	1.83436100	-0.27172100	-0.12185100
C	2.67563400	0.86761600	-0.20806200
C	3.90977800	0.87010600	0.45516300
C	-3.24582000	-0.14185100	0.01432200
C	-2.90341200	0.88197200	1.93333100
H	-2.33434700	1.05647100	2.83357800
C	-4.04818900	1.40237800	1.42934200
H	-4.66234900	2.16605600	1.88570600
C	-4.26998800	0.73634200	0.17714500
H	-5.08823200	0.89233300	-0.51238800
C	2.33661800	2.07517100	-0.96040800
C	4.32981400	-0.22025700	1.19718500
H	5.28725600	-0.20717600	1.70662300
C	3.49543200	-1.33447500	1.27584400
H	3.80537500	-2.20025600	1.85351400
C	2.26457600	-1.37048500	0.63036400
H	1.63091000	-2.24151900	0.70300100
C	-2.89147400	-1.11584200	-1.05579900
H	-2.86878500	-2.13377400	-0.65146700

H	-3.68522000	-1.08523900	-1.80669900
C	-1.54687800	-0.82819900	-1.74192900
H	-1.47450600	-1.44880100	-2.64240200
H	-1.49950900	0.21619800	-2.06332900
H	3.10109100	2.87063300	-0.92457000
H	4.53895400	1.75270200	0.37610700

(A₅)_N

O	-0.27511200	-2.30805300	-0.37310500
O	-2.30241800	-0.04947500	1.05116500
O	1.15392600	2.18606700	-1.65471600
H	0.50331000	0.66793800	-1.28142300
N	0.63711600	-0.24287500	-0.78657600
C	-0.36197800	-1.20990000	-0.90050200
C	1.81889300	-0.28156300	-0.11477600
C	2.64063500	0.93103500	-0.24036000
C	3.86051200	0.91429100	0.43693500
C	-3.20673900	-0.13561600	0.03073900
C	-2.77557400	0.86642900	1.94349800
H	-2.15721400	1.04309300	2.81011900
C	-3.96100200	1.36403700	1.51713300
H	-4.56517800	2.10523900	2.02124800
C	-4.24039600	0.71314800	0.26838100
H	-5.10091600	0.86032200	-0.36958500
C	2.24215400	2.07453900	-1.00396900
C	4.27776400	-0.19233700	1.19881700
H	5.23645900	-0.14562600	1.70560500
C	3.48290900	-1.34614100	1.31536900
H	3.81397900	-2.19128300	1.90622400
C	2.25650700	-1.38400200	0.65736900
H	1.61531400	-2.25122300	0.72312700
C	-2.88771600	-1.08438100	-1.07195200
H	-2.88388200	-2.11568200	-0.70166100
H	-3.68396600	-1.01280700	-1.81695500
C	-1.53921300	-0.80149000	-1.75622600
H	-1.47953800	-1.40193800	-2.67192100
H	-1.47121900	0.24895300	-2.05102500
H	2.95378200	2.91196800	-1.01072300
H	4.50753900	1.78456600	0.37352200

(A₅)_T

O	-0.23970700	-2.26620000	-0.43913100
O	-2.37525200	-0.12263400	1.08951400
O	1.16201100	2.23924300	-1.54866000

H	0.67230600	1.33751200	-1.42850200
N	0.64072100	-0.15209900	-0.81828300
C	-0.31430700	-1.13541800	-0.93052000
C	1.81172000	-0.27243500	-0.13647100
C	2.65734900	0.91711700	-0.18276400
C	3.87612900	0.88624400	0.49055700
C	-3.22001500	-0.16463500	0.01685700
C	-2.88435300	0.77410400	1.98050900
H	-2.31506300	0.91320700	2.88678400
C	-4.03581100	1.30489800	1.50318800
H	-4.65689700	2.04031200	1.99528500
C	-4.25332300	0.69433400	0.22229700
H	-5.07478100	0.87283900	-0.45792500
C	2.28708800	2.09347400	-0.87969500
C	4.30141400	-0.25748800	1.20465300
H	5.25931000	-0.23348600	1.71369000
C	3.50476800	-1.39141400	1.25332700
H	3.82513700	-2.27102100	1.79982600
C	2.26645100	-1.39725300	0.58550000
H	1.63382000	-2.27239800	0.61455800
C	-2.85830200	-1.08325900	-1.09848200
H	-2.82349500	-2.11848600	-0.74109300
H	-3.65637200	-1.02601700	-1.84368300
C	-1.51650400	-0.74888600	-1.77197400
H	-1.44701700	-1.32689900	-2.70223200
H	-1.47471900	0.30905200	-2.04139500
H	2.94412900	2.95826100	-0.89119800
H	4.51836600	1.76224200	0.46818800

(A₅)_b

O	-0.23394300	-2.30921400	-0.35204100
O	-2.31114800	-0.05304500	1.09122400
O	1.07168100	2.00744300	-1.71345400
H	0.63981000	0.97273100	-1.43129000
N	0.64799300	-0.22727200	-0.82352400
C	-0.32170700	-1.20652400	-0.89146300
C	1.80462200	-0.28065500	-0.11119800
C	2.63579100	0.91142700	-0.26815800
C	3.85172800	0.94722400	0.40570600
C	-3.18765300	-0.14521300	0.04708000
C	-2.78913800	0.89333600	1.94788700
H	-2.19276200	1.07636400	2.82853600
C	-3.95098400	1.40606400	1.47633900
H	-4.55322200	2.17108100	1.94614800

C	-4.20912000	0.73088900	0.23603500
H	-5.04860700	0.87998800	-0.42898400
C	2.21356000	1.99877800	-1.08202600
C	4.26881200	-0.12321000	1.22909900
H	5.22338500	-0.04933600	1.73993900
C	3.47368000	-1.25465500	1.39138000
H	3.79629700	-2.07120200	2.02662000
C	2.24363000	-1.33275400	0.72190200
H	1.61133600	-2.20276100	0.82675800
C	-2.86075800	-1.12406000	-1.02723200
H	-2.83511100	-2.14093900	-0.61980200
H	-3.66914200	-1.09179500	-1.76241900
C	-1.52548800	-0.84339000	-1.73724400
H	-1.47523300	-1.46756500	-2.63813700
H	-1.47401600	0.19952000	-2.05951200
H	2.85289500	2.87239800	-1.20016500
H	4.49385000	1.81740500	0.30251200

(K₀)_G

C	-1.55302300	1.44610800	0.00212900
C	-1.03297700	0.15030100	-0.01974700
C	0.37779600	-0.04964700	-0.06412100
C	1.22957300	1.07832600	-0.08283600
C	0.68430200	2.35807200	-0.05816600
C	-0.69201300	2.53477200	-0.01834100
C	0.97959100	-1.40406000	-0.09690200
C	2.73153100	0.93016600	-0.14337000
C	3.20751500	-0.35881300	0.51033800
C	2.48375700	-1.53489100	-0.12902300
H	-2.62302300	1.58654100	0.03609900
H	-1.10836300	3.53755000	0.00285400
H	1.34548700	3.21936700	-0.06557100
H	3.04611600	0.93656800	-1.19690400
H	3.19691600	1.80367300	0.32260400
H	4.28927100	-0.47332500	0.39324800
H	2.99955400	-0.33085400	1.58696700
H	2.73666800	-2.49189300	0.33484400
H	2.76795200	-1.61177000	-1.18901800
O	0.30100000	-2.43507200	-0.11878500
N	-1.87451100	-0.96860500	-0.00185600
H	-1.37405300	-1.85790800	-0.04454800
C	-3.23000200	-1.02891200	0.06178100
O	-4.01191300	-0.08932100	0.11939400
H	-3.58394400	-2.07110500	0.05709700

(K₀)_N

C	-1.57220200	1.48306900	-0.04085700
C	-1.03342200	0.17125300	-0.02995200
C	0.41292800	-0.06832100	-0.07910100
C	1.22981200	1.07904900	-0.07159100
C	0.65774700	2.36971600	-0.05932500
C	-0.73035400	2.58771800	-0.05807700
C	0.97130400	-1.38795700	-0.14083200
C	2.72375800	0.93170500	-0.13225300
C	3.18328000	-0.35574900	0.54818800
C	2.47189400	-1.55661200	-0.06710600
H	-2.64632300	1.59754700	-0.00256800
H	-1.13534800	3.59213200	-0.05460400
H	1.32962400	3.22348000	-0.06910000
H	3.03678800	0.90929100	-1.18782300
H	3.20269000	1.81006900	0.31261900
H	4.26807100	-0.46520400	0.45288600
H	2.95663700	-0.30047100	1.62008200
H	2.67337000	-2.47144300	0.50028200
H	2.84946900	-1.73660900	-1.08532100
O	0.25378000	-2.44261500	-0.25714300
N	-1.81409800	-0.94180300	0.04705500
H	-1.23642700	-1.81886400	-0.01780500
C	-3.18902300	-1.06983700	0.10421900
O	-3.98569600	-0.14844900	0.16471200
H	-3.49886000	-2.12300900	0.10153000

(K₀)_T

C	-1.58882100	1.45736500	-0.07184500
C	-1.06545200	0.14388600	-0.05883500
C	0.38453200	-0.05192600	-0.07625900
C	1.20426900	1.08881100	-0.07016300
C	0.62679700	2.38547200	-0.06953700
C	-0.74653200	2.57755100	-0.07565200
C	0.98619200	-1.33837200	-0.11442200
C	2.70096000	0.95733500	-0.10172100
C	3.17651900	-0.33616900	0.55375000
C	2.46399400	-1.53229300	-0.07071100
H	-2.66280100	1.57735300	-0.07319900
H	-1.16723400	3.57641800	-0.08156700
H	1.29479100	3.24196400	-0.07110200
H	3.02971600	0.97396800	-1.15288100
H	3.15816800	1.83095100	0.37380100

H	4.25955900	-0.44077400	0.44281900
H	2.96177100	-0.30074500	1.62841700
H	2.67304600	-2.45630200	0.47978300
H	2.83299100	-1.69818200	-1.09587500
O	0.27941600	-2.45836100	-0.21792300
N	-1.80440000	-0.99571800	-0.04943600
H	-0.70180100	-2.17346300	-0.19447900
C	-3.16412700	-1.05945900	0.05941800
O	-3.95170600	-0.14543900	0.31182000
H	-3.53906700	-2.08396200	-0.08498200

(K₀)_b

C	-1.55671600	1.51204200	0.00283800
C	-1.04111900	0.19371600	-0.01200900
C	0.40220100	-0.04349600	-0.05820500
C	1.24280100	1.07906700	-0.08089200
C	0.68646500	2.38084700	-0.05157300
C	-0.69250400	2.60773500	-0.01490700
C	0.93202800	-1.36612200	-0.09932900
C	2.73141800	0.89362400	-0.16962900
C	3.17775000	-0.40867400	0.49529300
C	2.41227100	-1.59797100	-0.08323200
H	-2.62877600	1.64565800	0.04172000
H	-1.08594700	3.61701400	0.00415500
H	1.36726700	3.22739500	-0.06507300
H	3.02161700	0.87393800	-1.23170500
H	3.24217900	1.75563600	0.27170500
H	4.25420500	-0.54958200	0.35962500
H	2.99381400	-0.34478700	1.57462500
H	2.60905200	-2.51264400	0.48679000
H	2.75039400	-1.79956400	-1.11192000
O	0.14935300	-2.40963900	-0.16034100
N	-1.78195400	-0.94328500	0.01173900
H	-0.97483200	-1.89647100	-0.07782100
C	-3.14900700	-1.06150000	0.05040800
O	-3.95888400	-0.14515600	0.13341700
H	-3.47257400	-2.11084900	0.00854500

(K₁)_g

C	-0.88167900	1.87758600	0.00443100
C	-0.65950600	0.49813900	-0.02207900
C	0.67642500	-0.00306500	-0.06533200
C	1.75393900	0.91304300	-0.08093900
C	1.50152700	2.28032800	-0.05163400

C	0.19604100	2.75163500	-0.01134500
C	0.97231500	-1.45470300	-0.09937300
C	3.18794800	0.44226200	-0.14395900
C	3.37411100	-0.91828000	0.51093800
C	2.41267400	-1.90880500	-0.12884300
H	-1.89497900	2.24734400	0.03826000
H	0.00806500	3.82108000	0.01354000
H	2.33444400	2.97701200	-0.05612100
H	3.49402900	0.37768200	-1.19806600
H	3.83299800	1.19478800	0.31911700
H	4.40543100	-1.26447700	0.39395200
H	3.17681700	-0.84555400	1.58747800
H	2.45063600	-2.89765600	0.33565200
H	2.67481900	-2.04615000	-1.18844400
O	0.08879100	-2.31741100	-0.12382700
N	-1.71792100	-0.41568700	-0.01085400
H	-1.40594100	-1.38529900	-0.05569900
C	-3.06500600	-0.18902700	0.04740700
O	-3.58118300	0.92401900	0.10658600
C	-3.91285500	-1.44025500	0.03125300
H	-3.33019800	-2.36344200	0.00737800
H	-4.55097400	-1.44264300	0.91897900
H	-4.56615800	-1.40889600	-0.84526000

(K₁)_N

C	-0.87847600	1.93663100	-0.04053100
C	-0.65837000	0.53739900	-0.03276500
C	0.69677000	-0.02851700	-0.07994800
C	1.75520400	0.89958600	-0.07192700
C	1.49593700	2.28807200	-0.05822200
C	0.19703200	2.81881100	-0.05559700
C	0.93925700	-1.44220300	-0.14146000
C	3.17624200	0.41354900	-0.13111100
C	3.32835700	-0.94339900	0.55183100
C	2.36090700	-1.94940300	-0.06329900
H	-1.89698100	2.29515500	-0.00298500
H	0.03363000	3.88948900	-0.05041700
H	2.34684700	2.96367400	-0.06579100
H	3.47713800	0.31817200	-1.18611600
H	3.84339600	1.15944700	0.31329400
H	4.35924800	-1.29917300	0.45867700
H	3.11908300	-0.83581300	1.62335100
H	2.34631500	-2.88527400	0.50558500
H	2.68992500	-2.21356600	-1.08016600

O	0.00141900	-2.30745000	-0.26494100
N	-1.66739800	-0.37243200	0.03774600
H	-1.29357000	-1.35314600	-0.03429700
C	-3.04944600	-0.19158600	0.08846600
O	-3.57103400	0.91100700	0.17139800
C	-3.82240000	-1.48032400	0.03050400
H	-3.45789000	-2.19392700	0.77617900
H	-4.87772400	-1.27287600	0.20623000
H	-3.70679300	-1.94529100	-0.95506400

(K₁)_T

C	-0.89531800	1.91018700	-0.07649800
C	-0.69031700	0.51290500	-0.04597100
C	0.67740000	-0.01033100	-0.07073400
C	1.73827600	0.90844300	-0.08327900
C	1.47624000	2.30425000	-0.09711700
C	0.18483900	2.80585200	-0.10114500
C	0.96352700	-1.40320600	-0.09927900
C	3.16342300	0.43177800	-0.12166400
C	3.33006100	-0.92724800	0.55258600
C	2.35592000	-1.93455400	-0.05146500
H	-1.91186200	2.27579300	-0.06841900
H	0.00517700	3.87472000	-0.11893600
H	2.32378400	2.98342300	-0.11181300
H	3.47822200	0.35569400	-1.17441900
H	3.81604400	1.18124700	0.33756700
H	4.35862900	-1.28212100	0.44102900
H	3.13551300	-0.82721000	1.62706600
H	2.34652300	-2.87316200	0.51408100
H	2.67220300	-2.19884600	-1.07380700
O	0.01410100	-2.32534500	-0.19948800
N	-1.66455000	-0.43070100	-0.01250500
H	-0.87416700	-1.80669800	-0.16647100
C	-3.01335700	-0.18955400	0.11136100
O	-3.52389700	0.89857800	0.39749400
C	-3.86106100	-1.41876100	-0.11315800
H	-3.53830600	-2.23269900	0.54390200
H	-4.91016800	-1.18807800	0.07627100
H	-3.74917000	-1.77158300	-1.14438200

(K₁)_b

C	-0.85207700	1.95918700	-0.00090500
C	-0.66301400	0.55807300	-0.00896300
C	0.68865100	-0.00375600	-0.05678800

C	1.76826200	0.88925200	-0.08481800
C	1.53238500	2.28658400	-0.06238000
C	0.24666200	2.82464600	-0.02631200
C	0.90109500	-1.41299500	-0.09546600
C	3.17312800	0.36176300	-0.17293300
C	3.30562400	-1.00482500	0.49896800
C	2.28338900	-1.98602200	-0.07300500
H	-1.86201800	2.34095100	0.04196300
H	0.09723400	3.89784300	-0.01236700
H	2.39219400	2.95041600	-0.08057000
H	3.45071800	0.27065800	-1.23460100
H	3.87037600	1.08348500	0.26505400
H	4.31924300	-1.39380200	0.36387600
H	3.14292200	-0.89430100	1.57792000
H	2.26007000	-2.91753300	0.50359300
H	2.56633700	-2.26956000	-1.09938200
O	-0.10386800	-2.25064200	-0.16380100
N	-1.64090900	-0.38116300	0.02403700
H	-1.04282700	-1.52174600	-0.07926800
C	-3.00829200	-0.17708900	0.06265200
O	-3.54040500	0.92668100	0.16753800
C	-3.80343200	-1.45375800	-0.02727800
H	-3.50072200	-2.15277300	0.75920100
H	-4.86685700	-1.23313000	0.06817900
H	-3.62040500	-1.94703900	-0.98838000

(K₂)_G

C	0.76651000	-1.71019200	0.04386700
C	1.32866300	-0.43095600	0.01226500
C	0.47533400	0.70973900	-0.02953700
C	-0.93296400	0.53991900	-0.01345100
C	-1.43956300	-0.75596400	0.00128400
C	-0.60667700	-1.86485600	0.02968100
C	1.02773400	2.08736000	-0.12031900
C	-1.87221000	1.72275800	-0.00842900
C	-1.22375900	2.99708400	0.50763000
C	0.07325400	3.24587500	-0.24265500
H	1.41356500	-2.57325200	0.07253700
H	-1.03210600	-2.86216000	0.04586600
H	-2.24068100	1.88153000	-1.03206800
H	-2.75040700	1.47850400	0.59226500
H	-1.90583100	3.84269400	0.38105600
H	-1.02105600	2.90471800	1.58163000
H	0.59853700	4.14181700	0.09673300

H	-0.13614400	3.37969500	-1.31424200
O	2.23928700	2.31801700	-0.12323600
N	2.71190200	-0.24673600	0.00828100
H	2.98417600	0.73496400	-0.02674700
C	3.71385300	-1.17960200	0.03355400
O	3.53129900	-2.39288500	0.07135900
C	5.10933800	-0.60136500	0.01037400
H	5.13028400	0.49022200	-0.00108700
H	5.65164500	-0.96062900	0.88906800
H	5.62871900	-0.97724100	-0.87551300
Br	-3.31388000	-1.07753100	-0.03994400

(K₂)_N

C	0.71130500	-1.77443400	-0.02048600
C	1.29562300	-0.49234500	-0.02559600
C	0.47143200	0.72682400	-0.07940000
C	-0.92947200	0.55459900	-0.01333400
C	-1.45666000	-0.75809100	-0.01809700
C	-0.66730200	-1.92244000	-0.03387700
C	1.05950100	2.03628800	-0.18754800
C	-1.83072700	1.75985300	0.00406500
C	-1.13942100	2.98038000	0.60064500
C	0.16874600	3.25203300	-0.12719400
H	1.35797600	-2.63916700	0.01188200
H	-1.12561400	-2.90210700	-0.03956500
H	-2.14370600	1.98340100	-1.02732100
H	-2.74526800	1.53551200	0.55623100
H	-1.80364700	3.84775800	0.53752200
H	-0.94097600	2.80271600	1.66472800
H	0.73856300	4.05421900	0.35265400
H	-0.03502500	3.58817800	-1.15540500
O	2.31430600	2.22440200	-0.33978300
N	2.64033800	-0.29173800	0.03427900
H	2.87497600	0.72644700	-0.06752500
C	3.68685700	-1.20967900	0.09599900
O	3.50789800	-2.41547200	0.18832900
C	5.04693800	-0.57011600	0.03484300
H	5.13557100	0.24239100	0.76266600
H	5.80642100	-1.32578400	0.23399500
H	5.21822700	-0.14314900	-0.95967900
Br	-3.31138300	-1.01991200	-0.03653200

(K₂)_T

C	0.71478800	-1.76721300	0.07442100
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C	1.32659600	-0.49923700	0.02784700
C	0.48182800	0.69998400	-0.03452100
C	-0.91835900	0.55073600	-0.03872100
C	-1.46091100	-0.76317500	-0.00020100
C	-0.67411600	-1.90687800	0.05329200
C	1.04375600	2.00855300	-0.10893600
C	-1.80295000	1.76509800	-0.11128900
C	-1.15611400	2.98248000	0.54051600
C	0.21191700	3.24360800	-0.07384100
H	1.34789000	-2.64004100	0.13710300
H	-1.12898600	-2.88880100	0.08054400
H	-2.01436700	1.98207100	-1.16979000
H	-2.76801500	1.55557400	0.35200900
H	-1.80173500	3.85677200	0.41918000
H	-1.04978200	2.80479100	1.61717300
H	0.76346200	4.01431800	0.47619500
H	0.10077500	3.62592000	-1.10152900
O	2.34266300	2.21337300	-0.23872000
N	2.66040500	-0.25715600	0.03923200
H	2.77554900	1.26790100	-0.16106600
C	3.65426700	-1.21061400	0.05901800
O	3.47623600	-2.42813100	0.16062200
C	5.04231000	-0.63297000	-0.07266200
H	5.15038500	0.28423700	0.51218200
H	5.78287500	-1.36909400	0.24365200
H	5.23188600	-0.37782500	-1.12239300
Br	-3.32405800	-1.01199700	-0.05207600

(K₂)_b

C	0.69305700	-1.78733300	0.05299800
C	1.30527600	-0.51984100	0.01315700
C	0.47602700	0.68930600	-0.04215700
C	-0.92344100	0.55404200	-0.03081900
C	-1.47295800	-0.75564900	-0.00049100
C	-0.69562700	-1.91267800	0.04048100
C	1.07555100	1.98317200	-0.11781900
C	-1.79318400	1.78049200	-0.08558800
C	-1.10855700	2.99881500	0.52789800
C	0.25446100	3.22920600	-0.11388800
H	1.32182100	-2.66468900	0.09720200
H	-1.16202200	-2.88903000	0.06315700
H	-2.04169300	1.98782600	-1.13777600
H	-2.74285700	1.59024900	0.41729700
H	-1.74278300	3.88093800	0.40151400

H	-0.98491800	2.84117200	1.60593300
H	0.81949700	4.01079900	0.40534700
H	0.13028800	3.57733600	-1.15173300
O	2.37546200	2.12930600	-0.20318700
N	2.63847300	-0.27510000	0.01258700
H	2.76041300	1.06270300	-0.11941800
C	3.65404300	-1.20967200	0.04953700
O	3.48363200	-2.42402500	0.15952500
C	5.02846600	-0.59809800	-0.04894300
H	5.18399400	0.12528900	0.75836600
H	5.78625900	-1.37972400	0.01040600
H	5.13761400	-0.05680900	-0.99506300
Br	-3.33618100	-0.98609100	-0.04457800

(K₃)_G

O	1.46012700	2.35750900	-0.78522100
O	3.12192000	0.05839000	1.07579400
O	-1.00676100	-1.86195700	-1.15074300
H	0.10839300	-0.49661400	-1.12691200
N	0.14254800	0.47510600	-0.81984600
C	1.27874400	1.18292800	-1.09185400
C	-1.02655100	0.88290600	-0.17075700
C	-2.10548500	-0.04481900	-0.05748000
C	-3.29229000	0.35788900	0.59781800
C	3.90444400	-0.27868400	0.00785800
C	3.43263300	-0.78790400	2.09754200
H	2.88646400	-0.63817300	3.01625400
C	4.39624100	-1.65691100	1.70798400
H	4.83805800	-2.43869100	2.30991200
C	4.70213200	-1.32601600	0.34505400
H	5.42447400	-1.80720600	-0.29991000
C	-2.02001300	-1.42141500	-0.59887100
C	-3.39345500	1.64273300	1.12025400
H	-4.31074200	1.94671500	1.61558200
C	-2.33297500	2.53170500	1.00592300
H	-2.42073400	3.53348300	1.41628200
C	-1.15634200	2.16585500	0.36771300
H	-0.33504900	2.86028400	0.27876100
C	3.73107500	0.51808200	-1.23905700
H	3.94554100	1.57512000	-1.04704100
H	4.47078200	0.16543900	-1.96262600
C	2.33170600	0.40490800	-1.86428400
H	2.36195300	0.84490200	-2.86766000
H	2.05096200	-0.64602900	-1.97891800

C	-3.20922500	-2.34130100	-0.45242100
C	-4.53787300	-1.60518800	-0.36432800
C	-4.46196100	-0.58398500	0.76098900
H	-3.17267600	-3.05347500	-1.28096200
H	-4.75063200	-1.09985900	-1.31435200
H	-4.36020300	-1.11330400	1.71932200
H	-5.38508700	-0.00068600	0.82737000
H	-5.35138600	-2.31497500	-0.18670100
H	-3.04507000	-2.91890500	0.46937500

(K₃)_N

O	1.45552800	2.40772900	-0.85206800
O	2.93595200	0.02475600	1.04209900
O	-0.80915900	-1.85422600	-1.07301400
H	0.05106500	-0.47393000	-1.13236100
N	0.12321900	0.53439700	-0.84523200
C	1.29124600	1.23017800	-1.13974100
C	-0.97890700	0.91831800	-0.14603500
C	-2.05096800	-0.08280300	-0.06049700
C	-3.23559300	0.33254700	0.57710600
C	3.80522700	-0.30534000	0.04098100
C	3.17641500	-0.81477700	2.08897600
H	2.55541900	-0.67195100	2.95994700
C	4.18005400	-1.67034000	1.77997100
H	4.58272300	-2.44511000	2.41728300
C	4.58776900	-1.34022400	0.44364100
H	5.36372700	-1.81479400	-0.14108000
C	-1.90850500	-1.41055300	-0.58680100
C	-3.33680500	1.62476800	1.13709700
H	-4.26563100	1.89195800	1.63367800
C	-2.28747100	2.55634100	1.09486100
H	-2.39602300	3.53674600	1.54223600
C	-1.10965300	2.19765500	0.44901400
H	-0.28539300	2.89046600	0.36015500
C	3.71452600	0.48821100	-1.21592900
H	3.96430900	1.53792800	-1.02465900
H	4.46272800	0.10105400	-1.91205500
C	2.33108700	0.42560700	-1.88753400
H	2.40972200	0.87100300	-2.88627400
H	2.01501700	-0.61301900	-2.01518400
C	-3.09951400	-2.34096200	-0.56801900
C	-4.43317900	-1.61013500	-0.45050500
C	-4.38766300	-0.62314900	0.71328700

H	-3.05784700	-2.94848400	-1.47841700
H	-4.63978400	-1.06556500	-1.38020100
H	-4.27546300	-1.18469500	1.65392100
H	-5.32573300	-0.06473700	0.79802800
H	-5.24932200	-2.32524700	-0.30724200
H	-2.97899900	-3.04052700	0.27348000

(K₃)_T

O	1.39122100	1.43401700	-2.00831100
O	3.07407300	0.56603400	0.83324400
O	-1.22477000	-2.26897100	-0.39974500
H	-0.45850000	-1.64437200	-0.67337900
N	0.09150800	-0.15834200	-0.93876000
C	1.22193200	0.28952600	-1.57225900
C	-0.88993900	0.63854100	-0.44298000
C	-2.10165300	-0.05684200	-0.01015100
C	-3.16963700	0.71428500	0.47517100
C	3.87423900	-0.28447100	0.12400100
C	3.40235300	0.43962700	2.14997000
H	2.84480000	1.05824500	2.83643500
C	4.39467000	-0.47058200	2.29869100
H	4.85506400	-0.77303200	3.22892900
C	4.70057300	-0.94387300	0.97832200
H	5.44207100	-1.68089100	0.70200000
C	-2.22890900	-1.47203600	-0.05410200
C	-3.04086100	2.12397400	0.58696900
H	-3.88361600	2.68492900	0.98067400
C	-1.87840900	2.78344600	0.22163300
H	-1.79469700	3.85916500	0.32602300
C	-0.80467800	2.03913400	-0.29057900
H	0.11073800	2.53116500	-0.58688400
C	3.68611700	-0.32079200	-1.35343100
H	3.88899500	0.66573200	-1.78524200
H	4.42932000	-1.01039800	-1.76293600
C	2.28376300	-0.77339500	-1.79300000
H	2.31038000	-0.97440100	-2.87144000
H	2.00618100	-1.70354200	-1.29139500
C	-3.49162400	-2.17200500	0.31714900
C	-4.70512400	-1.25524000	0.19206300
C	-4.44653500	0.05905200	0.92310200
H	-3.59155300	-3.06008400	-0.31691600
H	-4.90291900	-1.05078600	-0.86690900
H	-4.37650800	-0.13487100	2.00513800

H	-5.28314300	0.75297200	0.79218400
H	-5.59381600	-1.74607300	0.59900600
H	-3.40520400	-2.54410300	1.35113200
(K ₃) _b			
O	1.43189200	2.30648600	-0.99766900
O	2.98380200	0.10288200	1.04574200
O	-0.84092700	-1.80106300	-1.11612600
H	-0.15848200	-0.76199500	-1.12388500
N	0.07613500	0.44412900	-0.88947000
C	1.24438500	1.10983600	-1.20587700
C	-0.99539100	0.91680300	-0.20440900
C	-2.07844500	-0.05893400	-0.06064400
C	-3.23721900	0.35132700	0.61409500
C	3.82515900	-0.29223700	0.04448600
C	3.27202100	-0.64794900	2.14629200
H	2.67838100	-0.44460000	3.02432600
C	4.27879600	-1.51166200	1.87164900
H	4.71492900	-2.22786500	2.55392400
C	4.63738300	-1.28152600	0.50071700
H	5.40236100	-1.78905200	-0.07066500
C	-1.95260500	-1.38437600	-0.57296200
C	-3.32629600	1.66493900	1.13448100
H	-4.23877300	1.94876000	1.65157200
C	-2.28654800	2.58986000	1.01474400
H	-2.38352100	3.58657600	1.42857300
C	-1.11931500	2.21392300	0.34590900
H	-0.29981400	2.90666000	0.21883200
C	3.68400700	0.39740500	-1.26825600
H	3.91553600	1.46353700	-1.16530600
H	4.42557300	-0.02876200	-1.94892100
C	2.28719400	0.25487600	-1.89609200
H	2.33826000	0.60168100	-2.93558600
H	1.98048200	-0.79390800	-1.91652100
C	-3.09776200	-2.34783800	-0.49360000
C	-4.44070400	-1.64006000	-0.32055100
C	-4.36704000	-0.61967600	0.81513800
H	-3.08749800	-2.96617700	-1.39812800
H	-4.70643100	-1.12539700	-1.25192600
H	-4.21247800	-1.15048000	1.76742200
H	-5.31204700	-0.07610700	0.91689100
H	-5.23009400	-2.37044900	-0.11926300
H	-2.92316400	-3.03601300	0.34865900

(K₄)_G

O	-2.12280200	-1.96112400	-1.55894500
O	-3.81238000	-0.77720100	1.11178200
O	-0.58459600	2.59245900	-0.65855400
H	-1.39691100	1.09081800	-1.05728600
N	-1.19912900	0.09133500	-1.09362500
C	-2.21663600	-0.74124300	-1.47178600
C	0.10994300	-0.22135700	-0.72667900
C	1.00181600	0.83044900	-0.36719200
C	2.33874900	0.52923700	-0.00113700
C	-4.83208500	-0.33894100	0.31521900
C	-4.09158700	-0.39079500	2.38836500
H	-3.36467400	-0.67090000	3.13528100
C	-5.26667900	0.28230200	2.42625000
H	-5.73742600	0.70439800	3.30313000
C	-5.74805400	0.31794900	1.07423200
H	-6.66011100	0.77450500	0.71505200
C	0.55464600	2.24814500	-0.33545000
C	2.72650700	-0.80663400	0.03405600
C	1.85295100	-1.82946900	-0.30493700
H	2.18649100	-2.86077400	-0.27186200
C	0.55708600	-1.54519600	-0.69140400
H	-0.12010900	-2.34108600	-0.96037800
C	-4.73572900	-0.64772100	-1.13908700
H	-4.71608800	-1.73163100	-1.29686200
H	-5.64130600	-0.26830600	-1.61958300
C	-3.50991800	-0.02801200	-1.82829000
H	-3.62868900	-0.13335800	-2.91268100
H	-3.45181800	1.04211700	-1.61004600
C	3.33045400	1.61657100	0.33934800
C	1.52015600	3.30249700	0.13826300
C	2.95363400	2.97095000	-0.23909800
H	1.18308100	4.26138700	-0.26262800
H	3.05676700	2.95267100	-1.33089200
H	3.63453300	3.74086700	0.13496200
H	4.32022500	1.32013800	-0.01343500
H	3.40853400	1.68852500	1.43364900
H	1.42699800	3.35765400	1.23291200
Br	4.47946000	-1.30548100	0.57765000

(K₄)_N

O	-2.11179000	-1.93328900	-1.78939000
O	-3.54335600	-0.78239200	1.05819700

O	-0.79882400	2.51096100	-0.43746000
H	-1.38119200	1.09469800	-0.99054400
N	-1.20310700	0.07003800	-1.12508200
C	-2.23774800	-0.73301500	-1.58908900
C	0.04277100	-0.26985200	-0.69582900
C	0.91546000	0.85412000	-0.31812600
C	2.26282800	0.54539400	-0.02562700
C	-4.65267200	-0.33604200	0.39675600
C	-3.67932200	-0.43641800	2.36978600
H	-2.86743100	-0.72447800	3.01978600
C	-4.85041200	0.21689400	2.56076400
H	-5.22219600	0.60840500	3.49728700
C	-5.48340900	0.28493300	1.27397300
H	-6.43493000	0.73958400	1.03507200
C	0.42970700	2.20744200	-0.26415000
C	2.65045200	-0.81268800	0.03994700
C	1.78902900	-1.89171100	-0.23343100
H	2.13927800	-2.91230600	-0.15903600
C	0.48960100	-1.60427800	-0.61983200
H	-0.19450100	-2.39695000	-0.88560900
C	-4.71228400	-0.60473800	-1.06692000
H	-4.74460500	-1.68384800	-1.25573100
H	-5.64505700	-0.18316200	-1.44984500
C	-3.53464400	-0.00202200	-1.85573300
H	-3.74211700	-0.11236200	-2.92594700
H	-3.44176700	1.06643600	-1.64420900
C	3.24067600	1.65203700	0.26686100
C	1.40124300	3.32582000	0.01930500
C	2.82594000	2.96910300	-0.37882000
H	1.04410500	4.21478800	-0.51030200
H	2.89248600	2.87729900	-1.46990900
H	3.52035500	3.76024800	-0.07978000
H	4.23980400	1.36545200	-0.06804100
H	3.31114000	1.78367500	1.35734800
H	1.35892600	3.56483200	1.09300400
Br	4.39536900	-1.26013400	0.55377800
(K ₄) _T			
O	-2.15975100	-1.15503000	-2.32588000
O	-3.45815700	-1.13643200	0.82792800
O	-0.63038900	2.78790300	-0.06684900
H	-1.17205600	2.00796600	-0.48585800
N	-1.24520900	0.56670700	-1.07165800
C	-2.26737900	-0.08850100	-1.71110700

C	-0.02761600	0.03668100	-0.79496300
C	0.94109700	0.97000300	-0.21180800
C	2.24342700	0.51459000	0.06863900
C	-4.57898700	-0.47857600	0.40606800
C	-3.52058700	-1.22887200	2.18612500
H	-2.69238300	-1.73025500	2.66312200
C	-4.65684700	-0.64861500	2.64181900
H	-4.97112400	-0.57399600	3.67352400
C	-5.34534500	-0.15768400	1.48162400
H	-6.29014800	0.36755600	1.45365300
C	0.59708000	2.32132200	0.08342200
C	2.53923600	-0.86103700	-0.13857300
C	1.61905700	-1.76573100	-0.65213500
H	1.88538400	-2.80565000	-0.79211300
C	0.34326200	-1.30748000	-0.98656500
H	-0.38530400	-1.98878100	-1.40152900
C	-4.71725900	-0.25185400	-1.05977300
H	-4.73413500	-1.21063800	-1.59039500
H	-5.68399600	0.22897400	-1.23234700
C	-3.60515400	0.62578900	-1.66222100
H	-3.88081500	0.86520300	-2.69615600
H	-3.52244500	1.56578900	-1.11153000
C	3.28054200	1.45918100	0.61292800
C	1.58707200	3.30065100	0.61021000
C	3.00788600	2.90890200	0.22779900
H	1.32234600	4.29373300	0.23155800
H	3.14410200	3.03104700	-0.85318100
H	3.73033400	3.56512400	0.72114600
H	4.27205100	1.15968000	0.26804300
H	3.29999100	1.36270000	1.70943500
H	1.49044800	3.35385700	1.70672800
Br	4.23581900	-1.52924000	0.31848500

(K₄)_b

O	-2.13432300	-1.66075800	-2.01329800
O	-3.51708400	-0.95612400	1.01079300
O	-0.77176100	2.55026400	-0.43283300
H	-1.22316500	1.57588100	-0.80712900
N	-1.20497100	0.27112700	-1.14807100
C	-2.23743700	-0.48705000	-1.65346600
C	0.03016300	-0.17189600	-0.80455000
C	0.92942500	0.87966700	-0.31918900
C	2.24791900	0.53789200	0.02989300
C	-4.61950700	-0.39778700	0.42797800

C	-3.62657900	-0.77601600	2.35725400
H	-2.81738600	-1.16995300	2.95288300
C	-4.77469200	-0.11848900	2.64836300
H	-5.12361300	0.16015200	3.63290200
C	-5.42049200	0.13019000	1.39047800
H	-6.36088000	0.63792900	1.22569900
C	0.47598500	2.22724300	-0.19446600
C	2.62977800	-0.82748800	-0.04316200
C	1.77494900	-1.84171300	-0.47545500
H	2.11321500	-2.86916200	-0.51160100
C	0.47864700	-1.50549400	-0.86176100
H	-0.20130300	-2.26611100	-1.21710600
C	-4.70665600	-0.47054900	-1.05727300
H	-4.72944900	-1.51606400	-1.38496300
H	-5.65528600	-0.01807100	-1.35814200
C	-3.55596900	0.24913500	-1.78379800
H	-3.79558000	0.28724200	-2.85303300
H	-3.46457900	1.27794600	-1.42693300
C	3.19769900	1.60496500	0.50260400
C	1.39316600	3.32636300	0.22674400
C	2.84859300	2.97882100	-0.06322900
H	1.08623300	4.24492300	-0.28495300
H	3.01655200	2.97852000	-1.14679700
H	3.51339100	3.73387200	0.36605200
H	4.22237100	1.33872300	0.23660600
H	3.16822000	1.63969500	1.60237700
H	1.25541700	3.51307500	1.30377900
Br	4.35503000	-1.34115100	0.49222200

(K₅)_G

C	2.57112900	2.72731900	0.20820800
C	1.30217800	2.19287100	0.03809700
C	1.14248100	0.81330900	-0.12292100
C	2.29012200	-0.03651000	-0.11207700
C	3.57062900	0.53871000	0.06323700
C	3.69673300	1.91404900	0.22344200
H	2.67804400	3.80061200	0.33595900
H	0.43007000	2.82828700	0.02853000
H	4.68248600	2.34695000	0.36484900
C	2.18428500	-1.50382100	-0.28368500
O	1.10881700	-2.07965000	-0.47810800
C	-1.35527900	0.82419300	-0.31988800
N	-0.11731800	0.23661300	-0.29988600
O	-1.54490500	2.03122200	-0.19930400

H	-0.07759800	-0.77500200	-0.42267700
C	-2.48955100	-0.17810300	-0.45883100
C	-3.72757600	0.37692700	-1.21259900
C	-3.09575900	-0.54577300	0.95368600
C	-4.88560900	0.19564900	-0.18338600
H	-3.58961100	1.43655100	-1.44146400
C	-3.99472500	-1.74133900	0.69391400
H	-2.35033000	-0.66193700	1.74282500
C	-5.05988000	-1.29942100	0.01662200
H	-5.78786500	0.75968300	-0.42678500
H	-3.73523300	-2.76989300	0.92269600
H	-5.85539700	-1.89650100	-0.41768500
C	-4.14878400	0.56584700	1.11736800
H	-3.72499200	1.57366200	1.10377700
H	-4.76317500	0.42771100	2.01158900
H	-3.91226500	-0.15788000	-2.14747000
H	-2.10206400	-1.08325400	-0.93283700
C	3.44225600	-2.33966000	-0.24492200
C	4.55964700	-1.71664000	0.57853300
C	4.82165700	-0.30815100	0.06668700
H	3.15951100	-3.33517700	0.10724900
H	4.27245900	-1.68284400	1.63661700
H	5.21332300	-0.36649500	-0.95909400
H	5.59109000	0.19155000	0.66253900
H	5.46510800	-2.32692000	0.50889200
H	3.77264800	-2.45470800	-1.28791500

(K₅)_N

C	2.65923700	2.74449100	0.30490500
C	1.37225100	2.25571100	0.10525200
C	1.15335100	0.87139800	-0.10182200
C	2.26843200	-0.08683300	-0.13886100
C	3.55182900	0.45032900	0.07781000
C	3.72722400	1.83461700	0.29744900
H	2.82946900	3.80090400	0.47264400
H	0.51394700	2.91143000	0.12584000
H	4.73854200	2.19987300	0.45393000
C	2.07498700	-1.48713400	-0.39117200
O	0.93597400	-1.99361200	-0.68841200
C	-1.34221000	0.93824600	-0.30471300
N	-0.08398300	0.33317000	-0.26947900
O	-1.49848900	2.13746700	-0.11961100
H	-0.02012400	-0.70023800	-0.45171200
C	-2.46092400	-0.05270900	-0.52855700

C	-3.75681800	0.58174300	-1.09679400
C	-2.95858800	-0.65839200	0.85032000
C	-4.83188200	0.22040300	-0.02645600
H	-3.64745500	1.66624200	-1.17335600
C	-3.86387600	-1.81378400	0.46620400
H	-2.15689400	-0.88454500	1.55563800
C	-4.97955200	-1.29057500	-0.05308300
H	-5.75363500	0.79845800	-0.11144300
H	-3.57878300	-2.85968200	0.50974300
H	-5.80110200	-1.82648100	-0.51736300
C	-4.00280200	0.39616300	1.25951400
H	-3.59006000	1.40280100	1.37559600
H	-4.54747100	0.11071800	2.16370200
H	-4.00327500	0.18878800	-2.08590700
H	-2.08536300	-0.85983200	-1.16259400
C	3.26125900	-2.42007900	-0.31088600
C	4.41793800	-1.85779700	0.50899100
C	4.75684700	-0.44723100	0.03391700
H	2.90582800	-3.36995100	0.10263200
H	4.13946500	-1.82641800	1.56969700
H	5.12610600	-0.49833600	-1.00227500
H	5.56654200	-0.01149500	0.62834900
H	5.29617400	-2.50565600	0.42519900
H	3.59970700	-2.63893500	-1.33541100

(K₅)_T

C	2.66712000	2.76939300	0.06982600
C	1.36339300	2.26607900	-0.06125900
C	1.11619000	0.87764600	-0.13450000
C	2.24696000	-0.05275100	-0.10222500
C	3.53844500	0.47788900	0.04116500
C	3.72973700	1.88235300	0.12524100
H	2.83407000	3.83890000	0.12848700
H	0.51739900	2.93674600	-0.10106200
H	4.74488300	2.25481100	0.22861800
C	2.08327800	-1.46028700	-0.22517700
O	0.90508000	-2.02365200	-0.46089400
C	-1.31478600	0.94534400	-0.20352200
N	-0.10263900	0.29540500	-0.26226500
O	-1.47585700	2.11587200	0.15802100
H	0.22738700	-1.24786500	-0.45517000
C	-2.47768900	0.03486200	-0.55776400
C	-3.77905500	0.77401000	-0.95951000
C	-2.94099000	-0.79468000	0.70803900

C	-4.82482100	0.25440400	0.07515300
H	-3.64729800	1.85376600	-0.85481000
C	-3.88920200	-1.85055300	0.17069600
H	-2.11878000	-1.15273700	1.33007800
C	-5.01126700	-1.22665100	-0.20420300
H	-5.73529300	0.85433600	0.12919700
H	-3.62992200	-2.89368600	0.02065300
H	-5.86204700	-1.65974200	-0.72075600
C	-3.94421300	0.18957400	1.33747100
H	-3.50110800	1.15322100	1.60630300
H	-4.46260200	-0.23743000	2.20091200
H	-4.07410800	0.55980300	-1.99002700
H	-2.13494400	-0.65484600	-1.33292300
C	3.22912900	-2.40949500	-0.12753200
C	4.40689000	-1.80447000	0.63119700
C	4.73980200	-0.42551500	0.06851800
H	2.87363000	-3.32960400	0.34979200
H	4.15110700	-1.71259500	1.69349000
H	5.11762200	-0.53476100	-0.96029600
H	5.54470500	0.04828300	0.63959800
H	5.27832800	-2.46201600	0.56339500
H	3.54328800	-2.69611900	-1.14453500

(K₅)_b

C	2.69332100	2.75513900	0.21484400
C	1.38790800	2.28289700	0.05334300
C	1.14013800	0.89919000	-0.10062200
C	2.24932000	-0.05905000	-0.10253700
C	3.54697600	0.44908000	0.05274700
C	3.74856800	1.84121500	0.21634100
H	2.88024100	3.81508100	0.34030500
H	0.54469400	2.95846500	0.05633700
H	4.76713000	2.19850600	0.34046600
C	2.02026200	-1.45705900	-0.27625400
O	0.82435200	-1.92907000	-0.50281100
C	-1.31693800	0.93936300	-0.32280500
N	-0.07689400	0.32296800	-0.26070500
O	-1.48313100	2.14678500	-0.16458000
H	0.12773800	-0.90123000	-0.41945800
C	-2.44537700	-0.04521800	-0.54584700
C	-3.75114500	0.59091700	-1.08649800
C	-2.92079800	-0.67184500	0.82948000
C	-4.80955400	0.21623900	-0.00377700
H	-3.64440000	1.67637400	-1.15235200

C	-3.83238800	-1.82300700	0.44710900
H	-2.10728500	-0.90622700	1.51831400
C	-4.95733300	-1.29449900	-0.04640900
H	-5.73319000	0.79453400	-0.06572900
H	-3.54659700	-2.86947500	0.47223400
H	-5.78608400	-1.82527800	-0.50398800
C	-3.95916200	0.37604300	1.27052600
H	-3.54471200	1.38155700	1.39129200
H	-4.48885800	0.07967500	2.18029900
H	-4.01458700	0.20890100	-2.07584600
H	-2.07318400	-0.84239700	-1.19441300
C	3.15632500	-2.43241600	-0.21228800
C	4.36129800	-1.87190700	0.54145000
C	4.72492300	-0.48417700	0.01404400
H	2.78964400	-3.35418300	0.25288400
H	4.12505200	-1.80207300	1.61023400
H	5.07179000	-0.57395900	-1.02714000
H	5.55874700	-0.05507700	0.57916000
H	5.21635700	-2.54758700	0.44384300
H	3.44793100	-2.70352900	-1.23946400

(K₆)_G

C	-2.55062300	2.64211700	0.43798100
C	-1.27366800	2.21923700	0.09718700
C	-1.02703700	0.86257300	-0.12999100
C	-2.09177500	-0.08041900	-0.00838400
C	-3.38218500	0.38129900	0.34081300
C	-3.59747300	1.73792600	0.55811500
H	-2.72808200	3.70013800	0.60754500
H	-0.46247100	2.92470000	0.00267100
H	-4.59272300	2.08527400	0.81876800
C	-1.88815700	-1.53113500	-0.23147900
O	-0.78669600	-2.01813900	-0.50512500
C	1.40372700	1.09337300	-0.67991900
C	5.03826700	-0.37326100	-0.58204700
C	3.58131400	0.08605600	1.25408000
C	5.08351300	-1.53750800	0.43393400
H	4.97952500	-0.71868800	-1.61885800
C	4.25199300	-1.01836200	1.58072600
H	4.64675600	-2.46069900	0.02899400
H	4.19610900	-1.51994100	2.54294400
N	0.24582600	0.39634300	-0.47276600
O	1.50843900	2.31297600	-0.57381500
C	2.59255900	0.23611800	-1.07186000

H	2.33748600	-0.82859200	-1.05123100
C	3.82200800	0.49945100	-0.18207500
H	5.95171900	0.22304700	-0.49065300
H	4.05663700	1.56614600	-0.25841800
H	6.10769100	-1.78610100	0.73343400
H	2.89902800	0.62021800	1.91010800
H	2.83996100	0.49420000	-2.10857200
H	0.28188300	-0.61648700	-0.58430000
C	-4.54404900	-0.57085700	0.50053100
C	-3.06730500	-2.46573800	-0.09713000
C	-4.40477000	-1.79995900	-0.38518000
H	-4.45941100	-1.50839600	-1.44122300
H	-5.22320700	-2.50241700	-0.20127000
H	-4.59871200	-0.89031000	1.55120700
H	-5.47596500	-0.03736900	0.29140400
H	-2.87403400	-3.32691800	-0.74210800
H	-3.05496200	-2.83638200	0.93862600

(K₆)_N

C	-2.61861100	2.55601300	0.77234400
C	-1.33687700	2.09083600	0.49547600
C	-1.12990600	0.74556300	0.10281300
C	-2.24615300	-0.20536100	-0.00586000
C	-3.52568800	0.31013100	0.27598000
C	-3.69316000	1.66242400	0.64959400
H	-2.78185200	3.58627300	1.06384200
H	-0.47887600	2.74503200	0.55099700
H	-4.70097900	2.01025700	0.85908000
C	-2.05488100	-1.58252500	-0.36407100
O	-0.89788600	-2.10773200	-0.53182800
C	1.35295800	0.84988300	-0.20183900
C	4.97765500	-0.54347900	-0.75592000
C	4.11523800	0.52338600	1.20053600
C	5.43145500	-1.30906600	0.50785900
H	4.63849000	-1.21014400	-1.55483300
C	4.94760400	-0.42487000	1.63005600
H	4.97409400	-2.30555100	0.57744700
H	5.23240500	-0.58004600	2.66710100
N	0.09579800	0.24413200	-0.20645400
O	1.51812900	2.02943600	0.07205500
C	2.46398300	-0.08813800	-0.61399900
H	2.30397300	-1.06852300	-0.14866500
C	3.86877500	0.43546200	-0.29105000
H	5.81942500	0.03336500	-1.15168000

H	3.97924700	1.41288600	-0.77198700
H	6.51571900	-1.46483600	0.53002600
H	3.62164900	1.25810000	1.82928000
H	2.36529000	-0.24587900	-1.69773200
H	0.03452800	-0.78097300	-0.43463900
C	-4.72560700	-0.59332300	0.22073700
C	-3.26456400	-2.46876000	-0.55196600
C	-4.54764400	-1.69078900	-0.82547200
H	-4.50014200	-1.23668300	-1.82302900
H	-5.41121100	-2.36327400	-0.81800100
H	-4.86612200	-1.06053100	1.20799700
H	-5.62716900	-0.00252300	0.02830400
H	-3.03979300	-3.16400400	-1.36794500
H	-3.38565000	-3.08547800	0.35197300

(K₆)_T

C	-2.54079100	2.63573100	0.57518300
C	-1.26206800	2.23423400	0.16270800
C	-0.98125300	0.88585600	-0.15726300
C	-2.04923300	-0.11207800	-0.04697700
C	-3.31837700	0.31875100	0.37265600
C	-3.54678600	1.68691800	0.67242900
H	-2.73489300	3.67576100	0.81121000
H	-0.46150800	2.95362600	0.07180600
H	-4.54283900	1.98145400	0.99018700
C	-1.84294900	-1.49042300	-0.32665900
O	-0.65101000	-1.98510200	-0.63609300
C	1.36142700	1.13451400	-0.76974200
C	5.00120900	-0.29619500	-0.45444200
C	3.39423600	0.04056200	1.27957000
C	4.98697200	-1.51375100	0.49796300
H	5.02925900	-0.58504200	-1.50973500
C	4.05697700	-1.07044800	1.60012000
H	4.60108100	-2.41934800	0.01001700
H	3.93239400	-1.62595600	2.52565100
N	0.21919000	0.39616700	-0.56073800
O	1.43928000	2.36788900	-0.71310300
C	2.58966700	0.31501700	-1.10892600
H	2.33833000	-0.74808400	-1.16102300
C	3.74196600	0.53743400	-0.10713100
H	5.89487000	0.30561800	-0.25964500
H	3.96659800	1.60971300	-0.10344100
H	5.98849800	-1.76418700	0.86529000
H	2.65030900	0.52589900	1.90605600

H	2.92835900	0.63042900	-2.10387200
H	-0.02098400	-1.17197300	-0.66849000
C	-4.44260300	-0.66440400	0.54234000
C	-2.94479900	-2.49405100	-0.26951800
C	-4.31779200	-1.84512700	-0.41654000
H	-4.45004200	-1.49353200	-1.44671500
H	-5.10585100	-2.57779100	-0.22029300
H	-4.42828500	-1.03677400	1.57885300
H	-5.40252200	-0.15380300	0.41518200
H	-2.76849700	-3.24289600	-1.04984500
H	-2.88389200	-3.03391700	0.68949700

(K₆)_b

C	-2.54056400	2.76061400	0.12327800
C	-1.27241300	2.21073300	-0.08486200
C	-1.09843600	0.80825200	-0.13101800
C	-2.24313300	-0.08976600	0.04471200
C	-3.49962000	0.49425000	0.25873200
C	-3.63069800	1.90441200	0.28728500
H	-2.67303300	3.83568200	0.15156200
H	-0.40620000	2.84082800	-0.22735800
H	-4.62055400	2.32199500	0.44918200
C	-2.08259300	-1.50784200	0.01907100
O	-0.90438600	-2.05885300	-0.09455200
C	1.33556400	0.70517000	-0.51619400
C	4.91349600	-0.89916100	-0.78793900
C	4.19006100	0.76205300	0.76908500
C	5.44429000	-1.23203500	0.62520700
H	4.51637800	-1.77698600	-1.30721000
C	5.04145500	-0.02172100	1.43060100
H	4.98537400	-2.14074400	1.03853200
H	5.39161000	0.15473900	2.44406500
N	0.07639400	0.15992300	-0.32678600
O	1.55366200	1.91049000	-0.60163200
C	2.41714900	-0.34423800	-0.65396800
H	2.27033400	-1.10973400	0.11850500
C	3.84532700	0.20894800	-0.59782600
H	5.73239300	-0.50559800	-1.39850600
H	3.93556500	0.97876300	-1.37150600
H	6.52659500	-1.40296500	0.63124500
H	3.74239500	1.67200900	1.15655700
H	2.25072500	-0.85215100	-1.61486900
H	-0.17324300	-1.06402000	-0.24252500
C	-4.70060500	-0.38027400	0.48844400

C	-3.27060700	-2.41439000	0.13178400
C	-4.57425700	-1.71378600	-0.24778100
H	-4.59123800	-1.53231200	-1.32933200
H	-5.42988000	-2.35484700	-0.01508100
H	-4.79780400	-0.57236200	1.56833500
H	-5.61051500	0.14958200	0.18815900
H	-3.09221400	-3.29168900	-0.50001300
H	-3.33213600	-2.79005000	1.16555800

(K₇)_G

C	0.88318600	2.67276800	-0.00003700
C	-0.24487800	1.86486500	-0.00002500
C	-0.12067400	0.46924700	-0.00000800
C	1.17802400	-0.11271800	-0.00000200
C	2.29185200	0.74103700	-0.00001500
C	2.16086100	2.11918400	-0.00003200
H	0.75711100	3.75137900	-0.00005000
H	-1.23269500	2.30017000	-0.00003100
H	3.28730800	0.31456400	-0.00001200
H	3.04157700	2.75253900	-0.00004200
C	1.40524600	-1.58063200	0.00001700
O	0.47191200	-2.38647400	0.00000800
C	-2.56746400	-0.05407100	0.00000900
N	-1.23724500	-0.37209600	0.00000300
O	-3.00573000	1.09310500	-0.00001400
H	-0.98974500	-1.36044100	0.00001400
C	2.81623600	-2.11748600	0.00000900
H	3.36801200	-1.78325900	-0.88378400
H	3.36802500	-1.78324800	0.88379000
H	2.76731000	-3.20663400	0.00001600
C	-3.49806000	-1.24471100	0.00006200
H	-4.14137000	-1.18638800	-0.88214000
H	-2.97921100	-2.20540400	-0.00012100
H	-4.14104100	-1.18656200	0.88252000

(K₇)_N

C	0.92598000	2.72026900	-0.00002100
C	-0.21452500	1.92240800	0.00002700
C	-0.11199900	0.51133000	-0.00006400
C	1.20235300	-0.16520700	-0.00016600
C	2.30979400	0.69075200	-0.00022800
C	2.18208900	2.09197400	-0.00016000
H	0.84227000	3.80010200	0.00004400
H	-1.20154400	2.36171300	0.00012200

H	3.30900600	0.27263800	-0.00030900
H	3.08521500	2.69428700	-0.00020100
C	1.34635600	-1.59908500	-0.00011600
O	0.34030000	-2.39033800	0.00048000
C	-2.55387700	-0.02563800	0.00005200
N	-1.18902900	-0.31643900	-0.00008000
O	-2.98379200	1.11874900	0.00025400
H	-0.88584300	-1.32334000	-0.00035100
C	2.72709400	-2.20418700	0.00002900
H	3.30802400	-1.91006200	-0.88302500
H	3.30810100	-1.90950800	0.88284800
H	2.62512500	-3.29069800	0.00037500
C	-3.45049000	-1.23330100	-0.00009700
H	-4.09658200	-1.19271400	-0.88206100
H	-2.90313000	-2.17728300	-0.00050200
H	-4.09615900	-1.19324200	0.88220400

(K₇)_T

C	-0.94148800	2.71362800	-0.00014400
C	0.21330700	1.91421200	-0.00005300
C	0.13866200	0.50472500	-0.00003800
C	-1.18004600	-0.13969800	-0.00010700
C	-2.29824300	0.69265500	-0.00018100
C	-2.18574500	2.10208500	-0.00021600
H	-0.85208800	3.79399800	-0.00017100
H	1.19359600	2.36803000	-0.00004500
H	-3.29265100	0.26136700	-0.00017800
H	-3.09281200	2.69789900	-0.00029300
C	-1.34908900	-1.56044900	-0.00007100
O	-0.31469500	-2.38540100	0.00040000
C	2.52302300	-0.00634500	0.00012100
N	1.18898200	-0.35493600	-0.00004400
O	2.96173900	1.14713100	0.00019900
C	-2.68224400	-2.22458800	-0.00044300
H	-3.27467600	-1.95213100	0.88214200
H	-3.27455400	-1.95144800	-0.88288500
H	-2.54091100	-3.30659300	-0.00083000
C	3.44584100	-1.20066000	0.00040900
H	3.26146200	-1.82343800	0.88232200
H	3.26035200	-1.82489200	-0.88022400
H	4.48502500	-0.86967100	-0.00045600
H	0.52417200	-1.77579700	0.00049000

(K₇)_b

C	-1.04073400	2.69260300	0.00112300
C	0.13742000	1.94055800	0.00069800
C	0.09493000	0.52869600	-0.00005600
C	-1.19514800	-0.17890000	0.00015100
C	-2.34066200	0.61681300	0.00005800
C	-2.26768900	2.02591000	0.00062800
H	-0.99738200	3.77529400	0.00158400
H	1.10459100	2.42234800	0.00040900
H	-3.32056500	0.15339700	-0.00013400
H	-3.19284400	2.59358300	0.00076600
C	-1.26265700	-1.61223700	0.00021600
O	-0.17614800	-2.33237400	0.00107100
C	2.51088000	0.04120700	-0.00113400
N	1.16871300	-0.29969800	-0.00155100
O	2.92074700	1.19960900	-0.00275200
H	0.71573700	-1.46640500	0.00014000
C	-2.57067500	-2.33823600	-0.00127400
H	-3.17748900	-2.09144100	0.87911800
H	-3.17315800	-2.09519400	-0.88574900
H	-2.37807700	-3.41247500	0.00144300
C	3.45687000	-1.13122600	0.00220700
H	4.09298000	-1.07333900	0.89091700
H	2.94182600	-2.09294200	-0.00770900
H	4.11139200	-1.06394300	-0.87218700

(K₈)_G

C	-0.91539800	-1.56966400	0.00002100
C	0.46826700	-1.51105400	0.00003200
C	1.13778900	-0.27948800	-0.00001700
C	0.37460600	0.91900700	-0.00008100
C	-1.02414900	0.82936900	-0.00008600
C	-1.65864800	-0.39627900	-0.00004000
H	-1.41009000	-2.53468600	0.00005900
H	1.04785500	-2.42162800	0.00007700
H	-1.62156400	1.73098300	-0.00012600
C	0.99332100	2.27296600	-0.00012300
O	2.21514000	2.42520500	0.00013400
C	3.45924600	-1.20425800	0.00005400
N	2.53043400	-0.19757800	-0.00002100
O	3.18074200	-2.39943500	0.00014700
H	2.87393400	0.76135500	-0.00009500
C	0.11128300	3.49678100	0.00006900
H	-0.53271700	3.52225400	-0.88424500
H	-0.53281000	3.52193800	0.88432500

H	0.75198500	4.37872900	0.00025900
C	4.89512000	-0.73611800	0.00006400
H	5.39568800	-1.14410500	-0.88220800
H	5.00133000	0.35048200	-0.00018900
H	5.39553300	-1.14366800	0.88262900
Br	-3.55136700	-0.47921000	-0.00005600

(K₈)_N

C	-0.96907700	-1.62056300	-0.00000700
C	0.42078800	-1.56335100	0.00001500
C	1.10314600	-0.32966100	0.00000900
C	0.37047000	0.95274300	-0.00001000
C	-1.02466500	0.84714400	-0.00004100
C	-1.66645000	-0.40167900	-0.00003800
H	-1.49218300	-2.56741300	-0.00000300
H	1.00509100	-2.47195900	0.00003600
H	-1.63727900	1.73879400	-0.00006400
C	1.02644300	2.23594500	0.00001900
O	2.29722200	2.35382700	0.00014400
C	3.43663900	-1.21740300	0.00005200
N	2.45843200	-0.22453300	0.00001400
O	3.16577900	-2.40932600	0.00009800
H	2.75859300	0.77936800	-0.00004500
C	0.19282100	3.49270400	0.00003600
H	-0.45397200	3.55942800	-0.88343500
H	-0.45416400	3.55928900	0.88337600
H	0.86684800	4.35079100	0.00017500
C	4.85095800	-0.70541900	0.00004100
H	5.36659700	-1.09615900	-0.88208400
H	4.91655800	0.38380000	-0.00020400
H	5.36645800	-1.09574200	0.88243500
Br	-3.53148600	-0.43620600	-0.00007700

(K₈)_T

C	0.98149600	-1.60890200	0.00003300
C	-0.41862200	-1.56754600	0.00008700
C	-1.12989700	-0.35098400	0.00004800
C	-0.38061900	0.91150600	-0.00005300
C	1.00999300	0.83856000	-0.00007800
C	1.67293700	-0.40716400	-0.00004300
H	1.50465200	-2.55679100	0.00004900
H	-0.98462400	-2.48744800	0.00013000
H	1.60848000	1.74032500	-0.00011000
C	-1.02137000	2.19203700	-0.00009100

O	-2.33514600	2.30501200	0.00015200
C	-3.40014400	-1.22875000	0.00018700
N	-2.47697600	-0.20456600	0.00008600
O	-3.12926000	-2.43196000	-0.00013600
C	-0.27210300	3.47875900	-0.00033900
H	0.37203800	3.57528300	0.88263200
H	0.37261100	3.57465300	-0.88294600
H	-0.98429600	4.30530500	-0.00084100
C	-4.82768500	-0.74047600	0.00062900
H	-5.01662600	-0.11932700	0.88263800
H	-5.01670700	-0.11755000	-0.88009700
H	-5.51234100	-1.58929500	-0.00015100
H	-2.69712700	1.32457600	0.00007200
Br	3.54640300	-0.40869800	-0.00012500

(K₈)_b

C	-0.99942000	-1.60946300	0.00041500
C	0.39564900	-1.57831500	0.00051000
C	1.09882100	-0.35746500	0.00028200
C	0.37085700	0.92106600	0.00016400
C	-1.02145100	0.85193100	-0.00023200
C	-1.68231900	-0.39146000	-0.00002400
H	-1.53432300	-2.55026400	0.00059800
H	0.96263300	-2.49800100	0.00065100
H	-1.61703900	1.75576600	-0.00059500
C	1.06085000	2.17964500	0.00036000
O	2.35950900	2.22717500	0.00075200
C	3.40756700	-1.20963000	0.00020900
N	2.44638300	-0.21420000	-0.00001600
O	3.14457600	-2.40953600	0.00059100
H	2.67488700	1.01251300	0.00007100
C	0.32070000	3.47993000	0.00003800
H	-0.32135600	3.58489100	-0.88348900
H	-0.32314200	3.58438000	0.88230200
H	1.04435400	4.29662400	0.00097900
C	4.82936700	-0.71232400	-0.00049200
H	5.34249800	-1.10257400	-0.88475900
H	4.89898300	0.37644500	0.00341100
H	5.34591600	-1.10949200	0.87861900
Br	-3.55184200	-0.39530000	-0.00045200

(K₉)_G

O	-0.73279300	-2.34891900	-0.73033800
O	-2.64590400	-0.19080900	1.06282000

O	1.30636300	2.10972600	-1.13726700
H	0.31814800	0.62158400	-1.12406400
N	0.38105200	-0.34134100	-0.79674900
C	-0.67279400	-1.16929200	-1.06334000
C	1.57835600	-0.61316100	-0.12876700
C	2.54292200	0.42467400	0.00304000
C	3.74155500	0.14036500	0.67531900
C	-3.44605800	0.04016800	-0.02011300
C	-3.05217300	0.64356200	2.06057800
H	-2.50432200	0.57158800	2.98762000
C	-4.09427300	1.40088500	1.64113500
H	-4.61970000	2.14776400	2.21973200
C	-4.34942600	1.00883300	0.28398200
H	-5.10937600	1.39892500	-0.37906000
C	2.33662300	1.79220600	-0.53886800
C	4.00630300	-1.11000100	1.20733100
H	4.94267600	-1.29899300	1.72142000
C	3.05148700	-2.11438900	1.07075900
H	3.23774100	-3.10232700	1.48141400
C	1.85294400	-1.87552300	0.41390100
H	1.11617800	-2.65791400	0.31226400
C	-3.17863700	-0.76435700	-1.24510500
H	-3.28494500	-1.83273200	-1.02781500
H	-3.94328500	-0.50782400	-1.98296600
C	-1.79208500	-0.52283900	-1.86258100
H	-1.76674100	-0.98780000	-2.85473300
H	-1.61946800	0.54825000	-2.00141100
H	4.48615300	0.91923900	0.78417600
C	3.41238700	2.83614300	-0.35911900
H	4.35231300	2.52226300	-0.82292600
H	3.07334700	3.76031300	-0.82774200
H	3.60979400	3.02344200	0.70070500

(K₉)_N

O	-0.71718500	-2.38928400	-0.77338000
O	-2.49153400	-0.16106400	1.02881100
O	1.11879200	2.06667900	-1.16205000
H	0.37193800	0.62206600	-1.10747000
N	0.39921800	-0.38025800	-0.79099400
C	-0.67956800	-1.20994900	-1.09178000
C	1.54667400	-0.64141000	-0.11296100
C	2.49498100	0.48821900	-0.01900700
C	3.69620400	0.20091100	0.63941400
C	-3.37891400	0.04186400	0.00987800

C	-2.85313600	0.65679200	2.05798900
H	-2.23375000	0.60613900	2.94025700
C	-3.95113200	1.37433300	1.72004100
H	-4.45850000	2.10153400	2.33834800
C	-4.29194700	0.97571700	0.38364000
H	-5.11179700	1.33997800	-0.21993400
C	2.21754200	1.79229400	-0.56611800
C	3.96814700	-1.06105700	1.19856300
H	4.91696200	-1.20979500	1.70453900
C	3.04706200	-2.11833600	1.12097200
H	3.26779800	-3.08385100	1.55940600
C	1.84053200	-1.89997800	0.46216500
H	1.10564100	-2.68652200	0.36977200
C	-3.16926000	-0.75417900	-1.23114100
H	-3.30053300	-1.82279400	-1.02725700
H	-3.94099700	-0.46662400	-1.94942600
C	-1.78722400	-0.54130100	-1.87416600
H	-1.79000300	-1.00588300	-2.86726100
H	-1.58917400	0.52484900	-2.01194400
H	4.45065800	0.97221300	0.73567100
C	3.25033100	2.88333700	-0.43841300
H	4.19633800	2.61754800	-0.92658200
H	2.85823900	3.78500500	-0.91206200
H	3.48031300	3.11376000	0.60939600

(K₉)_T

O	-0.61913500	-2.39195400	-0.22793700
O	-2.69810800	-0.05891400	1.07024800
O	1.03447100	2.03362700	-1.13665200
H	0.53776000	1.12749500	-1.11266700
N	0.46072800	-0.39278400	-0.69740000
C	-0.57254800	-1.29548300	-0.79333500
C	1.66511600	-0.63372000	-0.11627000
C	2.55061200	0.53189900	-0.02551500
C	3.79014200	0.34613800	0.58575400
C	-3.47936400	-0.10707200	-0.04902500
C	-3.21087000	0.90107400	1.89040300
H	-2.68927900	1.05203700	2.82309200
C	-4.30288800	1.46665500	1.32197100
H	-4.91231300	2.25350200	1.74413100
C	-4.47635200	0.81097200	0.05679100
H	-5.24573400	0.99984500	-0.67921700
C	2.19085100	1.82105800	-0.52922100
C	4.20700300	-0.91426300	1.07069900

H	5.18845400	-0.99966000	1.52586000
C	3.38202300	-2.02357200	0.96247800
H	3.70126600	-2.99291900	1.32794600
C	2.11739200	-1.87858200	0.37013400
H	1.45742000	-2.72889600	0.27782600
C	-3.09986700	-1.09003400	-1.10176700
H	-3.13941300	-2.10923600	-0.70168000
H	-3.84774200	-1.02555500	-1.89675500
C	-1.70434400	-0.85173500	-1.70190100
H	-1.61746100	-1.44880600	-2.61881800
H	-1.57921300	0.19579700	-1.98614200
H	4.46964800	1.18368800	0.69420300
C	3.07600500	3.01473700	-0.43057100
H	4.01469400	2.87168100	-0.98116000
H	2.55832400	3.87775100	-0.85248500
H	3.34319600	3.24225800	0.60864000

(K₉)_b

O	-0.67872700	-2.30622600	-0.86511500
O	-2.56010500	-0.24535700	1.02956700
O	1.10214800	2.03457900	-1.08845600
H	0.54679700	0.92268300	-1.07067600
N	0.44935300	-0.29570500	-0.80202800
C	-0.62344000	-1.10730800	-1.12497000
C	1.58098800	-0.63300800	-0.13522100
C	2.52646400	0.48267100	0.02409600
C	3.71837400	0.19750800	0.69003600
C	-3.40183900	0.01225000	-0.01515200
C	-2.97869300	0.50231200	2.08969800
H	-2.40055400	0.40123000	2.99535500
C	-4.06901000	1.22937500	1.74673600
H	-4.61371800	1.91068500	2.38529300
C	-4.34312800	0.91179400	0.37379400
H	-5.13956500	1.30445600	-0.24325500
C	2.23027000	1.79222200	-0.48241900
C	3.99960900	-1.09044900	1.19276600
H	4.94247300	-1.25315300	1.70535500
C	3.09526200	-2.14407800	1.04563800
H	3.32152300	-3.12864400	1.43757600
C	1.88769400	-1.91127000	0.38115100
H	1.16616100	-2.70394100	0.24466400
C	-3.12753300	-0.69901700	-1.29473500
H	-3.23173700	-1.78126700	-1.15893400
H	-3.88810300	-0.39026800	-2.01650400

C	-1.73488800	-0.40714800	-1.87867600
H	-1.70301500	-0.78899900	-2.90663800
H	-1.55587500	0.66991400	-1.92568700
H	4.45615700	0.97813500	0.83590600
C	3.19376300	2.92768700	-0.33972400
H	4.15526700	2.71354500	-0.82333300
H	2.76272200	3.81638000	-0.80395500
H	3.40611400	3.15396700	0.71295700

(K₁₀)_G

O	-1.73328100	-2.04154100	-1.40190500
O	-3.51073400	-0.74290900	1.18067200
O	-0.48283800	2.68411100	-0.84386600
H	-1.22556500	1.08093900	-1.12996300
N	-0.95934000	0.09822500	-1.09409400
C	-1.91375900	-0.82847400	-1.41410200
C	0.36381100	-0.09702700	-0.69984500
C	1.17094800	1.03366500	-0.40156400
C	2.50017000	0.82916300	-0.00733100
C	-4.53875200	-0.40759500	0.34540300
C	-3.79919600	-0.23654500	2.41243100
H	-3.06780200	-0.42599700	3.18308900
C	-4.98802400	0.41245100	2.38423100
H	-5.46828100	0.90997900	3.21518200
C	-5.46889700	0.30256900	1.03608100
H	-6.39003700	0.70174900	0.63423400
C	0.66970600	2.43239400	-0.49183300
C	3.02600300	-0.44313800	0.09220000
C	2.23839200	-1.55002500	-0.19739100
H	2.64692900	-2.55156300	-0.11957700
C	0.92094500	-1.37827100	-0.58827900
H	0.30679800	-2.23710300	-0.81275100
C	-4.43266800	-0.85437400	-1.07178600
H	-4.35216300	-1.94578500	-1.12068800
H	-5.36060200	-0.57674900	-1.57845500
C	-3.24831700	-0.23774000	-1.83369200
H	-3.36263500	-0.46517800	-2.89953300
H	-3.25625900	0.85099200	-1.73037700
H	3.13043700	1.67738200	0.22332500
C	1.58759000	3.57831600	-0.14547600
H	2.46367000	3.59712000	-0.80087300
H	1.03240800	4.50867100	-0.26657800

H	1.94340900	3.50503000	0.88663200
Br	4.82749200	-0.68133100	0.62804300

(K₁₀)_N

O	-1.72924100	-2.10059600	-1.39314400
O	-3.39272100	-0.65483300	1.16551100
O	-0.60806900	2.58790700	-0.92841500
H	-1.14889500	1.04984700	-1.12506000
N	-0.92210800	0.02761200	-1.08482800
C	-1.91363100	-0.89280800	-1.41235300
C	0.36402000	-0.17363500	-0.69489700
C	1.14262500	1.05188900	-0.42678100
C	2.46876400	0.84663600	-0.03097800
C	-4.47904600	-0.38729200	0.38106800
C	-3.64306700	-0.14156200	2.40347900
H	-2.86270000	-0.27712800	3.13646600
C	-4.86395000	0.44457800	2.42742100
H	-5.32528300	0.93340300	3.27404100
C	-5.40762700	0.28691300	1.10809400
H	-6.36689200	0.63320900	0.74880300
C	0.59596600	2.37880900	-0.56163200
C	3.00378200	-0.44487400	0.10096000
C	2.26134100	-1.60975400	-0.15027200
H	2.70097800	-2.59174500	-0.03794300
C	0.93756900	-1.45285000	-0.54826000
H	0.32281200	-2.31694500	-0.75391700
C	-4.41903300	-0.85685400	-1.03093600
H	-4.36650400	-1.95073200	-1.06898300
H	-5.34898900	-0.56205500	-1.52339000
C	-3.23272200	-0.27821200	-1.82280800
H	-3.37058300	-0.51943600	-2.88316900
H	-3.20927900	0.81107600	-1.73479700
H	3.11007600	1.69168400	0.18117700
C	1.46836300	3.57179100	-0.26191900
H	2.34566000	3.61728600	-0.91897000
H	0.87643100	4.47585900	-0.41343800
H	1.83568800	3.56608100	0.77165600
Br	4.78292400	-0.61343400	0.63738800

(K₁₀)_T

O	-1.75848100	-1.26082600	-2.06800700
O	-3.42502300	-1.09790000	0.83685500
O	-0.44525200	2.90189800	-0.06650700

H	-0.92296400	2.07100200	-0.47896200
N	-0.91678500	0.60255600	-0.97396300
C	-1.90477900	-0.13591200	-1.58284300
C	0.33625400	0.16377800	-0.69721800
C	1.21691200	1.17123100	-0.09489200
C	2.52002000	0.78890400	0.21516100
C	-4.50510000	-0.52286400	0.22940200
C	-3.70215900	-1.19287800	2.16789200
H	-2.92957000	-1.63241300	2.78001000
C	-4.93500500	-0.69357300	2.42486700
H	-5.41787000	-0.63944800	3.39060100
C	-5.45710900	-0.25461500	1.16156300
H	-6.41900900	0.20213100	0.97331400
C	0.78922000	2.50914600	0.18008700
C	2.97079000	-0.52432400	-0.03399900
C	2.15015200	-1.49118300	-0.59526400
H	2.51100100	-2.49534100	-0.77872300
C	0.83606800	-1.13437700	-0.92220000
H	0.17444400	-1.86430300	-1.36513300
C	-4.42226500	-0.31487700	-1.24357000
H	-4.34522500	-1.27876300	-1.75909800
H	-5.35868100	0.14873600	-1.56535400
C	-3.24405700	0.57119400	-1.67882300
H	-3.38476700	0.83847100	-2.73378800
H	-3.22943500	1.50120700	-1.10544200
H	3.20972800	1.49517500	0.65937400
C	1.68383100	3.54824300	0.76017800
H	2.57199700	3.71502600	0.13854200
H	1.13421800	4.48731700	0.84073800
H	2.03719800	3.26691100	1.76038500
Br	4.73771000	-0.95161000	0.42001400

(K₁₀)_b

O	-1.73143000	-1.67563700	-1.83158000
O	-3.39383000	-0.94688400	1.01761800
O	-0.60145600	2.68793100	-0.48509900
H	-0.99526100	1.66735900	-0.81308300
N	-0.91358000	0.34619100	-1.06719800
C	-1.89610400	-0.48675200	-1.56028600
C	0.35010100	-0.00781800	-0.72709100
C	1.17036200	1.11425800	-0.25218600
C	2.48541200	0.83631400	0.11239700
C	-4.46857000	-0.47647900	0.31739500
C	-3.64686400	-0.75020200	2.34237100

H	-2.87565300	-1.07664300	3.02311500
C	-4.85891300	-0.16735700	2.50470000
H	-5.32038900	0.10486000	3.44364800
C	-5.39318900	0.01339000	1.18450200
H	-6.34453500	0.45239400	0.91710000
C	0.64363000	2.44410400	-0.16442900
C	2.99407600	-0.47579100	0.03044000
C	2.22616700	-1.54918000	-0.41175300
H	2.63969800	-2.54811300	-0.46467200
C	0.90274700	-1.30220200	-0.78822400
H	0.27839800	-2.11013200	-1.14093700
C	-4.40673700	-0.58251400	-1.16713800
H	-4.33993700	-1.63332800	-1.47056800
H	-5.34526000	-0.19052600	-1.56779900
C	-3.23264500	0.18786200	-1.79548100
H	-3.38263500	0.21946700	-2.88156100
H	-3.21562300	1.21974700	-1.43639000
H	3.13665000	1.62429700	0.46895900
C	1.46247700	3.60442000	0.29246700
H	2.35500100	3.74577500	-0.32933200
H	0.85524400	4.50951000	0.24011100
H	1.80592200	3.47683400	1.32713100
Br	4.77044200	-0.76629800	0.54403000

A₁(T₁)

C	-1.81879900	-2.01617700	0.19392300
C	-0.49680900	-1.56423100	0.17648000
C	-0.18578400	-0.19082700	0.05287300
C	-1.26886900	0.78128000	-0.02468200
C	-2.57159900	0.29022500	-0.02071300
C	-2.84332200	-1.09026900	0.08911400
H	-2.03148300	-3.07480900	0.28919600
H	0.31764000	-2.27307200	0.25779000
H	-3.40111100	0.98669500	-0.09858600
H	-3.87779100	-1.42010900	0.09699800
C	-1.05316700	2.18513800	-0.10886300
H	-1.88800600	2.87271800	-0.17447600
O	0.15146800	2.78017400	-0.11253700
C	2.20530000	-0.47942900	-0.13752900
N	1.07152500	0.29906700	0.04319600
O	2.25013300	-1.43026400	-0.90985300
H	0.83086000	2.05819400	-0.04423600
C	3.40616400	0.00750200	0.62793400
H	3.67116100	1.01689800	0.29743500
H	3.17712200	0.06570100	1.69672300
H	4.24943200	-0.66423700	0.46467900

K₁(T₁)

C	-0.97777200	1.82342300	-0.15489700
C	-0.70421000	0.43762300	-0.08579300
C	0.68246200	-0.02784100	-0.09371300
C	1.69394200	0.94448200	-0.12138800
C	1.35900900	2.32162100	-0.16872800
C	0.05106400	2.76783400	-0.19369500
C	1.03900400	-1.40601800	-0.07303100
C	3.14501200	0.53654000	-0.13332800
C	3.36927200	-0.79527900	0.57874100
C	2.45665200	-1.86868800	-0.01050300
H	-2.01124700	2.14497100	-0.17604100
H	-0.17678800	3.82641800	-0.24269200
H	2.17271400	3.04205300	-0.19402900
H	3.48177800	0.44914900	-1.17729700
H	3.75372300	1.32575100	0.32003400
H	4.41678800	-1.09908700	0.49229100
H	3.15250700	-0.67735200	1.64732400
H	2.49455400	-2.78805900	0.58501000
H	2.80407700	-2.14246700	-1.01956400

O	0.13041200	-2.40272800	-0.13259600
N	-1.67027700	-0.50131500	-0.06500900
H	-0.77048900	-1.98005500	-0.15124100
C	-3.00248600	-0.24377600	0.20673200
O	-3.37791900	0.59225000	1.02316400
C	-3.95901100	-1.14998700	-0.52254200
H	-3.77281000	-2.19093600	-0.24003300
H	-4.98713600	-0.88225200	-0.27689500
H	-3.80330200	-1.07470900	-1.60347700