Electronic supplementary information for

Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: The internal-coordinate multi-structural approximation

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Table S1. Calculated conformational-vibrational-rotational partition functions for the 1-D model potential of eqn (48)

T (K)	TES	MS-HO	MS-AS(M)	MS-AS(S)	MS-AS	MS-ASCB
60	0.5751	0.4776	0.4776	0.4758	0.5247	0.5356
100	1.266	1.083	1.081	1.059	1.236	1.229
150	2.159	1.935	1.917	1.821	2.174	2.132
200	3.025	2.863	2.786	2.581	3.078	3.006
300	4.600	4.848	4.45	4.015	4.703	4.596
400	5.979	6.922	5.93	5.316	6.106	5.983
600	8.303	11.18	8.395	7.575	8.447	8.315
1000	11.92	19.87	12.13	11.19	12.06	11.93
1500	15.42	30.83	15.66	14.73	15.55	15.44
2000	18.31	41.82	18.56	17.67	18.43	18.33
2400	20.34	50.62	20.59	19.74	20.46	20.36
3000	23.07	63.83	23.3	22.50	23.17	23.08
4000	27.02	85.87	27.24	26.51	27.11	27.03
7000	36.41	152.0	36.59	36.00	36.48	36.42
50000	99.40	1100	99.47	99.24	99.43	99.40

Table S2. Partition functions calculated by various methods compared to TES values using the 1-D model potential of H_2O_2.

T (K)	TES	MS-HO	MS-AS(M)	MS-AS(S)	MS-AS	MS-ASCB
60	0.03071	0.02036	0.02036	0.02036	0.02061	0.01999
100	0.1654	0.1281	0.1281	0.1281	0.1308	0.1281
150	0.3990	0.3276	0.3276	0.3276	0.3386	0.3364
200	0.6442	0.5395	0.5394	0.5394	0.5656	0.5655
300	1.116	0.9509	0.9498	0.9498	1.030	1.018
400	1.555	1.345	1.340	1.340	1.501	1.443
600	2.359	2.105	2.084	2.084	2.443	2.223
1000	3.787	3.588	3.468	3.468	4.199	3.616
1500	5.383	5.419	5.044	5.044	6.089	5.187
2000	6.827	7.244	6.475	6.475	7.707	6.621
2400	7.893	8.701	7.532	7.532	8.856	7.684
3000	9.366	10.88	8.995	8.995	10.40	9.158
4000	11.56	14.52	11.17	11.17	12.63	11.35
7000	16.83	25.43	16.45	16.45	17.86	16.65
50000	51.17	181.7	50.95	50.95	51.67	51.08

Table S3. Conformational-rovibrational partition function of ethanol calculated using multi-structural methods[a]

T (K)	MS-HO	MS-AS(M)	MS-AS(S)	MS-AS	MS-ASCB
100	4.12E-104	4.12E-104	4.12E-104	4.47E-104	4.37E-104
150	5.45E-68	5.44E-68	5.43E-68	6.21E-68	6.08E-68
200	8.13E-50	8.10E-50	8.08E-50	9.65E-50	9.46E-50
300	1.95E-31	1.92E-31	1.91E-31	2.43E-31	2.39E-31
400	4.77E-22	4.64E-22	4.60E-22	6.06E-22	6.00E-22
600	2.94E-12	2.74E-12	2.71E-12	3.73E-12	3.70E-12
1000	1.62E-03	1.38E-03	1.35E-03	1.90E-03	1.89E-03
1500	3.60E+02	2.71E+02	2.66E+02	3.65E+02	3.65E+02
2000	7.76E+05	5.22E+05	5.11E+05	6.84E+05	6.83E+05
2400	7.65E+07	4.72E+07	4.63E+07	6.06E+07	6.06E+07
3000	1.74E+10	9.56E+09	9.39E+09	1.19E+10	1.19E+10
4000	1.56E+13	7.19E+12	7.08E+12	8.67E+12	8.67E+12
7000	6.07E+18	1.90E+18	1.88E+18	2.15E+18	2.15E+18
50000	1.13E+38	6.20E+36	6.19E+36	6.34E+36	6.34E+36

[a]All ethanol calculations are for NS:SC = 2:0.

Table S4. Conformational-rovibrational partition function of 1-pentyl radical calculated using multi-structural methods

T (K)	MS-HO	MS-AS(M)	MS-AS(S)	MS-AS	MS-AS(M)	MS-AS(S)	MS-AS	MS-RS
		NS:SC = 2:2			NS:SC = 4:0			
100	5.11E-190	5.08E-190	5.00E-190	6.02E-190	5.07E-190	4.80E-190	5.53E-190	6.32E-190
150	1.83E-124	1.79E-124	1.73E-124	2.22E-124	1.78E-124	1.62E-124	1.93E-124	2.09E-124
200	2.04E-91	1.94E-91	1.87E-91	2.50E-91	1.93E-91	1.70E-91	2.11E-91	2.16E-91
300	6.69E-58	5.89E-58	5.67E-58	8.22E-58	5.83E-58	5.00E-58	6.72E-58	6.45E-58
400	1.05E-40	8.40E-41	8.22E-41	1.28E-40	8.31E-41	7.14E-41	1.04E-40	9.66E-41
600	1.14E-22	7.62E-23	7.81E-23	1.34E-22	7.53E-23	6.73E-23	1.12E-22	1.01E-22
1000	2.20E-06	1.08E-06	1.19E-06	2.21E-06	1.06E-06	1.04E-06	1.97E-06	1.78E-06
1500	2.74E+04	9.83E+03	1.14E+04	2.13E+04	9.71E+03	1.03E+04	1.99E+04	1.82E+04
2000	6.18E+10	1.72E+10	2.05E+10	3.71E+10	1.70E+10	1.88E+10	3.56E+10	3.29E+10
2400	4.06E+14	9.49E+13	1.14E+14	2.01E+14	9.39E+13	1.06E+14	1.95E+14	1.82E+14
3000	1.37E+19	2.54E+18	3.08E+18	5.17E+18	2.52E+18	2.90E+18	5.07E+18	4.78E+18
4000	6.57E+24	8.87E+23	1.07E+24	1.69E+24	8.80E+23	1.03E+24	1.67E+24	1.59E+24
7000	4.08E+35	2.70E+34	3.15E+34	4.37E+34	2.69E+34	3.09E+34	4.35E+34	4.22E+34
50000	7.38E+72	1.82E+70	1.85E+70	1.98E+70	1.82E+70	1.85E+70	1.97E+70	1.96E+70
90000	9.43E+83	7.56E+80	7.56E+80	7.83E+80	7.55E+80	7.54E+80	7.81E+80	7.80E+80

Table S5. Conformational-rovibrational partition function of 1-butanol calculated using multi-structural methods[a]

T (K)	MS-HO	MS-AS(M)	MS-AS(S)	MS-AS	MS-RS
100	1.09E-179	1.09E-179	1.09E-179	1.25E-179	1.10E-179
150	1.28E-117	1.28E-117	1.27E-117	1.58E-117	1.43E-117
200	2.44E-86	2.42E-86	2.41E-86	3.20E-86	2.95E-86
300	1.25E-54	1.21E-54	1.22E-54	1.80E-54	1.69E-54
400	2.26E-38	2.12E-38	2.14E-38	3.48E-38	3.31E-38
600	2.44E-21	2.09E-21	2.15E-21	3.98E-21	3.85E-21
1000	5.38E-06	3.79E-06	4.07E-06	8.20E-06	8.12E-06
1500	1.64E+04	9.08E+03	1.01E+04	1.99E+04	2.01E+04
2000	1.47E+10	6.57E+09	7.36E+09	1.39E+10	1.41E+10
2400	5.48E+13	2.09E+13	2.36E+13	4.27E+13	4.35E+13
3000	9.33E+17	2.87E+17	3.24E+17	5.53E+17	5.65E+17
4000	1.89E+23	4.22E+22	4.75E+22	7.49E+22	7.68E+22
7000	2.19E+33	2.36E+32	2.60E+32	3.55E+32	3.65E+32
50000	1.11E+68	3.99E+65	4.08E+65	4.31E+65	4.42E+65
90000	2.43E+78	2.81E+75	2.84E+75	2.93E+75	3.00E+75

[a]29 structures are used with NS:SC = 1:3 for the MS-AS(M), MS-AS(S), and MS-AS calculations, whereas the MS-RS calculations always treat all modes as nearly separable.

Table S6. Standard state entropies (cal mol^{-1} K^{-1}) of ethanol calculated by MS methods

T (K)	MS-HO	MS-AS
100	54.00	53.64
150	58.38	57.85
200	61.86	61.25
300	67.56	66.94
400	72.59	72.02
600	81.68	81.32
1000	96.85	97.05
1500	111.71	112.54
2000	123.48	124.82
2400	131.33	133.01
3000	141.25	143.35
4000	154.38	157.04
7000	180.53	184.30
50000	274.02	281.71

Table S7. Standard state entropies (cal mol^{-1} K^{-1}) of 1-pentyl radical calculated by MS methods

T (K)	SS-HO[a]	MS-HO	MS-AS		
			2:2	1:3	4:0
100	61.82	65.61	66.12	66.2	65.7
150	68.49	72.99	73.48	73.59	72.96
200	74.10	79.03	79.48	79.61	78.94
300	83.92	89.26	89.66	89.82	89.19
400	93.04	98.54	98.87	99.01	98.52
600	110.09	115.71	115.71	115.80	115.56
1000	139.20	144.88	143.95	143.99	143.98
1500	167.96	173.64	171.62	171.63	171.68
2000	190.72	196.41	193.46	193.46	193.51
2400	205.88	211.57	207.98	207.98	208.03
3000	224.99	230.67	226.27	226.27	226.31
4000	250.24	255.93	250.43	250.43	250.46
7000	300.47	306.15	298.44	298.44	298.45
50000	479.74	485.42	469.75	469.75	469.75

[a]SS-HO calculations use the global minimum structure P–a^{-}g^{+}t.

Table S8. Standard state entropies (cal mol^{-1} K^{-1}) of 1-butanol calculated by MS methods

T (K)	SS-HO[a]	MS-HO		MS-AS[b]	
		27 structures	29 structures	27 structures	29 structures
100	59.67	64.13	64.13	64.68	64.71
150	65.93	70.91	70.91	71.71	71.72
200	71.16	76.55	76.56	77.52	77.54
300	80.19	86.10	86.13	87.30	87.33
400	88.54	94.72	94.78	96.01	96.07
600	104.25	110.66	110.77	111.79	111.86
1000	131.29	137.84	138.00	138.07	138.14
1500	158.06	164.66	164.84	163.72	163.78
2000	179.28	185.89	186.08	183.97	184.02
2400	193.42	200.03	200.22	197.45	197.50
3000	211.25	217.87	218.06	214.44	214.48
4000	234.83	241.45	241.65	236.91	236.94
7000	281.75	288.38	288.57	281.59	281.61
50000	449.32	455.94	456.14	441.20	441.21

[a]SS-HO calculations use the global minimum structure B–tg^{+}t.

[b]The NS:SC = 4:0 scheme is used for the 27-structures MS-AS calculations, and the NS:SC = 1:3 scheme is used for the 29-structures calculations.

Table S9. Cartesian coordinates (in Å) of ethanol optimized by M06-2X/6-311+G(2df,2p)

E–t				E–g			
C	1.216605	-0.221763	0.000002	C	-1.206326	-0.240138	-0.021727
H	1.277392	-0.856203	-0.882979	H	-1.259186	-0.961169	0.796167
H	1.277394	-0.856193	0.882990	H	-1.264002	-0.785229	-0.962776
H	2.065916	0.460389	-0.000003	H	-2.072627	0.416905	0.055986
C	-0.084558	0.548269	-0.000002	C	0.082737	0.557533	0.046990
H	-0.142399	1.190146	0.884751	H	0.126311	1.278345	-0.768384
H	-0.142395	1.190145	-0.884757	H	0.132979	1.121132	0.984138
O	-1.143238	-0.394462	-0.000004	O	1.230319	-0.256916	-0.105646
H	-1.982289	0.068377	0.000031	H	1.235503	-0.919031	0.588459

Table S10. Cartesian coordinates (in Å) of 1-butanol optimized by MPW1K/6-311+G(2df,2p) [a]

B–ttt				B–ttg$^+$			
H	-3.202018	0.080509	0.000004	H	-2.907559	-0.761384	0.118415
O	-2.393019	-0.415789	0.000000	O	-2.311212	-0.089718	-0.188223
C	-1.301120	0.466488	0.000004	C	-1.021512	-0.346734	0.304966
C	-0.031641	-0.341128	-0.000005	C	-0.090226	0.699824	-0.247991
C	1.211806	0.523130	-0.000004	C	1.332568	0.589249	0.268286
C	2.489436	-0.288813	0.000004	C	2.063985	-0.662610	-0.175268
H	3.367690	0.349137	-0.000071	H	3.095483	-0.653483	0.163042
H	-1.326227	1.112519	0.880048	H	-0.692922	-1.343789	0.010947
H	-1.326234	1.112535	-0.880028	H	-1.009950	-0.305346	1.396620
H	-0.033929	-0.992495	-0.871725	H	-0.498898	1.674874	0.005951
H	-0.033931	-0.992510	0.871704	H	-0.099664	0.634241	-1.334372
H	1.198091	1.178361	0.869837	H	1.888369	1.460812	-0.068562
H	1.198095	1.178357	-0.869848	H	1.327750	0.642456	1.356375
H	2.545830	-0.929137	-0.875945	H	2.073718	-0.744219	-1.259057
H	2.545898	-0.929023	0.876033	H	1.604480	-1.564787	0.216473

B–tg$^+$t				B–tg$^+$g$^+$			
H	2.788855	-0.860117	0.044838	H	2.398032	-1.182666	-0.158230
O	1.900054	-0.720828	-0.257212	O	1.717465	-0.604712	-0.479786
C	1.426336	0.509986	0.228128	C	1.158017	0.106338	0.595525
C	0.001270	0.691334	-0.222906	C	0.067155	1.001377	0.065831
C	-0.952889	-0.335111	0.352346	C	-1.074498	0.266923	-0.614645
C	-2.374218	-0.147190	-0.132931	C	-1.874125	-0.626463	0.311303
H	-3.042335	-0.889019	0.293236	H	-2.709709	-1.081580	-0.211170
H	2.038693	1.330617	-0.147943	H	1.916166	0.716155	1.088655
H	1.473151	0.535192	1.319133	H	0.756930	-0.580911	1.341770
H	-0.320645	1.693336	0.057663	H	-0.316024	1.592860	0.896431
H	-0.024506	0.649033	-1.310578	H	0.516155	1.700628	-0.635979
H	-0.926247	-0.276317	1.439932	H	-1.738290	1.004151	-1.060702
H	-0.600561	-1.329239	0.092723	H	-0.674118	-0.320884	-1.435890
H	-2.432599	-0.235138	-1.214593	H	-2.277812	-0.065333	1.150713
H	-2.757235	0.834163	0.135456	H	-1.270338	-1.433775	0.714602

B–tg$^+$g$^-$

H	2.213949	-1.343129	0.251813
O	1.407646	-0.982258	-0.095777
C	1.344397	0.389501	0.205139
C	0.087129	0.990274	-0.370628
C	-1.213805	0.556978	0.286446
C	-1.680681	-0.839754	-0.072040
H	-2.631165	-1.063299	0.403587
H	2.209701	0.906752	-0.212234
H	1.359175	0.544778	1.286447
H	0.185947	2.070239	-0.277129
H	0.056251	0.774621	-1.437512
H	-1.109171	0.643717	1.367637
H	-1.988657	1.268031	0.006440
H	-0.960091	-1.589780	0.229426
H	-1.819345	-0.935860	-1.145766

B–g$^+$tt

H	-2.501002	-0.906525	0.639198
O	-2.468944	-0.296012	-0.087951
C	-1.306309	0.480705	0.014978
C	-0.037229	-0.336518	-0.029567
C	1.212337	0.517908	0.029279
C	2.487106	-0.297587	-0.009741
H	3.367272	0.336223	0.031314
H	-1.334562	1.167420	-0.825996
H	-1.326232	1.089132	0.921797
H	-0.038922	-0.935664	-0.938092
H	-0.034043	-1.040264	0.804369
H	1.194805	1.123119	0.934450
H	1.204705	1.221371	-0.801856
H	2.546762	-0.887196	-0.920392
H	2.537344	-0.986569	0.829125

B–g$^+$tg$^+$

H	-2.410763	-0.282998	-1.006790
O	-2.360511	-0.168791	-0.065019
C	-1.029787	-0.334036	0.347625
C	-0.097218	0.687310	-0.262128
C	1.330717	0.599501	0.247222
C	2.067586	-0.658605	-0.168781
H	3.098450	-0.637604	0.170611
H	-1.039663	-0.222794	1.428370
H	-0.688159	-1.347337	0.134865
H	-0.502877	1.674394	-0.053979
H	-0.101409	0.573125	-1.347531
H	1.880326	1.465982	-0.112446
H	1.328336	0.679184	1.333501
H	2.080626	-0.762327	-1.250843
H	1.611431	-1.554309	0.240767

B–g$^+$tg$^-$

H	2.676341	0.595652	0.020278
O	2.331285	-0.268328	-0.172503
C	1.021457	-0.360120	0.319521
C	0.099046	0.683184	-0.267850
C	-1.324674	0.606288	0.254304
C	-2.070299	-0.645986	-0.162597
H	-3.098980	-0.621030	0.182780
H	0.684575	-1.358671	0.062655
H	1.011064	-0.290421	1.409947
H	0.106263	0.584961	-1.351885
H	0.507688	1.668999	-0.043900
H	-1.314765	0.680365	1.341037
H	-1.871150	1.477743	-0.098048
H	-1.616088	-1.545133	0.241531
H	-2.088414	-0.746039	-1.244631

B–g$^+$g$^+$t

H	2.025387	-0.813569	-1.053979
O	1.983029	-0.738910	-0.107764
C	1.434710	0.508752	0.228895
C	0.008513	0.681525	-0.240296
C	-0.958548	-0.309470	0.373740
C	-2.371838	-0.151219	-0.144481
H	-3.046806	-0.867064	0.314096
H	1.478169	0.563848	1.313026
H	2.056225	1.317542	-0.157939
H	-0.307818	1.698698	-0.010167
H	-0.021354	0.598831	-1.328449
H	-0.948915	-0.187734	1.455972
H	-0.603161	-1.318477	0.182633
H	-2.414440	-0.302232	-1.220097
H	-2.758543	0.843903	0.059870

B–g$^+$g$^+$g$^+$

H	2.188282	-0.123672	-1.007235
O	1.761564	-0.708126	-0.391438
C	1.153735	0.053758	0.618596
C	0.077834	0.982134	0.100119
C	-1.063457	0.285356	-0.619041
C	-1.903287	-0.600922	0.277686
H	-2.734951	-1.033003	-0.269795
H	0.735884	-0.665577	1.315302
H	1.900060	0.628495	1.168814
H	-0.310051	1.555761	0.941771
H	0.539589	1.707958	-0.570231
H	-1.700269	1.041389	-1.072887
H	-0.658936	-0.305169	-1.437094
H	-2.315378	-0.039000	1.112339
H	-1.325687	-1.424130	0.686362

B–g$^+$g$^+$g$^-$

H	-1.510064	-1.184931	0.893485
O	-1.469803	-1.007193	-0.038974
C	-1.341949	0.376933	-0.235908
C	-0.101787	0.989449	0.377766
C	1.220770	0.577546	-0.247512
C	1.661637	-0.841648	0.051111
H	2.636860	-1.042436	-0.382252
H	-1.327528	0.518343	-1.313171
H	-2.225688	0.894867	0.140792
H	-0.209281	2.070201	0.295444
H	-0.088179	0.774047	1.448020
H	1.158277	0.720913	-1.325526
H	1.989966	1.264818	0.099150
H	0.959509	-1.567624	-0.340422
H	1.742521	-1.004328	1.123530

B–g$^+$g$^-$t

H	-1.604462	-1.419801	0.105070
O	-2.032825	-0.658621	-0.266791
C	-1.437516	0.505367	0.242824
C	-0.007541	0.698334	-0.206914
C	0.947945	-0.357446	0.311558
C	2.378203	-0.121705	-0.125457
H	3.044443	-0.889926	0.254088
H	-2.050319	1.327433	-0.112315
H	-1.488911	0.515648	1.333966
H	0.017932	0.714919	-1.295090
H	0.325091	1.680115	0.129103
H	0.632391	-1.340748	-0.035024
H	0.898037	-0.384401	1.399881
H	2.742406	0.837830	0.231402
H	2.459440	-0.119397	-1.208813

B–g$^+$x$^-$g$^+$

H	-0.864673	-1.493050	-0.063060
O	-1.604078	-0.908404	-0.172053
C	-1.278457	0.358889	0.335915
C	-0.096458	1.016729	-0.347360
C	1.275387	0.582930	0.142183
C	1.584666	-0.895068	-0.001177
H	2.623690	-1.099885	0.236672
H	-2.167525	0.961591	0.183216
H	-1.109092	0.311269	1.414662
H	-0.188281	0.840775	-1.417918
H	-0.181884	2.092399	-0.204292
H	1.385007	0.869245	1.187241
H	2.026564	1.151343	-0.401630
H	1.405774	-1.243842	-1.014935
H	0.992216	-1.503492	0.679107

B–g$^+$g$^-$g$^-$

H	-1.216861	-1.284351	-0.736280
O	-1.827372	-0.652803	-0.375762
C	-1.173681	0.128310	0.589536
C	-0.085044	1.006287	0.012831
C	1.071580	0.253642	-0.622554
C	1.872175	-0.592158	0.347349
H	2.710899	-1.069921	-0.149017
H	-1.943256	0.751124	1.033476
H	-0.778743	-0.501232	1.388137
H	-0.536139	1.664720	-0.725841
H	0.295072	1.642596	0.811760
H	0.700843	-0.367804	-1.437295
H	1.733257	0.974981	-1.095920
H	1.273389	-1.378617	0.797648
H	2.270335	0.014440	1.156448

B-g$^+$g-x$^+$

H	0.930174	1.457789	0.590947
O	1.485684	1.037827	-0.053756
C	1.415759	-0.354472	0.110659
C	0.120342	-0.979686	-0.357828
C	-1.124246	-0.530913	0.398494
C	-1.788606	0.712576	-0.162416
H	-2.660407	0.989865	0.422452
H	2.242438	-0.760935	-0.463709
H	1.592093	-0.621718	1.154866
H	-0.004993	-0.785862	-1.421524
H	0.239390	-2.056826	-0.252456
H	-0.872808	-0.378936	1.448923
H	-1.853109	-1.337501	0.390493
H	-2.118364	0.540540	-1.183180
H	-1.119369	1.565939	-0.190221

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[a] The coordinates for mirror image structures are only given for one structure.

Table S11. Cartesian coordinates (in Å) of 1-pentyl radical optimized by M06-2X/6-311+G(2df,2p)[a]

P–a⁻g⁺t				P–a⁻g⁺g⁺			
C	-2.090217	-0.735153	0.176272	C	-1.775936	-0.722562	0.428132
H	-1.890012	-1.157083	1.151497	H	-1.940371	-0.341172	1.426444
H	-2.880158	-1.178716	-0.409878	H	-2.229248	-1.668268	0.173254
H	0.561679	-1.336352	-0.169595	H	1.829493	1.027429	0.937213
C	-1.461188	0.553652	-0.216065	C	-1.172098	0.151223	-0.611490
H	-1.494020	0.669283	-1.302901	H	-0.784989	-0.458521	-1.430837
H	-2.045618	1.392061	0.187797	H	-1.945519	0.787044	-1.063992
C	-0.015728	0.686351	0.269401	C	-0.066504	1.060927	-0.064265
H	0.346635	1.696684	0.063501	H	0.329289	1.666851	-0.883280
H	0.009059	0.563777	1.356907	H	-0.506150	1.756510	0.655248
C	0.925514	-0.326504	-0.373820	C	1.081526	0.304864	0.605367
H	0.890915	-0.203216	-1.459863	H	0.711655	-0.193826	1.504188
C	2.360633	-0.182186	0.117445	C	1.736577	-0.727165	-0.306624
H	2.416996	-0.327954	1.197167	H	2.047523	-0.274255	-1.250155
H	3.021788	-0.909240	-0.352756	H	2.617811	-1.163688	0.161761
H	2.748654	0.813799	-0.101277	H	1.049113	-1.541827	-0.536565

P–a⁻g⁺g⁻				P–a⁺tg⁺			
C	1.649257	0.926046	0.130426	C	-2.456432	-0.179581	-0.111759
H	1.583309	1.175765	1.179846	H	-2.852523	0.821850	-0.202462
H	2.165157	1.617043	-0.518704	H	-3.153839	-1.002368	-0.147555
H	-1.371446	-0.792287	-1.222697	H	1.890815	1.467124	-0.101363
C	1.279227	-0.438214	-0.331867	C	-1.035660	-0.389826	0.266922
H	1.117920	-0.437952	-1.413982	H	-0.937396	-0.440286	1.362798
H	2.127278	-1.117007	-0.164333	H	-0.699265	-1.363212	-0.097898
C	0.049020	-1.030002	0.369053	C	-0.113274	0.717223	-0.246026
H	0.072249	-2.116307	0.264445	H	-0.118349	0.704906	-1.339678
H	0.117379	-0.820457	1.441096	H	-0.529152	1.682366	0.054400
C	-1.290695	-0.523522	-0.165771	C	1.323192	0.607675	0.260257
H	-2.090942	-1.061830	0.346832	H	1.324732	0.674759	1.351625
C	-1.518233	0.976621	-0.006241	C	2.024868	-0.676293	-0.172615
H	-0.817645	1.555522	-0.607230	H	1.983439	-0.792235	-1.257210
H	-2.527942	1.250157	-0.312252	H	3.073198	-0.671639	0.123490
H	-1.386766	1.281778	1.033380	H	1.562177	-1.556453	0.273184

P–a^+tt				P–a^+tg^-			
C	2.576312	-0.345454	-0.021135	C	2.455792	-0.165835	-0.122534
H	2.570542	-1.343341	0.393623	H	2.686850	0.401239	-1.012945
H	3.527248	0.074228	-0.311395	H	3.261246	-0.698737	0.359197
H	-1.180728	1.109833	0.959874	H	-1.343256	0.603143	1.381560
C	1.347607	0.488063	0.020354	C	1.042552	-0.380574	0.282223
H	1.332306	1.095784	0.937708	H	0.685868	-1.342151	-0.111838
H	1.358072	1.211149	-0.800890	H	0.974155	-0.473484	1.371547
C	0.060484	-0.332466	-0.035161	C	0.112336	0.734644	-0.195096
H	0.049805	-0.921863	-0.956332	H	0.513880	1.691784	0.145352
H	0.058870	-1.051648	0.789753	H	0.127478	0.763415	-1.289150
C	-1.197979	0.523557	0.037317	C	-1.328821	0.588550	0.288381
H	-1.189188	1.244614	-0.784297	H	-1.898576	1.460958	-0.037162
C	-2.474304	-0.307216	-0.021117	C	-2.018045	-0.676723	-0.214172
H	-2.513643	-1.015953	0.807216	H	-1.557730	-1.575673	0.194881
H	-3.364476	0.318537	0.031297	H	-3.070141	-0.690234	0.068228
H	-2.521528	-0.880239	-0.948106	H	-1.962666	-0.740627	-1.302482

P–stg^+				P–stt			
C	2.457274	-0.214481	0.087058	C	2.585902	-0.315573	0.000003
H	3.081579	0.537444	-0.372739	H	2.993955	-0.697730	0.923780
H	2.840235	-0.716634	0.962526	H	2.993483	-0.698457	-0.923686
H	-1.881413	1.463105	0.218984	H	-1.190100	1.173774	0.874709
C	1.039001	-0.372190	-0.327141	C	1.350864	0.510298	-0.000034
H	0.953220	-0.301652	-1.416174	H	1.332810	1.161804	0.877660
H	0.678589	-1.362172	-0.043426	H	1.332780	1.161677	-0.877827
C	0.119708	0.697840	0.292914	C	0.063878	-0.334168	0.000031
H	0.134905	0.589094	1.381031	H	0.065809	-0.989473	-0.875400
H	0.537076	1.683041	0.073611	H	0.065806	-0.989339	0.875561
C	-1.321039	0.630452	-0.210753	C	-1.199804	0.518326	-0.000039
H	-1.329082	0.780145	-1.293763	H	-1.190101	1.173633	-0.874892
C	-2.026270	-0.678975	0.129559	C	-2.470759	-0.322863	0.000031
H	-1.976713	-0.876963	1.201885	H	-2.510034	-0.965752	0.880373
H	-3.077076	-0.645890	-0.155863	H	-3.364855	0.299642	-0.000017
H	-1.573363	-1.525394	-0.385895	H	-2.510038	-0.965892	-0.880210

[a]The coordinates for mirror image structures are only given for only one of the two structures in each case.