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Overview of supplementary data

S1-S31. Cartesian coordinates of all structures in Å units. After delition of the first line with the file name heading the format corresponds to "Cartesian coordinates 1" of Chem3D Pro, version 5 (Cambridge Soft Corporation, Cambridge, U.S.A.).

Table S1. Molecular potential energies in Hartrees.

Figures S1-S4. Structural drawings of all stationary points obtained with MP2/6-31G(d,p). Bond distances indicated are in Å units.

Structure1.doc

8							
C	1	0.000000	-0.551300	0.000000	2	3	4
C	2	1.182251	0.166306	0.000000	1	5	6
C	3	-1.182251	0.166306	0.000000	1	7	8
H	4	0.000000	-1.632004	0.000000	1		
H	5	2.147507	-0.325150	0.000000	2		
H	6	1.173279	1.250534	0.000000	2		
H	7	-2.147507	-0.325150	0.000000	3		
H	8	-1.173279	1.250534	0.000000	3		

Structure2.doc

11								
C	1	0.199905	0.423157	0.274811	2	3	4	7
C	2	-0.878693	-0.561493	0.535400	1	3	8	9
C	3	-0.878662	0.260742	-0.730713	1	2	10	11
O	4	1.507050	-0.197830	-0.128464	1	5	6	
H	5	2.043777	-0.501556	0.630768	4			
H	6	2.043808	0.372223	-0.714752	4			
H	7	0.368866	1.316986	0.855255	1			
H	8	-1.562927	-0.323914	1.336212	2			
H	9	-0.640152	-1.609512	0.423691	2			
H	10	-0.640137	-0.267593	-1.642685	3			
H	11	-1.562897	1.088928	-0.839386	3			

Structure3.doc

11								
C	1	-1.476761	0.277069	0.905151	2	10	11	
C	2	-0.546265	-0.566452	0.429398	1	3	7	
C	3	0.213226	-0.231735	-0.784607	2	4	8	9
O	4	1.680847	0.079819	-0.309586	3	5	6	
H	5	1.686508	0.707062	0.440353	4			
H	6	2.281845	0.396988	-1.012436	4			
H	7	-0.357376	-1.524002	0.895172	2			
H	8	-0.122177	0.667145	-1.293915	3			
H	9	0.394241	-1.053925	-1.469025	3			
H	10	-2.064346	0.024963	1.775558	1			
H	11	-1.689682	1.223175	0.423859	1			

Structure4.doc

3						
O	1	-0.044800	0.438400	-0.020905	2	3
H	2	-0.818512	-0.145554	0.031281	1	
H	3	0.713257	-0.166626	0.019257	1	

Structure5.doc

14								
C	1	-0.579834	-0.539963	-0.073196	2	3	4	7
C	2	-1.327774	0.680405	-0.473068	1	3	8	9
C	3	-1.887604	-0.250366	0.573196	1	2	10	11
O	4	0.601288	-0.286606	0.759613	1	5	6	
H	5	1.481522	-0.048400	0.198837	4			
H	6	0.741669	-0.993988	1.412613	4			
H	7	-0.432251	-1.376328	-0.739822	1			
H	8	-1.756363	0.690674	-1.463638	2			
H	9	-0.950165	1.628738	-0.120209	2			
H	10	-1.869095	0.104279	1.593430	3			
H	11	-2.712051	-0.900681	0.323257	3			
O	12	2.535660	0.340134	-0.591400	13	14		
H	13	2.936905	1.211853	-0.481003	12			
H	14	3.218002	-0.259552	-0.918549	12			

Structure6.doc

14

C	1	-1.906235	-0.348618	0.249817	2	10	11	
C	2	-1.006592	-0.261017	-0.740600	1	3	7	
C	3	-0.129242	0.926651	-0.885910	2	4	8	9
O	4	1.290512	0.452972	-0.698593	3	5	6	
H	5	1.409836	-0.059555	0.235428	4	12		
H	6	1.931839	1.178421	-0.798004	4			
H	7	-0.928223	-1.029648	-1.498886	2			
H	8	-0.323288	1.692322	-0.137817	3			
H	9	-0.134552	1.349884	-1.886658	3			
H	10	-2.580963	-1.189377	0.318604	1			
H	11	-2.013794	0.433182	0.990875	1			
O	12	1.445862	-0.702011	1.457657	5	13	14	
H	13	0.698654	-1.289856	1.634964	12			
H	14	2.246094	-1.153198	1.759293	12			

Structure7.doc

14								
C	1	-0.670746	-0.455170	-1.644852	2	3	4	
C	2	-1.952393	0.341156	-1.577423	1	3	6	7
C	3	-1.499481	-0.779785	-0.676346	1	2	5	
H	4	0.189926	-0.713516	-2.238907	1			
H	5	-1.787827	-1.477615	0.091568	3			
H	6	-2.727478	0.134460	-2.305496	2			
H	7	-1.941681	1.364197	-1.218674	2			
O	8	0.624405	0.841385	0.746475	10	11	12	
O	9	2.166870	-0.443069	2.117996	13	14		
H	10	0.971710	1.635345	0.312256	8			
H	11	0.090637	0.292343	0.099625	8			
H	12	1.348755	0.295456	1.323929	8			
H	13	2.110779	-0.361633	3.078995	9			
H	14	3.076431	-0.673645	1.890976	9			

Structure8.doc

7								
C	1	0.598160	-0.435837	0.483902	2	3	4	
C	2	-0.759628	-0.000305	0.000275	1	3	6	7
C	3	0.596985	0.436218	-0.484482	1	2	5	
H	4	1.138092	-1.056824	1.173950	1			
H	5	1.135757	1.057846	-1.174927	3			
H	6	-1.354614	0.675232	0.609177	2			
H	7	-1.354660	-0.676422	-0.607880	2			

Structure9.doc

7							
O	1	-1.190063	-0.101288	-0.074982	2	3	7
H	2	-1.702866	0.032761	0.735367	1		
H	3	-1.641174	0.327500	-0.817596	1		
O	4	1.191711	-0.001114	-0.109756	5	6	7
H	5	1.649475	-0.854782	-0.133224	4		
H	6	1.692596	0.618927	0.440002	4		
H	7	0.000381	-0.022049	-0.039810	1	4	

Structure10.doc

15

C	1	1.669617	0.282898	0.284042	2	3	7	
C	2	0.694565	-0.097092	1.212173	1	3	4	9
C	3	1.089661	-0.750107	-0.459686	1	2	10	13
C	4	-0.588211	0.674011	1.022491	2	5	6	8
H	5	-0.398285	1.731415	0.834595	4			
H	6	-1.268448	0.568420	1.863892	4			
H	7	1.783997	1.295624	-0.084518	1			
C	8	-1.155212	-0.008347	-0.269714	4	11	12	13
H	9	0.691971	-1.038559	1.747742	2			
H	10	1.152893	-1.800476	-0.202911	3			
H	11	-1.926270	0.631149	-0.701691	8			
H	12	-1.609253	-0.962051	-0.004500	8			
C	13	-0.031006	-0.247009	-1.335587	3	8	14	15
H	14	0.229431	0.693878	-1.821762	13			
H	15	-0.335434	-0.973755	-2.084518	13			

S11

Structure11.doc

15

C	1	1.518143	0.566315	0.128647	2	3	7	
C	2	0.716400	0.918594	-0.948990	1	4	9	
C	3	1.049057	-0.414200	0.992691	1	10	13	
C	4	-0.663773	0.427231	-1.125229	2	5	6	8
H	5	-0.592026	-0.390793	-1.862274	4			
H	6	-1.262604	1.195053	-1.618881	4			
H	7	2.526047	0.945709	0.216309	1			
C	8	-1.280914	-0.052261	0.183563	4	11	12	13
H	9	1.145905	1.536621	-1.732422	2			
H	10	1.737595	-0.833755	1.720779	3			
H	11	-2.224518	-0.560059	-0.003326	8			
H	12	-1.494522	0.812607	0.813873	8			
C	13	-0.313843	-0.974548	0.917053	3	8	14	15
H	14	-0.204803	-1.942000	0.397552	13			
H	15	-0.656143	-1.234436	1.920593	13			

Structure12.doc

18								
C	1	1.226120	0.398376	0.268738	2	3	7	16
C	2	0.340759	-0.790543	0.383698	1	3	4	9
C	3	0.340744	0.059555	-0.876663	1	2	10	13
C	4	-0.984055	-0.547195	1.107697	2	5	6	8
H	5	-0.855881	0.168610	1.922333	4			
H	6	-1.360886	-1.470169	1.543427	4			
H	7	1.147095	1.291840	0.871368	1			
C	8	-1.904100	0.012558	0.008500	4	11	12	13
H	9	0.791870	-1.776062	0.378479	2			
H	10	0.791885	-0.314468	-1.788483	3			
H	11	-2.721985	0.608505	0.410477	8			
H	12	-2.337524	-0.816788	-0.550903	8			
C	13	-0.984055	0.822006	-0.922287	3	8	14	15
H	14	-0.855881	1.845459	-0.563782	13			
H	15	-1.360886	0.880264	-1.941284	13			
O	16	2.702621	0.129211	0.087219	1	17	18	
H	17	3.011932	-0.700836	0.497665	16			
H	18	3.012115	0.199463	-0.836029	16			

Structure13.doc

18								
C	1	1.476303	0.260452	0.162750	2	3	7	16
C	2	0.660233	-0.970169	0.295654	1	3	4	9
C	3	0.660233	-0.159546	-1.001602	1	2	10	13
C	4	-0.745193	-0.875015	0.895523	2	5	6	8
H	5	-0.789703	-0.161255	1.720398	4			
H	6	-1.033524	-1.841095	1.304352	4			
H	7	2.556885	0.263016	0.164352	1			
C	8	-1.640686	-0.439270	-0.274490	4	11	12	13
H	9	1.222122	-1.888306	0.403030	2			
H	10	1.222122	-0.465546	-1.873886	3			
H	11	-2.539749	0.082092	0.051300	8			
H	12	-1.952728	-1.325043	-0.827972	8			
C	13	-0.745193	0.421310	-1.179031	3	8	14	15
H	14	-0.789703	1.475586	-0.899109	13			
H	15	-1.033524	0.365265	-2.226563	13			
O	16	0.978867	1.473724	0.920883	1	17	18	
H	17	1.246521	1.467667	1.861328	16			
H	18	1.246521	2.316345	0.503159	16			

Structure14.doc

21

C	1	0.677872	0.391327	0.153839	2	3	7	16
C	2	-0.256683	-0.679413	-0.291885	1	3	4	9
C	3	0.000336	0.537064	-1.164276	1	2	10	13
C	4	-1.686981	-0.576950	0.234665	2	5	6	8
H	5	-1.701370	-0.185303	1.254639	4			
H	6	-2.164978	-1.554520	0.257400	4			
H	7	0.470825	1.042328	0.995026	1			
C	8	-2.373627	0.394500	-0.741211	4	11	12	13
H	9	0.172226	-1.636688	-0.556931	2			
H	10	0.612595	0.449661	-2.052200	3			
H	11	-3.240860	0.889343	-0.305878	8			
H	12	-2.710693	-0.161469	-1.616700	8			
C	13	-1.272675	1.381073	-1.167328	3	8	14	15
H	14	-1.192642	2.211746	-0.462189	13			
H	15	-1.452515	1.809906	-2.151230	13			
O	16	2.098541	0.019913	0.084167	1	17	18	
H	17	2.452927	-0.528046	0.926743	16			
H	18	2.663803	0.785629	-0.119995	16			
O	19	2.977539	-1.247879	1.986450	20	21		
H	20	2.631287	-1.192413	2.885971	19			
H	21	3.294785	-2.150055	1.850677	19			

Structure15.doc

21

C	1	1.048721	-0.203629	-0.786057	2	3	7	16
C	2	-0.176773	-1.043000	-0.676743	1	3	4	9
C	3	-0.130600	0.149460	-1.624298	1	2	10	13
C	4	-1.184448	-0.719666	0.426132	2	5	6	8
H	5	-0.686935	-0.424300	1.352173	4			
H	6	-1.779114	-1.601761	0.656158	4			
H	7	1.959579	-0.587326	-1.224716	1			
C	8	-2.036453	0.426163	-0.144821	4	11	12	13
H	9	-0.090332	-2.059036	-1.037262	2			
H	10	-0.008636	0.022980	-2.691330	3			
H	11	-2.473358	1.057251	0.628357	8			
H	12	-2.855331	-0.002258	-0.723312	8			
C	13	-1.107864	1.198883	-1.096191	3	8	14	15
H	14	-0.590775	2.007782	-0.577133	13			
H	15	-1.649094	1.651978	-1.924286	13			
O	16	1.344086	0.669952	0.359177	1	18	19	
O	17	2.282608	-0.454147	2.320938	20	21		
H	18	1.759232	0.160965	1.200470	16			
H	19	1.870758	1.444321	0.094116	16			
H	20	1.846680	-0.350906	3.177017	17			
H	21	2.658310	-1.343430	2.291473	17			

Structure16.doc
21

C	1	-0.274628	-0.929977	0.400757	2	3	7	
C	2	-1.528915	-1.084976	-0.054871	1	4	9	
C	3	0.620956	0.121124	-0.148315	1	10	13	16
C	4	-2.135132	-0.241409	-1.137344	2	5	6	8
H	5	-2.862259	0.443710	-0.689911	4			
H	6	-2.701218	-0.879913	-1.817093	4			
H	7	0.136749	-1.610748	1.135513	1			
C	8	-1.070435	0.541428	-1.901810	4	11	12	13
H	9	-2.134964	-1.877716	0.367538	2			
H	10	1.473175	-0.290039	-0.694305	3			
H	11	-1.525955	1.303848	-2.532104	8			
H	12	-0.520233	-0.133545	-2.561417	8			
C	13	-0.101500	1.202500	-0.919586	3	8	14	15
H	14	-0.664520	1.811523	-0.209244	13			
H	15	0.610413	1.846634	-1.439255	13			
O	16	1.251053	0.812256	1.072693	3	17	18	
H	17	1.774048	0.161621	1.696747	16			
H	18	1.818237	1.554443	0.797836	16			
O	19	2.392410	-0.800659	2.587875	20	21		
H	20	3.300110	-1.122864	2.525986	19			
H	21	2.142578	-0.827209	3.520248	19			

Structure17.doc

18								
C	1	1.317520	-0.463715	0.119690	2	3	7	
C	2	0.699310	-0.980194	1.198853	1	4	9	
C	3	0.555466	0.259247	-0.912933	1	10	13	16
C	4	-0.777588	-0.886581	1.435318	2	5	6	8
H	5	-0.966660	-0.137070	2.210892	4			
H	6	-1.135590	-1.834839	1.837708	4			
H	7	2.370422	-0.655609	-0.053772	1			
C	8	-1.525192	-0.527664	0.153900	4	11	12	13
H	9	1.296982	-1.528671	1.917328	2			
H	10	0.650818	-0.158646	-1.915512	3			
H	11	-2.562790	-0.272659	0.363846	8			
H	12	-1.534225	-1.386536	-0.520386	8			
C	13	-0.845000	0.664658	-0.527527	3	8	14	15
H	14	-0.782822	1.490250	0.183853	13			
H	15	-1.406372	0.998688	-1.400345	13			
O	16	1.335648	1.669342	-1.080276	3	17	18	
H	17	2.300674	1.553696	-1.175018	16			
H	18	1.009293	2.196152	-1.835770	16			

Structure18.doc

21

C	1	0.630554	1.966522	0.377625	2	3	7	
C	2	-0.087219	1.022308	1.111511	1	3	4	9
C	3	0.754639	0.877853	-0.494614	1	2	10	13
C	4	-1.560669	1.053680	0.774002	2	5	6	8
H	5	-1.941711	2.069611	0.664444	4			
H	6	-2.159210	0.507309	1.497955	4			
H	7	0.243378	2.936188	0.086243	1			
C	8	-1.539276	0.324800	-0.609467	4	11	12	13
H	9	0.308426	0.101791	1.542725	2			
H	10	1.326477	-0.024521	-0.304321	3			
H	11	-2.485794	0.495789	-1.124344	8			
H	12	-1.413681	-0.742325	-0.435089	8			
C	13	-0.364059	0.844025	-1.505508	3	8	14	15
H	14	-0.597458	1.837952	-1.890060	13			
H	15	-0.161514	0.169510	-2.333328	13			
O	16	2.226578	-2.075577	-0.524979	18	19		
O	17	0.322922	-1.851074	1.535309	20	21		
H	18	3.172821	-2.175415	-0.365707	16			
H	19	2.036911	-2.685257	-1.248093	16			
H	20	1.026200	-2.197327	0.963776	17			
H	21	0.261566	-2.456146	2.281647	17			

StructureTSa.doc

8								
C	1	0.000000	0.870087	0.153412	2	3	4	
C	2	-0.765213	-0.314270	-0.055420	1	3	5	6
C	3	0.765213	-0.314270	-0.055420	1	2	7	8
H	4	0.000000	1.938522	0.341797	1			
H	5	-1.314987	-0.386734	-0.993881	2			
H	6	-1.314987	-0.703323	0.801682	2			
H	7	1.314987	-0.703323	0.801682	3			
H	8	1.314987	-0.386734	-0.993881	3			

StructureTSb.doc

11

C	1	0.157242	0.200958	0.414352	2	3	4	7
C	2	-0.832275	-0.715210	0.756836	1	3	8	9
C	3	-0.884506	0.989960	-0.064072	1	2	10	11
O	4	1.498077	-0.491074	-1.045151	1	5	6	
H	5	2.181458	-1.131760	-0.801147	4			
H	6	1.929810	0.140060	-1.638718	4			
H	7	0.910141	0.556030	1.099426	1			
H	8	-0.933075	-1.031113	1.788437	2			
H	9	-1.471237	-1.182404	0.023331	2			
H	10	-1.534500	0.675430	-0.866150	3			
H	11	-1.021164	1.988983	0.332870	3			

StructureTSc.doc

14								
C	1	-0.942337	0.295868	-0.798660	2	3	7	
C	2	-1.646088	-0.506149	0.088608	1	3	8	9
C	3	-0.190750	-0.772369	-1.260391	1	2	10	11
O	4	1.646103	-0.433716	1.308167	5	6		
H	5	2.545471	-0.639526	1.023026	4			
H	6	1.680588	-0.519012	2.269150	4			
H	7	-1.402405	1.032288	-1.435959	1			
H	8	-2.730362	-0.506027	0.079391	2			
H	9	-1.144638	-1.152374	0.793991	2			
H	10	0.366470	-1.392380	-0.574005	3			
H	11	-0.140030	-0.986588	-2.320938	3			
O	12	0.505295	1.739900	-0.056580	13	14		
H	13	1.032043	1.212662	0.570297	12			
H	14	0.420624	2.627243	0.313950	12			

StructureTSd.doc

14

C	1	0.814941	-0.746338	-0.923600	2	3	5	
C	2	2.196640	-0.471802	-1.077896	1	3	6	7
C	3	0.838486	0.590805	-1.003922	1	2	8	9
O	4	-1.009903	1.339035	0.647568	8	10	11	
H	5	0.158188	-1.456238	-0.443359	1			
H	6	2.605820	-0.370026	-2.071838	2			
H	7	2.895645	-0.566208	-0.255692	2			
H	8	-0.110641	1.012268	-0.040924	3	4		
H	9	1.147522	1.454117	-1.567764	3			
H	10	-0.753952	1.928940	1.371567	4			
H	11	-1.495575	0.531311	1.002777	4	12		
O	12	-2.130569	-0.896255	1.286880	11	13	14	
H	13	-3.001526	-1.065979	0.905548	12			
H	14	-2.155136	-1.283691	2.170654	12			

StructureTSe.doc
14

C	1	-0.007126	0.308900	0.123123	2	3	4	5	12
C	2	0.454803	-0.598343	-0.927139	1	3	6	7	
C	3	-0.409973	-1.093948	0.224335	1	2	8	9	
O	4	-1.771393	0.931747	-0.883957	1	10	11		
H	5	-0.023621	1.296967	0.529526	1				
H	6	1.504822	-0.848709	-0.920563	2				
H	7	0.005264	-0.497635	-1.903412	2				
H	8	-1.448532	-1.310303	0.025833	3				
H	9	0.056808	-1.688309	0.994949	3				
H	10	-2.476807	1.353333	-0.373947	4				
H	11	-1.746246	1.391281	-1.734680	4				
O	12	1.735748	0.093353	1.335617	1	13	14		
H	13	2.477707	0.703200	1.220871	12				
H	14	1.648727	-0.041595	2.289505	12				

StructureTSf.doc

14

C	1	0.344055	0.683136	0.592880	2	3	4		
C	2	-0.061096	1.862823	0.068863	1	5	6		
C	3	-0.008835	-0.532944	-0.067398	1	7	8	9	12
H	4	0.936127	0.636490	1.495407	1				
H	5	0.195648	2.804977	0.532028	2				
H	6	-0.648987	1.899292	-0.839508	2				
H	7	0.341888	-1.484711	0.288223	3				
H	8	-0.646469	-0.516525	-0.935043	3				
O	9	-1.731613	-1.031403	1.172043	3	10	11		
H	10	-2.355789	-0.341049	1.429932	9				
H	11	-2.251984	-1.841522	1.088974	9				
O	12	1.597900	-0.605789	-1.525620	3	13	14		
H	13	2.407272	-0.112305	-1.339203	12				
H	14	1.881775	-1.420654	-1.961685	12				

StructureTSg.doc

14

C	1	-0.113663	-1.383560	0.046570	2	3	4	
C	2	-1.161819	-0.888718	-0.704620	1	5	6	12
C	3	1.166214	-1.052261	-0.345840	1	7	8	9
H	4	-0.290848	-1.941055	0.954132	1			
H	5	-2.191666	-1.097626	-0.454102	2			
H	6	-0.975266	-0.373917	-1.636002	2			
H	7	2.036209	-1.392166	0.196533	3			
H	8	1.338318	-0.530777	-1.276825	3			
O	9	1.397766	1.061447	0.699738	3	10	11	14
H	10	1.059753	1.763962	0.128204	9			
H	11	2.211746	1.412460	1.084671	9			
O	12	-1.336578	1.294403	0.127533	2	13	14	
H	13	-2.143280	1.826508	0.147583	12			
H	14	-0.996719	1.301163	1.032593	9	12		

StructureTSh.doc

14

C	1	0.018448	0.322357	-0.723404	2	3	4	
C	2	-1.180115	0.014938	-0.111206	1	5	6	12
C	3	1.183731	0.050446	-0.034836	1	7	8	9
H	4	0.043671	0.761475	-1.709686	1			
H	5	-2.130905	0.249603	-0.564636	2			
H	6	-1.193695	-0.358887	0.902313	2			
H	7	2.157303	0.211807	-0.471649	3			
H	8	1.146866	-0.452423	0.920609	3			
O	9	1.638641	1.930023	1.284454	3	10	11	
H	10	2.281479	1.943954	2.004486	9			
H	11	1.674973	2.817337	0.907227	9			
O	12	-1.654968	-2.214996	-0.644745	2	13	14	
H	13	-2.327744	-2.746857	-0.201584	12			
H	14	-1.657562	-2.528641	-1.557236	12			

SC7

StructureTSi.doc
15

C	1	0.234070	1.634521	0.373000	2	3	7	
C	2	0.255692	0.494095	1.181747	1	3	4	9
C	3	1.108658	0.635483	-0.121384	1	2	10	13
C	4	-1.020813	-0.311203	0.724533	2	5	6	8
H	5	-1.809067	0.334595	0.324738	4			
H	6	-1.423950	-0.835876	1.588318	4			
H	7	-0.409607	2.457794	0.078369	1			
C	8	-0.424164	-1.173447	-0.393463	4	11	12	13
H	9	0.683136	0.333191	2.161469	2			
H	10	2.184494	0.733017	-0.014709	3			
H	11	-1.222580	-1.589386	-1.010040	8			
H	12	0.155563	-1.987869	0.036957	8			
C	13	0.490067	-0.259232	-1.225006	3	8	14	15
H	14	-0.079971	0.323212	-1.950363	13			
H	15	1.278305	-0.789093	-1.754166	13			

StructureTSj.doc

21

C	1	1.032089	0.172729	0.317215	2	3	7	
C	2	0.234497	-1.016708	0.199921	1	3	4	9
C	3	0.427353	-0.015945	-0.972504	1	2	10	13
C	4	-1.264496	-0.959152	0.590637	2	5	6	8
H	5	-1.411102	-0.337402	1.469666	4			
H	6	-1.594223	-1.968216	0.828568	4			
H	7	1.692917	0.756592	0.924286	1			
C	8	-1.955536	-0.375778	-0.642426	4	11	12	13
H	9	0.752045	-1.961502	0.307678	2			
H	10	1.100220	-0.154526	-1.809204	3			
H	11	-2.905167	0.097778	-0.394409	8			
H	12	-2.152039	-1.175110	-1.357040	8			
C	13	-0.961441	0.613541	-1.251800	3	8	14	15
H	14	-1.038254	1.597412	-0.796997	13			
H	15	-1.075012	0.726105	-2.327866	13			
O	16	2.968048	-0.807114	-0.200729	18	19		
O	17	-0.192368	1.854813	1.551636	20	21		
H	18	3.643173	-0.322388	-0.694046	16			
H	19	3.452393	-1.312408	0.465775	16			
H	20	-0.281586	2.786758	1.317947	17			
H	21	-0.471695	1.800278	2.473648	17			

StructureTSk.doc

21

C	1	1.316574	-0.737274	-0.605804	2	3	7	
C	2	0.396286	-1.532532	0.102966	1	4	9	
C	3	0.322098	-0.485291	-1.570358	1	10	13	
C	4	-0.883224	-1.051102	0.728043	2	5	6	8
H	5	-0.655273	-0.211212	1.388168	4			
H	6	-1.309586	-1.852951	1.327606	4			
H	7	2.266312	-1.159393	-0.901352	1			
C	8	-1.840820	-0.581940	-0.370972	4	11	12	13
H	9	0.694382	-2.565964	0.254425	2			
H	10	0.559052	-0.786163	-2.586884	3			
H	11	-2.677872	-0.008972	0.027451	8			
H	12	-2.242767	-1.443085	-0.906219	8			
C	13	-0.963882	0.248474	-1.310898	3	8	14	15
H	14	-0.726639	1.203598	-0.834839	13			
H	15	-1.456467	0.456268	-2.258820	13			
O	16	0.360306	2.098938	1.885574	18	19		
O	17	2.126450	0.731873	0.375732	20	21		
H	18	0.550537	2.059952	2.831009	16			
H	19	0.046417	2.997528	1.729233	16			
H	20	1.491867	1.287216	0.893417	17			
H	21	2.625977	1.331894	-0.197632	17			

StructureTS1.doc

21

C	1	0.748505	0.411896	0.488220	2	3	7	
C	2	-0.284409	-0.519577	0.666214	1	3	4	9
C	3	0.104126	0.451767	-0.756454	1	2	10	13
C	4	-1.534744	0.109512	1.241516	2	5	6	8
H	5	-1.291031	0.835022	2.020126	4			
H	6	-2.222107	-0.628006	1.648483	4			
H	7	0.898834	1.278183	1.121841	1			
C	8	-2.126770	0.839264	-0.002304	4	11	12	13
H	9	-0.273148	-1.502014	0.210968	2			
H	10	0.202988	-0.343109	-1.485672	3			
H	11	-2.855591	1.588394	0.308990	8			
H	12	-2.635437	0.110382	-0.632355	8			
C	13	-0.978973	1.507095	-0.820038	3	8	14	15
H	14	-0.663864	2.434311	-0.338013	13			
H	15	-1.281860	1.724777	-1.841415	13			
O	16	1.270126	-2.218307	-1.310181	18	19		
O	17	2.807983	-0.462967	0.567352	20	21		
H	18	1.443542	-2.896774	-1.971191	16			
H	19	2.132339	-1.966675	-0.957184	16			
H	20	2.977661	-0.878143	1.425186	17			
H	21	3.561691	0.125198	0.415695	17			

StructureTSm.doc

21

C	1	0.640167	1.804245	0.224762	2	3	7	
C	2	-0.287491	0.925308	0.791092	1	3	4	9
C	3	0.869156	0.690506	-0.587280	1	2	10	13
C	4	-1.642532	1.067642	0.136978	2	5	6	8
H	5	-1.903244	2.112167	-0.039566	4			
H	6	-2.433411	0.584595	0.705063	4			
H	7	0.398575	2.793945	-0.146118	1			
C	8	-1.385712	0.341583	-1.225510	4	11	12	13
H	9	-0.046402	0.028122	1.363419	2			
H	10	1.319641	-0.249878	-0.265198	3			
H	11	-2.173096	0.608948	-1.931473	8			
H	12	-1.415283	-0.735260	-1.066025	8			
C	13	0.005127	0.733322	-1.826736	3	8	14	15
H	14	-0.042389	1.734300	-2.257980	13			
H	15	0.328079	0.024109	-2.584503	13			
O	16	2.058548	-2.005341	0.274384	18	19		
O	17	0.335510	-1.677444	2.351624	20	21		
H	18	1.382385	-2.648651	0.517532	16			
H	19	2.769104	-2.512421	-0.133865	16			
H	20	-0.064331	-1.931549	3.191284	17			
H	21	1.287552	-1.688156	2.508118	17			

Supplementary material Table S1. Molecular potential energies in Hartrees.

Molecule	*E*(MP2/6-31G(d,p)	E_{zpv}	E_{tot}
1	-116.58108	0.06747	-116.51361
TSa(**1->1**)	-116.52230	0.06372	-116.45858
2	-192.83704	0.09725	-192.73980
3	-192.84699	0.09587	-192.75111
4	-76.21979	0.02101	-76.19877
TSb(**2->3**)	-192.80548	0.09141	-192.71407
5	-269.10657	0.12047	-268.98609
6	-269.11357	0.11960	-268.99397
TSc (**5->6**)	-269.05196	0.11591	-268.93605
7	-269.04442	0.11440	-268.93002
TSd(**5->7**)	-269.01268	0.11032	-268.90236
8	-116.23746	0.05530	-116.18216
9	-152.78858	0.05649	-152.73208
TSe(**5->5´**)	-269.04035	0.11676	-268.92359
TSf(**6->6´**)	-269.07374	0.11588	-268.95786
TSg(**6->6´**)	-269.07119	0.11679	-268.95440
TSh(**6->6´**)	-269.06892	0.11514	-268.95378
10	-232.92376	0.13135	-232.79241
11	-232.99025	0.13182	-232.85843
TSi(**10->11**)	-232.90494	0.12810	-232.77684
12	-309.20232	0.16066	-309.04165
13	-309.20236	0.16119	-309.04117
14	-385.47014	0.18399	-385.28615
15	-385.47054	0.18467	-385.28587
TSj(**14->15**)	-385.40508	0.17894	-385.22615
TSk(**15->16**)	-385.43565	0.18119	-385.25446
16	-385.49337	0.18429	-385.30908
17	-309.22916	0.16005	-309.06911
TSl(**14->18**)	-385.40983	0.17905	-385.23077
18	-385.41041	0.17932	-385.23109
TSm(**18->18´**)	-385.40742	0.17894	-385.22848

a) Zero-point vibrational energy scaled by 0.9608 (E_{zpv}) are included in the total energies (E_{tot}) (see Methods).

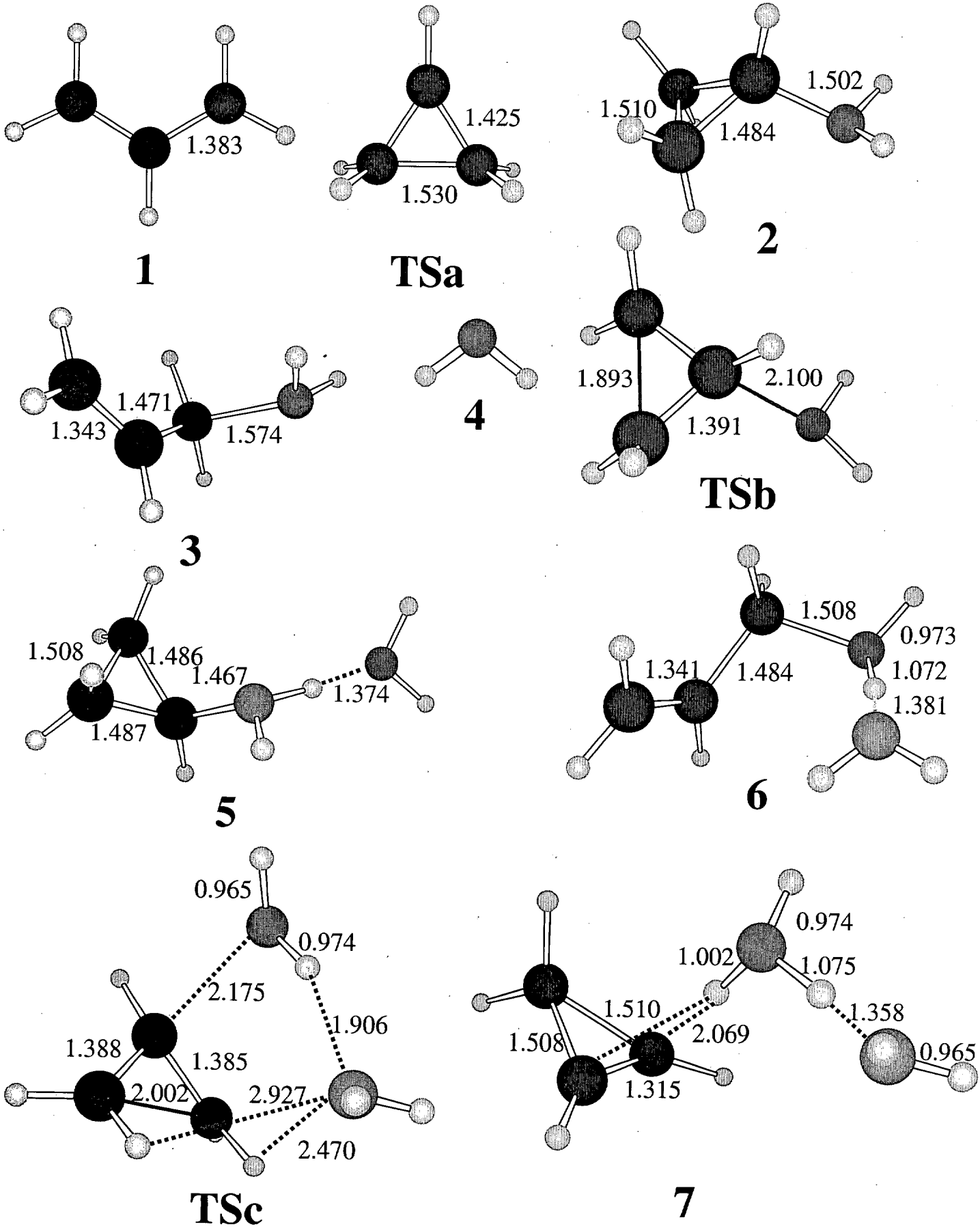

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TSa
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1.391
TSb
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1.467
1.374
1.487
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TSc
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1.315
7

Figure S1

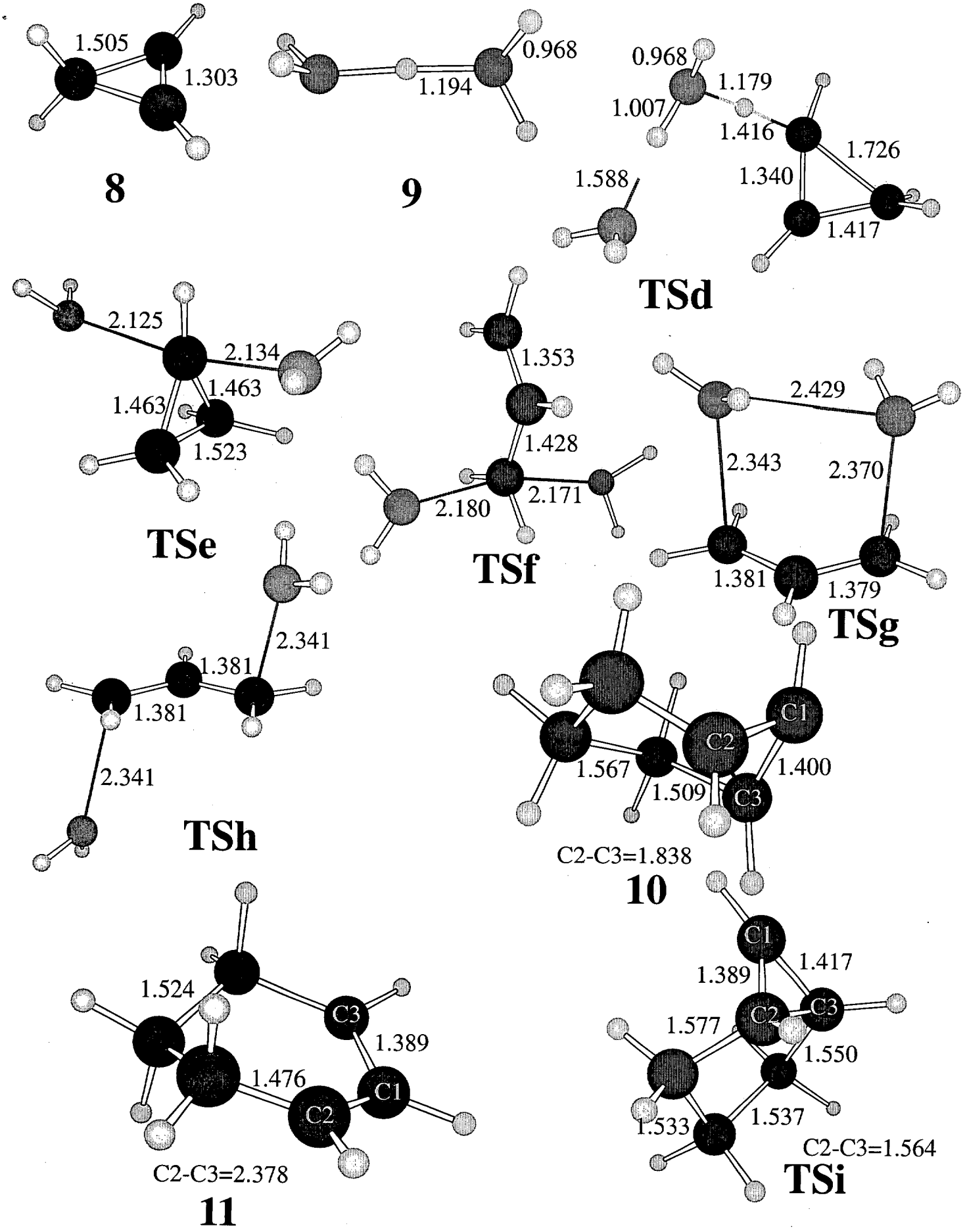
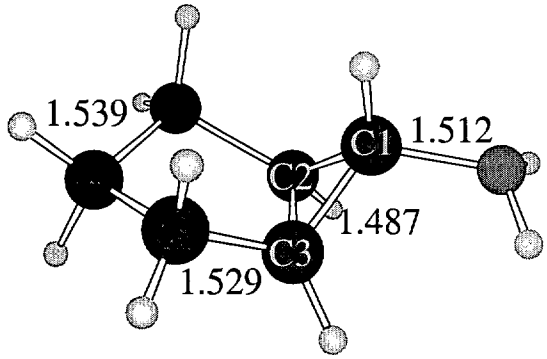
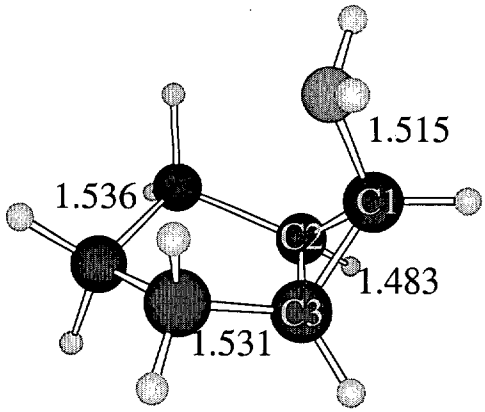

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1.417
TSd
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2.134
1.463
1.463
1.523
TSe
1.353
1.428
2.171
2.180
TSf
2.429
2.343
2.370
1.381
1.379
TSg
2.341
1.381
1.381
2.341
TSh
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C2
C3
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1.400
1.509
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C2
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C3
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1.537
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TSi

Figure S2

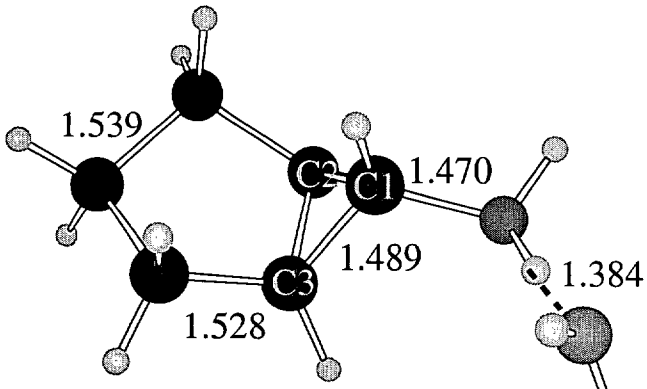


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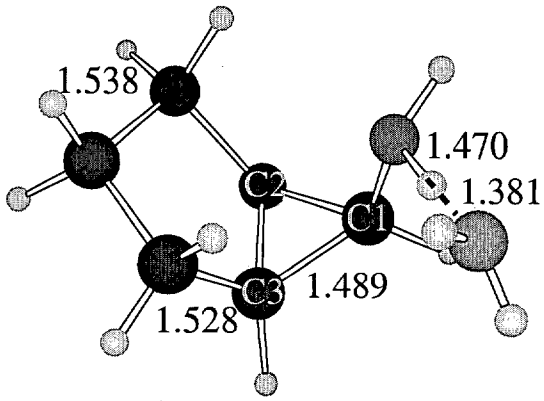
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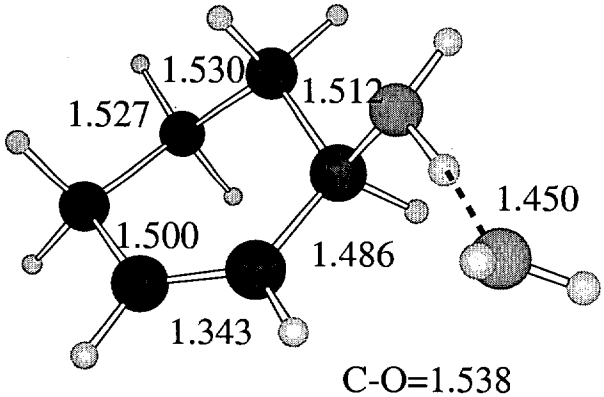
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14 C2-C3=1.519

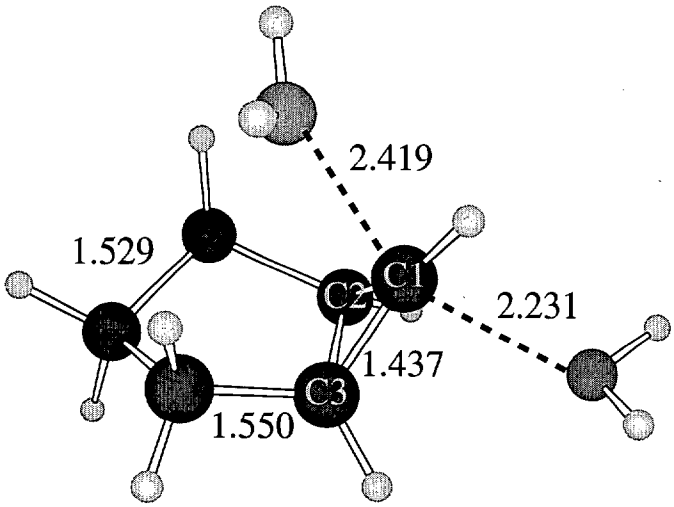


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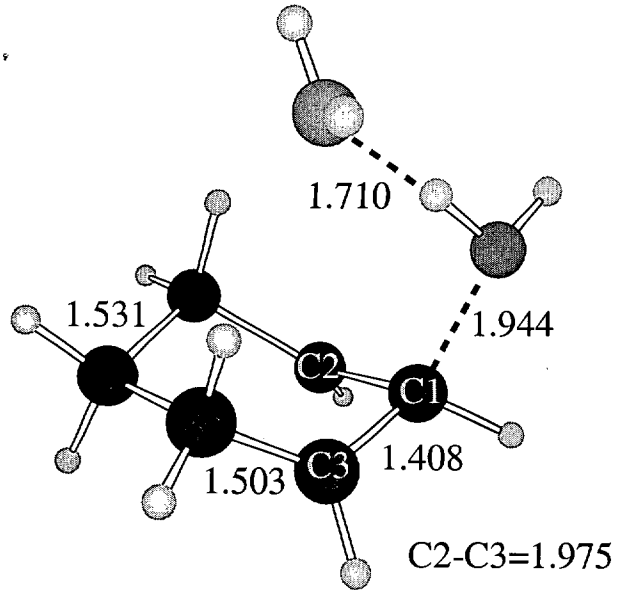


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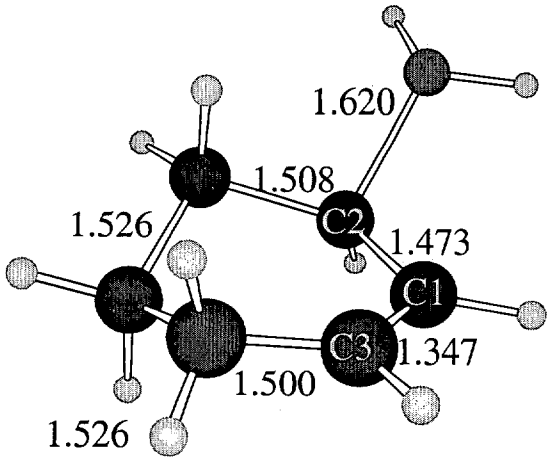
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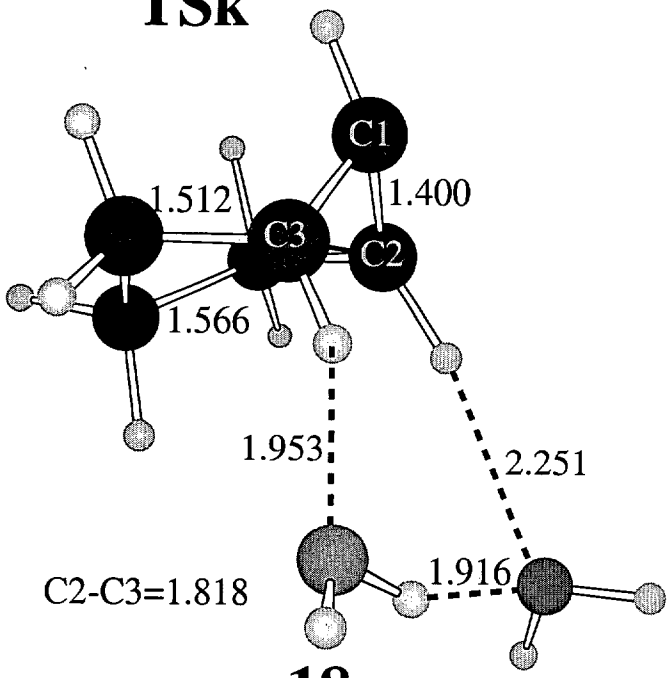
TSj C2-C3=1.553



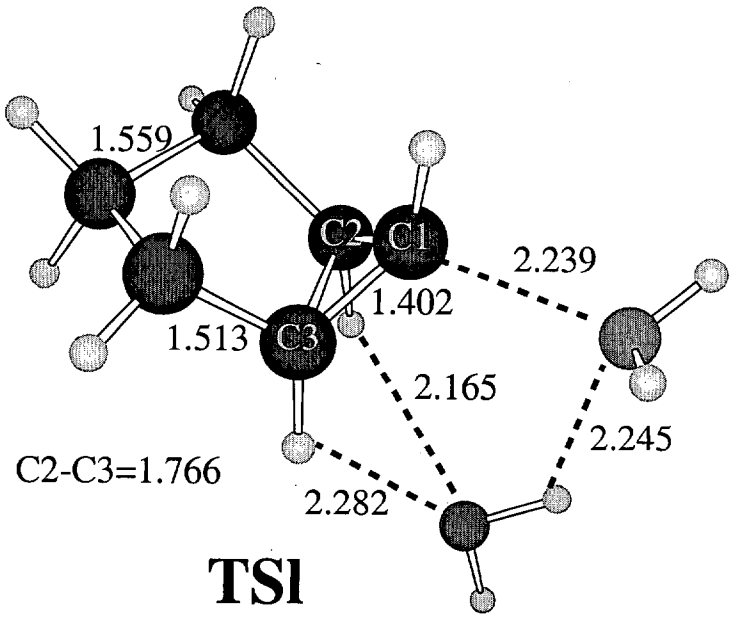
TSk



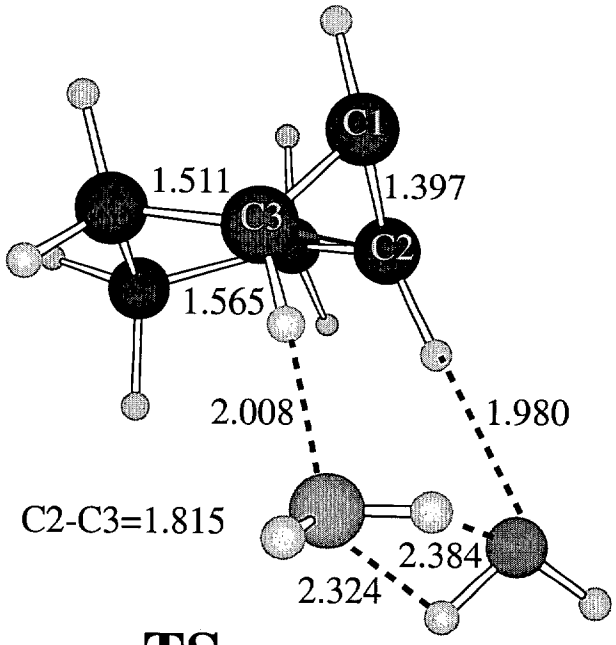
17



18



TSl



TSm

Figure S4