Determination of the Covalent Bond Orders and Atomic Valence Indices
Using Topological Features of the Experimental Electron Density

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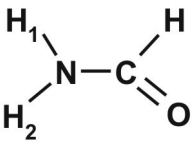
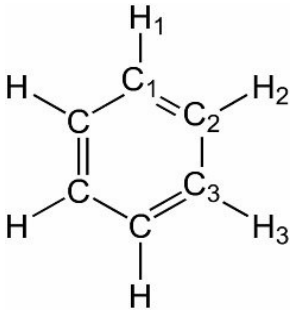
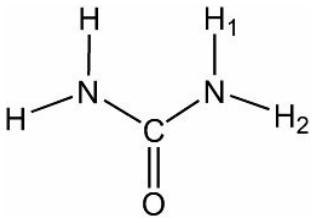
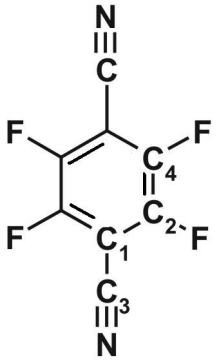
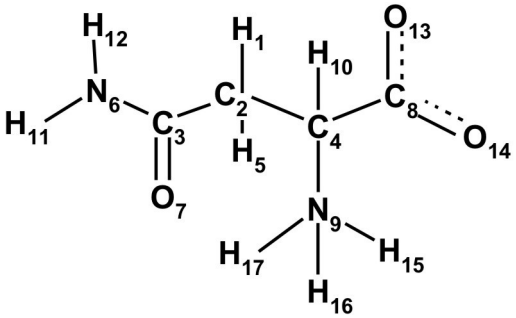
Deposit material

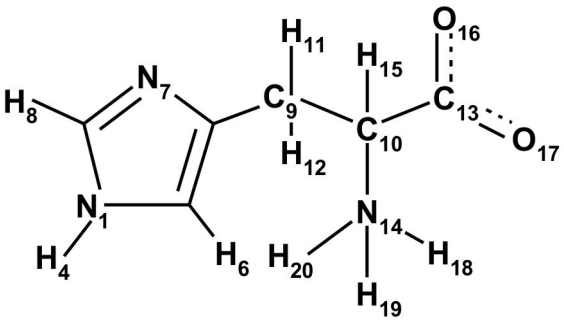
Table D1. The Cioslowski–Mixon bond orders, n_{CM}, and topological bond orders, n_{topo}, for different bonds computed using coefficients in model (4) derived by fit to the theoretical electron density features

Structure	Bond	n_{CM}	n_{topo}
 Formamide	C—O	1.361	1.260
	C—N	1.050	1.013
	C—H	0.867	0.885
	N—H1	0.832	0.819
	N—H2	0.819	0.803
 Benzene	C1—C2	1.390	1.277
	C1—C3	1.390	1.277
	C2—C3	1.390	1.277
	C1—H1	0.962	0.911
	C2—H2	0.962	0.911
	C3—H3	0.962	0.911
 Urea	C—O	1.231	1.321
	C—N	0.961	1.160
	N—H1	0.819	0.809
	N—H2	0.842	0.836
 Tetrafluoroterephthalonitrile	C1—C2	1.262	1.276
	C2—C4	1.276	1.289
	C1—C3	1.097	1.087
	C3—N	2.420	2.193
	C2—F	0.856	-



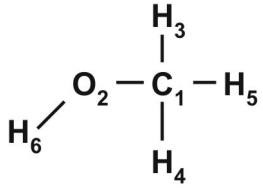
Asparagine

H1—C2	0.945	0.935
C2—C3	0.897	0.910
C2—C4	0.957	0.937
C2—H5	0.917	0.921
C3—N6	0.880	1.086
C3—O7	1.066	1.062
C4—C8	0.741	0.783
C4—N9	0.793	0.723
O7…H17	0.075	0.067
C4—H10	0.928	0.933
N6—H11	0.783	0.799
N6—H12	0.789	0.815
C8—O13	1.004	1.075
C8—O14	0.940	1.039
N9—H15	0.563	0.585
O14…H15	0.101	0.106
N9—H16	0.800	0.810
N9—H17	0.621	0.651



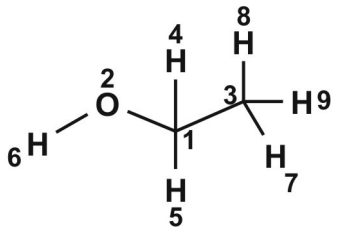
Histidine

N1—C2	1.023	1.074
N1—C3	1.006	1.165
N1—H4	0.765	0.759
C2—C5	1.381	1.406
C2—H6	0.960	0.907
C3—N7	1.267	1.202
C5—N7	1.126	1.233
C3—H8	0.911	0.878
C5—C9	0.964	0.936
C9—C10	0.942	0.913
C9—H11	0.933	0.908
C9—H12	0.907	0.883
C10—C13	0.856	0.842
C10—N14	0.767	0.775
C10—H15	0.899	0.892
C13—O16	1.165	1.075
C13—O17	1.154	0.899
N14—H18	0.684	0.674
N14—H19	0.759	0.754
N14—H20	0.757	0.761



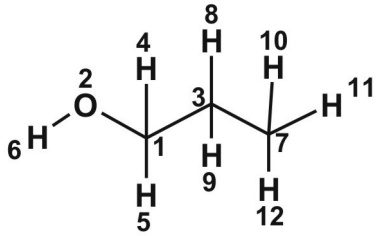
Methanol

C1—O2	0.828	0.794
C1—H3	0.931	0.919
C1—H4	0.935	0.927
O2—H6	0.638	0.631



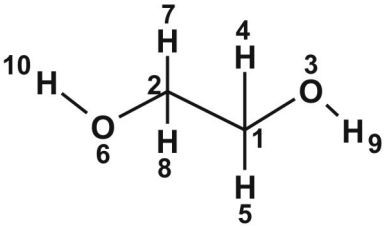
Ethanol

C1—O2	0.807	0.779
C1—C3	0.954	0.913
C1—H4	0.923	0.931
O2—H6	0.637	0.634
C3—H7	0.967	0.934
C3—H8	0.962	0.931



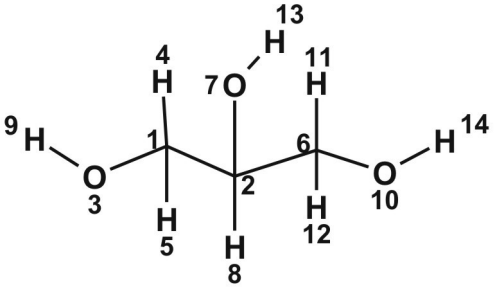
Propanol

C1—O2	0.803	0.777
C1—C3	0.938	0.912
C1—H4	0.919	0.932
O2—H6	0.636	0.637
C3—C7	0.979	0.921
C3—H8	0.948	0.936
C7—H10	0.966	0.934
C7—H11	0.965	0.936



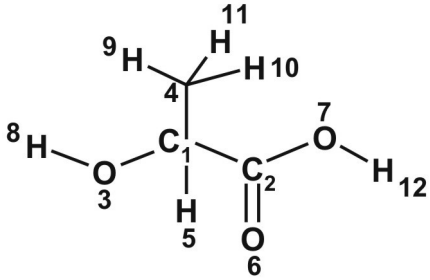
Ethylene glycol

C1—C2	0.906	0.884
C1—O3	0.805	0.777
C1—H4	0.919	0.929
O3—H9	0.630	0.623



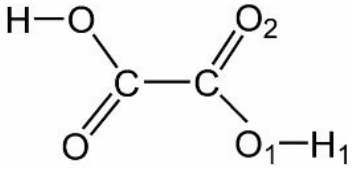
Glycerin

C1—C2	0.900	0.898
C1—O3	0.813	0.812
C1—H4	0.913	0.928
C1—H5	0.917	0.924
C2—O7	0.784	0.785
C2—H8	0.903	0.928
O3—H9	0.594	0.600
C6—O10	0.803	0.774
C6—H11	0.923	0.929
O7—H13	0.585	0.588
O10—H14	0.620	0.609



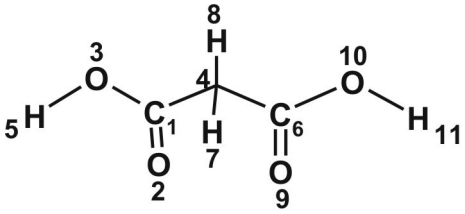
Lactic acid

C1—C2	0.849	0.875
C1—O3	0.805	0.833
C1—C4	0.932	0.920
C1—H5	0.897	0.925
C2—O6	1.117	1.059
C2—O7	0.729	0.800
O3—H8	0.567	0.578
C4—H9	0.956	0.930
C4—H10	0.959	0.931
C4—H11	0.958	0.932
O7—H12	0.561	0.552



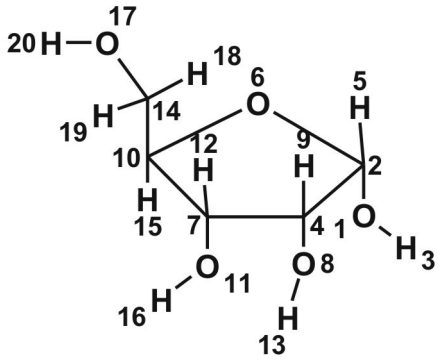
Oxalic acid

C—C	0.787	0.755
C—O1	0.740	0.836
C—O2	1.163	1.082
O1—H1	0.556	0.543



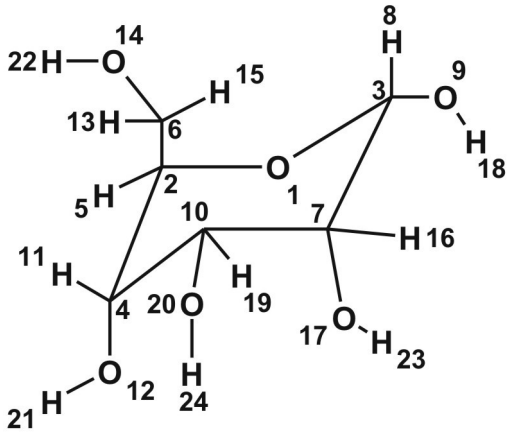
Malonic acid

C1—O2	1.140	1.076
C1—O3	0.728	0.812
C1—C4	0.886	0.910
O3—H5	0.562	0.547
C4—H7	0.935	0.922



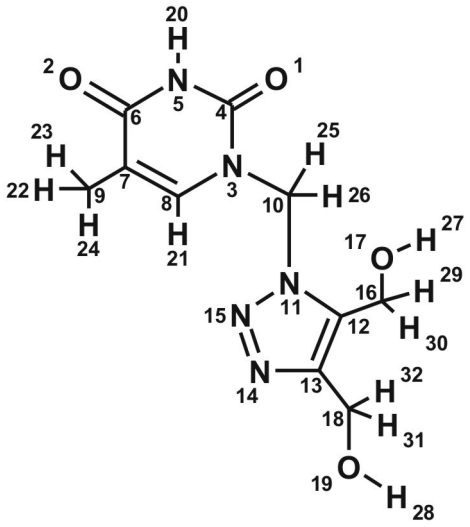
α-D-ribopiranose

O1—C2	0.722	0.775
O1—H3	0.602	0.596
C2—C4	0.852	0.884
C2—H5	0.884	0.915
C2—O6	0.723	0.811
C4—C7	0.880	0.915
C4—O8	0.813	0.829
C4—H9	0.899	0.929
O6—C10	0.757	0.757
C7—C10	0.898	0.914
O1…H16	0.030	0.039
C7—O11	0.800	0.805
C7—H12	0.910	0.923
O8—H13	0.578	0.581
C10—C14	0.908	0.898
C10—H15	0.907	0.922
O11—H16	0.562	0.578
C14—O17	0.810	0.809
C14—H18	0.910	0.930
C14—H19	0.917	0.923
O17—H20	0.600	0.605



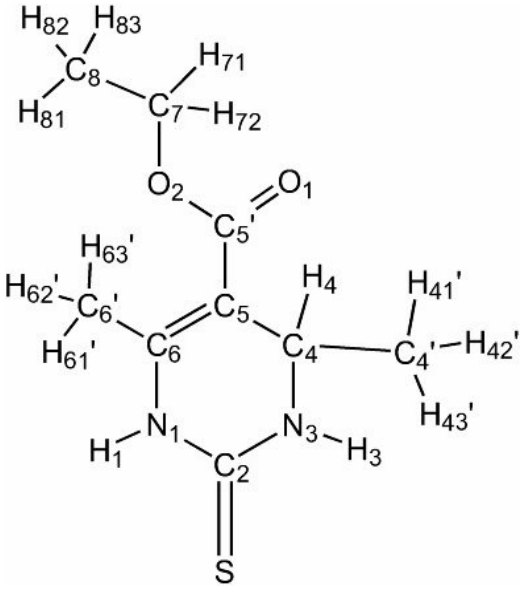
α-D-glucopiranose

O1—C2	0.760	0.751
O1—C3	0.727	0.813
C2—C4	0.893	0.897
C2—H5	0.896	0.928
C2—C6	0.896	0.893
C3—C7	0.863	0.879
C3—H8	0.876	0.915
C3—O9	0.724	0.784
C4—C10	0.895	0.915
C7—C10	0.894	0.917
C4—H11	0.896	0.931
C4—O12	0.788	0.780
C6—H13	0.912	0.929
C6—O14	0.817	0.814
C6—H15	0.912	0.923
C7—H16	0.898	0.926
C7—O17	0.795	0.800
O9—H18	0.600	0.579
C10—H19	0.895	0.931
C10—O20	0.788	0.788
O12—H21	0.578	0.576
O14—H22	0.547	0.558
O17—H23	0.580	0.591
O20—H24	0.589	0.588
O12…H22	0.035	0.036



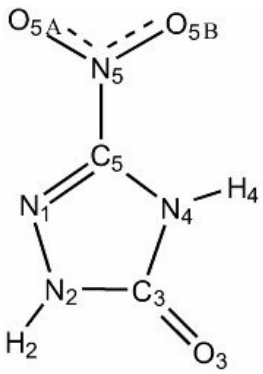
1-[(4,5-dihydroxymethyl-1,2,3-triazolyl)-1-methyl]-5-methyl-pyrimidine-2,4-dione (MTMT)

O1—C4	1.234	1.316
N5—C6	0.935	0.959
N3—C4	0.922	0.957
C4—N5	0.957	0.995
O2—C6	1.303	1.268
C6—C7	1.026	1.072
N3—C8	1.026	0.972
C7—C8	1.566	1.503
C7—C9	1.008	0.989
N3—C10	0.900	0.790
C8—H21	0.916	0.902
C10—N11	0.854	0.717
N11—C12	1.094	1.107
N11—N15	1.337	1.351
C12—C13	1.339	1.422
C13—N14	1.222	1.121
N14—N15	1.587	1.433
C12—C16	0.969	0.956
O17…H25	0.036	0.035
C10—H25	0.860	0.882
C16—O17	0.906	0.866
C13—C18	0.957	0.949
C18—O19	0.916	0.870
N5—H20	0.774	0.775
C9—H22	0.947	0.942
C9—H23	0.947	0.944
C9—H24	0.959	0.954
C10—H26	0.893	0.907
O17—H27	0.694	0.689
O19—H28	0.685	0.687
C16—H29	0.906	0.916
C16—H30	0.909	0.915
C18—H31	0.912	0.911
C18—H32	0.915	0.926



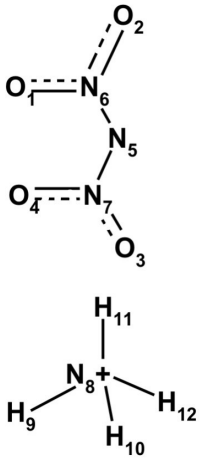
Ethyl 4,6-dimethyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (EDTTH)

S—C2	1.518	-
O1—C5'	1.264	1.259
O2—C5'	0.87	0.971
O2—C7	0.819	0.745
N1—C2	1.023	1.000
N1—C6	1.057	0.944
N1—H1	0.768	0.781
N3—C2	1.143	1.146
N3—C4	0.895	0.712
N3—H3	0.787	0.794
C4—C4'	0.948	0.918
C4—C5	0.967	0.953
C4—H4	0.895	0.917
C4'—H41'	0.952	0.938
C4'—H42'	0.961	0.948
C4'—H43'	0.959	0.945
C5—C5'	1.02	1.064
C5—C6	1.546	1.495
C6—C6'	0.992	0.973
C6'—H61'	0.94	0.933
C6'—H62'	0.956	0.948
C6'—H63'	0.931	0.934
C7—C8	0.984	0.936
C7—H71	0.911	0.904
C7—H72	0.913	0.905
C8—H81	0.959	0.944
C8—H82	0.96	0.946
C8—H83	0.962	0.945



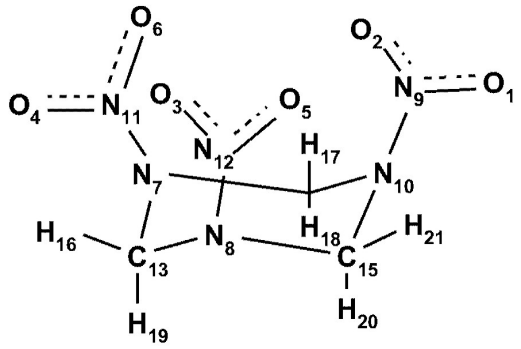
5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (*β*-form) (β-NTO)

O3—C3	1.324	1.392
O5B—N5	1.634	1.622
O5A—N5	1.664	1.629
N1—C5	1.403	1.367
N2—H2	0.741	0.739
N2—N1	1.302	1.254
N2—C3	0.953	1.004
N4—H4	0.727	0.721
N4—C3	0.941	0.967
N4—C5	1.045	1.079
N5—C5	0.85	0.811



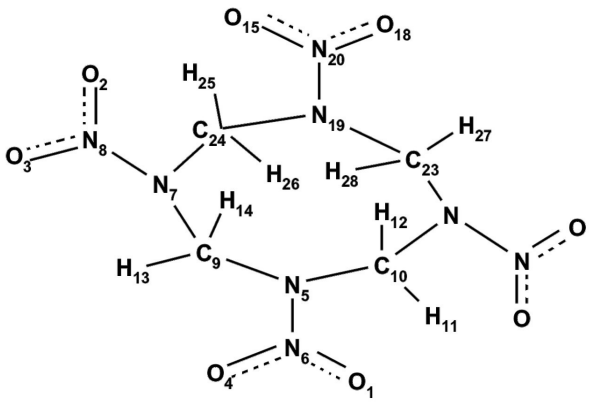
ammonium dinitramide (ADN)

N5—N6	1.177	1.183
O1—N6	1.618	1.606
O2—N6	1.554	1.520
N5—N7	1.210	1.272
O3—N7	1.485	1.518
O4—N7	1.621	1.592
N8—H9	0.703	0.673
N8—H12	0.697	0.669
N8—H10	0.753	0.739
N8—H11	0.689	0.660



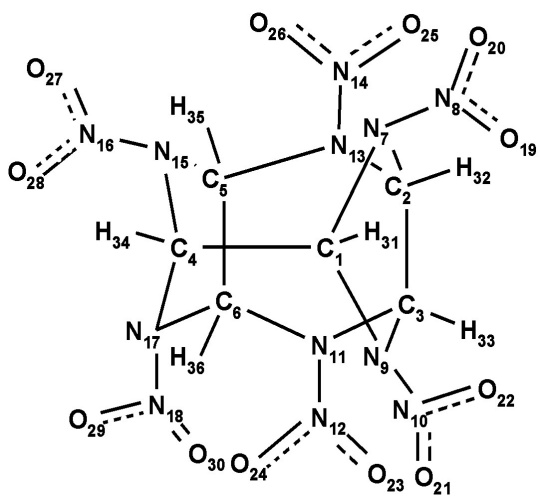
Hexahydro-1,3,5-trinitro-1,3,5-s-triazine, (RDX)

O1—N9	1.612	1.612
O2—N9	1.605	1.601
N10—C14	0.766	0.768
N10—C15	0.768	0.778
N9—N10	1.163	1.176
O4—N11	1.640	1.631
O6—N11	1.630	1.625
N7—N11	1.084	1.074
O3—N12	1.645	1.635
O5—N12	1.623	1.613
N8—N12	1.084	1.076
N7—C13	0.786	0.769
N8—C13	0.787	0.767
N7—C14	0.788	0.803
N8—C15	0.787	0.799
C13—H16	0.844	0.854
C14—H17	0.834	0.848
C14—H18	0.888	0.909
C13—H19	0.887	0.902
C15—H20	0.889	0.908
C15—H21	0.832	0.850
O6…H17	0.041	0.041
O5…H21	0.041	0.042



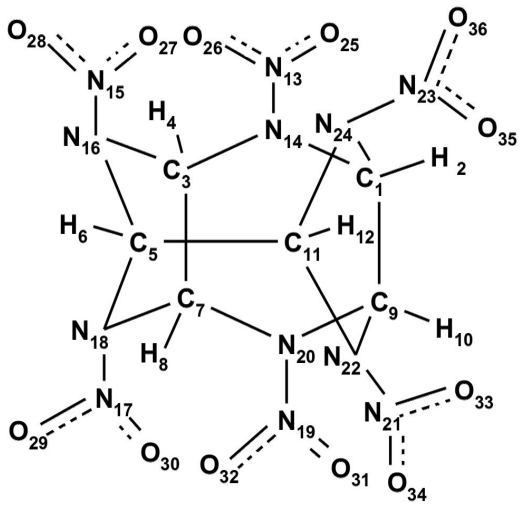
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, (β-HMX)

O1—N6	1.606	1.607
O4—N6	1.612	1.621
N5—N6	1.150	1.171
O2—N8	1.614	1.613
O3—N8	1.592	1.589
N7—C9	0.755	0.714
N7—N8	1.160	1.173
N5—C9	0.775	0.834
N5—C10	0.757	0.783
C10—H11	0.844	0.864
C10—H12	0.876	0.899
C9—H13	0.860	0.876
C9—H14	0.871	0.899
N21—N22	1.159	1.174
O15—N20	1.605	1.607
O18—N20	1.612	1.621
N19—N20	1.150	1.170
C10—N21	0.775	0.780
O16—N22	1.615	1.615
O17—N22	1.591	1.588
N21—C23	0.755	0.715
N19—C24	0.757	0.783
N19—C23	0.775	0.834
N7—C24	0.775	0.779
C24—H25	0.844	0.864
C24—H26	0.876	0.899
C23—H27	0.860	0.876
C23—H28	0.871	0.899
O16…H11	0.045	0.041
O2…H25	0.045	0.041



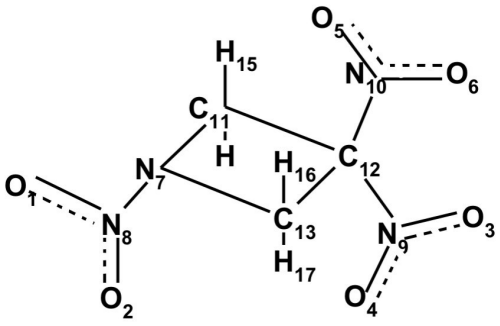
γ-hexanitrohexaazaisowurtzitane
(γ-HNIW)

C2—C3	0.817	0.843
C1—C4	0.819	0.814
C5—C6	0.815	0.844
C1—N7	0.775	0.819
C2—N7	0.762	0.778
N7—N8	1.085	1.078
C1—N9	0.773	0.790
C3—N9	0.770	0.748
N9—N10	1.052	1.034
C3—N11	0.779	0.869
C6—N11	0.770	0.843
N11—N12	1.089	1.086
C2—N13	0.775	0.825
C5—N13	0.785	0.831
N13—N14	1.052	1.025
C4—N15	0.782	0.822
C5—N15	0.770	0.724
N15—N16	1.029	1.001
C4—N17	0.751	0.781
C6—N17	0.763	0.758
N17—N18	1.114	1.106
N8—O19	1.649	1.648
N8—O20	1.633	1.624
N10—O21	1.648	1.647
N10—O22	1.653	1.648
N12—O23	1.631	1.639
N12—O24	1.644	1.659
N14—O25	1.652	1.651
N14—O26	1.649	1.643
N16—O27	1.669	1.661
C4—H34	0.895	0.889
N16—O28	1.638	1.624
N18—O29	1.617	1.621
N18—O30	1.629	1.628
C1—H31	0.891	0.881
C2—H32	0.897	0.891
C3—H33	0.882	0.878
C5—H35	0.902	0.900
C6—H36	0.897	0.891



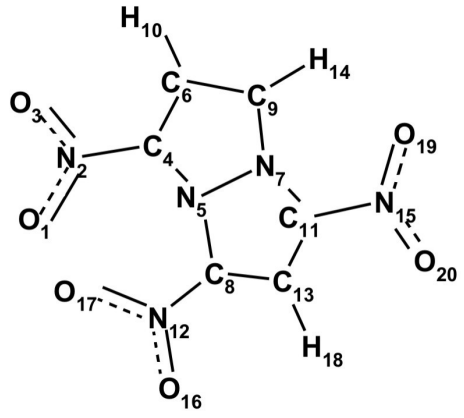
ε-hexanitrohexaazaisowurtzitane
(ε-HNIW)

C1—H2	0.894	0.889
C1—N14	0.778	0.849
C3—N14	0.774	0.815
C3—H4	0.905	0.894
C5—N16	0.752	0.802
C5—H6	0.907	0.900
C3—C7	0.812	0.832
C5—N18	0.752	0.811
C7—N18	0.758	0.762
C7—H8	0.900	0.887
C1—C9	0.819	0.846
C7—N20	0.766	0.849
C9—N20	0.770	0.821
C9—H10	0.873	0.869
C5—C11	0.808	0.811
C9—N22	0.783	0.762
C11—N24	0.767	0.795
C11—N22	0.765	0.805
C11—H12	0.906	0.898
N13—N14	1.064	1.045
C3—N16	0.761	0.744
N15—N16	1.103	1.096
N17—N18	1.112	1.108
N19—N20	1.104	1.109
N21—N22	1.041	1.013
C1—N24	0.766	0.757
N23—N24	1.051	1.030
N13—O25	1.647	1.641
N13—O26	1.639	1.646
N15—O27	1.631	1.629
N15—O28	1.616	1.618
N17—O29	1.603	1.604
N17—O30	1.642	1.640
N19—O31	1.635	1.651
N19—O32	1.632	1.641
N21—O33	1.653	1.654
N21—O34	1.657	1.648
N23—O35	1.658	1.659
N23—O36	1.648	1.644



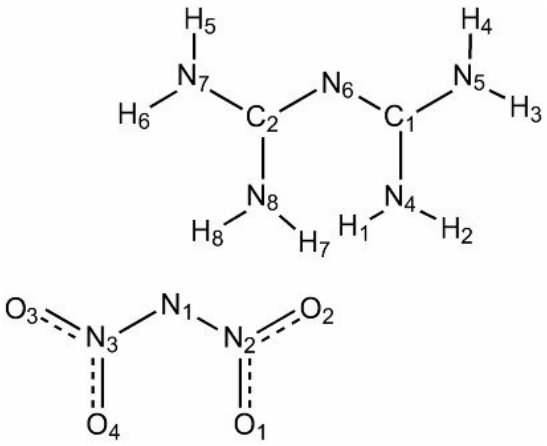
1,3,3-trinitroazetidine, (TNAZ)

N9—C12	0.795	0.650
O1—N8	1.603	1.628
O2—N8	1.601	1.624
N7—N8	1.141	1.213
O3—N9	1.691	1.643
O4—N9	1.664	1.635
N7—C11	0.900	0.709
N7—C13	0.898	0.716
O5—N10	1.671	1.635
O6—N10	1.673	1.636
N10—C12	0.791	0.673
C11—C12	0.892	0.902
C12—C13	0.894	0.905
C11—H14	0.897	0.895
C11—H15	0.906	0.892
C13—H16	0.907	0.894
C13—H17	0.891	0.893



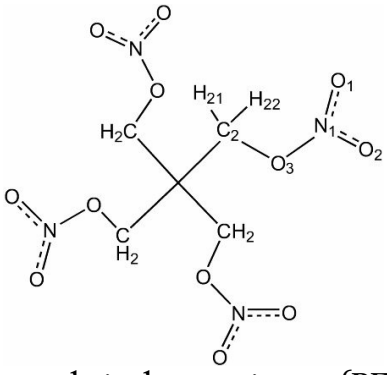
Trinitrodiazapentalene (TNDAP)

O1—N2	1.619	1.605
N2—O3	1.624	1.604
N2—C4	0.922	0.916
C4—N5	1.003	1.079
C4—C6	1.262	1.332
N5—N7	1.209	1.245
N5—C8	0.963	1.010
C6—C9	1.408	1.391
N7—C9	1.045	1.063
C6—H10	0.932	0.874
N7—C11	0.970	1.013
C8—N12	0.925	0.923
C8—C13	1.305	1.370
C11—C13	1.310	1.385
C9—H14	0.900	0.866
C11—N15	0.937	0.930
N12—O16	1.625	1.603
N12—O17	1.616	1.595
C13—H18	0.913	0.860
N15—O19	1.602	1.593
N15—O20	1.628	1.606



Biguanidinium dinitramide
(BIGH DN)

O1—N2	1.610	1.617
O2—N2	1.470	1.536
O3—N3	1.563	1.596
O4—N3	1.611	1.630
N1—N2	1.246	1.290
N1—N3	1.159	1.192
N4—C1	1.085	1.104
N4—H1	0.757	0.771
N4—H2	0.801	0.800
N5—C1	1.058	1.116
N5—H3	0.816	0.812
N5—H4	0.780	0.772
N6—C1	1.192	1.146
N6—C2	1.154	1.137
N7—C2	1.060	1.106
N7—H5	0.786	0.777
N7—H6	0.807	0.804
N8—C2	1.121	1.137
N8—H7	0.661	0.705
N8—H8	0.793	0.794
O2...H7	0.064	0.057



Pentaerythritol tetranitrate (PETN)

C1—C2	0.921	0.917
C2—O3	0.823	0.773
C2—H21	0.884	0.902
C2—H22	0.894	0.903
O1—N1	1.022	1.032
O2—N1	1.660	1.728
O3—N1	1.679	1.720