

Inorganic Chemistry

including bioinorganic chemistry

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HETATM	30	H	30	9.914	2.266	-6.574
HETATM	31	H	31	11.056	0.432	-8.830
HETATM	32	H	32	10.845	0.281	-7.078
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HETATM	49	H	49	13.437	5.058	-6.512
HETATM	50	H	50	10.541	4.781	-4.135
HETATM	51	H	51	10.545	3.012	-4.253
HETATM	52	H	52	11.886	3.880	-3.471
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CONNECT 51 37
CONNECT 52 37
END

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Pt (pmdien) (1-Me-Thymine-N3)

anti

HETATM	1	N1	1	-3.377	-0.765	1.202
HETATM	2	C6	2	-3.646	0.404	1.873
HETATM	3	H6	3	-4.602	0.517	2.364
HETATM	4	C5	4	-2.744	1.416	1.931
HETATM	5	C5M	5	-3.082	2.688	2.684
HETATM	6	1H5M	6	-2.552	2.694	3.637
HETATM	7	2H5M	7	-2.774	3.555	2.099
HETATM	8	3H5M	8	-4.153	2.758	2.872
HETATM	9	C4	9	-1.450	1.293	1.283
HETATM	10	O4	10	-0.568	2.150	1.299
HETATM	11	N3	11	-1.243	0.088	0.612
HETATM	12	C2	12	-2.163	-0.960	0.547
HETATM	13	O2	13	-1.912	-1.992	-0.073
HETATM	14	C	14	-4.379	-1.857	1.137
HETATM	15	H	15	-3.944	-2.782	1.516
HETATM	16	H	16	-5.258	-1.617	1.737
HETATM	17	H	17	-4.692	-2.003	0.102
HETATM	18	Pt	18	0.559	-0.108	-0.331
HETATM	19	N	19	2.343	-0.275	-1.274
HETATM	20	N	20	1.413	-1.008	1.302
HETATM	21	C	21	3.152	0.951	-1.062
HETATM	22	C	22	0.668	-2.241	1.646
HETATM	23	C	23	1.432	-0.070	2.445
HETATM	24	C	24	0.903	0.586	-3.070
HETATM	25	C	25	1.929	-0.474	-2.675
HETATM	26	C	26	2.911	-1.475	-0.630
HETATM	27	C	27	2.799	-1.357	0.889

HETATM	28	H		28	1.404	1.549	-3.155
HETATM	29	H		29	0.522	0.351	-4.065
HETATM	30	H		30	2.794	-0.429	-3.338
HETATM	31	H		31	1.456	-1.450	-2.786
HETATM	32	H		32	3.953	-1.607	-0.924
HETATM	33	H		33	2.349	-2.358	-0.935
HETATM	34	H		34	3.500	-0.601	1.237
HETATM	35	H		35	3.117	-2.299	1.339
HETATM	36	N		36	-0.201	0.661	-2.076
HETATM	37	C		37	-0.626	2.065	-1.880
HETATM	38	C		38	-1.339	-0.169	-2.533
HETATM	39	H		39	4.109	0.852	-1.575
HETATM	40	H		40	2.643	1.835	-1.437
HETATM	41	H		41	3.337	1.129	-0.006
HETATM	42	H		42	1.210	-2.809	2.402
HETATM	43	H		43	-0.308	-2.005	2.065
HETATM	44	H		44	0.543	-2.861	0.758
HETATM	45	H		45	2.036	-0.486	3.253
HETATM	46	H		46	1.859	0.884	2.135
HETATM	47	H		47	0.427	0.099	2.828
HETATM	48	H		48	-0.852	2.518	-2.846
HETATM	49	H		49	-1.522	2.121	-1.264
HETATM	50	H		50	0.172	2.631	-1.400
HETATM	51	H		51	-1.639	0.125	-3.540
HETATM	52	H		52	-1.053	-1.221	-2.542
HETATM	53	H		53	-2.208	-0.034	-1.893
CONECT	1	2	12	14			
CONECT	2	1	3	4			
CONECT	3	2					
CONECT	4	2	5	9			
CONECT	5	4	6	7	8		
CONECT	6	5					
CONECT	7	5					
CONECT	8	5					
CONECT	9	4	10	11			
CONECT	10	9					
CONECT	11	9	12	18			
CONECT	12	1	11	13			
CONECT	13	12					
CONECT	14	1	15	16	17		
CONECT	15	14					
CONECT	16	14					
CONECT	17	14					
CONECT	18	19	20	36	11		
CONECT	19	18	21	25	26		
CONECT	20	18	22	23	27		
CONECT	21	19	39	40	41		
CONECT	22	20	42	43	44		
CONECT	23	20	45	46	47		
CONECT	24	25	28	29	36		
CONECT	25	24	19	30	31		
CONECT	26	19	27	32	33		
CONECT	27	26	20	34	35		
CONECT	28	24					

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CONNECT 29 24
CONNECT 30 25
CONNECT 31 25
CONNECT 32 26
CONNECT 33 26
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CONNECT 35 27
CONNECT 36 18 24 37 38
CONNECT 37 36 48 49 50
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CONNECT 43 22
CONNECT 44 22
CONNECT 45 23
CONNECT 46 23
CONNECT 47 23
CONNECT 48 37
CONNECT 49 37
CONNECT 50 37
CONNECT 51 38
CONNECT 52 38
CONNECT 53 38
END

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syn

HETATM	1	N1	1	31.343	3.472	-2.415
HETATM	2	C6	2	30.181	2.815	-2.739
HETATM	3	H6	3	29.288	3.020	-2.166
HETATM	4	C5	4	30.131	1.917	-3.754
HETATM	5	C5M	5	28.831	1.200	-4.065
HETATM	6	1H5M	6	28.684	1.153	-5.144
HETATM	7	2H5M	7	28.877	0.187	-3.666
HETATM	8	3H5M	8	27.983	1.721	-3.620
HETATM	9	C4	9	31.316	1.612	-4.536
HETATM	10	O4	10	31.359	0.805	-5.463
HETATM	11	N3	11	32.465	2.306	-4.152
HETATM	12	C2	12	32.526	3.235	-3.113
HETATM	13	O2	13	33.583	3.794	-2.822
HETATM	14	C	14	31.387	4.442	-1.294
HETATM	15	H	15	31.738	5.409	-1.656
HETATM	16	H	16	30.399	4.575	-0.852
HETATM	17	H	17	32.067	4.077	-0.523
HETATM	18	Pt	18	34.229	1.957	-5.121
HETATM	19	N	19	35.984	1.638	-6.082
HETATM	20	N	20	34.700	0.390	-3.885
HETATM	21	C	21	37.064	2.460	-5.480
HETATM	22	C	22	33.638	-0.640	-3.950
HETATM	23	C	23	34.877	0.875	-2.499
HETATM	24	C	24	34.960	3.388	-7.469
HETATM	25	C	25	35.653	2.027	-7.465
HETATM	26	C	26	36.167	0.187	-5.884

HETATM	27	C	27	35.975	-0.168	-4.410
HETATM	28	H	28	35.689	4.156	-7.215
HETATM	29	H	29	34.625	3.608	-8.483
HETATM	30	H	30	36.556	2.058	-8.077
HETATM	31	H	31	34.964	1.301	-7.899
HETATM	32	H	32	37.157	-0.121	-6.223
HETATM	33	H	33	35.417	-0.360	-6.456
HETATM	34	H	34	36.821	0.215	-3.841
HETATM	35	H	35	36.003	-1.253	-4.304
HETATM	36	N	36	33.824	3.413	-6.510
HETATM	37	C	37	33.721	4.740	-5.864
HETATM	38	C	38	32.567	3.076	-7.219
HETATM	39	H	39	37.999	2.279	-6.010
HETATM	40	H	40	36.832	3.521	-5.530
HETATM	41	H	41	37.206	2.227	-4.428
HETATM	42	H	42	32.730	-0.298	-3.458
HETATM	43	H	43	33.421	-0.886	-4.989
HETATM	44	H	44	33.958	-1.545	-3.432
HETATM	45	H	45	35.296	0.080	-1.881
HETATM	46	H	46	35.554	1.729	-2.489
HETATM	47	H	47	33.924	1.173	-2.066
HETATM	48	H	48	33.673	5.518	-6.627
HETATM	49	H	49	32.821	4.810	-5.257
HETATM	50	H	50	34.592	4.915	-5.232
HETATM	51	H	51	32.427	3.738	-8.075
HETATM	52	H	52	32.603	2.045	-7.572
HETATM	53	H	53	31.704	3.209	-6.572
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CONNECT	7	5				
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CONNECT 44 22
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CONNECT 47 23
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CONNECT 49 37
CONNECT 50 37
CONNECT 51 38
CONNECT 52 38
CONNECT 53 38
END

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Pt (pmdien) (1-Me-Uracil-N3)

anti

HETATM	1	N1	1	30.104	1.502	-3.975
HETATM	2	C6	2	29.896	2.640	-3.234
HETATM	3	H6	3	28.931	2.811	-2.779
HETATM	4	C5	4	30.875	3.559	-3.060
HETATM	5	C4	5	32.187	3.376	-3.650
HETATM	6	O4	6	33.128	4.158	-3.528
HETATM	7	N3	7	32.334	2.205	-4.394
HETATM	8	C2	8	31.334	1.247	-4.579
HETATM	9	O2	9	31.535	0.237	-5.253
HETATM	10	C	10	29.022	0.502	-4.160
HETATM	11	H	11	29.336	-0.458	-3.749
HETATM	12	H	12	28.110	0.816	-3.652
HETATM	13	H	13	28.806	0.385	-5.223
HETATM	14	Pt	14	34.172	1.924	-5.242
HETATM	15	N	15	35.995	1.674	-6.089
HETATM	16	N	16	34.846	0.846	-3.633
HETATM	17	C	17	36.886	2.810	-5.745
HETATM	18	C	18	33.985	-0.341	-3.428
HETATM	19	C	19	34.863	1.697	-2.423
HETATM	20	C	20	34.746	2.773	-7.898
HETATM	21	C	21	35.658	1.606	-7.523
HETATM	22	C	22	36.424	0.390	-5.503

HETATM	23	C	23	36.224	0.413	-3.987
HETATM	24	H	24	35.325	3.695	-7.877
HETATM	25	H	25	34.415	2.643	-8.929
HETATM	26	H	26	36.565	1.625	-8.129
HETATM	27	H	27	35.117	0.683	-7.734
HETATM	28	H	28	37.469	0.194	-5.743
HETATM	29	H	29	35.816	-0.421	-5.904
HETATM	30	H	30	36.959	1.083	-3.544
HETATM	31	H	31	36.438	-0.580	-3.591
HETATM	32	N	32	33.588	2.866	-6.970
HETATM	33	C	33	33.253	4.283	-6.705
HETATM	34	C	34	32.427	2.154	-7.551
HETATM	35	H	35	37.858	2.669	-6.218
HETATM	36	H	36	36.470	3.759	-6.075
HETATM	37	H	37	37.029	2.895	-4.670
HETATM	38	H	38	34.431	-1.009	-2.691
HETATM	39	H	39	33.007	-0.056	-3.046
HETATM	40	H	40	33.866	-0.881	-4.367
HETATM	41	H	41	35.382	1.180	-1.615
HETATM	42	H	42	35.379	2.634	-2.636
HETATM	43	H	43	33.851	1.918	-2.088
HETATM	44	H	44	33.116	4.812	-7.649
HETATM	45	H	45	32.329	4.367	-6.136
HETATM	46	H	46	34.060	4.757	-6.145
HETATM	47	H	47	31.530	2.313	-6.958
HETATM	48	H	48	32.638	1.086	-7.614
HETATM	49	H	49	32.215	2.532	-8.552
HETATM	50	H	50	30.675	4.443	-2.471
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CONNECT 28 22
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CONNECT 49 34
CONNECT 50 4
END

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syn

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HETATM	2	C6	2	30.179	2.817	-2.741
HETATM	3	H6	3	29.278	3.026	-2.183
HETATM	4	C5	4	30.133	1.911	-3.747
HETATM	5	C4	5	31.316	1.594	-4.525
HETATM	6	O4	6	31.348	0.792	-5.456
HETATM	7	N3	7	32.467	2.288	-4.143
HETATM	8	C2	8	32.529	3.220	-3.107
HETATM	9	O2	9	33.587	3.775	-2.815
HETATM	10	C	10	31.382	4.466	-1.317
HETATM	11	H	11	31.716	5.429	-1.706
HETATM	12	H	12	30.395	4.594	-0.872
HETATM	13	H	13	32.073	4.133	-0.542
HETATM	14	Pt	14	34.230	1.949	-5.117
HETATM	15	N	15	35.985	1.642	-6.082
HETATM	16	N	16	34.709	0.379	-3.886
HETATM	17	C	17	37.057	2.479	-5.487
HETATM	18	C	18	33.659	-0.661	-3.975
HETATM	19	C	19	34.865	0.854	-2.493
HETATM	20	C	20	34.943	3.378	-7.474
HETATM	21	C	21	35.642	2.020	-7.466
HETATM	22	C	22	36.188	0.195	-5.879
HETATM	23	C	23	35.995	-0.159	-4.404
HETATM	24	H	24	35.671	4.153	-7.237
HETATM	25	H	25	34.594	3.588	-8.486
HETATM	26	H	26	36.539	2.052	-8.085
HETATM	27	H	27	34.952	1.290	-7.889

HETATM	28	H	28	37.184	-0.100	-6.211
HETATM	29	H	29	35.450	-0.367	-6.453
HETATM	30	H	30	36.831	0.241	-3.832
HETATM	31	H	31	36.040	-1.243	-4.293
HETATM	32	N	32	33.818	3.407	-6.501
HETATM	33	C	33	33.733	4.733	-5.850
HETATM	34	C	34	32.552	3.081	-7.196
HETATM	35	H	35	37.994	2.302	-6.015
HETATM	36	H	36	36.816	3.537	-5.545
HETATM	37	H	37	37.200	2.255	-4.433
HETATM	38	H	38	33.982	-1.568	-3.464
HETATM	39	H	39	32.742	-0.334	-3.491
HETATM	40	H	40	33.456	-0.896	-5.020
HETATM	41	H	41	35.288	0.058	-1.878
HETATM	42	H	42	35.531	1.716	-2.468
HETATM	43	H	43	33.904	1.136	-2.067
HETATM	44	H	44	33.695	5.515	-6.610
HETATM	45	H	45	32.834	4.813	-5.241
HETATM	46	H	46	34.607	4.894	-5.218
HETATM	47	H	47	32.406	3.747	-8.048
HETATM	48	H	48	32.579	2.052	-7.554
HETATM	49	H	49	31.696	3.216	-6.539
HETATM	50	H	50	29.200	1.417	-3.974
CONNECT	1	2	8	10		
CONNECT	2	1	3	4		
CONNECT	3	2				
CONNECT	4	2	5	50		
CONNECT	5	4	6	7		
CONNECT	6	5				
CONNECT	7	5	8	14		
CONNECT	8	1	7	9		
CONNECT	9	8				
CONNECT	10	1	11	12	13	
CONNECT	11	10				
CONNECT	12	10				
CONNECT	13	10				
CONNECT	14	15	16	32	7	
CONNECT	15	14	17	21	22	
CONNECT	16	14	18	19	23	
CONNECT	17	15	35	36	37	
CONNECT	18	16	38	39	40	
CONNECT	19	16	41	42	43	
CONNECT	20	21	24	25	32	
CONNECT	21	20	15	26	27	
CONNECT	22	15	23	28	29	
CONNECT	23	22	16	30	31	
CONNECT	24	20				
CONNECT	25	20				
CONNECT	26	21				
CONNECT	27	21				
CONNECT	28	22				
CONNECT	29	22				
CONNECT	30	23				
CONNECT	31	23				

```
CONNECT 32 14 20 33 34
CONNECT 33 32 44 45 46
CONNECT 34 32 47 48 49
CONNECT 35 17
CONNECT 36 17
CONNECT 37 17
CONNECT 38 18
CONNECT 39 18
CONNECT 40 18
CONNECT 41 19
CONNECT 42 19
CONNECT 43 19
CONNECT 44 33
CONNECT 45 33
CONNECT 46 33
CONNECT 47 34
CONNECT 48 34
CONNECT 49 34
CONNECT 50 4
END
```