Supplementary Data

X-Ray Crystal Structure and Hirshfeld Analysis of Gem-Aminals Based Morpholine , Pyrrolidine, and Piperidine Moieties

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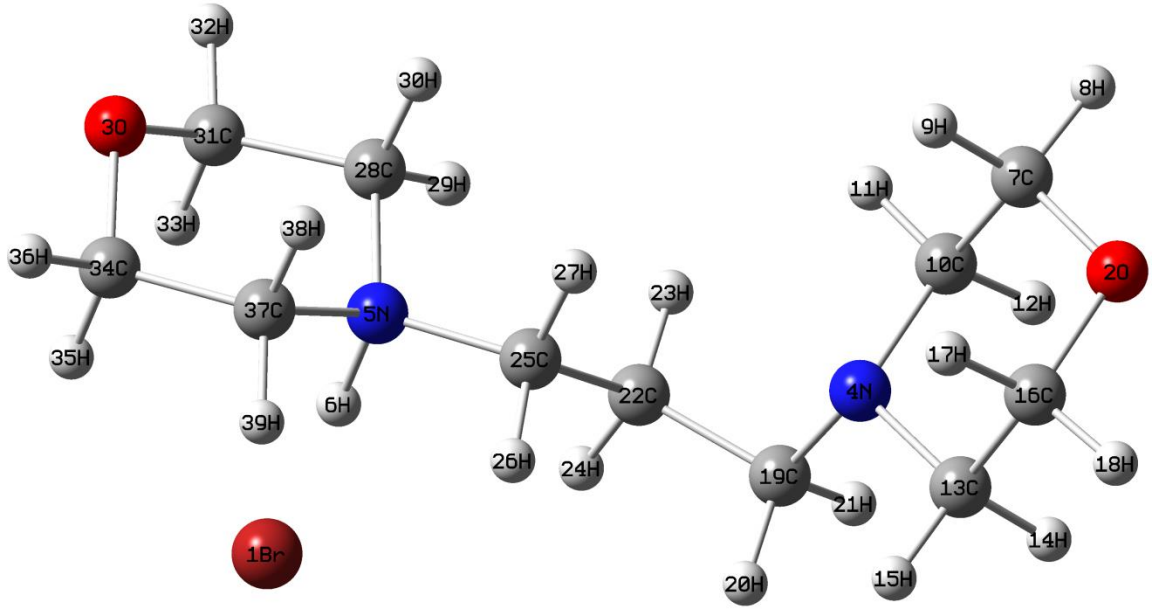
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23H
12H
37C
5N
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25C
17H
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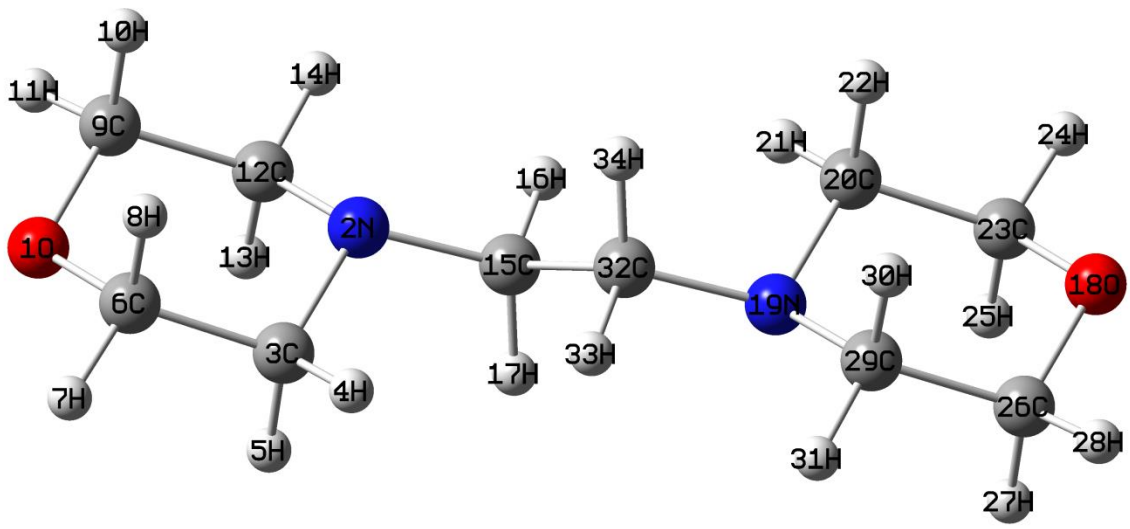
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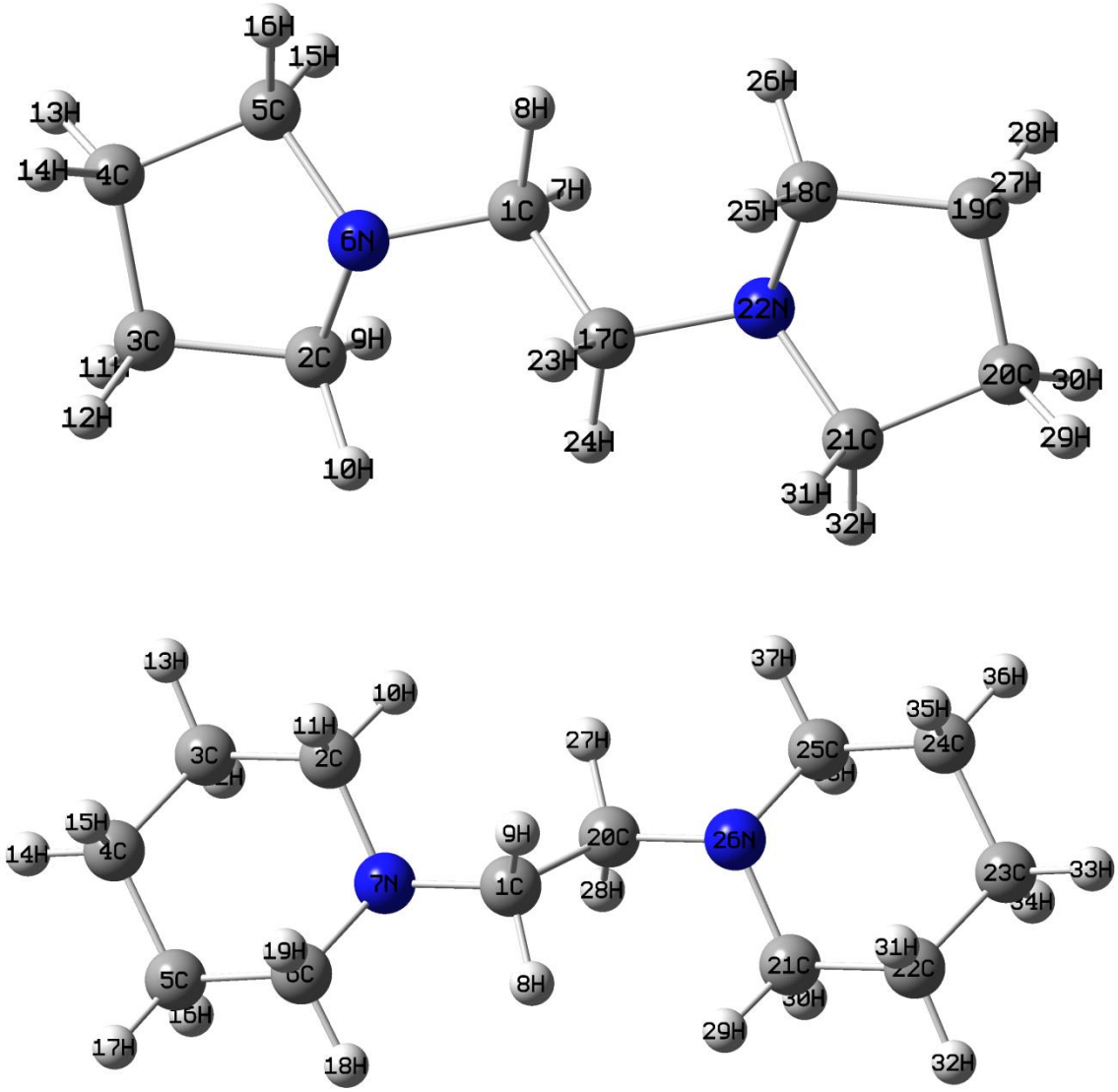

Fig. S1 Atom numbering of the optimized structures of the studied systems. Bond distances and angles are listed in Table S1.

Table S1 The calculated bond distances and angles compared to X-ray data.

Parameter	Calc	Exp	Parameter	Calc	Exp	Parameter	Calc	Exp	Parameter	Calc	Exp
1			**2**			**3**			**4**		
R(1-6)	1.421	1.428	R(2-7)	1.42	1.424	R(1-6)	1.457	1.457	R(1-7)	1.464	1.467
R(1-9)	1.422	1.425	R(2-16)	1.422	1.431	R(1-17)	1.533	1.525	R(1-20)	1.536	1.534
R(2-3)	1.465	1.463	R(3-31)	1.422	1.42	R(2-3)	1.541	1.528	R(2-3)	1.532	1.526
R(2-12)	1.465	1.465	R(3-34)	1.422	1.425	R(2-6)	1.465	1.47	R(2-7)	1.466	1.469
R(2-15)	1.463	1.465	R(4-10)	1.467	1.462	R(2-10)	1.094	0.996	R(3-4)	1.534	1.531
R(3-6)	1.527	1.515	R(4-13)	1.467	1.467	R(3-4)	1.555	1.545	R(4-5)	1.534	1.52
R(9-12)	1.526	1.513	R(4-19)	1.466	1.466	R(4-5)	1.539	1.528	R(5-6)	1.532	1.526
R(15-32)	1.535	1.522	R(5-25)	1.498	1.498	R(5-6)	1.464	1.467	R(6-7)	1.466	1.471
R(18-23)	1.421	1.428	R(5-28)	1.497	1.498	R(17-22)	1.457	1.457	R(20-26)	1.464	1.467
R(18-26)	1.422	1.425	R(5-37)	1.497	1.497	R(18-19)	1.541	1.528	R(21-22)	1.532	1.526
R(19-20)	1.465	1.463	R(7-10)	1.527	1.511	R(18-22)	1.465	1.47	R(21-26)	1.466	1.469
R(19-29)	1.465	1.465	R(13-16)	1.526	1.514	R(19-20)	1.555	1.545	R(22-23)	1.534	1.531
R(19-32)	1.463	1.465	R(19-22)	1.534	1.527	R(20-21)	1.539	1.528	R(23-24)	1.534	1.52
R(20-23)	1.527	1.515	R(22-25)	1.531	1.521	R(21-22)	1.464	1.467	R(24-25)	1.532	1.526
R(26-29)	1.526	1.513	R(28-31)	1.529	1.517	A(6-1-17)	112.3	111.9	R(25-26)	1.466	1.471
A(6-1-9)	110.6	109.4	R(34-37)	1.528	1.513	A(1-6-2)	115.3	113.8	A(7-1-20)	112.3	112.5
A(1-6-3)	111.5	111.8	A(7-2-16)	110.724	109.816	A(1-6-5)	113.6	112.2	A(1-7-2)	112.6	111.4
A(1-9-12)	111.3	111.2	A(2-7-10)	111.438	111.565	A(1-17-22)	112.3	111.9	A(1-7-6)	112.3	109.4
A(3-2-12)	109.5	108.6	A(2-16-13)	111.299	111.269	A(3-2-6)	103.9	104	A(1-20-26)	112.3	112.5
A(3-2-15)	113.2	112.0	A(31-3-34)	110.077	110.756	A(2-3-4)	104.4	104.5	A(1-20-27)	109.1	110.9
A(2-3-6)	110.0	110.8	A(3-31-28)	110.878	112.187	A(2-6-5)	104.4	103.4	A(1-20-28)	108.8	106.6
A(12-2-15)	112.4	109.1	A(3-34-37)	110.725	111.435	A(3-4-5)	104.2	104.3	A(3-2-7)	111.3	111.2
A(2-12-9)	110.0	110.6	A(10-4-13)	109.479	108.719	A(4-5-6)	103.9	103.9	A(2-3-4)	110.9	110.8
A(2-15-32)	112.3	112.2	A(10-4-19)	112.74	111.224	A(17-22-18)	115.3	113.8	A(2-7-6)	110.7	109.7
A(15-32-19)	112.3	112.2	A(4-10-7)	110.037	109.857	A(17-22-21)	113.6	112.2	A(3-4-5)	110.1	109.9

A(23-18-26)	110.6	109.4	A(13-4-19)	112.097	110.077	A(19-18-22)	103.9	104	A(4-5-6)	111.0	111.2
A(18-23-20)	111.5	111.8	A(4-13-16)	109.886	110.499	A(18-19-20)	104.4	104.5	A(5-6-7)	111.2	111.3
A(18-26-28)	106.6	109.4	A(4-19-22)	113.256	112.21	A(18-22-21)	104.4	103.4	A(20-26-21)	112.6	111.4
A(18-26-29)	111.3	111.2	A(25-5-28)	114.304	113.735	A(19-20-21)	104.2	104.3	A(20-26-25)	112.3	109.4
A(20-19-29)	109.5	108.6	A(25-5-37)	112.097	110.402	A(20-21-22)	103.9	103.9	A(22-21-26)	111.3	111.2
A(20-19-32)	113.2	112.0	A(5-25-22)	112.87	112.888				A(21-22-23)	110.9	110.8
A(19-20-23)	110.0	110.8	A(28-5-37)	110.925	109.093				A(21-26-25)	110.7	109.7
A(29-19-32)	112.4	109.1	A(5-28-29)	107.887	109.925				A(22-23-24)	110.1	109.9
A(19-29-26)	110.0	110.6	A(5-28-30)	108.231	109.88				A(23-24-25)	111.0	111.2
A(19-32-33)	107.1	109.2	A(5-28-31)	109.645	109.01				A(24-25-26)	111.2	111.3
A(20-23-25)	109.3	109.3	A(5-37-34)	109.855	109.828						
			A(5-37-38)	108.367	109.683						
			A(5-37-39)	107.221	109.68						
			A(8-7-10)	110.515	109.3						
			A(19-22-25)	110.981	109.497						